ETH Zurich

Advanced Graph Algorithms and Optimization

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These notes will be updated throughout the course. They are likely to contain typos, and they may have mistakes or lack clarity in places. Feedback and comments are welcome. Please send to kyng@inf.ethz.ch or, even better, submit a pull request at

`https://github.com/rjkyng/agao22_script`.

We want to thank scribes from the 2020 edition of the course who contributed to these notes: Hongjie Chen, Meher Chaitanya, Timon Knigge, and Tim Taubner – and we're grateful to all the readers who've submitted corrections, including Martin Kucera, Alejandro Cassis, and Luke Volpatti.

A important note: If you're a student browsing these notes to decide whether to take this course, please note that the current notes are incomplete. We will release Parts III and IV later in the semester. You can take a look at last year's notes for an impression of the what the rest of the course will look like. Find them here:

`https://kyng.inf.ethz.ch/courses/AGAO21/agao21_script.pdf`

There will, however, be some changes to the content compared to last year.

Contents

Chapter 1

Course Introduction

1.1 Overview

This course will take us quite deep into modern approaches to graph algorithms using convex optimization techniques. By studying convex optimization through the lens of graph algorithms, we'll try to develop an understanding of fundamental phenomena in optimization. Much of our time will be devoted to flow problems on graphs. We will not only be studying these problems for their own sake, but also because they often provide a useful setting for thinking more broadly about optimization.

The course will cover some traditional discrete approaches to various graph problems, especially flow problems, and then contrast these approaches with modern, asymptotically faster methods based on combining convex optimization with spectral and combinatorial graph theory.

1.2 Electrical Flows and Voltages - a Graph Problem from Middle School?

We will dive right into graph problems by considering how electrical current moves through a network of resistors.

First, let us recall some middle school physics. If some of these things don't make sense two you, don't worry, in less than paragraph from here, we'll be make to safely doing math.

Recall that a typical battery that buy from Migros has two endpoints, and produces what is called a *voltage difference* between these endpoints.

One end of the battery will have a positive charge (I think that means an excess of positrons[1]), and the other a negative charge. If we connect the two endpoints with a wire, then a current will flow from one end of the battery to the other in an attempt to even out this imbalance of charge.

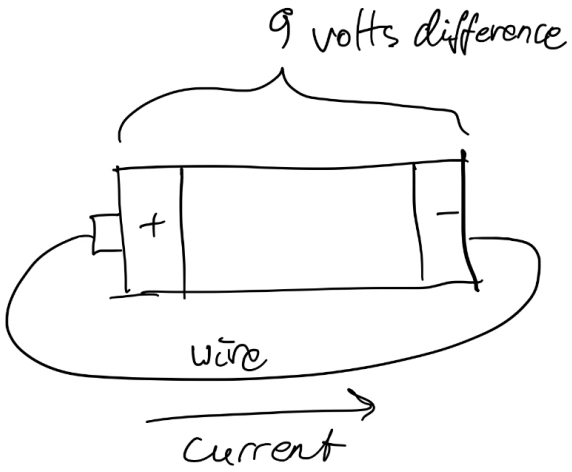


Figure 1.1: A 9 volts battery with a wire attached.

We can also imagine a kind of battery that tries to send a certain amount of current the wires between its endpoints, e.g. 1 unit of charge per unit of time. This will be a little more convenient to work with, so let us focus on that case.

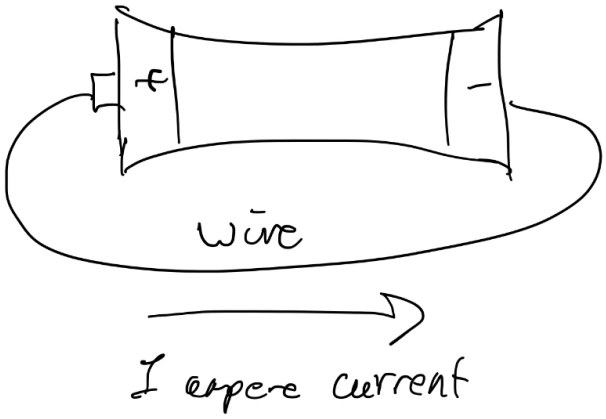


Figure 1.2: A 1 ampere battery with a wire attached.

A *resistor* is a piece of wire that connects two points u and v, and is completely described by a single number r called its *resistance*.

[1] I'm joking, of course! Try Wikipedia if you want to know more. However, you will not need it for this class.

If the voltage difference between the endpoints of the resistor is x, and the resistance is r then this will create a flow of charge per unit of time of $f = x/r$. This is called Ohm's Law.

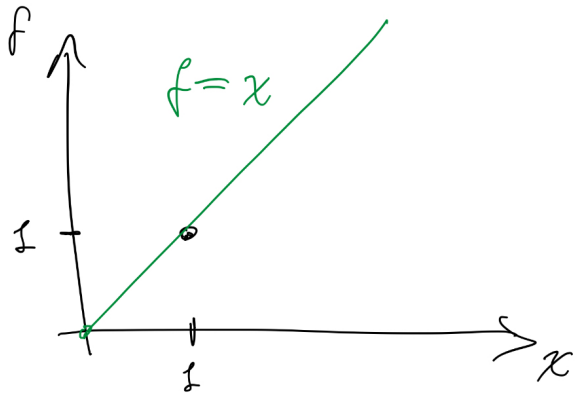


Figure 1.3: Ohm's Law for a resistor with resistance $r = 1$.

Suppose we set up a bunch of wires that route electricity from our current source s to our current sink t in some pattern:

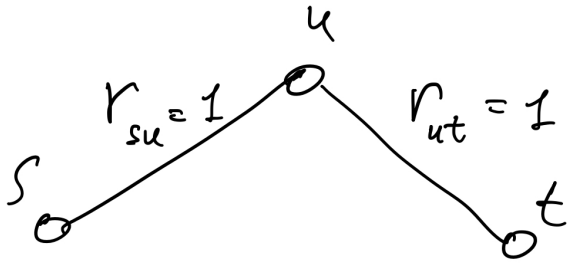


Figure 1.4: A path of two resistors.

We have one unit of charge flowing out of s per unit of time, and one unit coming into t. Because charge is conserved, the current flowing into any other point u must equal the amount flowing out of it. This is called Kirchoff's Current Law.

To send one unit of current from s to t, we must be sending it first form s to u and then from u to t. So the current on edge (s, u) is 1 and the current on (u, t) is 1. By Ohm's Law, the voltage difference must also be 1 across each of the two wires. Thus if the voltage is x at s, it must be $x + 1$ at u and $x + 2$ at t. What is x? It turns out it doesn't matter: We only care about the differences. So let us set $x = 0$.

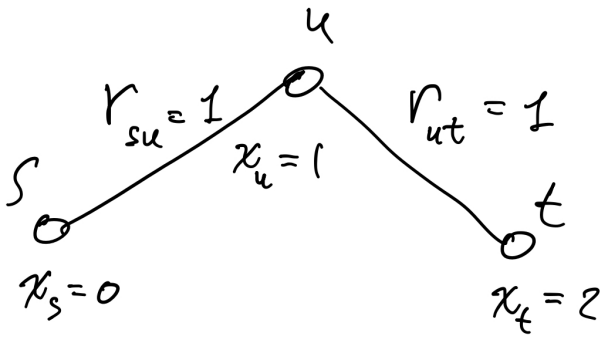


Figure 1.5: A path of two resistors.

Let us try one more example:

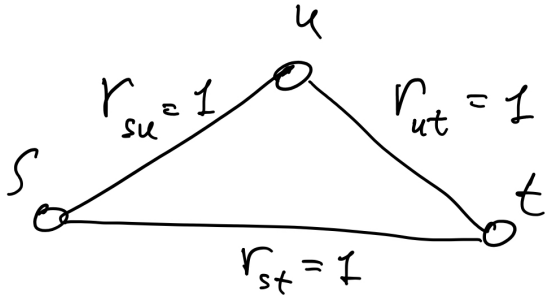


Figure 1.6: A network with three resistors.

How much flow will go directly from s to t and how much via u?

Well, we know what the net current flowing into and out of each vertex must be, and we can use to set up some equations. Let us say the voltage at s is x_s, at u is x_u and at t is x_t.

- Net current at s: $-1 = (x_s - x_t) + (x_s - x_u)$
- Net current at u: $0 = (x_u - x_s) + (x_u - x_t)$
- Net current at t: $1 = (x_t - x_s) + (x_t - x_u)$

The following is a solution: $x_s = 0$, $x_u = \frac{1}{3}$, $x_t = \frac{2}{3}$. And as before, we can shift all the voltages by some constant x and get another solution $a = x + 0$, $x_u = x + \frac{1}{3}$, $x_t = x + \frac{2}{3}$. You might want to convince yourself that these are the only solutions.

Electrical flows in general graphs. Do we know enough to calculate the electrical flow in some other network of resistors? To answer this, let us think about the network as a graph. Consider a undirected graph $G = (V, E)$ with $|V| = n$ vertices and $|E| = m$ edges, and let us assume G is connected. Let's associate a resistance $\boldsymbol{r}(e) > 0$ with every edge $e \in E$.

To keep track of the direction of the flow on each edge, it will be useful to assign an arbitrary direction to every edge. So let's do that, but remember that this is just a bookkeeping tool that helps us track where flow is going.

A *flow* in the graph is a vector $\boldsymbol{f} : \mathbb{R}^E$. The *net flow* of $\boldsymbol{f}$ at a vertex $u \in V$ is defined as $\sum_{v \to u} \boldsymbol{f}(v,u) - \sum_{u \to v} \boldsymbol{f}(u,v)$.

We say a flow routes the demands $\boldsymbol{d} \in \mathbb{R}^V$ if the net flow at every vertex v is $\boldsymbol{d}(v)$.

We can assign a voltage to every vertex $\boldsymbol{x} \in R^V$. Ohm's Law says that the electrical flow induced by these voltages will be $\boldsymbol{f}(u,v) = \frac{1}{\boldsymbol{r}(u,v)}(\boldsymbol{x}(u) - \boldsymbol{x}(v))$.

Say we want to route unit of current from vertex $s \in V$ to vertex $t \in V$. As before, we can write an equation for every vertex saying that the voltage differences must produce the desired net current:

- Net current at s: $-1 = \sum_{(s,v)} \frac{1}{\boldsymbol{r}(s,v)}(\boldsymbol{x}(s) - \boldsymbol{x}(v))$
- Net current at $u \in V \setminus \{s,t\}$: $0 = \sum_{(u,v)} \frac{1}{\boldsymbol{r}(u,v)}(\boldsymbol{x}(u) - \boldsymbol{x}(v))$
- Net current at t: $1 = \sum_{(t,v)} \frac{1}{\boldsymbol{r}(t,v)}(\boldsymbol{x}(t) - \boldsymbol{x}(v))$

This gives us n constraints, exactly as many as we have voltage variables. However we have to be a little careful when trying to conclude that a solution exists, yielding voltages $\boldsymbol{x}$ that gives induce an electrical flow routing the desired demand.

You will prove in the exercises (Week 1, Exercise 3) that a solution $\boldsymbol{x}$ exists. The proof requires two important observations: Firstly that the graph is connected, and secondly that summed over all vertices, the net demand is zero, i.e. as much flow is coming into the network as is leaving it.

The incidence matrix and the Laplacian matrix. To have a more compact notation for net flow constraints, we also introduce the *edge-vertex incidence matrix* of the graph, $\boldsymbol{B} \in \mathbb{R}^{V \times E}$.

$$\boldsymbol{B}(v,e) = \begin{cases} 1 & \text{if } e = (u,v) \\ -1 & \text{if } e = (v,u) \\ 0 & \text{o.w.} \end{cases}$$

Now we can express the net flow constraint that $\boldsymbol{f}$ routes $\boldsymbol{d}$ by

$$\boldsymbol{B}\boldsymbol{f} = \boldsymbol{d}.$$

This is also called a conservation constraint. In our examples so far, we have $\boldsymbol{d}(s) = -1$, $\boldsymbol{d}(t) = 1$ and $\boldsymbol{d}(u) = 0$ for all $u \in V \setminus \{s,t\}$.

If we let $\boldsymbol{R} = \mathrm{diag}_{e \in E}\, \boldsymbol{r}(e)$ then Ohm's law tells us that $\boldsymbol{f} = \boldsymbol{R}^{-1}\boldsymbol{B}^\top \boldsymbol{x}$. Putting these observations together, we have $\boldsymbol{B}\boldsymbol{R}^{-1}\boldsymbol{B}^\top \boldsymbol{x} = \boldsymbol{d}$. The voltages $\boldsymbol{x}$ that induce $\boldsymbol{f}$ must solve this system of linear equations, and we can use that to compute both $\boldsymbol{x}$ and $\boldsymbol{f}$. It is exactly

the same linear equation as the one we considered earlier. We can show a that for a connected graph, a solution $\boldsymbol{x}$ exists if and only if the flow into the graph equals the net flow out, which we can express as $\sum_v \boldsymbol{d}(v) = 0$ or $\mathbf{1}^\top \boldsymbol{d} = 0$. You will show this as part of Exercise 3. This also implies that an electrical flow routing $\boldsymbol{d}$ exists if and only if the net flow into the graph equals the net flow out, which we can express as $\mathbf{1}^\top \boldsymbol{d} = 0$.

The matrix $\boldsymbol{B}\boldsymbol{R}^{-1}\boldsymbol{B}^\top$ is called the *Laplacian* of the graph and is usually denoted by $\boldsymbol{L}$.

An optimization problem in disguise. So far, we have looked at electrical voltages and flows as arising from a set of linear equations – and it might not be apparent that this has anything to do with optimization. But transporting current through a resistor requires energy, which will be dissipated as heat by the resistor (i.e. it will get hot!). If we send a current of f across a resistor with a potential drop of x, then the amount of energy spent per unit of time by the resistor will be $f \cdot x$. This is called Joule's Law. Applying Ohm's law to a resistor with resistance r, we can also express this energy per unit of time as $f \cdot x = x^2/r = r \cdot f^2$. Since we aren't bothering with units, we will even forget about time, and refer to these quantities as "energy", even though a physicist would call them "power".

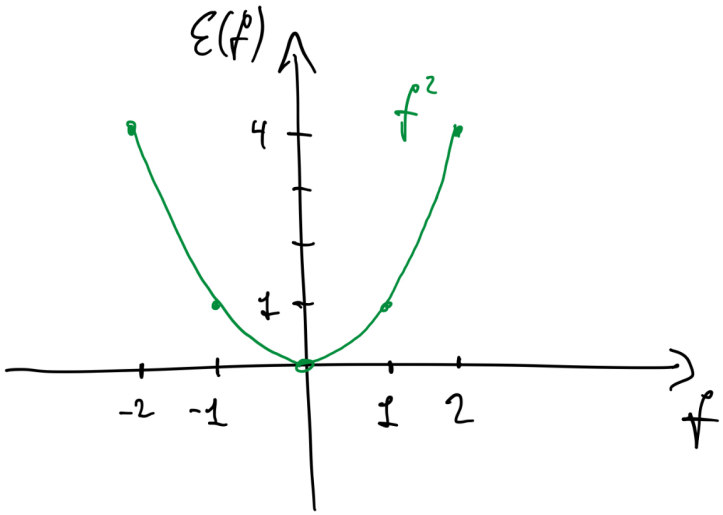


Figure 1.7: Energy has a function of flow in a resistor with resistance $r = 1$.

Now, another interesting question would seem to be: If we want to find a flow routing a certain demand $\boldsymbol{d}$, how should the flow behave in order to minimize the electrical energy spent routing the flow? The electrical energy of a flow vector $\boldsymbol{f}$ is $\mathcal{E}(\boldsymbol{f}) \stackrel{\text{def}}{=} \sum_e \boldsymbol{r}(e)\boldsymbol{f}(e)^2$. We can phrase this as an optimization problem:

$$\begin{aligned} &\min_{\boldsymbol{f} \in \mathbb{R}^E} \mathcal{E}(\boldsymbol{f}) \\ &\text{s.t. } \boldsymbol{B}\boldsymbol{f} = \boldsymbol{d}. \end{aligned}$$

We call this problem *electrical energy-minimizing flow*. As we will prove later, the flow $\boldsymbol{f}^*$ that minimizes the electrical energy among all flows that satisfy $\boldsymbol{B}\boldsymbol{f} = \boldsymbol{d}$ is precisely the electrical flow.

A pair of problems. What about our voltages, can we also get them from some optimization problem? Well, we can work backwards from the fact that our voltages solve the equation $\boldsymbol{L}\boldsymbol{x} = \boldsymbol{d}$. Consider the function $c(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^\top \boldsymbol{L}\boldsymbol{x} - \boldsymbol{x}^\top \boldsymbol{d}$. We should ask ourselves some questions about this function $c : \mathbb{R}^V \to \mathbb{R}$. Is it continuous and continuously differentiable? The answer to this is yes, and that is not hard to see. Does the function have a minimum? This is maybe not immediately clear, but the minimum does indeed exist.

When this is minimized, the derivative of $c(\boldsymbol{x})$ with respect to each coordinate of $\boldsymbol{x}$ must be zero. This condition yields exactly the system of linear equations $\boldsymbol{L}\boldsymbol{x} = \boldsymbol{d}$. You will confirm this in Exercise 4 of the first exercise sheet.

Based on our derivative condition for the optimum, we can also express the electrical voltages as the solution to an optimization problem, namely

$$\min_{\boldsymbol{x}\in\mathbb{R}^V} c(\boldsymbol{x})$$

As you are probably aware, having the derivative of each coordinate equal zero is not a sufficient condition for being at the optimum of a function[2].

It is also interesting to know whether *all* solutions to $\boldsymbol{L}\boldsymbol{x} = \boldsymbol{d}$ are in fact minimizers of c. The answer is yes, and will see some very general tools for proving statements like this in Chapter 2.

Altogether, we can see that routing electrical current through a network of resistors leads to a *pair* of optimization problems, let's call them $\boldsymbol{f}^*$ and $\boldsymbol{x}^*$, and that the solutions to the two problems are related, in our case through the equation $\boldsymbol{f}^* = \boldsymbol{R}^{-1}\boldsymbol{B}^\top \boldsymbol{x}^*$ (Ohm's Law). But, why and how are these two optimization problems related?

Instead of minimizing $c(\boldsymbol{x})$, we can equivalently think about maximizing $-c(\boldsymbol{x})$, which gives the following optimization problem: $\max_{\boldsymbol{x}\in\mathbb{R}^V} -c(\boldsymbol{x})$. In fact, as you will show in the exercises for Week 1, we have $\mathcal{E}(\boldsymbol{f}^*) = -c(\boldsymbol{x}^*)$, so the minimum electrical energy is exactly the maximum value of $-\boldsymbol{c}(\boldsymbol{x})$. More generally for *any* flow that routes $\boldsymbol{d}$ and *any* voltages $\boldsymbol{x}$, we have $\mathcal{E}(\boldsymbol{f}) \geq -c(\boldsymbol{x})$. So, for any $\boldsymbol{x}$, the value of $-c(\boldsymbol{x})$ is a lower bound on the minimum energy $\mathcal{E}(\boldsymbol{f}^*)$.

This turns out to be an instance of a much broader phenomenon, known as Lagrangian duality, which allows us to learn a lot about many optimization problems by studying two related pairs of problems, a minimization problem, and a related maximization problem that gives lower bounds on the optimal value of the minimization problem.

[2]Consider the function in one variable $c(x) = x^3$.

Solving $\boldsymbol{Lx} = \boldsymbol{d}$. Given a graph G with resistances for the edges, and some net flow vector $\boldsymbol{d}$, how quickly can we compute $\boldsymbol{x}$? Broadly speaking, there are two very different families of algorithms we could use to try to solve this problem.

Either, we could solve the linear equation using something like *Gaussian Elimination* to compute an exact solution.

Alternatively, we could start with a guess at a solution, e.g. $\boldsymbol{x}_0 = \mathbf{0}$, and then we could try to make a change to $\boldsymbol{x}_0$ to reach a new point $\boldsymbol{x}_1$ with a lower value of $c(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^\top \boldsymbol{L}\boldsymbol{x} - \boldsymbol{x}^\top \boldsymbol{d}$, i.e. $c(\boldsymbol{x}_1) < c(\boldsymbol{x}_0)$. If we repeat a process like that for enough steps, say t, hopefully we eventually reach $\boldsymbol{x}_t$ with $c(\boldsymbol{x}_t)$ close to $c(\boldsymbol{x}^*)$, where $\boldsymbol{x}^*$ is a minimizer of $c(\boldsymbol{x})$ and hence $\boldsymbol{L}\boldsymbol{x}^* = \boldsymbol{d}$. Now, we also need to make sure that $c(\boldsymbol{x}_t) \approx c(\boldsymbol{x}^*)$ implies that $\boldsymbol{L}\boldsymbol{x}_t \approx \boldsymbol{d}$ in some useful sense.

One of the most basic algorithms in this framework of "guess and adjust" is called *Gradient Descent*, which we will study in Week 2. The rough idea is the following: if we make a very small step from $\boldsymbol{x}$ to $\boldsymbol{x} + \boldsymbol{\delta}$, then a multivariate Taylor expansion suggests that $c(\boldsymbol{x} + \boldsymbol{\delta}) - c(\boldsymbol{x}) \approx \sum_{v \in V} \boldsymbol{\delta}(v) \frac{\partial c(\boldsymbol{x})}{\partial \boldsymbol{x}(v)}$.

If we are dealing with smooth convex function, this quantity is negative if we let $\boldsymbol{\delta}(v) = -\epsilon \cdot \frac{\partial c(\boldsymbol{x})}{\partial \boldsymbol{x}(v)}$ for some small enough ϵ so the approximation holds well. So we should be able to make progress by taking a small step in this direction. That's Gradient Descent! The name comes from the vector of partial derivatives, which is called the gradient.

As we will see later in this course, understanding electrical problems from an optimization perspective is crucial to develop fast algorithms for computing electrical flows and voltages, but to do very well, we also need to borrow some ideas from Gaussian Elimination.

What running times do different approaches get?

1. Using Gaussian Elimination, we can find $\boldsymbol{x}$ s.t. $\boldsymbol{L}\boldsymbol{x} = \boldsymbol{d}$ in $O(n^3)$ time and with asymptotically faster algorithms based on matrix multiplication, we can bring this down to roughly $O(n^{2.372})$.

2. Meanwhile Gradient Descent will get a running time of $O(n^3 m)$ or so – at least this is a what a simple analysis suggests.

3. However, we can do much better: By combining ideas from both algorithms, and a bit more, we can get $\boldsymbol{x}$ up to very high accuracy in time $O(m \log^c n)$ where c is some small constant.

1.3 Convex Optimization

Recall our plot in Figure 1.7 of the energy required to route a flow f across a resistor with resistance r, which was $\mathcal{E}(f) = r \cdot f^2$. We see that the function has a special structure: the

graph of the function sits below the line joining any two points $(f, \mathcal{E}(f))$ and $(g, \mathcal{E}(g))$. A function $\mathcal{E} : \mathbb{R} \to \mathbb{R}$ that has this property is said to be convex.

Figure 1.8 shows the energy as a function of flow, along with two points $(f, \mathcal{E}(f))$ and $(g, \mathcal{E}(g))$. We see the function sits below the line segment between these points.

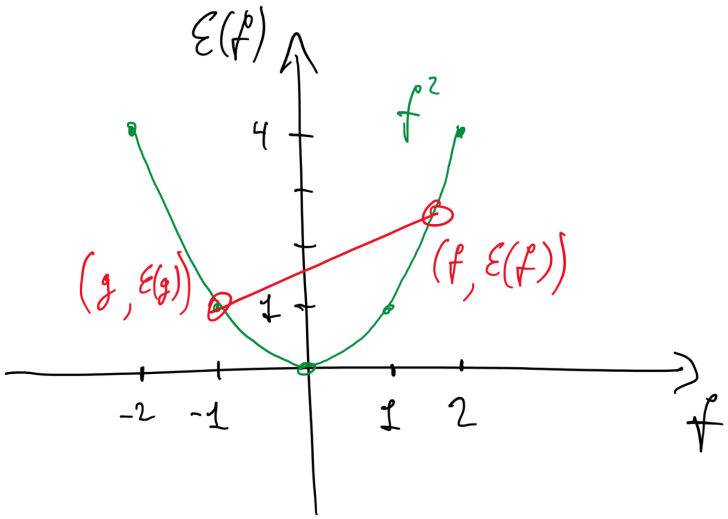


Figure 1.8: Energy has a function of flow in a resistor with resistance $r = 1$. The function is convex.

We can also interpret this condition as saying that for all $\theta \in [0, 1]$

$$\mathcal{E}(\theta f + (1 - \theta)g) \leq \theta \mathcal{E}(f) + (1 - \theta)\mathcal{E}(g).$$

This immediately generalizes to functions $\mathcal{E} : \mathbb{R}^m \to \mathbb{R}$.

A *convex set* is a subset of $S \subseteq \mathbb{R}^m$ s.t. if $\boldsymbol{f}, \boldsymbol{g} \in S$ then for all $\theta \in [0, 1]$ we have $\theta \boldsymbol{f} + (1-\theta)\boldsymbol{g} \in S$.

Figure 1.9 shows some examples of sets that are and aren't convex.

Convex functions and convex sets are central to optimization, because for most problems of minimization a convex function over a convex set, we can develop fast algorithms [3].

So why convex functions and convex sets? One important reason is that for a convex function defined over a convex feasible set, any local minimum is also a global minimum, and this fact makes searching for an optimal solution computationally easier. In fact, this is closely related to why Gradient Descent works well on many convex functions.

Notice that the set $\{\boldsymbol{f} : \boldsymbol{B}\boldsymbol{f} = \boldsymbol{d}\}$ is convex, i.e. the set of all flows that route a fixed demand

[3] There are some convex optimization problems that are NP-hard. That said, polynomial time algorithms exist for almost any convex problem you can come up with. The most general polynomial time algorithm for convex optimization is probably the Ellipsoid Method.

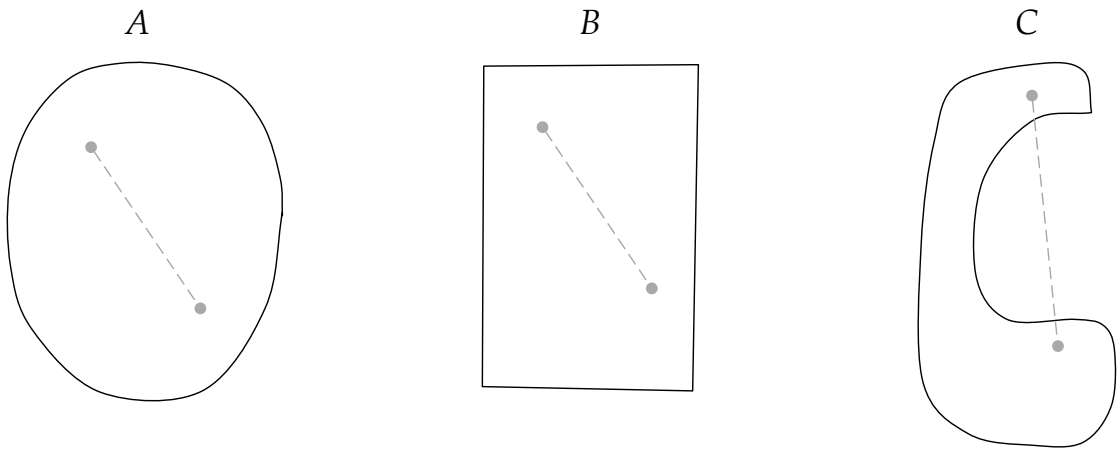


Figure 1.9: A depiction of convex and non-convex sets. The sets A and B are convex since the straight line between any two points inside them is also in the set. The set C is not convex.

$\boldsymbol{d}$ is convex. It is also easy to verify that $\mathcal{E}(\boldsymbol{f}) = \sum_e \boldsymbol{r}(e)\boldsymbol{f}(e)^2$ is a convex function, and hence finding an electrical flow is an instance of convex minmization:

1.4 More Graph Optimization Problems

Maximum flow. Again, let $G = (V, E)$ be an undirected, connected graph with n vertices and m edges. Suppose we want to find a flow $\boldsymbol{f} \in \mathbb{R}^E$ that routes $\boldsymbol{d}$, but instead of trying to minimize electrical energy, we try to pick an $\boldsymbol{f}$ that minimizes the largest amount of flow on any edge, i.e. $\max_e |\boldsymbol{f}_e|$ – which we also denote by $\|\boldsymbol{f}\|_\infty$. We can write this problem as

$$\begin{aligned} &\min_{\boldsymbol{f} \in \mathbb{R}^E} \|\boldsymbol{f}\|_\infty \\ &\text{s.t. } \boldsymbol{B}\boldsymbol{f} = \boldsymbol{d} \end{aligned}$$

This problem is known as the Minimum Congested Flow Problem[4]. It is equivalent to the more famous Maximum Flow Problem.

The behavior of this kind of flow is very different than electrical flow. Consider the question of whether a certain demand can be routed $\|\boldsymbol{f}\|_\infty \leq 1$. Imagine sending goods from a source s to a destination t using a network of train lines that all have the same capacity and asking whether the network is able to route the goods at the rate you want: This boils down to whether routing exists with $\|\boldsymbol{f}\|_\infty \leq 1$, if we set it up right.

We have a very fast, convex optimization-based algorithm for Minimum Congested Flow: In $m\epsilon^{-1}\log^{O(1)} n$ time, we can find a flow $\tilde{\boldsymbol{f}}$ s.t. $\boldsymbol{B}\tilde{\boldsymbol{f}} = \boldsymbol{d}$ and $\left\|\tilde{\boldsymbol{f}}\right\|_\infty \leq (1+\epsilon)\|\boldsymbol{f}^*\|_\infty$, where $\boldsymbol{f}^*$

[4]This version is called undirected, because the graph is undirected, and *uncapacitated* because we are aiming for the same bound on the flow on all edges.

is an optimal solution, i.e. an actual minimum congestion flow routing $\boldsymbol{d}$.

But what if we want ϵ to be very small, e.g. $1/m$? Then this running time isn't so good anymore. But, in this case, we can use other algorithms that find flow $\boldsymbol{f}^*$ *exactly*. Unfortunately, these algorithms take time roughly $m^{4/3+o(1)}$.

Just as the electrical flow problem had a dual voltage problem, so maximum flow has a dual voltage problem, which is know as the s-t minimum cut problem.

Maximum flow, with directions and capacities. We can make the maximum flow problem harder by introducing directed edges: To do so, we allow edges to exist in both directions between vertices, and we require that the flow on a directed edge is always non-negative. So now $G = (V, E)$ is a directed graph. We can also make the problem harder by introducing capacities. We define a capacity vector $\boldsymbol{c} \in \mathbb{R}^E \geq \mathbf{0}$ and try to minimize $\left\| \boldsymbol{C}^{-1}\boldsymbol{f} \right\|_\infty$, where $\boldsymbol{C} = \operatorname{diag}_{e \in E} \boldsymbol{c}(e)$. Then our problem becomes

$$\begin{aligned} \min_{\boldsymbol{f} \in \mathbb{R}^E} & \left\| \boldsymbol{C}^{-1}\boldsymbol{f} \right\|_\infty \\ \text{s.t. } & \boldsymbol{B}\boldsymbol{f} = \boldsymbol{d} \\ & \boldsymbol{f} \geq \mathbf{0}. \end{aligned}$$

For this capacitated, directed maximum flow problem, our best algorithms run in about $O(m\sqrt{n})$ time in sparse graphs and $O(m^{1.483})$ in dense graphs[5], even if we are willing to accept fairly low accuracy solution. If the capacities are allowed to be exponentially large, the best running time we can get is $O(mn)$. For this problem, we do not yet know how to improve over classical combinatorial algorithms using convex optimization.

Multi-commodity flow. We can make the even harder still, by simultaneously trying to route two types of flow (imagine pipes with Coke and Pepsi). Our problem now looks like

$$\begin{aligned} \min_{\boldsymbol{f}_1, \boldsymbol{f}_2 \in \mathbb{R}^E} & \left\| \boldsymbol{C}^{-1}(\boldsymbol{f}_1 + \boldsymbol{f}_2) \right\|_\infty \\ \text{s.t. } & \boldsymbol{B}\boldsymbol{f}_1 = \boldsymbol{d}_1 \\ & \boldsymbol{B}\boldsymbol{f}_2 = \boldsymbol{d}_2 \\ & \boldsymbol{f}_1, \boldsymbol{f}_2 \geq \mathbf{0}. \end{aligned}$$

Solving this problem to high accuracy is essentially as hard as solving a general linear program! We should see later in the course how to make this statement precise.

If we in the above problem additionally require that our flows must be integer valued, i.e. $\boldsymbol{f}_1, \boldsymbol{f}_2 \in \mathbb{N}_0$, then the problem becomes NP-complete.

[5]Provided the capacities are integers satisfying a condition like $\boldsymbol{c} \leq n^{100}\mathbf{1}$.

Random walks in a graph. Google famously uses[6] the PageRank problem to help decide how to rank their search results. This problem essentially boils down to computing the *stable distribution* of a random walk on a graph. Suppose $G = (V, E)$ is a directed graph where each outgoing edge (v, u), which we will define as going from u to v, has a transition probability $p_{(v,u)} > 0$ s.t. $\sum_{z \leftarrow u} p_{(z,u)} = 1$. We can take a step of a random walk on the vertex set by starting at some vertex $u_0 = u$, and then randomly pick one of the outgoing edges (v, u) with probability $p_{(v,u)}$ and move to the chosen vertex $u_1 = v$. Repeating this procedure, to take a step from the next vertex u_1, gives us a *random walk* in the graph, a sequence of vertices $u_0, u_1, u_2 \ldots, u_k$.

We let $\boldsymbol{P} \in \mathbb{R}^{V \times V}$ be the matrix of transition probabilities given by

$$\boldsymbol{P}_{vu} = \begin{cases} p_{(v,u)} & \text{for } (u, v) \in E \\ 0 & \text{o.w.} \end{cases}$$

Any probability distribution over the vertices can be specified by a vector $\boldsymbol{p} \in \mathbb{R}^V$ where $\boldsymbol{p} \geq \boldsymbol{0}$ and $\sum_v \boldsymbol{p}(v) = 1$. We say that probability distribution $\boldsymbol{\pi}$ on the vertices is a *stable distribution* of the random walk if $\boldsymbol{\pi} = \boldsymbol{P}\boldsymbol{\pi}$. A strongly connected graph always has exactly one stable distribution.

How quickly can we compute the stable distribution of a general random walk? Under some mild conditions on the stable distribution[7], we can find a high accuracy approximation of $\boldsymbol{\pi}$ in time $O(m \log^c n)$ for some constant c.

This problem does not easily fit in a framework of convex optimization, but nonetheless, our fastest algorithms for it use ideas from convex optimization.

Topics in this Course

In this course, we will try to address the following questions.

1. What are the fundamental tools of fast convex optimization?
2. What are some problems we can solve quickly on graphs using optimization?
3. What can graphs teach us about convex optimization?
4. What algorithm design techniques are good for getting algorithms that quickly find a crude approximate solution? And what techniques are best when we need to get a highly accurate answer?
5. What is special about flow problems?

[6] At least they did at some point.

[7] Roughly something like $\max_v 1/\boldsymbol{\pi}(v) \leq n^{100}$.

Part I

Introduction to Convex Optimization

Chapter 2

Some Basic Optimization, Convex Geometry, and Linear Algebra

2.1 Overview

In this chapter, we will

1. Start with an overview (i.e. this list).
2. Learn some basic terminology and facts about optimization.
3. Recall our definition of convex functions and see how convex functions can also be understood in terms of a characterization based on first derivatives.
4. See how the first derivatives of a convex function can certify that we are at a global minimum.

2.2 Optimization Problems

Focusing for now on optimization over $\boldsymbol{x} \in \mathbb{R}^n$, we usually write optimization problems as:

$$\begin{aligned} \min_{\boldsymbol{x}\in\mathbb{R}^n} \text{ (or } \max) \; & f(\boldsymbol{x}) \\ s.t. \; & g_1(\boldsymbol{x}) \leq b_1 \\ & . \\ & . \\ & . \\ & g_m(\boldsymbol{x}) \leq b_m \end{aligned}$$

where $\{g_i(\boldsymbol{x})\}_{i=1}^m$ encode the constraints. For example, in the following optimization problem from the previous chapter

$$\min_{\boldsymbol{f} \in \mathbb{R}^E} \sum_e \boldsymbol{r}(e)\boldsymbol{f}(e)^2$$
$$\text{s.t. } \boldsymbol{B}\boldsymbol{f} = \boldsymbol{d}$$

we have the constraint $\boldsymbol{B}\boldsymbol{f} = \boldsymbol{d}$. Notice that we can rewrite this constraint as $\boldsymbol{B}\boldsymbol{f} \leq \boldsymbol{d}$ and $-\boldsymbol{B}\boldsymbol{f} \leq -\boldsymbol{d}$ to match the above setting. The set of points which respect the constraints is called the *feasible set*.

Definition 2.2.1. For a given optimization problem the set $\mathcal{F} = \{\boldsymbol{x} \in \mathbb{R}^n \ : \ g_i(\boldsymbol{x}) \leq b_i, \forall i \in [m]\}$ is called the **feasible set**. A point $\boldsymbol{x} \in \mathcal{F}$ is called a **feasible point**, and a point $\boldsymbol{x}' \notin \mathcal{F}$ is called an **infeasible point**.

Ideally, we would like to find optimal solutions for the optimization problems we consider. Let's define what we mean exactly.

Definition 2.2.2. For a *maximization* problem $\boldsymbol{x}^\star$ is called an **optimal solution** if $f(\boldsymbol{x}^\star) \geq f(\boldsymbol{x}), \forall \boldsymbol{x} \in \mathcal{F}$. Similarly, for a *minimization* problem $\boldsymbol{x}^\star$ is an optimal solution if $f(\boldsymbol{x}^\star) \leq f(\boldsymbol{x}), \forall \boldsymbol{x} \in \mathcal{F}$.

What happens if there are *no feasible points*? In this case, an optimal solution cannot exist, and we say the problem is infeasible.

Definition 2.2.3. If $\mathcal{F} = \emptyset$ we say that the optimization problem is **infeasible**. If $\mathcal{F} \neq \emptyset$ we say the optimization problem is **feasible**.

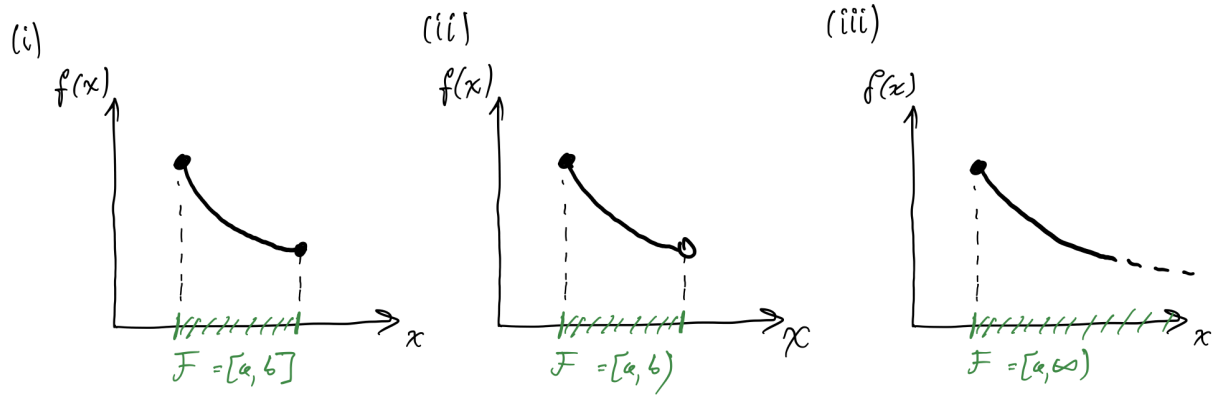


Figure 2.1

Consider three examples depicted in Figure 2.1:

(i) $\mathcal{F} = [a, b]$

(ii) $\mathcal{F} = [a, b)$

(iii) $\mathcal{F} = [a, \infty)$

In the first example, the minimum of the function is attained at b. In the second case the region is open and therefore there is no minimum function value, since for every point we will choose, there will always be another point with a smaller function value. Lastly, in the third example, the region is unbounded and the function decreasing, thus again there will always be another point with a smaller function value.

Sufficient Condition for Optimality. The following theorem, which is a fundamental theorem in real analysis, gives us a sufficient (though not necessary) condition for optimality.

Theorem (Extreme Value Theorem)**.** Let $f : \mathbb{R}^n \to \mathbb{R}$ be a continuous function and $\mathcal{F} \subseteq \mathbb{R}^n$ be nonempty, bounded, and closed. Then, the optimization problem $\min f(\boldsymbol{x}) : \boldsymbol{x} \in \mathcal{F}$ has an optimal solution.

2.3 A Characterization of Convex Functions

Recall the definitions of convex sets and convex functions that we introduced in Chapter 1:

Definition 2.3.1. A set $S \subseteq \mathbb{R}^n$ is called a **convex set** if any two points in S contain their line, i.e. for any $\boldsymbol{x}, \boldsymbol{y} \in S$ we have that $\theta\boldsymbol{x} + (1-\theta)\boldsymbol{y} \in S$ for any $\theta \in [0, 1]$.

Definition 2.3.2. For a convex set $S \subseteq \mathbb{R}^n$, we say that a function $f : S \to \mathbb{R}$ is **convex on** S if for any two points $\boldsymbol{x}, \boldsymbol{y} \in S$ and any $\theta \in [0, 1]$ we have that:

$$f\left(\theta\boldsymbol{x} + (1-\theta)\boldsymbol{y}\right) \leq \theta f(\boldsymbol{x}) + \Big(1-\theta\Big) f(\boldsymbol{y}).$$

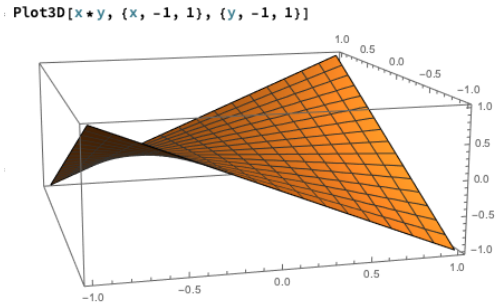


Figure 2.2: This plot shows the function $f(x, y) = xy$. For any fixed y_0, the function $h(x) = f(x, y_0) = xy_0$ is this is linear in x, and so is a convex function in x. But is f convex?

We will first give an important characterization of convex function. To do so, we need to characterize multivariate functions via their Taylor expansion.

Notation for this section. In the rest of this section, we frequently consider a multivariate function f whose domain is a set $S \subseteq \mathbb{R}^n$, which we will require to be open. When we additionally require that S is convex, we will specify this. Note that $S = \mathbb{R}^n$ is both open and convex and it suffices to keep this case in mind. Things sometimes get more complicated if S is not open, e.g. when the domain of f has a boundary. We will leave those complications for another time.

2.3.1 First-order Taylor Approximation

Definition 2.3.3. The **gradient** of a function $f : S \to \mathbb{R}$ at point $\boldsymbol{x} \in S$ is denoted $\boldsymbol{\nabla} f(\boldsymbol{x})$ is:

$$\boldsymbol{\nabla} f(\boldsymbol{x}) = \left[\frac{\partial f(\boldsymbol{x})}{\partial \boldsymbol{x}(1)}, \ldots, \frac{\partial f(\boldsymbol{x})}{\partial \boldsymbol{x}(n)}\right]^\top$$

First-order Taylor expansion. For a function $f : \mathbb{R} \to \mathbb{R}$ of a single variable, differentiable at $x \in \mathbb{R}$

$$f(x + \delta) = f(x) + f'(x)\delta + o(|\delta|)$$

where by definition:

$$\lim_{\delta \to 0} \frac{o(|\delta|)}{|\delta|} = 0.$$

Similarly, a multivariate function $f : S \to \mathbb{R}$ is said to be *(Fréchet) differentiable* at $\boldsymbol{x} \in S$ when there exists $\boldsymbol{\nabla} f(\boldsymbol{x}) \in \mathbb{R}^n$ s.t.

$$\lim_{\boldsymbol{\delta} \to \mathbf{0}} \frac{\left\| f(\boldsymbol{x} + \boldsymbol{\delta}) - f(\boldsymbol{x}) - \boldsymbol{\nabla} f(\boldsymbol{x})^\top \boldsymbol{\delta} \right\|_2}{\|\boldsymbol{\delta}\|_2} = 0.$$

Note that this is equivalent to saying that $f(\boldsymbol{x} + \boldsymbol{\delta}) = f(\boldsymbol{x}) + \boldsymbol{\nabla} f(\boldsymbol{x})^\top \boldsymbol{\delta} + o(\|\boldsymbol{\delta}\|_2)$.

We say that f is *continuously differentiable* on a set $S \subseteq \mathbb{R}^n$ if it is differentiable and in addition the gradient is continuous on S. A differentiable convex function whose domain is an open convex set $S \subseteq \mathbb{R}^n$ is always continuously differentiable[1].

Remark. In this course, we will generally err on the side of being informal about functional analysis when we can afford to, and we will not worry too much about the details of different notions of differentiability (e.g. Fréchet and Gateaux differentiability), except when it turns out to be important.

Theorem 2.3.4 (Taylor's Theorem, multivariate first-order remainder form)**.** *If $f : S \to \mathbb{R}$ is continuously differentiable over $[\boldsymbol{x}, \boldsymbol{y}]$, then for some $\boldsymbol{z} \in [\boldsymbol{x}, \boldsymbol{y}]$,*

$$f(\boldsymbol{y}) = f(\boldsymbol{x}) + \boldsymbol{\nabla} f(\boldsymbol{z})^\top (\boldsymbol{y} - \boldsymbol{x}).$$

[1] See p. 248, Corollary 25.5.1 in *Convex Analysis* by Rockafellar (my version is the Second print, 1972). Rockefellar's corollary concerns finite convex functions, because he otherwise allows convex functions that may take on the values $\pm\infty$.

This theorem is useful for showing that the function f can be approximated by the affine function $\boldsymbol{y} \to f(\boldsymbol{x}) + \boldsymbol{\nabla} f(\boldsymbol{x})^\top (\boldsymbol{y} - \boldsymbol{x})$ when $\boldsymbol{y}$ is "close to" $\boldsymbol{x}$ in some sense.

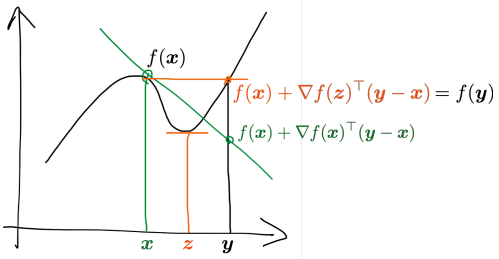


Figure 2.3: The convex function $f(\boldsymbol{y})$ sits above the linear function in $\boldsymbol{y}$ given by $f(\boldsymbol{x}) + \boldsymbol{\nabla} f(\boldsymbol{x})^\top (\boldsymbol{y} - \boldsymbol{x})$.

2.3.2 Directional Derivatives

Definition 2.3.5. Let $f : S \to \mathbb{R}$ be a function differentiable at $\boldsymbol{x} \in S$ and let us consider $\boldsymbol{d} \in \mathbb{R}^n$. We define the **derivative of f at $\boldsymbol{x}$ in direction $\boldsymbol{d}$** as:

$$Df(\boldsymbol{x})[\boldsymbol{d}] = \lim_{\lambda \to \boldsymbol{0}} \frac{f(\boldsymbol{x} + \lambda \boldsymbol{d}) - f(\boldsymbol{x})}{\lambda}$$

Proposition 2.3.6. $Df(\boldsymbol{x})[\boldsymbol{d}] = \boldsymbol{\nabla} f(\boldsymbol{x})^\top \boldsymbol{d}$.

Proof. Using the first order expansion of f at $\boldsymbol{x}$:

$$f(\boldsymbol{x} + \lambda \boldsymbol{d}) = f(\boldsymbol{x}) + \boldsymbol{\nabla} f(\boldsymbol{x})^\top (\lambda \boldsymbol{d}) + o(\|\lambda \boldsymbol{d}\|_2)$$

hence, dividing by λ (and noticing that $\|\lambda \boldsymbol{d}\|_2 = \lambda \|\boldsymbol{d}\|_2$):

$$\frac{f(\boldsymbol{x} + \lambda \boldsymbol{d}) - f(\boldsymbol{x})}{\lambda} = \boldsymbol{\nabla} f(\boldsymbol{x})^\top \boldsymbol{d} + \frac{o(\lambda \|\boldsymbol{d}\|_2)}{\lambda}$$

letting λ go to 0 concludes the proof. □

2.3.3 Lower Bounding Convex Functions with Affine Functions

In order to prove the characterization of convex functions in the next section we will need the following lemma. This lemma says that any differentiable convex function can be lower bounded by an affine function.

Theorem 2.3.7. *Let S be an open convex subset of $\mathbb{R}^n$, and let $f : S \to \mathbb{R}$ be a differentiable function. Then, f is convex if and only if for any $\boldsymbol{x}, \boldsymbol{y} \in S$ we have that $f(\boldsymbol{y}) \geq f(\boldsymbol{x}) + \boldsymbol{\nabla} f(\boldsymbol{x})^\top (\boldsymbol{y} - \boldsymbol{x})$.*

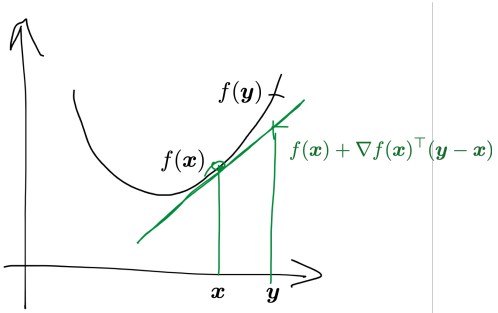


Figure 2.4: The convex function $f(\boldsymbol{y})$ sits above the linear function in $\boldsymbol{y}$ given by $f(\boldsymbol{x}) + \boldsymbol{\nabla} f(\boldsymbol{x})^\top(\boldsymbol{y} - \boldsymbol{x})$.

Proof. [$\implies$] Assume f is convex, then for all $\mathbf{x}, \mathbf{y} \in S$ and $\theta \in [0, 1]$, if we let $\mathbf{z} = \theta\boldsymbol{y} + (1-\theta)\boldsymbol{x}$, we have that

$$f(\mathbf{z}) = f((1-\theta)\boldsymbol{x} + \theta\boldsymbol{y}) \leq (1-\theta)f(\boldsymbol{x}) + \theta f(\boldsymbol{y})$$

and therefore by subtracting $f(\boldsymbol{x})$ from both sides we get:

$$\begin{aligned} f\left(\boldsymbol{x} + \theta(\boldsymbol{y} - \boldsymbol{x})\right) - f(\boldsymbol{x}) &\leq \theta f(\boldsymbol{y}) + (1-\theta)f(\boldsymbol{x}) - f(\boldsymbol{x}) \\ &= \theta f(\boldsymbol{y}) - \theta f(\boldsymbol{x}). \end{aligned}$$

Thus we get that (for $\theta > 0$):

$$\frac{f\left(\boldsymbol{x} + \theta(\boldsymbol{y} - \boldsymbol{x})\right) - f(\boldsymbol{x})}{\theta} \leq f(\boldsymbol{y}) - f(\boldsymbol{x})$$

Applying Proposition 2.3.6 with $\boldsymbol{d} = \boldsymbol{x} - \boldsymbol{y}$ we have that:

$$\boldsymbol{\nabla} f(\boldsymbol{x})^\top(\boldsymbol{y} - \boldsymbol{x}) = \lim_{\theta \to 0^+} \frac{f(\boldsymbol{x} + \theta(\boldsymbol{y} - \boldsymbol{x})) - f(\boldsymbol{x})}{\theta} \leq f(\boldsymbol{y}) - f(\boldsymbol{x}).$$

[$\impliedby$] Assume that $f(\boldsymbol{y}) \geq f(\boldsymbol{x}) + \boldsymbol{\nabla} f(\boldsymbol{x})^\top(\boldsymbol{y} - \boldsymbol{x})$ for all $\mathbf{x}, \mathbf{y} \in S$ and show that f is convex. Let $\mathbf{x}, \mathbf{y} \in S$ and $\mathbf{z} = \theta\boldsymbol{y} + (1-\theta)\boldsymbol{x}$. By our assumption we have that:

$$f(\boldsymbol{y}) \geq f(\boldsymbol{z}) + \boldsymbol{\nabla} f(\boldsymbol{z})^\top(\boldsymbol{y} - \mathbf{z}) \tag{2.1}$$

$$f(\boldsymbol{x}) \geq f(\boldsymbol{z}) + \boldsymbol{\nabla} f(\boldsymbol{z})^\top(\boldsymbol{x} - \mathbf{z}) \tag{2.2}$$

Observe that $\boldsymbol{y} - \boldsymbol{z} = (1-\theta)(\boldsymbol{y} - \boldsymbol{x})$ and $\boldsymbol{x} - \boldsymbol{z} = \theta(\boldsymbol{y} - \boldsymbol{x})$. Thus adding θ times (2.1) to $(1-\theta)$ times (2.2) gives cancellation of the vectors multiplying the gradient, yielding

$$\begin{aligned} \theta f(\boldsymbol{y}) + (1-\theta)f(\boldsymbol{x}) &\geq f(\boldsymbol{z}) + \boldsymbol{\nabla} f(\boldsymbol{z})^\top \mathbf{0} \\ &= f(\theta\boldsymbol{y} + (1-\theta)\boldsymbol{x}) \end{aligned}$$

This is exactly the definition of convexity. □

2.4 Conditions for Optimality

We now want to find necessary and sufficient conditions for local optimality.

Definition 2.4.1. Consider a differentiable function $f : S \to \mathbb{R}$. A point $\boldsymbol{x} \in S$ at which $\boldsymbol{\nabla} f(\boldsymbol{x}) = \mathbf{0}$ is called a **stationary point**.

Proposition 2.4.2. *If $\boldsymbol{x}$ is a local extremum of a differentiable function $f : S \to \mathbb{R}$ then $\boldsymbol{\nabla} f(\boldsymbol{x}) = \mathbf{0}$.*

Proof. Let us assume that $\boldsymbol{x}$ is a local minimum for f. Then for all $\boldsymbol{d} \in \mathbb{R}^n$, $f(\boldsymbol{x}) \leq f(\boldsymbol{x}+\lambda \boldsymbol{d})$ for λ small enough. Hence:

$$0 \leq f(\boldsymbol{x} + \lambda \boldsymbol{d}) - f(\boldsymbol{x}) = \lambda \boldsymbol{\nabla} f(\boldsymbol{x})^\top \boldsymbol{d} + o(\|\lambda \boldsymbol{d}\|)$$

dividing by $\lambda > 0$ and letting $\lambda \to 0^+$, we obtain $0 \leq \boldsymbol{\nabla} f(\boldsymbol{x})^\top \boldsymbol{d}$. But, taking $\boldsymbol{d} = -\boldsymbol{\nabla} f(\boldsymbol{x})$, we get $0 \leq -\|\boldsymbol{\nabla} f(\boldsymbol{x})\|_2^2$. This implies that $\boldsymbol{\nabla} f(\boldsymbol{x}) = \mathbf{0}$.

The case where $\boldsymbol{x}$ is a local maximum can be dealt with similarly. □

Remark 2.4.3. For this proposition to hold, it is important that S is open.

For convex functions however it turns out that a stationary point necessarily implies that the function is at its minimum. Together with the proposition above, this says that for a convex function on $\mathbb{R}^n$ a point is optimal if and only if it is stationary.

Proposition 2.4.4. *Let $S \subseteq \mathbb{R}^n$ be an open convex set and let $f : S \to \mathbb{R}$ be a differentiable and convex function. If $\boldsymbol{x}$ is a stationary point then $\boldsymbol{x}$ is a global minimum.*

Proof. From Theorem 3.3.5 we know that for all $\boldsymbol{x}, \boldsymbol{y} \in S$: $f(\boldsymbol{y}) \geq f(\boldsymbol{x}) + \boldsymbol{\nabla} f(\boldsymbol{x})(\boldsymbol{y} - \boldsymbol{x})$. Since $\boldsymbol{\nabla} f(\boldsymbol{x}) = \mathbf{0}$ this implies that $f(\boldsymbol{y}) \geq f(\boldsymbol{x})$. As this holds for any $\boldsymbol{y} \in S$, $\boldsymbol{x}$ is a global minimum.

□

Chapter 3

Convexity and Second Derivatives, Gradient Descent and Acceleration

Notation for this chapter. In this chapter, we sometimes consider a multivariate function f whose domain is a set $S \subseteq \mathbb{R}^n$, which we will require to be open. When we additionally require that S is convex, we will specify this. Note that $S = \mathbb{R}^n$ is both open and convex and it suffices to keep this case in mind. Things sometimes get more complicated if S is not open, e.g. when the domain of f has a boundary. We will leave those complications for another time.

3.1 A Review of Linear Algebra

Semi-definiteness of a matrix. The following classification of symmetric matrices will be useful.

Definition 3.1.1. Let $\boldsymbol{A}$ by a symmetric matrix in $\mathbb{R}^{n\times n}$. We say that $\boldsymbol{A}$ is:

1. *positive definite* iff $\boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x} > 0$ for all $x \in \mathbb{R}^n \setminus \{0\}$;
2. *positive semidefinite* iff $\boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x} \geq 0$ for all $x \in \mathbb{R}^n$;
3. If neither $\boldsymbol{A}$ nor $-\boldsymbol{A}$ is positive semi-definite, we say that $\boldsymbol{A}$ is *indefinite*.

Example: indefinite matrix. Consider the following matrix $\boldsymbol{A}$:

$$\boldsymbol{A} := \begin{bmatrix} +4 & -1 \\ -1 & -2 \end{bmatrix}$$

For $\boldsymbol{x} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, we have $\boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x} = 4 > 0$. For $\boldsymbol{x} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ we have $\boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x} = -2 < 0$. $\boldsymbol{A}$ is therefore indefinite.

The following theorem gives a useful characterization of (semi)definite matrices.

Theorem 3.1.2. *Let $\boldsymbol{A}$ be a symmetric matrix in $\mathbb{R}^{n\times n}$.*

1. *$\boldsymbol{A}$ is positive definite iff all its eigenvalues are positive;*
2. *$\boldsymbol{A}$ is positive semidefinite iff all its eigenvalues are non-negative;*

In order to prove this theorem, let us first recall the Spectral Theorem for symmetric matrices.

Theorem 3.1.3 (The Spectral Theorem for Symmetric Matrices)**.** *For all symmetric $\boldsymbol{A} \in \mathbb{R}^{n\times n}$ there exist $\boldsymbol{V} \in \mathbb{R}^{n\times n}$ and a diagonal matrix $\boldsymbol{\Lambda} \in \mathbb{R}^{n\times n}$ s.t.*

1. *$\boldsymbol{A} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^\top$.*
2. *$\boldsymbol{V}^\top\boldsymbol{V} = \boldsymbol{I}$ (the $n \times n$ identity matrix). I.e. the columns of $\boldsymbol{V}$ form an orthonormal basis. Furthermore, $\boldsymbol{v}_i$ is an eigenvector of $\lambda_i(\boldsymbol{A})$, the ith eigenvalue of $\boldsymbol{A}$.*
3. *$\boldsymbol{\Lambda}_{ii} = \lambda_i(\boldsymbol{A})$.*

Using the Spectral Theorem, we can show the following result:

Theorem 3.1.4 (The Courant-Fischer Theorem)**.** *Let $\boldsymbol{A}$ be a symmetric matrix in $\mathbb{R}^{n\times n}$, with eigenvalues $\lambda_1 \le \lambda_2 \le \ldots \le \lambda_n$. Then*

1. $$\lambda_i = \min_{\substack{\text{subspace } W\subseteq\mathbb{R}^n \\ \dim(W)=i}} \max_{\boldsymbol{x}\in W, \boldsymbol{x}\neq\boldsymbol{0}} \frac{\boldsymbol{x}^\top\boldsymbol{A}\boldsymbol{x}}{\boldsymbol{x}^\top\boldsymbol{x}}$$
2. $$\lambda_i = \max_{\substack{\text{subspace } W\subseteq\mathbb{R}^n \\ \dim(W)=n+1-i}} \min_{\boldsymbol{x}\in W, \boldsymbol{x}\neq\boldsymbol{0}} \frac{\boldsymbol{x}^\top\boldsymbol{A}\boldsymbol{x}}{\boldsymbol{x}^\top\boldsymbol{x}}$$

Theorem 3.1.2 is an immediate corollary of Theorem 4.1.1, since we can see that the minimum value of the quadratic form $\boldsymbol{x}^\top\boldsymbol{A}\boldsymbol{x}$ over $\boldsymbol{x} \in W = \mathbb{R}^n$ is $\lambda_1(\boldsymbol{A})\|\boldsymbol{x}\|_2^2$.

Proof of Theorem 4.1.1. We start by showing Part 1.

Consider letting $W = \operatorname{span}\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_i\}$, and normalize $\boldsymbol{x} \in W$ so that $\|\boldsymbol{x}\|_2 = 1$. Then $\boldsymbol{x} = \sum_{j=1}^{i} \boldsymbol{c}(j)\boldsymbol{v}_j$ for some vector $\boldsymbol{c} \in \mathbb{R}^i$ with $\|\boldsymbol{c}\|_2 = 1$.

Using the decomposition from Theorem 3.1.3 $\boldsymbol{A} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^\top$ where $\boldsymbol{\Lambda}$ is a diagonal matrix of eigenvalues of $\boldsymbol{A}$, which we take to be sorted in increasing order. Then $\boldsymbol{x}^\top\boldsymbol{A}\boldsymbol{x} = \boldsymbol{x}^\top\boldsymbol{V}^\top\boldsymbol{\Lambda}\boldsymbol{V}\boldsymbol{x} = (\boldsymbol{V}\boldsymbol{x})^\top\boldsymbol{\Lambda}(\boldsymbol{V}\boldsymbol{x}) = \sum_{j=1}^{i}\lambda_j\boldsymbol{c}(j)^2 \le \lambda_i\|\boldsymbol{c}\|_2^2 = \lambda_i$. So this choice of W ensures the maximizer cannot achieve a value above λ_i.

But is it possible that the "minimizer" can do better by choosing a different W? Let $T = \text{span}\{\boldsymbol{v}_i, \ldots, \boldsymbol{v}_n\}$. As $\dim(T) = n+1-i$ and $\dim(W) = i$, we must have $\dim(W \cap T) \geq 1$, by a standard property of subspaces. Hence for any W of this dimension,

$$\begin{aligned}\max_{\boldsymbol{x} \in W, \boldsymbol{x} \neq \boldsymbol{0}} \frac{\boldsymbol{x}^\top \boldsymbol{A} \boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}} &\geq \max_{\boldsymbol{x} \in W \cap T, \boldsymbol{x} \neq \boldsymbol{0}} \frac{\boldsymbol{x}^\top \boldsymbol{A} \boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}} \\ &\geq \min_{\substack{\text{subspace } V \subseteq T \\ \dim(V)=1}} \max_{\boldsymbol{x} \in V, \boldsymbol{x} \neq \boldsymbol{0}} \frac{\boldsymbol{x}^\top \boldsymbol{A} \boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}} = \lambda_i,\end{aligned}$$

where the last equality follows from a similar calculation to our first one. Thus, λ_i can always be achieved by the "maximizer" for all W of this dimension.

Part 2 can be dealt with similarly.

□

Example: a positive semidefinite matrix. Consider the following matrix $\boldsymbol{A}$:

$$\boldsymbol{A} := \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

For $\boldsymbol{x} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, we have $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{0}$, so $\lambda = 0$ is an eigenvalue of $\boldsymbol{A}$. For $\boldsymbol{x} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$, we have $\boldsymbol{A}\boldsymbol{x} = \begin{pmatrix} 2 \\ -2 \end{pmatrix} = 2\boldsymbol{x}$, so $\lambda = 2$ is the other eigenvalue of $\boldsymbol{A}$. As both are non-negative, by the theorem above, $\boldsymbol{A}$ is positive semidefinite.

Since we are learning about symmetric matrices, there is one more fact that everyone should know about them. We'll use $\lambda_{\max}(\boldsymbol{A})$ denote maximum eigenvalue of a matrix $\boldsymbol{A}$, and $\lambda_{\min}(\boldsymbol{A})$ the minimum.

Claim 3.1.5. *For a symmetric matrix $\boldsymbol{A} \in \mathbb{R}^{n \times n}$, $\|\boldsymbol{A}\| = \max(|\lambda_{\max}(\boldsymbol{A})|, |\lambda_{\min}(\boldsymbol{A})|)$.*

3.2 Characterizations of Convexity and Optimality via Second Derivatives

We will now use the second derivatives of a function to obtain characterizations of convexity and optimality. We will begin by introducing the *Hessian*, the matrix of pairwise second derivatives of a function. We will see that it plays a role in approximating a function via a second-order Taylor expansion. We will then use *semi-definiteness* of the Hessian matrix to characterize both conditions of optimality as well as the convexity of a function.

Definition 3.2.1. Given a function $f : S \to \mathbb{R}$ its **Hessian** matrix at point $\boldsymbol{x} \in S$ denoted $\boldsymbol{H}_f(\boldsymbol{x})$ (also sometimes denoted $\boldsymbol{\nabla}^2 f(\boldsymbol{x})$) is:

$$\boldsymbol{H}_f(\boldsymbol{x}) := \begin{bmatrix} \frac{\partial^2 f(\boldsymbol{x})}{\partial \boldsymbol{x}(1)^2} & \frac{\partial^2 f(\boldsymbol{x})}{\partial \boldsymbol{x}(1)\partial \boldsymbol{x}(2)} & \cdots & \frac{\partial^2 f(\boldsymbol{x})}{\partial \boldsymbol{x}(1)\partial \boldsymbol{x}(n)} \\ \frac{\partial^2 f(\boldsymbol{x})}{\partial \boldsymbol{x}(2)\partial \boldsymbol{x}(1)} & \frac{\partial^2 f(\boldsymbol{x})}{\partial \boldsymbol{x}(2)^2} & \cdots & \frac{\partial^2 f(\boldsymbol{x})}{\partial \boldsymbol{x}(2)\partial \boldsymbol{x}(n)} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(\boldsymbol{x})}{\partial \boldsymbol{x}(n)\partial \boldsymbol{x}(1)} & \frac{\partial^2 f(\boldsymbol{x})}{\partial \boldsymbol{x}(n)\partial \boldsymbol{x}(2)} & \cdots & \frac{\partial^2 f(\boldsymbol{x})}{\partial \boldsymbol{x}(n)^2} \end{bmatrix}$$

Second-order Taylor expansion. When f is twice differentiable it is possible to obtain an approximation of f by quadratic functions. Our definition of $f : S \to \mathbb{R}$ being twice (Fréchet) differentiable at $\boldsymbol{x} \in S$ is that there exists $\boldsymbol{\nabla} f(\boldsymbol{x}) \in \mathbb{R}^n$ and $\boldsymbol{H}_f(\boldsymbol{x}) \in R^{n \times n}$ s.t.

$$\lim_{\boldsymbol{\delta} \to \boldsymbol{0}} \frac{\left\| f(\boldsymbol{x} + \boldsymbol{\delta}) - f(\boldsymbol{x}) - \left(\boldsymbol{\nabla} f(\boldsymbol{x})^\top \boldsymbol{\delta} + \frac{1}{2} \boldsymbol{\delta}^\top \boldsymbol{H}_f(\boldsymbol{x}) \boldsymbol{\delta} \right) \right\|_2}{\|\boldsymbol{\delta}\|_2^2} = 0.$$

This is equivalent to saying that for all $\boldsymbol{\delta}$

$$f(\boldsymbol{x} + \boldsymbol{\delta}) = f(\boldsymbol{x}) + \boldsymbol{\nabla} f(\boldsymbol{x})^\top \boldsymbol{\delta} + \frac{1}{2} \boldsymbol{\delta}^\top \boldsymbol{H}_f(\boldsymbol{x}) \boldsymbol{\delta} + o(\|\boldsymbol{\delta}\|_2^2).$$

where by definition:

$$\lim_{\boldsymbol{\delta} \to \boldsymbol{0}} \frac{o(\|\boldsymbol{\delta}\|^2)}{\|\boldsymbol{\delta}\|_2^2} = 0$$

We say that f is *continuously differentiable* on a set $S \subseteq \mathbb{R}^n$ if it is twice differentiable and in addition the gradient and Hessian are continuous on S.

As for first order expansions, we have a Taylor's Theorem, which we state in the so-called remainder form.

Theorem 3.2.2 (Taylor's Theorem, multivariate second-order remainder form)**.** *If $f : S \to \mathbb{R}$ is twice continuously differentiable over $[\boldsymbol{x}, \boldsymbol{y}]$, then for some $\boldsymbol{z} \in [\boldsymbol{x}, \boldsymbol{y}]$,*

$$f(\boldsymbol{y}) = f(\boldsymbol{x}) + \boldsymbol{\nabla} f(\boldsymbol{x})^\top (\boldsymbol{y} - \boldsymbol{x}) + \frac{1}{2} (\boldsymbol{y} - \boldsymbol{x})^\top \boldsymbol{H}_f(\boldsymbol{z}) (\boldsymbol{y} - \boldsymbol{x})$$

3.2.1 A Necessary Condition for Local Extrema

Recall that in the previous chapter, we show the following proposition.

Proposition 3.2.3. *If $\boldsymbol{x}$ is a local extremum of a differentiable function $f : S \to \mathbb{R}$ then $\boldsymbol{\nabla} f(\boldsymbol{x}) = \boldsymbol{0}$.*

We can now give the second-order necessary conditions for local extrema via the Hessian.

Theorem 3.2.4. *Let $f : S \to \mathbb{R}$ be a function twice differentiable at $\boldsymbol{x} \in S$. If $\boldsymbol{x}$ is a local minimum, then $\boldsymbol{H}_f(\boldsymbol{x})$ is positive semidefinite.*

Proof. Let us assume that $\boldsymbol{x}$ is a local minimum. We know from Proposition 3.2.3 that $\boldsymbol{\nabla} f(\boldsymbol{x}) = \boldsymbol{0}$, hence the second-order expansion at $\boldsymbol{x}$ takes the form:

$$f(\boldsymbol{x} + \lambda \boldsymbol{d}) = f(\boldsymbol{x}) + \lambda^2 \frac{1}{2} \boldsymbol{d}^\top \boldsymbol{H}_f(\boldsymbol{x}) \boldsymbol{d} + o(\lambda^2 \left\| \boldsymbol{d} \right\|_2^2)$$

Because $\boldsymbol{x}$ is a local minimum, we can then derive

$$0 \leq \lim_{\lambda \to 0^+} \frac{f(\boldsymbol{x} + \lambda \boldsymbol{d}) - f(\boldsymbol{x})}{\lambda^2} = \frac{1}{2} \boldsymbol{d}^\top \boldsymbol{H}_f(\boldsymbol{x}) \boldsymbol{d}$$

This is true for any $\boldsymbol{d}$, hence $\boldsymbol{H}_f(\boldsymbol{x})$ is positive semidefinite. □

Remark 3.2.5. Again, for this proposition to hold, it is important that S is open.

3.2.2 A sufficient condition for local extrema

A local minimum thus is a stationary point and has a positive semi-definite Hessian. The converse is almost true, but we need to strengthen the Hessian condition slightly.

Theorem 3.2.6. *Let $f : S \to \mathbb{R}$ be a function twice differentiable at a stationary point $\boldsymbol{x} \in S$. If $\boldsymbol{H}_f(\boldsymbol{x})$ is positive definite then $\boldsymbol{x}$ is a local minimum.*

Proof. Let us assume that $\boldsymbol{H}_f(\boldsymbol{x})$ is positive definite. We know that $\boldsymbol{x}$ is a stationary point. We can write the second-order expansion at $\boldsymbol{x}$:

$$f(\boldsymbol{x} + \boldsymbol{\delta}) = f(\boldsymbol{x}) + \frac{1}{2} \boldsymbol{\delta}^\top \boldsymbol{H}_f(\boldsymbol{x}) \boldsymbol{\delta} + o(\left\| \boldsymbol{\delta} \right\|_2^2)$$

Because the Hessian is positive definite, it has a strictly positive minimum eigenvalue $\lambda_{\min}$, we can conclude that $\boldsymbol{\delta}^\top \boldsymbol{H}_f(\boldsymbol{x}) \boldsymbol{\delta} \geq \lambda_{\min} \left\| \boldsymbol{\delta} \right\|_2^2$. From this, we conclude that when $\left\| \boldsymbol{\delta} \right\|_2^2$ is small enough, $f(\boldsymbol{x} + \boldsymbol{\delta}) - f(\boldsymbol{x}) \geq \frac{1}{4} \lambda_{\min} \left\| \boldsymbol{\delta} \right\|_2^2 > 0$. This proves that $\boldsymbol{x}$ is a local minimum. □

Remark 3.2.7. When $\boldsymbol{H}_f(\boldsymbol{x})$ is indefinite at a stationary point $\boldsymbol{x}$, we have what is known as a *saddle point*: $\boldsymbol{x}$ will be a minimum along the eigenvectors of $\boldsymbol{H}_f(\boldsymbol{x})$ for which the eigenvalues are positive and a maximum along the eigenvectors of $\boldsymbol{H}_f(\boldsymbol{x})$ for which the eigenvalues are negative.

3.2.3 Characterization of convexity

Definition 3.2.8. For a convex set $S \subseteq R^n$, we say that a function $f : S \to \mathbb{R}$ is **strictly convex on** S if for any two points $\boldsymbol{x}_1, \boldsymbol{x}_2 \in S$ and any $\theta \in (0, 1)$ we have that:

$$f\left(\theta \boldsymbol{x}_1 + (1 - \theta) \boldsymbol{x}_2\right) < \theta f(\boldsymbol{x}_1) + \Big(1 - \theta\Big) f(\boldsymbol{x}_2).$$

Theorem 3.2.9. *Let $S \subseteq \mathbb{R}^n$ be open and convex, and let $f : S \to \mathbb{R}$ be twice continuously differentiable.*

1. *If $H_f(\boldsymbol{x})$ is positive semi-definite for any $\boldsymbol{x} \in S$ then f is convex on S.*
2. *If $H_f(\boldsymbol{x})$ is positive definite for any $\boldsymbol{x} \in S$ then f is **strictly** convex on S.*
3. *If f is convex, then $H_f(\boldsymbol{x})$ is positive semi-definite $\forall \boldsymbol{x} \in S$.*

Proof.

1. By applying Theorem 3.2.2, we find that for some $\boldsymbol{z} \in [\boldsymbol{x}, \boldsymbol{y}]$:

$$f(\boldsymbol{y}) = f(\boldsymbol{x}) + \boldsymbol{\nabla} f(\boldsymbol{x})^\top (\boldsymbol{y} - \boldsymbol{x}) + \frac{1}{2}\Big((\boldsymbol{y} - \boldsymbol{x})^\top H_f(\boldsymbol{z})(\boldsymbol{y} - \boldsymbol{x})\Big)$$

   If $H_f(\boldsymbol{z})$ is positive semi-definite, this necessarily implies that:

$$f(\boldsymbol{y}) \geq f(\boldsymbol{x}) + \boldsymbol{\nabla} f(\boldsymbol{x})^\top (\boldsymbol{y} - \boldsymbol{x})$$

   and from Theorem 3.3.5 we get that f is convex.

2. if $H_f(\boldsymbol{x})$ is positive definite, we have that:

$$f(\boldsymbol{y}) > f(\boldsymbol{x}) + \boldsymbol{\nabla} f(\boldsymbol{x})^\top (\boldsymbol{y} - \boldsymbol{x}).$$

   Applying the same idea as in Theorem 3.3.5 we can show that in this case f is **strictly** convex.

3. Let f be a convex function. For $\boldsymbol{x} \in S$, and some small $\lambda > 0$, for any $\mathbf{d} \in \mathbb{R}^n$ we have that $\boldsymbol{x} + \lambda \mathbf{d} \in S$. From the Taylor expansion of f we get:

$$f(\boldsymbol{x} + \lambda \mathbf{d}) = f(\boldsymbol{x}) + \lambda \boldsymbol{\nabla} f(\boldsymbol{x})^\top \mathbf{d} + \frac{\lambda^2}{2} \mathbf{d}^\top H_f(\boldsymbol{x}) \mathbf{d} + o(\lambda^2 \left\| \boldsymbol{d} \right\|_2^2).$$

   From Lemma 3.3.5 we get that if f is convex then:

$$f(\boldsymbol{x} + \lambda \mathbf{d}) \geq f(\boldsymbol{x}) + \lambda \boldsymbol{\nabla} f(\boldsymbol{x})^\top \mathbf{d}.$$

   Therefore, we have that for any $\mathbf{d} \in \mathbb{R}^n$:

$$\frac{\lambda^2}{2} \mathbf{d}^\top H_f(\boldsymbol{x}) \mathbf{d} + o(||\lambda \mathbf{d}||^2) \geq 0$$

   Dividing by λ^2 and taking $\lambda \to 0^+$ gives us that for any $\mathbf{d} \in \mathbb{R}^n$: $\mathbf{d}^\top H_f(\boldsymbol{x}) \mathbf{d} \geq 0$. □

Remark 3.2.10. It is important to note that if S is open and f is strictly convex, then $\boldsymbol{H}_f(\boldsymbol{x})$ may still (only) be positive semi-definite $\forall \boldsymbol{x} \in S$. Consider $f(x) = x^4$ which is strictly convex, then the Hessian is $\boldsymbol{H}_f(x) = 12x^2$ which equals 0 at $x = 0$.

3.3 Gradient Descent - An Approach to Optimization?

We have begun to develop an understanding of convex functions, and what we have learned already suggests a way for us to try to find an approximate minimizer of a given convex function.

Suppose $f : \mathbb{R}^n \to \mathbb{R}$ is convex and differentiable, and we want to solve

$$\min_{\boldsymbol{x} \in \mathbb{R}^n} f(\boldsymbol{x})$$

We would like to find $\boldsymbol{x}^*$, a global minimizer of f. Suppose we start with some initial guess $\boldsymbol{x}_0$, and we want to update it to $\boldsymbol{x}_1$ with $f(\boldsymbol{x}_1) < f(\boldsymbol{x}_0)$. If we can repeatedly make updates like this, maybe we eventually find a point with nearly minimum function value, i.e. some $\tilde{\boldsymbol{x}}$ with $f(\tilde{\boldsymbol{x}}) \approx f(\boldsymbol{x}^*)$?

Recall that $f(\boldsymbol{x}_0 + \boldsymbol{\delta}) = f(\boldsymbol{x}_0) + \boldsymbol{\nabla} f(\boldsymbol{x}_0)^\top \boldsymbol{\delta} + o(\|\boldsymbol{\delta}\|_2)$. This means that if we choose $\boldsymbol{x}_1 = \boldsymbol{x}_0 - \lambda \boldsymbol{\nabla} f(\boldsymbol{x}_0)$, we get

$$f(\boldsymbol{x}_0 - \lambda \boldsymbol{\nabla} f(\boldsymbol{x}_0)) = f(\boldsymbol{x}_0) - \lambda \|\boldsymbol{\nabla} f(\boldsymbol{x}_0)\|_2^2 + o(\lambda \|\boldsymbol{\nabla} f(\boldsymbol{x}_0)\|_2)$$

And because f is convex, we know that $\boldsymbol{\nabla} f(\boldsymbol{x}_0) \neq \mathbf{0}$ unless we are already at a global minimum. So, for some small enough $\lambda > 0$, we should get $f(\boldsymbol{x}_1) < f(\boldsymbol{x}_0)$ unless we're already at a global minimizer. This idea of taking a step in the direction of $-\boldsymbol{\nabla} f(\boldsymbol{x}_0)$ is what is called *Gradient Descent*. But how do we choose λ each time? And does this lead to an algorithm that quickly reaches a point with close to minimal function value? To get good answers to these questions, we need to assume more about the function f that we are trying to minimize.

In the following subsection, we will see some conditions that suffice. But there are also many other settings where one can show that some form of gradient descent converges.

3.3.1 A Quantitative Bound on Changes in the Gradient

Definition 3.3.1. Let $f : S \to \mathbb{R}$ be a differentiable function, where $S \subseteq \mathbb{R}^n$ is convex and open. We say that f is *β-gradient Lipschitz* iff for all $\boldsymbol{x}, \boldsymbol{y} \in S$

$$\|\boldsymbol{\nabla} f(\boldsymbol{x}) - \boldsymbol{\nabla} f(\boldsymbol{y})\|_2 \leq \beta \|\boldsymbol{x} - \boldsymbol{y}\|_2 .$$

We also refer to this as f being *β-smooth*.

Proposition 3.3.2. *Consider a twice continuously differentiable $f : S \to \mathbb{R}$. Then f is β-gradient Lipschitz if and only if for all $\boldsymbol{x} \in S$, $\|\boldsymbol{H}_f(\boldsymbol{x})\| \leq \beta$.*

You will prove this in Exercise 13 (Week 2) of the first exercise set.

Proposition 3.3.3. *Let $f : S \to \mathbb{R}$ be a β-gradient Lipschitz function. Then for all $\boldsymbol{x}, \boldsymbol{y} \in S$,*

$$f(\boldsymbol{y}) \leq f(\boldsymbol{x}) + \boldsymbol{\nabla} f(\boldsymbol{x})^\top (\boldsymbol{y} - \boldsymbol{x}) + \frac{\beta}{2} \|\boldsymbol{x} - \boldsymbol{y}\|_2^2$$

To prove this proposition, we need the following result from multi-variate calculus. This is a restricted form of the fundamental theorem of calculus for line integrals.

Proposition 3.3.4. *Let $f : S \to \mathbb{R}$ be a differentiable function, and consider $\boldsymbol{x}, \boldsymbol{y}$ such that $[\boldsymbol{x}, \boldsymbol{y}] \in S$. Let $\boldsymbol{x}_\theta = \boldsymbol{x} + \theta(\boldsymbol{y} - \boldsymbol{x})$. Then*

$$f(\boldsymbol{y}) = f(\boldsymbol{x}) + \int_{\theta=0}^{1} \boldsymbol{\nabla} f(\boldsymbol{x}_\theta)^\top (\boldsymbol{y} - \boldsymbol{x}) d\theta$$

Now, we're in a position to show Proposition 3.3.3

Proof of Proposition 3.3.3. Let $f : S \to \mathbb{R}$ be a β-gradient Lipschitz function. Consider arbitrary $\boldsymbol{x}, \boldsymbol{y} \in S$ such that $[\boldsymbol{x}, \boldsymbol{y}] \in S$

$$\begin{aligned}
f(\boldsymbol{y}) &= f(\boldsymbol{x}) + \int_{\theta=0}^{1} \boldsymbol{\nabla} f(\boldsymbol{x}_\theta)^\top (\boldsymbol{y} - \boldsymbol{x}) d\theta \\
&= f(\boldsymbol{x}) + \int_{\theta=0}^{1} \boldsymbol{\nabla} f(\boldsymbol{x})^\top (\boldsymbol{y} - \boldsymbol{x}) d\theta + \int_{\theta=0}^{1} (\boldsymbol{\nabla} f(\boldsymbol{x}_\theta) - \boldsymbol{\nabla} f(\boldsymbol{x}))^\top (\boldsymbol{y} - \boldsymbol{x}) d\theta \\
&\qquad \text{Next we use Cauchy-Schwarz pointwise.} \\
&\qquad \text{We also evaluate the first integral.} \\
&\leq f(\boldsymbol{x}) + \boldsymbol{\nabla} f(\boldsymbol{x})^\top (\boldsymbol{y} - \boldsymbol{x}) + \int_{\theta=0}^{1} \|\boldsymbol{\nabla} f(\boldsymbol{x}_\theta) - \boldsymbol{\nabla} f(\boldsymbol{x})\| \, \|\boldsymbol{y} - \boldsymbol{x}\| \, d\theta \\
&\qquad \text{Then we apply } \beta\text{-gradient Lipschitz and note } \boldsymbol{x}_\theta - \boldsymbol{x} = \theta(\boldsymbol{y} - \boldsymbol{x}). \\
&\leq f(\boldsymbol{x}) + \boldsymbol{\nabla} f(\boldsymbol{x})^\top (\boldsymbol{y} - \boldsymbol{x}) + \int_{\theta=0}^{1} \beta\theta \, \|\boldsymbol{y} - \boldsymbol{x}\|^2 \, d\theta. \\
&= f(\boldsymbol{x}) + \boldsymbol{\nabla} f(\boldsymbol{x})^\top (\boldsymbol{y} - \boldsymbol{x}) + \frac{\beta}{2} \|\boldsymbol{y} - \boldsymbol{x}\|^2 .
\end{aligned}$$

□

3.3.2 Analyzing Gradient Descent

It turns out that just knowing a function $f : \mathbb{R}^n \to \mathbb{R}$ is convex and β-gradient Lipschitz is enough to let us figure out a reasonable step size for Gradient Descent and let us analyze its convergence.

We start at a point $\boldsymbol{x}_0 \in \mathbb{R}^n$, and we try to find a point $\boldsymbol{x}_1 = \boldsymbol{x}_0 + \boldsymbol{\delta}$ with lower function value. We will let our upper bound from Proposition 3.3.3 guide us, in fact, we could ask, what is the *best* update for minimizing this upper bound, i.e. a $\boldsymbol{\delta}$ solving

$$\min_{\boldsymbol{\delta} \in \mathbb{R}^n} f(\boldsymbol{x}_0) + \boldsymbol{\nabla} f(\boldsymbol{x}_0)^\top \boldsymbol{\delta} + \frac{\beta}{2} \|\boldsymbol{\delta}\|^2$$

We can compute the best according to this upper bound by noting first that function is convex and continuously differentiable, and hence will be minimized at any point where the gradient is zero. Thus we want $\mathbf{0} = \boldsymbol{\nabla}_{\boldsymbol{\delta}} \left(f(\boldsymbol{x}_0) + \boldsymbol{\nabla} f(\boldsymbol{x}_0)^\top \boldsymbol{\delta} + \frac{\beta}{2} \|\boldsymbol{\delta}\|^2 \right) = \boldsymbol{\nabla} f(\boldsymbol{x}_0) + \beta \boldsymbol{\delta}$, which occurs at $\boldsymbol{\delta} = -\frac{1}{\beta} \boldsymbol{\nabla} f(\boldsymbol{x}_0)$.

Plugging in this value into the upper bound, we get that $f(\boldsymbol{x}_1) \leq f(\boldsymbol{x}_0) - \|\boldsymbol{\nabla} f(\boldsymbol{x}_0)\|_2^2 / 2\beta$.

Now, as our algorithm, we will start with some guess $\boldsymbol{x}_0$, and then at every step we will update our guess using the best step based on our Proposition 3.3.3 upper bound on f at $\boldsymbol{x}_i$, and so we get

$$\boldsymbol{x}_{i+1} = \boldsymbol{x}_i - \frac{1}{\beta} \boldsymbol{\nabla} f(\boldsymbol{x}_i) \text{ and } f(\boldsymbol{x}_{i+1}) \leq f(\boldsymbol{x}_i) - \frac{\|\boldsymbol{\nabla} f(\boldsymbol{x}_i)\|_2^2}{2\beta}. \tag{3.1}$$

Let us try to prove that our algorithm converges toward an $\boldsymbol{x}$ with low function value.

We will measure this by looking at

$$\text{gap}_i = f(\boldsymbol{x}_i) - f(\boldsymbol{x}^*)$$

where $\boldsymbol{x}^*$ is a global minimizer of f (note that there may not be a unique minimizer of f). We will try to show that this function value gap grows small. Using $f(\boldsymbol{x}_{i+1}) - f(\boldsymbol{x}_i) = \text{gap}_{i+1} - \text{gap}_i$, we get

$$\text{gap}_{i+1} - \text{gap}_i \leq -\frac{\|\boldsymbol{\nabla} f(\boldsymbol{x}_i)\|_2^2}{2\beta} \tag{3.2}$$

If the gap_i value is never too much bigger than $\frac{\|\boldsymbol{\nabla} f(\boldsymbol{x}_i)\|_2^2}{2\beta}$, then this should help us show we are making progress. But how much can they differ? We will now try to show a limit on this.

Recall that in the previous chapter we showed the following theorem.

Theorem 3.3.5. *Let S be an open convex subset of $\mathbb{R}^n$, and let $f : S \to \mathbb{R}$ be a differentiable function. Then, f is convex if and only if for any $\boldsymbol{x}, \boldsymbol{y} \in S$ we have that $f(\boldsymbol{y}) \geq f(\boldsymbol{x}) + \boldsymbol{\nabla} f(\boldsymbol{x})^\top (\boldsymbol{y} - \boldsymbol{x})$.*

Using the convexity of f and the lower bound on convex functions given by Theorem 3.3.5, we have that

$$f(\boldsymbol{x}^*) \geq f(\boldsymbol{x}_i) + \boldsymbol{\nabla} f(\boldsymbol{x}_i)^\top (\boldsymbol{x}^* - \boldsymbol{x}_i) \tag{3.3}$$

Rearranging gets us

$$\begin{aligned} \text{gap}_i &\leq \nabla f(\boldsymbol{x}_i)^\top (\boldsymbol{x}_i - \boldsymbol{x}^*) && (3.4) \\ &\leq \|\nabla f(\boldsymbol{x}_i)\|_2 \|\boldsymbol{x}_i - \boldsymbol{x}^*\|_2 && \text{by Cauchy-Schwarz.} \end{aligned}$$

At this point, we are essentially ready to connect Equation (3.2) with Equation (3.4) and analyze the convergence rate of our algorithm.

However, at the moment, we see that the change $\text{gap}_{i+1} - \text{gap}_i$ in how close we are to the optimum function value is governed by the norm of the gradient $\|\nabla f(\boldsymbol{x}_i)\|_2$, while the size of the gap is related to *both* this quantity and the distance $\|\boldsymbol{x}_i - \boldsymbol{x}^*\|_2$ between the current solution $\boldsymbol{x}_i$ and an optimum $\boldsymbol{x}^*$. Do we need both or can we get rid of, say, the distance? Unfortunately, with this algorithm and for this class of functions, a dependence on the distance is necessary. However, we can simplify things considerably using the following observation, which you will prove in the exercises (Exercise 2):

Claim 3.3.6. *When running Gradient Descent as given by the step in Equation* (3.1)*, for all* i $\|\boldsymbol{x}_i - \boldsymbol{x}^*\|_2 \leq \|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2$.

Combining this Claim with Equation (3.2) and Equation (3.4),

$$\text{gap}_{i+1} - \text{gap}_i \leq -\frac{1}{2\beta} \cdot \left(\frac{\text{gap}_i}{\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2} \right)^2 \tag{3.5}$$

At this point, a simple induction will complete the proof of following result.

Theorem 3.3.7. *Let* $f : \mathbb{R}^n \to \mathbb{R}$ *be a* β*-gradient Lipschitz, convex function. Let* $\boldsymbol{x}_0$ *be a given starting point, and let* $\boldsymbol{x}^* \in \arg\min_{\boldsymbol{x} \in \mathbb{R}^n} f(\boldsymbol{x})$ *be a minimizer of* f*. The Gradient Descent algorithm given by*

$$\boldsymbol{x}_{i+1} = \boldsymbol{x}_i - \frac{1}{\beta} \nabla f(\boldsymbol{x}_i)$$

ensures that the k*th iterate satisfies*

$$f(\boldsymbol{x}_k) - f(\boldsymbol{x}^*) \leq \frac{2\beta \|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2^2}{k+1}.$$

Carrying out this induction is one of the Week 2 exercises (Exercise 15 in the first exercise set).

3.4 Accelerated Gradient Descent

It turns out that we can get an algorithm that converges substantially faster than Gradient Descent, using an approach known as *Accelerated Gradient Descent*, which was developed by Nesterov [Nes83]. This algorithm in turn improved on some earlier results by Nemirovski

and Yudin [NY83]. The phenomenon of acceleration was perhaps first understood in the context of quadratic functions, minimizing $\boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x} - \boldsymbol{x}^\top \boldsymbol{b}$ when $\boldsymbol{A}$ is positive definite – for this case, the Conjugate Gradient algorithm was developed independently by Hestenes and Stiefel [HS$^+$52] (here at ETH!), and by Lanczos [Lan52]. In the past few years, providing more intuitive explanations of acceleration has been a popular research topic. This presentation is based on an analysis of Nesterov's algorithm developed by Diakonikolas and Orecchia [DO19].

We will adopt a slightly different approach to analyzing this algorithm than what we used in the previous section for Gradient Descent.

We will use $\boldsymbol{x}_0$ to denote the starting point of our algorithm, and we will produce a sequence of iterates $\boldsymbol{x}_0, \boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_k$. At each iterate $\boldsymbol{x}_i$, we will compute the gradient $\boldsymbol{\nabla} f(\boldsymbol{x}_i)$. However, the way we choose $\boldsymbol{x}_{i+1}$ based on what we know so far will now be a little more involved than what we did for Gradient Descent.

To help us understand the algorithm, we are going to introduce two more sequences of iterates $\boldsymbol{y}_0, \boldsymbol{y}_1, \boldsymbol{y}_2, \ldots, \boldsymbol{y}_k \in \mathbb{R}^n$ and $\boldsymbol{v}_0, \boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_k \in \mathbb{R}^n$.

The sequence of $\boldsymbol{y}_i$'s will be constructed to help us get as low a function value as possible at $f(\boldsymbol{y}_i)$, which we will consider our current solution and the last iterate $\boldsymbol{y}_k$ will be the output solution of our algorithm.

The sequence of $\boldsymbol{v}_i$'s will be constructed to help us get a lower bound on $f(\boldsymbol{x}^*)$.

By combining the upper bound on the function value of our current solution $f(\boldsymbol{y}_i)$ with a lower bound on the function value at an optimal solution $f(\boldsymbol{x}^*)$, we get an upper bound on the gap $f(\boldsymbol{y}_i) - f(\boldsymbol{x}^*)$ between the value of our solution and the optimal one. Finally, each iterate $\boldsymbol{x}_i$, which will be where we evaluate gradient $\boldsymbol{\nabla} f(\boldsymbol{x}_i)$, is chosen through a trade-off between wanting to reduce the upper bound and wanting to increase the lower bound.

The upper bound sequence: $\boldsymbol{y}_i$'s. The point $\boldsymbol{y}_i$ will be chosen from $\boldsymbol{x}_i$ to minimize an upper bound on f based at $\boldsymbol{x}_i$. This is similar to what we did in the previous section. We let $\boldsymbol{y}_i = \boldsymbol{x}_i + \boldsymbol{\delta}_i$ and choose $\boldsymbol{\delta}_i$ to minimize the upper bound $\boldsymbol{f}(\boldsymbol{y}_i) \leq f(\boldsymbol{x}_i) + \boldsymbol{\nabla} f(\boldsymbol{x}_i)^\top \boldsymbol{\delta}_i + \frac{\beta}{2} \|\boldsymbol{\delta}_i\|^2$, which gives us

$$\boldsymbol{y}_i = \boldsymbol{x}_i - \frac{1}{\beta} \boldsymbol{\nabla} f(\boldsymbol{x}_i) \text{ and } f(\boldsymbol{y}_i) \leq f(\boldsymbol{x}_i) - \frac{\|\boldsymbol{\nabla} f(\boldsymbol{x}_i)\|_2^2}{2\beta}.$$

We will introduce a notation for this upper bound

$$U_i = f(\boldsymbol{y}_i) \leq f(\boldsymbol{x}_i) - \frac{\|\boldsymbol{\nabla} f(\boldsymbol{x}_i)\|_2^2}{2\beta}. \tag{3.6}$$

Philosophizing about lower bounds[1]**.** A crucial ingredient to establishing an upper bound on gap_i was a lower bound on $f(\boldsymbol{x}^*)$.

In our analysis of Gradient Descent, in Equation (3.4), we used the lower bound $f(\boldsymbol{x}^*) \geq f(\boldsymbol{x}_i) - \|\boldsymbol{\nabla} f(\boldsymbol{x}_i)\|_2 \|\boldsymbol{x}_i - \boldsymbol{x}^*\|_2$. We can think of the Gradient Descent analysis as being based on a tension between two statements: Firstly that "a large gradient implies we quickly approach the optimum" and secondly "the function value gap to optimum cannot exceed the magnitude of the current gradient (scaled by distance to opt)".

This analysis does not use that we have seen many different function values and gradients, and each of these can be used to construct a lower bound on the optimum value $f(\boldsymbol{x}^*)$, and, in particular, it is not clear that the last gradient provides the best bound. To do better, we will try to use lower bounds that take advantage of all the gradients we have seen.

Definition 3.4.1. We will adopt a new notation for inner products that sometimes is more convenient when dealing with large expressions: $\langle \boldsymbol{a}, \boldsymbol{b} \rangle \stackrel{\text{def}}{=} \boldsymbol{a}^\top \boldsymbol{b}$.

The lower bound sequence: $\boldsymbol{v}_i$'s. We can introduce weights $a_i > 0$ for each step and combine the gradients we have observed into one lower bound based on a weighted average. Let us use $A_i = \sum_{j \leq i} a_j$ to denote the sum of the weights. Now a general lower bound on the function value at any $\boldsymbol{v} \in \mathbb{R}^n$ is :

$$f(\boldsymbol{v}) \geq \frac{1}{A_i} \sum_{j \leq i} a_j \left(f(\boldsymbol{x}_j) + \langle \boldsymbol{\nabla} f(\boldsymbol{x}_j), \boldsymbol{v} - \boldsymbol{x}_j \rangle \right)$$

However, to use Cauchy-Schwarz on each individual term here to instantiate this bound at $\boldsymbol{x}^*$ does not give us anything useful. Instead, we will employ a somewhat magical trick: we introduce a regularization term

$$\phi(\boldsymbol{v}) \stackrel{\text{def}}{=} \frac{\sigma}{2} \|\boldsymbol{v} - \boldsymbol{x}_0\|_2^2 .$$

We will choose the value $\sigma > 0$ later. Now we derive our lower bound L_i

$$\begin{aligned} f(\boldsymbol{x}^*) &\geq \frac{1}{A_i} \left(\phi(\boldsymbol{x}^*) + \sum_{j \leq i} a_j f(\boldsymbol{x}_j) + \langle a_j \boldsymbol{\nabla} f(\boldsymbol{x}_j), \boldsymbol{x}^* - \boldsymbol{x}_j \rangle \right) - \frac{\phi(\boldsymbol{x}^*)}{A_i} \\ &\geq \min_{\boldsymbol{v} \in \mathbb{R}^n} \left\{ \frac{1}{A_i} \left(\phi(\boldsymbol{v}) + \sum_{j \leq i} a_j f(\boldsymbol{x}_j) + \langle a_j \boldsymbol{\nabla} f(\boldsymbol{x}_j), \boldsymbol{v} - \boldsymbol{x}_j \rangle \right) \right\} - \frac{\phi(\boldsymbol{x}^*)}{A_i} \\ &= L_i \end{aligned}$$

We will let $\boldsymbol{v}_i$ be the $\boldsymbol{v}$ obtaining the minimum in the optimization problem appearing in the definition of L_i, so that

$$L_i = \frac{1}{A_i} \left(\phi(\boldsymbol{v}_i) + \sum_{j \leq i} a_i f(\boldsymbol{x}_i) + \langle a_i \boldsymbol{\nabla} f(\boldsymbol{x}_i), \boldsymbol{v}_i - \boldsymbol{x}_i \rangle \right) - \frac{\phi(\boldsymbol{x}^*)}{A_i}$$

[1] YMMV. People have a lot of different opionions about how to understand acceleration, and you should take my thoughts with a grain of salt.

How we will measure convergence. We have designed the upper bound U_i and the lower bound L_i such that $\text{gap}_i = f(\boldsymbol{y}_i) - f(\boldsymbol{x}^*) \leq U_i - L_i$.

As you will show in Exercise 3, we can prove the convergence of Gradient Descent directly by an induction that establishes $1/\text{gap}_i \leq C \cdot i$ for some constant C depending on the Lipschitz gradient parameter β and the distance $\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2$.

To analyze Accelerated Gradient Descent, we will adopt a similar, but slightly different strategy, namely trying to show that $(U_i - L_i)r(i)$ is non-increasing for some positive "rate function" $r(i)$. Ideally $r(i)$ should grow quickly, which would imply that gap_i quickly gets small. We will also need to show that $(U_0 - L_0)r(0) \leq C$ for some constant C again depending on β and $\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|_2$. Then, we'll be able to conclude that

$$\text{gap}_i \cdot r(i) \leq (U_i - L_i)r(i) \leq (U_{i-1} - L_{i-1})r(i-1) \leq \cdots \leq (U_0 - L_0)r(0) \leq C,$$

and hence $\text{gap}_i \leq C/r(i)$.

This framework is fairly general. We could have also used it to analyze Gradient Descent, and it works for many other optimization algorithms too.

We are going to choose our rate function $r(i)$ to be exactly A_i, which of course is no accident! As we will see, this interacts nicely with our lower bound L_i. Hence, our goals are to

1. provide an upper bound on $A_0(U_0 - L_0)$,
2. and show that $A_{i+1}(U_{i+1} - L_{i+1}) \leq A_i(U_i - L_i)$,

Establishing the convergence rate. Let's start by looking at the change in the upper bound scaled by our rate function:

$$A_{i+1}U_{i+1} - A_iU_i = A_{i+1}\left(f(\boldsymbol{y}_{i+1}) - f(\boldsymbol{x}_{i+1})\right) - A_i\left(f(\boldsymbol{y}_i) - f(\boldsymbol{x}_{i+1})\right) + (A_{i+1} - A_i)f(\boldsymbol{x}_{i+1}) \tag{3.7}$$

$$\begin{aligned}
&\leq A_{i+1}\left(-\frac{\|\boldsymbol{\nabla} f(\boldsymbol{x}_{i+1})\|_2^2}{2\beta}\right) && \text{First term controlled by Equation (3.6).}\\
&\quad - A_i\left\langle \boldsymbol{\nabla} f(\boldsymbol{x}_{i+1}), \boldsymbol{y}_i - \boldsymbol{x}_{i+1}\right\rangle && \text{Second term bounded by Theorem 3.3.5.}\\
&\quad + a_{i+1}f(\boldsymbol{x}_{i+1}) && \text{Third term uses } a_{i+1} = A_{i+1} - A_i.
\end{aligned}$$

The solution $\boldsymbol{v}_i$ to the minimization in the lower bound L_i turns out to be relatively simple to characterize. By using derivatives to find the optimum, we first analyze the initial value of the lower bound L_0.

Claim 3.4.2.

1. $\boldsymbol{v}_0 = \boldsymbol{x}_0 - \frac{a_0}{\sigma}\boldsymbol{\nabla} f(\boldsymbol{x}_0)$
2. $L_0 = f(\boldsymbol{x}_0) - \frac{a_0}{2\sigma}\left\|\boldsymbol{\nabla} f(\boldsymbol{x}_0)\right\|_2^2 - \frac{\sigma}{2a_0}\left\|\boldsymbol{x}^* - \boldsymbol{x}_0\right\|_2^2$.

You will prove Claim 3.4.2 in Exercise 17 (Week 2) of the first exercise sheet. Noting $A_0 = a_0$, we see from Equation (3.6) and Part 2 of Claim 3.4.2, that

$$A_0(U_0 - L_0) \leq \left(\frac{a_0^2}{2\sigma} - \frac{a_0}{2\beta}\right)\left\|\boldsymbol{\nabla} f(\boldsymbol{x}_0)\right\|_2^2 + \frac{\sigma}{2}\left\|\boldsymbol{x}^* - \boldsymbol{x}_0\right\|_2^2 \tag{3.8}$$

It will be convenient to introduce notation for the rescaled lower bound $A_i L_i$ *without* optimizing over $\boldsymbol{v}$.

$$m_i(\boldsymbol{v}) = \phi(\boldsymbol{v}) - \phi(\boldsymbol{x}^*) + \sum_{j \leq i} a_j f(\boldsymbol{x}_j) + \langle a_j \boldsymbol{\nabla} f(\boldsymbol{x}_j), \boldsymbol{v} - \boldsymbol{x}_j \rangle$$

Thus $A_i L_i - A_{i+1} L_{i+1} = m_i(\boldsymbol{v}_i) - m_{i+1}(\boldsymbol{v})$. Now, it is not too hard to show the following relationships.

Claim 3.4.3.

1. $m_i(\boldsymbol{v}) = m_i(\boldsymbol{v}_i) + \frac{\sigma}{2}\left\|\boldsymbol{v} - \boldsymbol{v}_i\right\|_2^2$
2. $m_{i+1}(\boldsymbol{v}) = m_i(\boldsymbol{v}) + a_{i+1} f(\boldsymbol{x}_{i+1}) + \langle a_{i+1}\boldsymbol{\nabla} f(\boldsymbol{x}_{i+1}), \boldsymbol{v} - \boldsymbol{x}_{i+1}\rangle$
3. $\boldsymbol{v}_{i+1} = \boldsymbol{v}_i - \frac{a_{i+1}}{\sigma}\boldsymbol{\nabla} f(\boldsymbol{x}_{i+1})$

And again, you will prove Claim 3.4.3 in Exercise 18 (Week 2) of the first exercise sheet. *Hint for Part 1: note that $m_i(v)$ is a quadratic function, miminimized at v_i and its Hessian equals σI at all v.*

Given Claim 3.4.3, we see that

$$\begin{aligned} A_i L_i - A_{i+1} L_{i+1} & \\ &= m_i(\boldsymbol{v}_i) - m_{i+1}(\boldsymbol{v}_{i+1}) && (3.9)\\ &= -a_{i+1} f(\boldsymbol{x}_{i+1}) - \langle a_{i+1}\boldsymbol{\nabla} f(\boldsymbol{x}_{i+1}), \boldsymbol{v}_{i+1} - \boldsymbol{x}_{i+1}\rangle - \frac{\sigma}{2}\left\|\boldsymbol{v}_{i+1} - \boldsymbol{v}_i\right\|_2^2 && (3.10)\\ &= -a_{i+1} f(\boldsymbol{x}_{i+1}) - \langle a_{i+1}\boldsymbol{\nabla} f(\boldsymbol{x}_{i+1}), \boldsymbol{v}_i - \boldsymbol{x}_{i+1}\rangle + \frac{a_{i+1}^2}{2\sigma}\left\|\boldsymbol{\nabla} f(\boldsymbol{x}_{i+1})\right\|_2^2 && (3.11) \end{aligned}$$

This means that by combining Equation (3.7) and (3.11) we get

$$\begin{aligned} A_{i+1}(U_{i+1} - L_{i+1}) - A_i(U_i - L_i) \leq \left(\frac{-A_{i+1}}{2\beta} + \frac{a_{i+1}^2}{2\sigma}\right)\left\|\boldsymbol{\nabla} f(\boldsymbol{x}_{i+1})\right\|_2^2 & \\ + \langle \boldsymbol{\nabla} f(\boldsymbol{x}_{i+1}), A_{i+1}\boldsymbol{x}_{i+1} - a_{i+1}\boldsymbol{v}_i - A_i \boldsymbol{y}_i\rangle\,. & \end{aligned}$$

Now, this means that $A_{i+1}(U_{i+1} - L_{i+1}) - A_i(U_i - L_i) \leq 0$ if

$$A_{i+1}\boldsymbol{x}_{i+1} - a_{i+1}\boldsymbol{v}_i - A_i\boldsymbol{y}_i = \mathbf{0} \text{ and } A_{i+1}/\beta \geq a_{i+1}^2/\sigma$$

We can get this by letting $\boldsymbol{x}_{i+1} = \frac{A_i\boldsymbol{y}_i + a_{i+1}\boldsymbol{v}_i}{A_{i+1}}$, and $\sigma = \beta$ and $a_i = \frac{i+1}{2}$, which implies that $A_i = \frac{(i+1)(i+2)}{4} > a_i^2$.

By Equation (3.8), these parameter choices also imply that

$$A_0(U_0 - L_0) \leq \frac{\beta}{2}\left\|\boldsymbol{x}^* - \boldsymbol{x}_0\right\|_2^2.$$

Finally, by induction, we get $A_i(U_i - L_i) \leq \frac{\beta}{2}\left\|\boldsymbol{x}^* - \boldsymbol{x}_0\right\|_2^2$. Dividing through by A_i and using $\text{gap}_i \leq U_i - L_i$ results in the following theorem.

Theorem 3.4.4. *Let $f : \mathbb{R}^n \to \mathbb{R}$ be a β-gradient Lipschitz, convex function. Let $\boldsymbol{x}_0$ be a given starting point, and let $\boldsymbol{x}^* \in \arg\min_{\boldsymbol{x}\in\mathbb{R}^n} f(\boldsymbol{x})$ be a minimizer of f.*

The Accelerated Gradient Descent algorithm given by

$$\begin{aligned}
a_i &= \frac{i+1}{2}, A_i = \frac{(i+1)(i+2)}{4} \\
\boldsymbol{v}_0 &= \boldsymbol{x}_0 - \frac{1}{2\beta}\boldsymbol{\nabla} f(\boldsymbol{x}_0) \\
\boldsymbol{y}_i &= \boldsymbol{x}_i - \frac{1}{\beta}\boldsymbol{\nabla} f(\boldsymbol{x}_i) \\
\boldsymbol{x}_{i+1} &= \frac{A_i\boldsymbol{y}_i + a_{i+1}\boldsymbol{v}_i}{A_{i+1}} \\
\boldsymbol{v}_{i+1} &= \boldsymbol{v}_i - \frac{a_{i+1}}{\beta}\boldsymbol{\nabla} f(\boldsymbol{x}_{i+1})
\end{aligned}$$

ensures that the kth iterate satisfies

$$f(\boldsymbol{x}_k) - f(\boldsymbol{x}^*) \leq \frac{2\beta\left\|\boldsymbol{x}_0 - \boldsymbol{x}^*\right\|_2^2}{(k+1)(k+2)}.$$

Part II

Spectral Graph Theory

Chapter 4

Introduction to Spectral Graph Theory

In this chapter, we will study graphs through linear algebra. This approach is known as Spectral Graph Theory and turns out to be surprisingly powerful. An in-depth treatment of many topics in this area can be found in [Spi19].

4.1 Recap: Incidence and Adjacency Matrices, the Laplacian Matrix and Electrical Energy

In Chapter 1, we looked at undirected graphs and we introduce the incidence matrix and the Laplacian of the graph. Let us recall these.

We consider an undirected weighted graph $G = (V, E, \boldsymbol{w})$, with $n = |V|$ vertices and $m = |E|$ edges, where $\boldsymbol{w} \in \mathbb{R}_+^E$ assigns positive weight for every edge. Let's assume G is connected.

To introduce the *edge-vertex incidence matrix* of the graph, we first have to associate an arbitrary direction to every edge. We then let $\boldsymbol{B} \in \mathbb{R}^{V \times E}$.

$$\boldsymbol{B}(v, e) = \begin{cases} 1 & \text{if } e = (u, v) \\ -1 & \text{if } e = (v, u) \\ 0 & \text{o.w.} \end{cases}$$

The edge directions are only there to help us track the meaning of signs of quantities defined on edges: The math we do should not depend on the choice of sign.

Let $\boldsymbol{W} \in \mathbb{R}^{E \times E}$ be the diagonal matrix given by $\boldsymbol{W} = \text{diag}(\boldsymbol{w})$, i.e $\boldsymbol{W}(e, e) = \boldsymbol{w}(e)$. We define the Laplacian of the graph as $\boldsymbol{L} = \boldsymbol{B}\boldsymbol{W}\boldsymbol{B}^\top$. Note that in the first chapter, we defined the Laplacian as $\boldsymbol{B}\boldsymbol{R}^{-1}\boldsymbol{B}^\top$, where $\boldsymbol{R}$ is the diagonal matrix with edge resistances on the diagonal. We want to think of high *weight* on an edge as expressing that two vertices are

highly connected, whereas we think of high resistance on an edge as expressing that the two vertices are poorly connected, so we let $\boldsymbol{w}(e) = 1/\boldsymbol{R}(e,e)$.

The weighted adjacency matrix $\boldsymbol{A} \in \mathbb{R}^{V \times V}$ of a graph is given by

$$\boldsymbol{A}(u,v) = \begin{cases} \boldsymbol{w}(u,v) & \text{if } \{u,v\} \in E \\ 0 & \text{otherwise.} \end{cases}$$

Note that we treat the edges as undirected here, so $\boldsymbol{A}^\top = \boldsymbol{A}$. The weighted degree of a vertex is defined as $\boldsymbol{d}(v) = \sum_{\{u,v\} \in E} w(u,v)$. Again we treat the edges as undirected. Let $\boldsymbol{D} = \mathrm{diag}(\boldsymbol{d})$ be the diagonal matrix in $\mathbb{R}^{V \times V}$ with weighted degrees on the diagonal.

In Problem Set 1, you showed that $\boldsymbol{L} = \boldsymbol{D} - \boldsymbol{A}$, and that for $\boldsymbol{x} \in \mathbb{R}^V$,

$$\boldsymbol{x}^\top \boldsymbol{L} \boldsymbol{x} = \sum_{\{a,b\} \in E} \boldsymbol{w}(a,b)(\boldsymbol{x}(a) - \boldsymbol{x}(b))^2.$$

Now we can express the net flow constraint that $\boldsymbol{f}$ routes $\boldsymbol{d}$ by

$$\boldsymbol{B}\boldsymbol{f} = \boldsymbol{d}.$$

This is also called a conservation constraint. In our examples so far, we have $\boldsymbol{d}(s) = -1$, $\boldsymbol{d}(t) = 1$ and $\boldsymbol{d}(u) = 0$ for all $u \in V \setminus \{s,t\}$.

If we let $\boldsymbol{R} = \mathrm{diag}_{e \in E}\, \boldsymbol{r}(e)$ then Ohm's law tells us that electrical voltages $\boldsymbol{x}$ will induce an electrical flow $\boldsymbol{f} = \boldsymbol{R}^{-1}\boldsymbol{B}^\top \boldsymbol{x}$. We defined the electrical energy of a flow $\boldsymbol{f} \in \mathbb{R}^E$ to be

$$\mathcal{E}(\boldsymbol{f}) = \sum_e \boldsymbol{r}(e)\boldsymbol{f}(e)^2 = \boldsymbol{f}^\top \boldsymbol{R}\boldsymbol{f}.$$

And, from Ohm's Law, we can then see that

$$\mathcal{E}(\boldsymbol{f}) = \boldsymbol{f}^\top \boldsymbol{R}\boldsymbol{f} = \boldsymbol{x}^\top \boldsymbol{L}\boldsymbol{x}.$$

Hence, define the electrical energy associated with a set of voltages to be

$$\mathcal{E}(\boldsymbol{x}) = \boldsymbol{x}^\top \boldsymbol{L}\boldsymbol{x}.$$

The Courant-Fisher Theorem. Let us also recall the Courant-Fischer theorem, which we proved in Chapter 3 (Theorem 4.1.1).

Theorem 4.1.1 (The Courant-Fischer Theorem)**.** *Let $\boldsymbol{A}$ be a symmetric matrix in $\mathbb{R}^{n \times n}$, with eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$. Then*

1.

$$\lambda_i = \min_{\substack{\text{subspace } W \subseteq \mathbb{R}^n \\ \dim(W) = i}} \max_{\boldsymbol{x} \in W, \boldsymbol{x} \neq \boldsymbol{0}} \frac{\boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}}$$

2.

$$\lambda_i = \max_{\substack{\text{subspace } W \subseteq \mathbb{R}^n \\ \dim(W)=n+1-i}} \min_{\boldsymbol{x} \in W, \boldsymbol{x} \neq \boldsymbol{0}} \frac{\boldsymbol{x}^\top \boldsymbol{A} \boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}}$$

In fact, from our proof of the Courant-Fischer theorem in Chapter 3, we can also extract a slightly different statement:

Theorem 4.1.2 (The Courant-Fischer Theorem, eigenbasis version)**.** *Let $\boldsymbol{A}$ be a symmetric matrix in $\mathbb{R}^{n \times n}$, with eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$, and corresponding eigenvectors $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n$ which form an othernormal basis. Then*

1.

$$\lambda_i = \min_{\substack{\boldsymbol{x} \perp \boldsymbol{x}_1, \ldots \boldsymbol{x}_{i-1} \\ \boldsymbol{x} \neq \boldsymbol{0}}} \frac{\boldsymbol{x}^\top \boldsymbol{A} \boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}}$$

2.

$$\lambda_i = \max_{\substack{\boldsymbol{x} \perp \boldsymbol{x}_{i+1}, \ldots \boldsymbol{x}_n \\ \boldsymbol{x} \neq \boldsymbol{0}}} \frac{\boldsymbol{x}^\top \boldsymbol{A} \boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}}$$

Of course, we also have $\lambda_i(\boldsymbol{A}) = \frac{\boldsymbol{x}_i^\top \boldsymbol{A} \boldsymbol{x}_i}{\boldsymbol{x}_i^\top \boldsymbol{x}_i}$.

4.2 Understanding Eigenvalues of the Laplacian

We would like to understand the eigenvalues of the Laplacian matrix of a graph.

But first, why should we care? It turns out that Laplacian eigenvalues can help us understand many properties of a graph. But we are going to start off with simple motivating observation: Electrical voltages $\boldsymbol{x} \in \mathbb{R}^V$ consume electrical energy $\mathcal{E}(\boldsymbol{x}) = \boldsymbol{x}^\top \boldsymbol{L} \boldsymbol{x}$. This means that by the Courant-Fischer Theorem

$$\mathcal{E}(\boldsymbol{x}) = \boldsymbol{x}^\top \boldsymbol{L} \boldsymbol{x} \leq \lambda_n(L) \boldsymbol{x}^\top \boldsymbol{x}$$

And, for any voltages $\boldsymbol{x} \perp \boldsymbol{1}$,

$$\mathcal{E}(\boldsymbol{x}) = \boldsymbol{x}^\top \boldsymbol{L} \boldsymbol{x} \geq \lambda_2(L) \boldsymbol{x}^\top \boldsymbol{x}.$$

Thus, we can use the eigenvalues to give upper and lower bounds on how much electrical energy will be consumed by the flow induced by $\boldsymbol{x}$, in terms compared to $\boldsymbol{x}^\top \boldsymbol{x} = \|\boldsymbol{x}\|_2^2$.

In a couple of chapters, we will also prove the following claim, which shows that the Laplacian eigenvalues can directly tell us about the electrical energy that is required to route a given demand.

Claim 4.2.1. *Given a demand vector $\boldsymbol{d} \in \mathbb{R}^V$ such that $\boldsymbol{d} \perp \boldsymbol{1}$, the electrical voltages $\boldsymbol{x}$ that route $\boldsymbol{d}$ satisfy $\boldsymbol{L}\boldsymbol{x} = \boldsymbol{d}$ and the electrical energy of these voltages satifies*

$$\frac{\|\boldsymbol{d}\|_2^2}{\lambda_n} \leq \mathcal{E}(\boldsymbol{x}) \leq \frac{\|\boldsymbol{d}\|_2^2}{\lambda_2}$$

Eigenvalues of the Laplacian of a Complete Graph. To get a sense of how Laplacian eigenvalues behave, let us start by considering the n vertex complete graph with unit weights, which we denote by K_n. The adjacency matrix of K_n is $\boldsymbol{A} = \mathbf{1}\mathbf{1}^\top - \boldsymbol{I}$, since it has ones everywhere, except for the diagonal, where entries are zero. The degree matrix $\boldsymbol{D} = (n-1)\boldsymbol{I}$. Thus the Laplacian is $\boldsymbol{L} = \boldsymbol{D} - \boldsymbol{A} = n\boldsymbol{I} - \mathbf{1}\mathbf{1}^\top$.

Thus for any $\boldsymbol{y} \perp \mathbf{1}$, we have $\boldsymbol{y}^\top \boldsymbol{L}\boldsymbol{y} = n\boldsymbol{y}^\top\boldsymbol{y} - (\mathbf{1}^\top\boldsymbol{y})^2 = n\boldsymbol{y}^\top\boldsymbol{y}$.

From this, we can conclude that any $\boldsymbol{y} \perp \mathbf{1}$ is an eigenvector of eigenvalue n, and that all $\lambda_2 = \lambda_3 = \ldots = \lambda_n = n$.

Next, let us try to understand λ_2 and λ_n for P_n, the n vertex path graph with unit weight edges. I.e. the graph has edges $E = \{\{i, i+1\} \text{ for } i = 1 \text{ to } (n-1)\}$.

This is in a sense the least well-connected unit weight graph on n vertices, whereas K_n is the most well-connected.

4.2.1 Test Vector Bounds on λ_2 and λ_n

We can use the eigenbasis version of the Courant-Fisher theorem to observe that the second-smallest eigenvalue of the Laplacian is given by

$$\lambda_2(\boldsymbol{L}) = \min_{\substack{\boldsymbol{x}\neq\mathbf{0} \\ \boldsymbol{x}^\top\mathbf{1}=0}} \frac{\boldsymbol{x}^\top\boldsymbol{L}\boldsymbol{x}}{\boldsymbol{x}^\top\boldsymbol{x}}. \tag{4.1}$$

We can get a better understanding of this particular case through a couple of simple observations. Suppose $\boldsymbol{x} = \boldsymbol{y} + \alpha\mathbf{1}$, where $\boldsymbol{y} \perp \mathbf{1}$. Then $\boldsymbol{x}^\top\boldsymbol{L}\boldsymbol{x} = \boldsymbol{y}^\top\boldsymbol{L}\boldsymbol{y}$, and $\|\boldsymbol{x}\|_2^2 = \|\boldsymbol{y}\|^2 + \alpha^2\|\mathbf{1}\|^2$. So for any given vector, you can increase the value of $\frac{\boldsymbol{x}^\top\boldsymbol{L}\boldsymbol{x}}{\boldsymbol{x}^\top\boldsymbol{x}}$, by instead replacing $\boldsymbol{x}$ with the component orthogonal to $\mathbf{1}$, which we denoted by $\boldsymbol{y}$.

We can conclude from Equation (4.1) that for *any* vector $\boldsymbol{y} \perp \mathbf{1}$,

$$\lambda_2 \leq \frac{\boldsymbol{y}^\top\boldsymbol{L}\boldsymbol{y}}{\boldsymbol{y}^\top\boldsymbol{y}}$$

When we use a vector $\boldsymbol{y}$ in this way to prove a bound on an eigenvalue, we call it a *test vector*.

Now, we'll use a test vector to give an upper bound on $\lambda_2(\boldsymbol{L}_{P_n})$. Let $\boldsymbol{x} \in \mathbb{R}^V$ be given by $\boldsymbol{x}(i) = (n+1) - 2i$, for $i \in [n]$. This vector satisfies $\boldsymbol{x} \perp \mathbf{1}$. We picked this because we wanted a sequence of values growing linearly along the path, while also making sure that the vector

is orthogonal to $\mathbf{1}$. Now

$$\begin{aligned}\lambda_2(\boldsymbol{L}_{P_n}) &\leq \frac{\sum_{i\in[n-1]}(\boldsymbol{x}(i)-\boldsymbol{x}(i+1))^2}{\sum_{i=1}^n \boldsymbol{x}(i)^2} \\ &= \frac{\sum_{i=1}^{n-1} 2^2}{\sum_{i=1}^n (n+1-2i)^2} \\ &= \frac{4(n-1)}{(n+1)n(n-1)/3} \\ &= \frac{12}{n(n+1)} \leq \frac{12}{n^2}.\end{aligned}$$

Later, we will prove a lower bound that shows this value is right up to a constant factor. But the test vector approach based on the Courant-Fischer theorem doesn't immediately work when we want to prove lower bounds on $\lambda_2(\boldsymbol{L})$.

We can see from either version of the Courant-Fischer theorem that

$$\lambda_n(\boldsymbol{L}) = \max_{\boldsymbol{v}\neq\mathbf{0}} \frac{\boldsymbol{v}^\top \boldsymbol{L}\boldsymbol{v}}{\boldsymbol{v}^\top \boldsymbol{v}}. \tag{4.2}$$

Thus for *any* vector $\boldsymbol{y} \neq 0$,

$$\lambda_n \geq \frac{\boldsymbol{y}^\top \boldsymbol{L}\boldsymbol{y}}{\boldsymbol{y}^\top \boldsymbol{y}}.$$

This means we can get a test vector-based lower bound on λ_n. Let us apply this to the Laplacian of P_n. We'll try the vector $\boldsymbol{x} \in \mathbb{R}^V$ given by $\boldsymbol{x}(1) = -1$, and $\boldsymbol{x}(n) = 1$ and $\boldsymbol{x}(i) = 0$ for $i \neq 1, n$.

Here we get

$$\lambda_n(\boldsymbol{L}_{P_n}) \geq \frac{\boldsymbol{x}^\top \boldsymbol{L}\boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}} = \frac{2}{2} = 1.$$

Again, it's not clear how to use the Courant-Fischer theorem to prove an upper bound on $\lambda_n(\boldsymbol{L})$. But, later we'll see how to prove an upper that shows that for P_n, the lower bound we obtained is right up to constant factors.

4.2.2 Eigenvalue Bounds Beyond Test Vectors

In the previous sections, we first saw a complete characterization of the eigenvalues and eigenvectors of the unit weight complete graph on n vertices, K_n. Namely, $\boldsymbol{L}_{K_n} = n\boldsymbol{I} - \mathbf{1}\mathbf{1}^\top$, and this means that *every* vector $\boldsymbol{y} \perp \mathbf{1}$ is an eigenvector of eigenvalue n.

We then looked at eigenvalues of P_n, the unit weight path on n vertices, and we showed using *test vector* bounds that

$$\lambda_2(\boldsymbol{L}_{P_n}) \leq \frac{12}{n^2} \text{ and } 1 \leq \lambda_n(\boldsymbol{L}_{P_n}). \tag{4.3}$$

Ideally we would like to prove an almost matching lower bound on λ_2 and an almost matching upper bound on λ_n, but it is not clear how to get that from the Courant-Fischer theorem.

To get there, we start we need to introduce some more tools.

4.2.3 The Loewner Order, aka. the Positive Semi-Definite Order

We'll now introduce an ordering on symmetric matrices called the *Loewner order*, which I also like to just call the positive semi-definite order. As we will see in a moment, it is a partial order on symmetric matrices, we denote it by "$\preceq$". For conveniece, we allow ourselves to both write $\boldsymbol{A} \preceq \boldsymbol{B}$ and equivalently $\boldsymbol{B} \succeq \boldsymbol{A}$.

For a symmetric matrix $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ we define that

$$\boldsymbol{A} \succeq \boldsymbol{0}$$

if and only if $\boldsymbol{A}$ is positive semi-definite.

More generally, when we have two symmetric matrices $\boldsymbol{A}, \boldsymbol{B} \in \mathbb{R}^{n \times n}$, we will write

$$\boldsymbol{A} \preceq \boldsymbol{B} \text{ if and only if for all } \boldsymbol{x} \in \mathbb{R}^n \text{ we have } \boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x} \leq \boldsymbol{x}^\top \boldsymbol{B}\boldsymbol{x} \tag{4.4}$$

This is a partial order, because it satisfies the three requirements of

1. Reflexivity: $\boldsymbol{A} \preceq \boldsymbol{A}$.
2. Anti-symmetry: $\boldsymbol{A} \preceq \boldsymbol{B}$ and $\boldsymbol{B} \preceq \boldsymbol{A}$ implies $\boldsymbol{A} = \boldsymbol{B}$
3. Transitivity: $\boldsymbol{A} \preceq \boldsymbol{B}$ and $\boldsymbol{B} \preceq \boldsymbol{C}$ implies $\boldsymbol{A} \preceq \boldsymbol{C}$

Check for yourself that these properties hold!

The PSD order has other very useful properties: $\boldsymbol{A} \preceq \boldsymbol{B}$ implies $\boldsymbol{A} + \boldsymbol{C} \preceq \boldsymbol{B} + \boldsymbol{C}$ for any symmetric matrix $\boldsymbol{C}$. Convince yourself of this too!

And, combining this observation with transitivity, we can see that $\boldsymbol{A} \preceq \boldsymbol{B}$ and $\boldsymbol{C} \preceq \boldsymbol{D}$ implies $\boldsymbol{A} + \boldsymbol{C} \preceq \boldsymbol{B} + \boldsymbol{D}$.

Here is another useful property: If $\boldsymbol{0} \preceq \boldsymbol{A}$ then for all $\alpha \geq 1$

$$\frac{1}{\alpha}\boldsymbol{A} \preceq \boldsymbol{A} \preceq \alpha \boldsymbol{A}.$$

Here is another one:

Claim 4.2.2. *If $\boldsymbol{A} \preceq \boldsymbol{B}$, then for all i*

$$\lambda_i(\boldsymbol{A}) \leq \lambda_i(\boldsymbol{B}).$$

Proof. We can prove this Claim by applying the subspace version of the Courant-Fischer theorem.

$$\lambda_i(\boldsymbol{A}) = \min_{\substack{\text{subspace } W \subseteq \mathbb{R}^n \\ \dim(W)=i}} \max_{\boldsymbol{x} \in W, \boldsymbol{x} \neq \boldsymbol{0}} \frac{\boldsymbol{x}^\top \boldsymbol{A} \boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}} \leq \min_{\substack{\text{subspace } W \subseteq \mathbb{R}^n \\ \dim(W)=i}} \max_{\boldsymbol{x} \in W, \boldsymbol{x} \neq \boldsymbol{0}} \frac{\boldsymbol{x}^\top \boldsymbol{B} \boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}} = \lambda_i(\boldsymbol{B}).$$

□

Note that the converse of Clam 4.2.2 is very much false, for example the matrices $\boldsymbol{A} = \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}$ and $\boldsymbol{B} = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$ have equal eigenvalues, but both $\boldsymbol{A} \not\preceq \boldsymbol{B}$ and $\boldsymbol{B} \not\preceq \boldsymbol{A}$.

Remark 4.2.3. It's useful to get used to and remember some of the properties of the Loewner order, but all the things we have established so far are almost immediate from the basic characterization in Equation (4.4). So, ideally, don't memorize all these facts, instead, try to see that they are simple consequences of the definition.

4.2.4 Upper Bounding a Laplacian's λ_n Using Degrees

In an earlier chapter, we observed that for any graph $G = (V, E, \boldsymbol{w})$, $\boldsymbol{L} = \boldsymbol{D} - \boldsymbol{A} \succeq \boldsymbol{0}$. We can see this from $\boldsymbol{x}^\top(\boldsymbol{D} - \boldsymbol{A})\boldsymbol{x} = \sum_{(u,v)\in E} \boldsymbol{w}(u,v)(\boldsymbol{x}(u) - \boldsymbol{x}(v))^2 \geq 0$. Similarly $\boldsymbol{D} + \boldsymbol{A} \succeq \boldsymbol{0}$. because $\boldsymbol{x}^\top(\boldsymbol{D} + \boldsymbol{A})\boldsymbol{x} = \sum_{(u,v)\in E} \boldsymbol{w}(u,v)(\boldsymbol{x}(u) + \boldsymbol{x}(v))^2 \geq 0$. But this means that $-\boldsymbol{A} \preceq \boldsymbol{D}$ and hence $\boldsymbol{L} = \boldsymbol{D} - \boldsymbol{A} \preceq 2\boldsymbol{D}$.

So, for the path graph P_n, we have $\boldsymbol{L}_{P_n} \preceq \boldsymbol{D} - \boldsymbol{A} \preceq 2\boldsymbol{D} \preceq 4\boldsymbol{I}$. So by Claim 4.2.2

$$\lambda_n(\boldsymbol{L}_{P_n}) \leq 4. \tag{4.5}$$

We can see that our test vector-based lower bound on $\lambda_n(\boldsymbol{L}_{P_n})$ from Equation (4.3) is tight up to a factor 4.

Since this type of argument works for any unit weight graph, it proves the following claim.

Claim 4.2.4. *For any unit weight graph G, $\lambda_n(\boldsymbol{L}_G) \leq 2 \max_{v \in V} \mathit{degree}(v)$.*

This is tight on a graph consisting of a single edge.

4.2.5 The Loewner Order and Laplacians of Graphs.

It's sometimes convenient to overload the for the PSD order to also apply to graphs. We will write

$$G \preceq H$$

if $\boldsymbol{L}_G \preceq \boldsymbol{L}_H$.

For example, given two unit weight graphs $G = (V, E)$ and $H = (V, F)$, if $H = (V, F)$ is a subgraph of G, then

$$\boldsymbol{L}_H \preceq \boldsymbol{L}_G.$$

We can see this from the Laplacian quadratic form:

$$\boldsymbol{x}^\top \boldsymbol{L}_G \boldsymbol{x} = \sum_{(u,v)\in E} \boldsymbol{w}(u, v)(\boldsymbol{x}(u) - \boldsymbol{x}(v))^2.$$

Dropping edges will only decrease the value of the quadratic form. The same is for decreasing the weights of edges. The graph order notation is especially useful when we allow for scaling a graph by a constant, say $c > 0$,

$$c \cdot H \preceq G$$

What is $c \cdot H$? It is the same graph as H, but the weight of every edge is multiplied by c. Now we can make statements like $\frac{1}{2}H \preceq G \preceq 2H$, which turn out to be useful notion of the two graphs approximating each other.

4.2.6 The Path Inequality

Now, we'll see a general tool for comparing two graphs G and H to prove inequalities like $cH \preceq G$ for some constant c. Our tools won't necessarily work well for all cases, but we'll see some examples where they do.

In the rest of the chapter, we will often need to compare two graphs defined on the same vertex set $V = \{1, \ldots, n\} = [n]$.

We use $G_{i,j}$ to denote the unit weight graph on vertex set $[n]$ consisting of a single edge between vertices i and j.

Lemma 4.2.5 (The Path Inequality)**.**

$$(n - 1) \cdot P_n \succeq G_{1,n},$$

Proof. We want to show that for every $\boldsymbol{x} \in \mathbb{R}^n$,

$$(n - 1) \cdot \sum_{i=1}^{n-1} (\boldsymbol{x}(i + 1) - \boldsymbol{x}(i))^2 \geq (\boldsymbol{x}(n) - \boldsymbol{x}(1))^2.$$

For $i \in [n - 1]$, set

$$\boldsymbol{\Delta}(i) = \boldsymbol{x}(i + 1) - \boldsymbol{x}(i).$$

The inequality we want to prove then becomes

$$(n-1)\sum_{i=1}^{n-1}(\boldsymbol{\Delta}(i))^2 \geq \left(\sum_{i=1}^{n-1}\boldsymbol{\Delta}(i)\right)^2.$$

But, this is immediate from the Cauchy-Schwarz inequality $\boldsymbol{a}^\top \boldsymbol{b} \leq \|\boldsymbol{a}\|_2 \|\boldsymbol{b}\|_2$:

$$\begin{aligned}(n-1)\sum_{i=1}^{n-1}(\boldsymbol{\Delta}(i))^2 &= \|\mathbf{1}_{n-1}\|^2 \cdot \|\boldsymbol{\Delta}\|^2 \\ &= (\|\mathbf{1}_{n-1}\| \cdot \|\boldsymbol{\Delta}\|)^2 \\ &\geq (\mathbf{1}_{n-1}^\top \boldsymbol{\Delta})^2 \\ &= (\sum_{i=1}^{n-1}\boldsymbol{\Delta}(i))^2\end{aligned}$$

□

4.2.7 Lower Bounding λ_2 of a Path Graph

We will now use Lemma 4.2.5 to prove a lower bound on $\lambda_2(\boldsymbol{L}_{P_n})$. Our strategy will be to prove that the path P_n is at least some multiple of the complete graph K_n, measured by the Loewner order, i.e. $K_n \preceq f(n)P_n$ for some function $f : \mathbb{N} \to \mathbb{R}$. We can combine this with our observation earlier that $\lambda_2(\boldsymbol{L}_{K_n}) = n$ to show that

$$f(n)\lambda_2(\boldsymbol{L}_{P_n}) \geq \lambda_2(\boldsymbol{L}_{K_n}) = n, \tag{4.6}$$

and this will give our lower bound on $\lambda_2(\boldsymbol{L}_{P_n})$. When establishing the inequality between P_n and K_n, we can treat each edge of the complete graph separately, by first noting that

$$\boldsymbol{L}_{K_n} = \sum_{i<j}\boldsymbol{L}_{G_{i,j}}$$

For every edge (i, j) in the complete graph, we apply the Path Inequality, Lemma 4.2.5:

$$\begin{aligned}G_{i,j} &\preceq (j-i)\sum_{k=i}^{j-1}G_{k,k+1} \\ &\preceq (j-i)P_n\end{aligned}$$

This inequality says that $G_{i,j}$ is at most $(j-i)$ times the part of the path connecting i to j, and that this part of the path is less than the whole.

Summing inequality (4.3) over all edges $(i, j) \in K_n$ gives

$$K_n = \sum_{i<j}G_{i,j} \preceq \sum_{i<j}(j-i)P_n.$$

To finish the proof, we compute

$$\sum_{i<j}(j-i) \leq \sum_{i<j} n \leq n^3$$

So

$$L_{K_n} \preceq n^3 \cdot L_{P_n}.$$

Plugging this into Equation (4.6) we obtain

$$\frac{1}{n^2} \leq \lambda_2(P_n).$$

This only differs from our test vector-based upper bound in Equation (4.3) by a factor 12.

We could make this considerably tighter by being more careful about the sums.

4.2.8 Laplacian Eigenvalues of the Complete Binary Tree

Let's do the same analysis with the complete binary tree with unit weight edges on $n = 2^{d+1} - 1$ vertices, which we denote by T_d.

T_d is the balanced binary tree on this many vertices, i.e. it consists of a root node, which has two children, each of those children have two children and so on until we reach a depth of d from the root, at which point the child vertices have no more children. A simple induction shows that indeed $n = 2^{d+1} - 1$.

We can also describe the edge set by saying that each node i has edges to its children $2i$ and $2i + 1$ whenever the node labels do not exceed n. We emphasize that we still think of the graph as undirected.

The largest eigenvalue. We'll start by above bounding $\lambda_n(\boldsymbol{L}_{T_d})$ using a test vector.

We let $\boldsymbol{x}(i) = 0$ for all nodes that have a child node, and $\boldsymbol{x}(i) = -1$ for even-numbered leaf nodes and $\boldsymbol{x}(i) = +1$ for odd-numbered leaf nodes. Note that there are $(n+1)/2$ leaf nodes, and every leaf node has a single edge, connecting it to a parent with value 0. Thus

$$\lambda_n(\boldsymbol{L}) = \max_{\boldsymbol{v} \neq \boldsymbol{0}} \frac{\boldsymbol{v}^\top \boldsymbol{L} \boldsymbol{v}}{\boldsymbol{v}^\top \boldsymbol{v}} \geq \frac{\boldsymbol{x}^\top \boldsymbol{L} \boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}} = \frac{(n+1)/2}{(n+1)/2} = 1. \tag{4.7}$$

Meanwhile, every vertex has degree at most 3, so by Claim 4.2.4, $\lambda_n(\boldsymbol{L}) \leq 6$. So we can bound the largest eigenvalue above and below by a constant.

λ_2 and diameter in any graph. The following lemma gives a simple lower bound on λ_2 for any graph.

Lemma 4.2.6. *For any unit weight graph G with diameter D,*

$$\lambda_2(\boldsymbol{L}_G) \geq \frac{1}{nD}.$$

Proof. We will again prove a lower bound comparing G to the complete graph. For each edge $(i,j) \in K_n$, let $G^{i,j}$ denote a shortest path in G from i to j. This path will have length at most D. So, we have

$$\begin{aligned} K_n &= \sum_{i<j} G_{i,j} \\ &\preceq \sum_{i<j} DG^{i,j} \\ &\preceq \sum_{i<j} DG \\ &\preceq n^2 DG. \end{aligned}$$

So, we obtain the bound

$$n^2 D\lambda_2(G) \geq n,$$

which implies our desired statement. □

λ_2 in a tree. Since a complete binary tree T_d has diameter $2d \leq 2\log_2(n)$, by Lemma 4.2.6, $\lambda_2(\boldsymbol{L}_{T_d}) \geq \frac{1}{2n\log_2(n)}$.

Let us give an upper bound on λ_2 of the tree using a test vector. Let $\boldsymbol{x} \in \mathbb{R}^v$ have $\boldsymbol{x}(1) = 0$ and $\boldsymbol{x}(i) = -1$ for i in the left subtree and $\boldsymbol{x}(i) = +1$ in the right subtree. Then

$$\lambda_2(\boldsymbol{L}_{T_d}) = \min_{\substack{\boldsymbol{v}\neq\boldsymbol{0} \\ \boldsymbol{v}^\top\boldsymbol{1}=0}} \frac{\boldsymbol{v}^\top\boldsymbol{L}\boldsymbol{v}}{\boldsymbol{v}^\top\boldsymbol{v}} \leq \frac{\boldsymbol{x}^\top\boldsymbol{L}\boldsymbol{x}}{\boldsymbol{x}^\top\boldsymbol{x}} = \frac{2}{n-1}.$$

So, we have shown $\frac{1}{2n\log_2(n)} \leq \lambda_2(\boldsymbol{L}_{T_d}) \leq \frac{2}{n-1}$, and unlike the previous examples, the gap is more than a constant.

In the exercises for Week 3, I will ask you to improve the lower bound to $1/(cn)$ for some constant c.

Chapter 5

Conductance, Expanders and Cheeger's Inequality

A common algorithmic problem that arises is the problem of partitioning the vertex set V of a graph G into clusters $X_1, X_2, \ldots, X_k$ such that

- for each i, the *induced* graph $G[X_i] = (X_i, E \cap (X_i \times X_i))$ is "well-connected", and
- only an ϵ-fraction of edges e are not contained in any induced graph $G[X_i]$ (where ϵ is a very small constant).

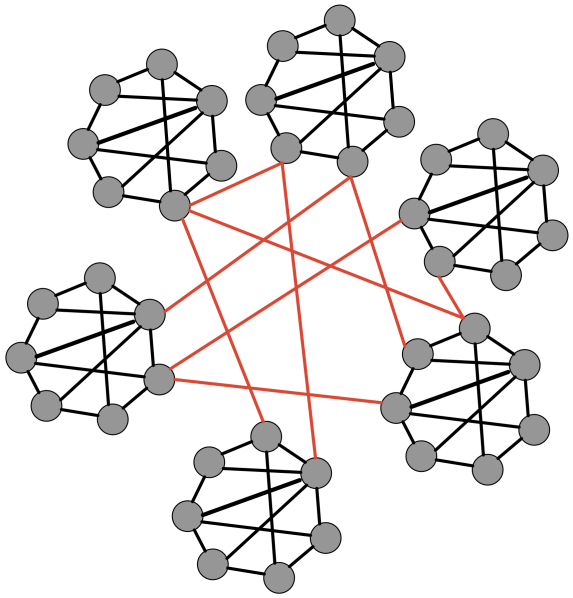


Figure 5.1: After removing the red edges (of which there are few in relation to the total number of edges), each connected component in G is "well-connected".

In this lecture, we make precise what "well-connected" means by introducing the notions of *conductance* and *expanders*.

Building on the last two lectures, we show that the second eigenvalue of the Laplacian L associated with graph G can be used to certify that a graph is "well-connected" (more precisely the second eigenvalue of a normalized version of the Laplacian). This result, called Cheeger's inequality, is one of the key tools in Spectral Graph Theory. Moreover, it can be turned into an algorithm that computes the partition efficiently!

5.1 Conductance and Expanders

Graph Definitions. In this lecture, we let $G = (V, E)$ be unweighted[1] and always be *connected*, and let $\boldsymbol{d}(v)$ be the degree of a vertex v in G. We define the *volume* $\mathrm{vol}(S)$ for any vertex subset $S \subseteq V$, to be the sum of degrees, i.e. $\mathrm{vol}(S) = \sum_{v \in S} \boldsymbol{d}(v)$.

For any $A, B \subseteq V$, we define $E(A, B)$ to be the set of edges in $E \cap (A \times B)$, i.e. with one endpoint in A and one endpoint in B. We let $G[A]$ be the *induced* graph G by $A \subseteq V$, which is the graph G restricted to the vertices A, i.e. an edge e in G is in $G[A]$ iff both endpoints are in A.

Conductance. Given set $\emptyset \subset S \subset V$, then we define the conductance $\phi(S)$ of S by

$$\phi(S) = \frac{|E(S, V \setminus S)|}{\min\{\mathrm{vol}(S), \mathrm{vol}(V \setminus S)\}}.$$

It can be seen that $\phi(\cdot)$ is symmetric in the sense that $\phi(S) = \phi(V \setminus S)$. We define the conductance of the graph G denoted $\phi(G)$ by

$$\phi(G) = \min_{\emptyset \subset S \subset V} \phi(S).$$

We note that finding the conductance of a graph G is NP-hard. However, good approximations can be found as we will see today (and in a later lecture).

Expander and Expander Decomposition. For any $\phi \in (0, 1]$, we say that a graph G is a *ϕ-expander* if $\phi(G) \geq \phi$. We say that the partition $X_1, X_2, \ldots, X_k$ of the vertex set V is a *ϕ-expander decomposition* of quality q if

- each induced graph $G[X_i]$ is a ϕ-expander, and
- the number of edges not contained in any $G[X_i]$ is at most $q \cdot \phi \cdot m$.

[1] Everything we present here also works for weighted graphs, however, we focus on unweighted graphs for simplicity.

Today, we obtain a ϕ-expander decomposition of quality $q = O(\phi^{-1/2} \cdot \log n)$. In a few lectures, we revisit the problem and obtain quality $q = O(\log^c n)$ for some small constant c. In practice, we mostly care about values $\phi \approx 1$.

An Algorithm to Compute Conductance and Expander Decomposition. In this lecture, the main focus is *not* to obtain an algorithm to compute conductance but rather only to show that the conductance of a graph can be approximated using the eigenvalues of the "normalized" Laplacian.

However, this proof gives then rise to an algorithm CertifyOrCut(G, ϕ) that given a graph G and a parameter ϕ either:

- *Certifies* that G is a ϕ-expander, or
- Presents a *cut* S such that $\phi(S) \leq \sqrt{2\phi}$.

In the graded homework, we ask you to make the procedure CertifyOrCut(G, ϕ) explicit, and then to show how to use it to compute a ϕ-expander decomposition.

5.2 A Lower Bound for Conductance via Eigenvalues

An Alternative Characterization of Conductance. Let us now take a closer look at the definition of conductance and observe that if a set S has $\text{vol}(S) \leq \text{vol}(V)/2$ then

$$\phi(S) = \frac{|E(S, V \setminus S)|}{\min\{\text{vol}(S), \text{vol}(V \setminus S)\}} = \frac{|E(S, V \setminus S)|}{\text{vol}(S)} = \frac{\mathbf{1}_S^\top \boldsymbol{L} \mathbf{1}_S}{\mathbf{1}_S^\top \boldsymbol{D} \mathbf{1}_S}.$$

To see this, observe that we can rewrite the numerator above using the Laplacian of G as

$$|E(S, V \setminus S)| = \sum_{(u,v) \in E} (\mathbf{1}_S(u) - \mathbf{1}_S(v))^2 = \mathbf{1}_S^\top \boldsymbol{L} \mathbf{1}_S$$

where $\mathbf{1}_S$ is the characteristic vector of S. Further, we can rewrite the denominator as

$$\text{vol}(S) = \mathbf{1}_S^\top \boldsymbol{d} = \mathbf{1}_S^\top \boldsymbol{D} \mathbf{1}_S$$

where $\boldsymbol{D} = \text{diag}(\boldsymbol{d})$ is the degree-matrix. We can now alternatively define the graph conductance of G by

$$\phi(G) = \min_{\substack{\emptyset \subset S \subset V, \\ \text{vol}(S) \leq \text{vol}(V)/2}} \frac{\mathbf{1}_S^\top \boldsymbol{L} \mathbf{1}_S}{\mathbf{1}_S^\top \boldsymbol{D} \mathbf{1}_S} \tag{5.1}$$

where we use that $\phi(S) = \phi(V \setminus S)$ such that the objective value is unchanged as long as for each set $\emptyset \subset S \subset V$ either S or $V \setminus S$ is in the set that we minimize over.

The Normalized Laplacian. Let us next define the *normalized* Laplacian

$$\boldsymbol{N} = \boldsymbol{D}^{-1/2}\boldsymbol{L}\boldsymbol{D}^{-1/2} = \boldsymbol{I} - \boldsymbol{D}^{-1/2}\boldsymbol{A}\boldsymbol{D}^{-1/2}.$$

To learn a bit about this new matrix, let us first look at the first eigenvalue where we use the test vector $y = \boldsymbol{D}^{1/2}\mathbf{1}$, to get by Courant-Fischer (see Theorem 4.1.2) that

$$\lambda_1(\boldsymbol{N}) = \min_{\boldsymbol{x}\neq\mathbf{0}} \frac{\boldsymbol{x}^\top \boldsymbol{N}\boldsymbol{x}}{\boldsymbol{x}^\top\boldsymbol{x}} \leq \frac{\boldsymbol{y}^\top \boldsymbol{D}^{-1/2}\boldsymbol{L}\boldsymbol{D}^{-1/2}\boldsymbol{y}}{\boldsymbol{y}^\top\boldsymbol{y}} = \frac{\mathbf{1}^\top\boldsymbol{L}\mathbf{1}}{\boldsymbol{y}^\top\boldsymbol{y}} = 0 \tag{5.2}$$

because $\boldsymbol{D}^{-1/2}\boldsymbol{D}^{1/2} = I$ and $\boldsymbol{L}\mathbf{1} = 0$ (for the former we use the assumption that G is connected). Since $\boldsymbol{N}$ is PSD (as you will show in the exercises), we also know $\lambda_1(\boldsymbol{N}) \geq 0$, so $\lambda_1(\boldsymbol{N}) = 0$.

Let us use Courant-Fischer again to reason a bit about the second eigenvalue of $\boldsymbol{N}$:

$$\lambda_2(\boldsymbol{N}) = \min_{\substack{\boldsymbol{x}\perp\boldsymbol{D}^{1/2}\mathbf{1}\\ \boldsymbol{x}\neq\mathbf{0}}} \frac{\boldsymbol{x}^\top\boldsymbol{N}\boldsymbol{x}}{\boldsymbol{x}^\top\boldsymbol{x}} = \min_{\substack{\boldsymbol{z}\perp\boldsymbol{d}\\ \boldsymbol{z}\neq\mathbf{0}}} \frac{\boldsymbol{z}^\top\boldsymbol{D}^{1/2}\boldsymbol{N}\boldsymbol{D}^{1/2}\boldsymbol{z}}{\boldsymbol{z}^\top\boldsymbol{D}^{1/2}\boldsymbol{D}^{1/2}\boldsymbol{z}} = \min_{\substack{\boldsymbol{z}\perp\boldsymbol{d}\\ \boldsymbol{z}\neq\mathbf{0}}} \frac{\boldsymbol{z}^\top\boldsymbol{L}\boldsymbol{z}}{\boldsymbol{z}^\top\boldsymbol{D}\boldsymbol{z}}. \tag{5.3}$$

Relating Conductance to the Normalized Laplacian. At this point, it might become clearer why $\boldsymbol{N}$ is a natural matrix to consider when arguing about conductance: if we could argue that for every $\emptyset \subset S \subset V, \mathrm{vol}(S) \leq \mathrm{vol}(V)/2$, we have $\mathbf{1}_S \perp \boldsymbol{d}$, then it would be easy to see that taking the second eigenvalue of $\boldsymbol{N}$ in equation 5.3 is a relaxation of the minimization problem 5.1 defining $\phi(G)$.

While this is clearly not true, we can still argue along these lines.

Theorem 5.2.1 (Cheeger's Inequality, Lower Bound)**.** *We have* $\frac{\lambda_2(\boldsymbol{N})}{2} \leq \phi(G)$.

Proof. Instead of using $\mathbf{1}_S$ directly, we shift $\mathbf{1}_S$ by $\mathbf{1}$ such that it is orthogonal to $\boldsymbol{d}$: we define $\boldsymbol{z}_S = \mathbf{1}_S - \alpha\mathbf{1}$ where α is the scalar that solves

$$\begin{aligned}
&0 = \boldsymbol{d}^\top\boldsymbol{z}_S\\
\iff\ &0 = \boldsymbol{d}^\top(\mathbf{1}_S - \alpha\mathbf{1})\\
\iff\ &0 = \boldsymbol{d}^\top\mathbf{1}_S - \alpha\boldsymbol{d}^\top\mathbf{1}\\
\iff\ &\alpha = \frac{\boldsymbol{d}^\top\mathbf{1}_S}{\boldsymbol{d}^\top\mathbf{1}} = \frac{\mathrm{vol}(S)}{\mathrm{vol}(V)}.
\end{aligned}$$

To conclude the proof, it remains to argue that $\frac{\mathbf{1}_S^\top\boldsymbol{L}\mathbf{1}_S}{\mathbf{1}_S^\top\boldsymbol{D}\mathbf{1}_S} \geq \frac{1}{2}\cdot\frac{\boldsymbol{z}_S^\top\boldsymbol{L}\boldsymbol{z}_S}{\boldsymbol{z}_S^\top\boldsymbol{D}\boldsymbol{z}_S}$:

- Numerator: since $\mathbf{1}^\top\boldsymbol{L}\mathbf{1} = 0$, we have that $\mathbf{1}_S^\top\boldsymbol{L}\mathbf{1}_S = \boldsymbol{z}_S^\top\boldsymbol{L}\boldsymbol{z}_S$.

- Denominator: observe by straight-forward calculations that

$$\begin{aligned}\boldsymbol{z}_S^\top \boldsymbol{D}\boldsymbol{z}_S &= \mathrm{vol}(S)\cdot(1-\alpha)^2 + \mathrm{vol}(V\setminus S)\cdot(-\alpha)^2 \\ &= \mathrm{vol}(S) - 2\,\mathrm{vol}(S)\cdot\alpha + \mathrm{vol}(V)\cdot\alpha^2 \\ &= \mathrm{vol}(S) - \frac{\mathrm{vol}(S)^2}{\mathrm{vol}(V)} \\ &= \mathrm{vol}(S) - \mathrm{vol}(S)\cdot\frac{\mathrm{vol}(S)}{\mathrm{vol}(V)} \\ &\geq \frac{1}{2}\,\mathrm{vol}(S) = \frac{1}{2}\mathbf{1}_S^\top \boldsymbol{D}\mathbf{1}_S\end{aligned}$$

  where we use the assumption that $\mathrm{vol}(S) \leq \mathrm{vol}(V)/2$.

□

5.3 An Upper Bound for Conductance via Eigenvalues

Slightly more surprisingly, we can also show that the second eigenvalue $\lambda_2(\boldsymbol{N})$ can be used to upper bound the conductance.

Theorem 5.3.1 (Cheeger's Inequality, Upper Bound)**.** *We have* $\phi(G) \leq \sqrt{2\cdot\lambda_2(\boldsymbol{N})}$.

Proof. To prove the theorem, we want to show that for *any* $\boldsymbol{z} \perp \boldsymbol{d}$, we can find a set $\emptyset \subset S \subset V$ with $\mathrm{vol}(S) \leq \mathrm{vol}(V)/2$, such that

$$\frac{\mathbf{1}_S^\top \boldsymbol{L}\mathbf{1}_S}{\mathbf{1}_S^\top \boldsymbol{D}\mathbf{1}_S} \leq \sqrt{2\cdot\frac{\boldsymbol{z}^\top\boldsymbol{L}\boldsymbol{z}}{\boldsymbol{z}^\top\boldsymbol{D}\boldsymbol{z}}}. \tag{5.4}$$

As a first step, we would like to change $\boldsymbol{z}$ slightly to make it more convenient to work with:

- we *renumber* the vertices in V such that we have

$$\boldsymbol{z}(1) \leq \boldsymbol{z}(2) \leq \cdots \leq \boldsymbol{z}(n).$$

- we *center* $\boldsymbol{z}$, that is we let $\boldsymbol{z}_c = \boldsymbol{z} - \alpha\mathbf{1}$ where α is chosen such that

$$\sum_{\boldsymbol{z}_c(i)<0} \boldsymbol{d}(i) < \mathrm{vol}(V)/2 \text{ and } \sum_{\boldsymbol{z}_c(i)\leq 0} \boldsymbol{d}(i) \geq \mathrm{vol}(V)/2$$

  i.e. $\sum_{\boldsymbol{z}_c(i)>0} \boldsymbol{d}(i) \leq \mathrm{vol}(V)/2$.

- we *scale*, let $\boldsymbol{z}_{sc} = \beta\boldsymbol{z}_c$ for some scalar β such that $\boldsymbol{z}_{sc}(1)^2 + \boldsymbol{z}_{sc}(n)^2 = 1$.

In the exercises, you will show that changing $\boldsymbol{z}$ to $\boldsymbol{z}_{sc}$ can only make the ratio we are interested in smaller, i.e. that $\frac{\boldsymbol{z}^\top \boldsymbol{L}\boldsymbol{z}}{\boldsymbol{z}^\top \boldsymbol{D}\boldsymbol{z}} \geq \frac{\boldsymbol{z}_{sc}^\top \boldsymbol{L}\boldsymbol{z}_{sc}}{\boldsymbol{z}_{sc}^\top \boldsymbol{D}\boldsymbol{z}_{sc}}$. Thus, if we can show that equation 5.4 holds for $\boldsymbol{z}_{sc}$ in place of $\boldsymbol{z}$, then it also follows for $\boldsymbol{z}$ itself.

We now arrive at the main idea of the proof: we define the set $S_\tau = \{i \in V \mid \boldsymbol{z}_{sc}(i) < \tau\}$ for some random variable τ with probability density function

$$p(t) = \begin{cases} 2 \cdot |t| & t \in [\boldsymbol{z}_{sc}(1), \boldsymbol{z}_{sc}(n)], \\ 0 & \text{otherwise.} \end{cases} \tag{5.5}$$

So, we have probability $\mathbb{P}[a < \tau < b] = \int_{t=a}^{b} p(t)\, dt$.

Since the volume incident to S_τ might be quite large, let us define S for convenience by

$$S = \begin{cases} S_\tau & \mathrm{vol}(S_\tau) < \mathrm{vol}(V)/2, \\ V \setminus S_\tau & \text{otherwise.} \end{cases}$$

Claim 5.3.2. *We have* $\frac{\mathbb{E}_\tau\left[\mathbf{1}_S^\top \boldsymbol{L}\mathbf{1}_S\right]}{\mathbb{E}_\tau\left[\mathbf{1}_S^\top \boldsymbol{D}\mathbf{1}_S\right]} \leq \sqrt{2 \cdot \frac{\boldsymbol{z}_{sc}^\top \boldsymbol{L}\boldsymbol{z}_{sc}}{\boldsymbol{z}_{sc}^\top \boldsymbol{D}\boldsymbol{z}_{sc}}}$.

Proof. Recall $\mathbf{1}_S^\top \boldsymbol{L}\mathbf{1}_S = E(S_\tau, V \setminus S_\tau)$, and by choice of τ, we have for any edge $e = \{i, j\} \in E$ where $\boldsymbol{z}_{sc}(i) \leq \boldsymbol{z}_{sc}(j)$,

$$\begin{aligned} \mathbb{P}_\tau[e \in E(S_\tau, V \setminus S_\tau)] &= \mathbb{P}_\tau[\boldsymbol{z}_{sc}(i) < \tau \leq \boldsymbol{z}_{sc}(j)] \\ &= \int_{t=i}^{j} 2|t|\, dt = \mathrm{sgn}(j) \cdot \boldsymbol{z}_{sc}(j)^2 - \mathrm{sgn}(i) \cdot \boldsymbol{z}_{sc}(i)^2. \end{aligned}$$

Distinguishing by cases, we get

$$\mathrm{sgn}(j) \cdot \boldsymbol{z}_{sc}(j)^2 - \mathrm{sgn}(i) \cdot \boldsymbol{z}_{sc}(i)^2 = \begin{cases} |\boldsymbol{z}_{sc}(i)^2 - \boldsymbol{z}_{sc}(j)^2| & \mathrm{sgn}(i) = \mathrm{sgn}(j), \\ \boldsymbol{z}_{sc}(i)^2 + \boldsymbol{z}_{sc}(j)^2 & \text{otherwise.} \end{cases}$$

We can further upper bound either case by $|\boldsymbol{z}_{sc}(i) - \boldsymbol{z}_{sc}(j)| \cdot (|\boldsymbol{z}_{sc}(i)| + |\boldsymbol{z}_{sc}(j)|)$ (we leave this as an exercise).

Using our new upper bound, we can sum over all edges $e \in E$ to conclude that

$$\begin{aligned} \mathbb{E}_\tau[|E(S_\tau, V \setminus S_\tau)|] &\leq \sum_{i \sim j} |\boldsymbol{z}_{sc}(i) - \boldsymbol{z}_{sc}(j)| \cdot (|\boldsymbol{z}_{sc}(i)| + |\boldsymbol{z}_{sc}(j)|) \\ &\leq \sqrt{\sum_{i \sim j} (\boldsymbol{z}_{sc}(i) - \boldsymbol{z}_{sc}(j))^2 \cdot \sum_{i \sim j} (|\boldsymbol{z}_{sc}(i)| + |\boldsymbol{z}_{sc}(j)|)^2} \end{aligned}$$

where the last line follows from $\langle \boldsymbol{x}, \boldsymbol{y} \rangle^2 \leq \langle \boldsymbol{x}, \boldsymbol{x} \rangle \cdot \langle \boldsymbol{y}, \boldsymbol{y} \rangle$ (i.e. Cauchy-Schwarz).

The first sum should look familiar by now: it is simply the Quadratic Laplacian Form $\sum_{i\sim j}(\boldsymbol{z}_{sc}(i)-\boldsymbol{z}_{sc}(j))^2 = \boldsymbol{z}_{sc}^\top \boldsymbol{L}\boldsymbol{z}_{sc}$.

It is not hard to reason about the second term either

$$\sum_{i\sim j}(|\boldsymbol{z}_{sc}(i)|+|\boldsymbol{z}_{sc}(j)|)^2 \leq 2\sum_{i\sim j}\boldsymbol{z}_{sc}(i)^2+\boldsymbol{z}_{sc}(j)^2 = 2\sum_{i\in V}\boldsymbol{d}(i)\boldsymbol{z}_{sc}(i)^2 = 2\boldsymbol{z}_{sc}^\top \boldsymbol{D}\boldsymbol{z}_{sc}.$$

Putting everything together, we obtain

$$\mathbb{E}_\tau[|E(S_\tau, V\setminus S_\tau)|] \leq \sqrt{\boldsymbol{z}_{sc}^\top \boldsymbol{L}\boldsymbol{z}_{sc}\cdot 2\boldsymbol{z}_{sc}^\top \boldsymbol{D}\boldsymbol{z}_{sc}} = \sqrt{2\cdot\frac{\boldsymbol{z}_{sc}^\top \boldsymbol{L}\boldsymbol{z}_{sc}}{\boldsymbol{z}_{sc}^\top \boldsymbol{D}\boldsymbol{z}_{sc}}}\cdot \boldsymbol{z}_{sc}^\top \boldsymbol{D}\boldsymbol{z}_{sc} \tag{5.6}$$

While this almost looks like what we want, we still have to argue that $\boldsymbol{z}_{sc}^\top \boldsymbol{D}\boldsymbol{z}_{sc} = \mathbb{E}_\tau[\mathbf{1}_S^\top \boldsymbol{D}\mathbf{1}_S]$ to finish the proof.

To this end, when unrolling the expectation, we use a simple trick that splits by cases:

$$\begin{aligned}
\mathbb{E}_\tau[\mathbf{1}_S^\top \boldsymbol{D}\mathbf{1}_S] &= \sum_{i\in V}\boldsymbol{d}(i)\cdot\mathbb{P}[i\in S] \\
&= \sum_{i\in V,\boldsymbol{z}_{sc}(i)<0}\boldsymbol{d}(i)\cdot\mathbb{P}[i\in S\wedge S=S_\tau] + \sum_{i\in V,\boldsymbol{z}_{sc}(i)\geq 0}\boldsymbol{d}(i)\cdot\mathbb{P}[i\in S\wedge S\neq S_\tau] \\
&= \sum_{i\in V,\boldsymbol{z}_{sc}(i)<0}\boldsymbol{d}(i)\cdot\mathbb{P}[\boldsymbol{z}_{sc}(i)<\tau\wedge\tau<0] + \sum_{i\in V,\boldsymbol{z}_{sc}(i)\geq 0}\boldsymbol{d}(i)\cdot\mathbb{P}[\boldsymbol{z}_{sc}(i)\geq\tau\wedge\tau\geq 0]
\end{aligned}$$

where we use the centering of $\boldsymbol{z}_{sc}$ the definition of S and that the event $\{i\in S\wedge S=S_\tau\}$ can be rewritten as the event $\{i<\tau\wedge\tau<0\}$ (the other case is analogous).

Let i be a vertex with $\boldsymbol{z}_{sc}(i)<0$, then the probability $\mathbb{P}[i\in S\wedge S=S_\tau]$ is exactly $\boldsymbol{z}_{sc}(i)^2$ by choice of the density function of τ (again the case for i with $\boldsymbol{z}_{sc}(i)$ non-negative is analgous). Thus, summing over all vertices, we obtain

$$\begin{aligned}
\mathbb{E}_\tau[\mathbf{1}_S^\top \boldsymbol{D}\mathbf{1}_S] &= \sum_{i\in V,\boldsymbol{z}_{sc}(i)<0}\boldsymbol{d}(i)\cdot\mathbb{P}[\boldsymbol{z}_{sc}(i)<\tau\wedge\tau<0] + \sum_{i\in V,\boldsymbol{z}_{sc}(i)\geq 0}\mathbb{P}[\boldsymbol{z}_{sc}(i)\geq\tau\wedge\tau\geq 0] \\
&= \sum_{i\in V}\boldsymbol{d}(i)\cdot\boldsymbol{z}_{sc}(i)^2 = \boldsymbol{z}_{sc}^\top \boldsymbol{D}\boldsymbol{z}_{sc}.
\end{aligned}$$

Therefore, we can plug in our result directly into Equation 5.6 and the proof is completed by dividing both sides by $\mathbb{E}_\tau[\mathbf{1}_S^\top \boldsymbol{D}\mathbf{1}_S]$. □

While Theorem 5.3.2 only ensures our claim in expectation, this is already sufficient to conclude that there exists some set S that satisfies the same guarantees deterministically, as you will prove in Problem Set 4. This is often called the *probabilistic method of expectation* and can be seen from the definition of expectation. We have thus proven the upper bound of Cheeger's inequality. □

5.4 Conclusion

Today, we have introduced the concepts of conductance and formalized expanders and expander decompositions. These are crucial concepts that you will encounter often in literature and also again in this course. They are a key tool in many recent breakthroughs in Theoretical Computer Science.

In the second part of the lecture (the main part), we discussed Cheeger's inequality which allows to relate the second eigenvalue of the normalized Laplacian to a graphs conductance. We summarize the full statement here.

Theorem 5.4.1 (Cheeger's Inequality)**.** *We have* $\frac{\lambda_2(\boldsymbol{N})}{2} \leq \phi(G) \leq \sqrt{2 \cdot \lambda_2(\boldsymbol{N})}$.

We point out that this Theorem is tight as you will show in the exercises. The proof for Cheeger's inequality is probably the most advanced proof, we have seen so far in the course. The many tricks that make the proof work might sometimes seem a bit magical but it is important to remember that they are a result of many people polishing this proof over and over. The proof techniques used are extremely useful and can be re-used in various contexts. We therefore strongly encourage you to really understand the proof yourself!

Chapter 6

Random Walks

Today, we talk about random walks on graphs and how the spectrum of the Laplacian guides convergence of random walks. We start by giving the definition of a random walk on a weighted graph $G = (V, E, w)$.

6.1 A Primer on Random Walks

Random Walk Basics. We call a random sequence of vertices $v_0, v_1, \ldots$ a *random walk* on G, if v_0 is a vertex in G chosen according to some probability distribution $\boldsymbol{p}_0 \in \mathbb{R}^V$; and for any $t \geq 0$, we have

$$\mathbb{P}[v_{t+1} = v \mid v_t = u] = \begin{cases} \boldsymbol{w}(u,v)/\boldsymbol{d}(u) & \text{if } \{u,v\} \in E, \\ 0 & \text{otherwise.} \end{cases}$$

To gain some intuition for the definition, assume first that the graph G is undirected. Consider a particle that is placed at a random vertex v_0 initially. Then at each step the particle is moved to a neighbor of the current vertex it is resting at, where the neighbor is chosen uniformly at random.

If the graph is weighted, then instead of choosing a neighbor v_{t+1} of a vertex v_t at each step uniformly at random, one chooses a neighbor v of v_t with probability $\boldsymbol{w}(v, v_t)$ divided by the degree $\boldsymbol{d}(v_t)$.

The Random Walk Matrix. We now define the random walk matrix $\boldsymbol{W}$ by

$$\boldsymbol{W} = \boldsymbol{A}\boldsymbol{D}^{-1}$$

and observe that for all vertices $u, v \in V$ (and any t), we have that

$$\boldsymbol{W}_{vu} = \begin{cases} \boldsymbol{w}(u,v)/\boldsymbol{d}(u) & \text{if } \{u,v\} \in E, \\ 0 & \text{otherwise.} \end{cases}$$

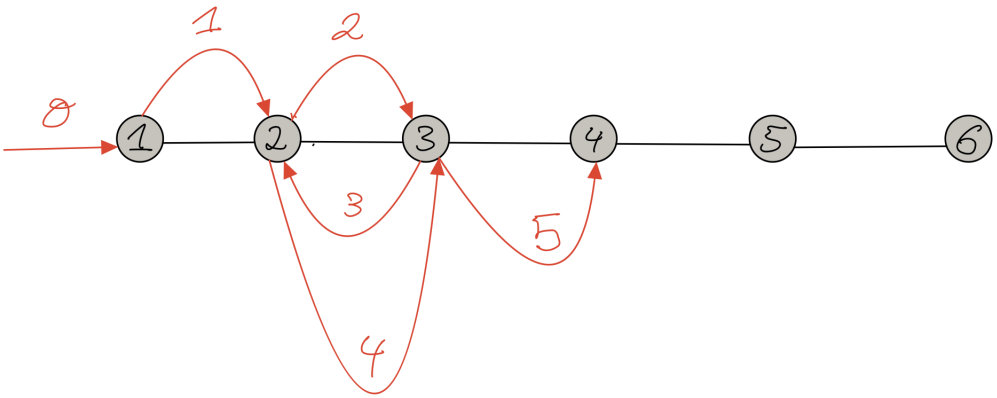


Figure 6.1: A (possibly random) walk where the red edges indicate the edges that the particle moves along. Here the walk visits the vertices $v_0 = 1, v_1 = 2, v_2 = 3, v_3 = 2, v_4 = 3, v_5 = 4$.

Thus, $\boldsymbol{W}_{vu} = \mathbb{P}[v_{t+1} = v \mid v_t = u]$ (for any t).

Therefore, $W\mathbf{1}_u$ is the distribution over the vertices that the random walk visits them at the next time step, given that it currently is at u. More generally, we can now compute the distribution $\boldsymbol{p}_1$ over the vertices that they are visited at time 1 by $\boldsymbol{W}\boldsymbol{p}_0$, the distribution $\boldsymbol{p}_2$ by $\boldsymbol{W}\boldsymbol{p}_1 = \boldsymbol{W}(\boldsymbol{W}\boldsymbol{p}_0)$ and so on. Another way of writing this is $\boldsymbol{p}_t = \boldsymbol{W}^t\boldsymbol{p}_0$.

6.2 Convergence Results for Random Walks

In this first part of the chapter, we are interested mostly in convergence of random walks that is the two questions:

- How does a random walk behave after a large number of steps are taken?
- How many steps does it take asymptotically until the random walk behaves as if an infinite number of steps were taken?

To start shedding some light on these questions, we introduce stationary distributions.

Stationary Distribution. We call a distribution $\boldsymbol{\pi} \in \mathbb{R}^V$, a *stationary distribution* if $\boldsymbol{W}\boldsymbol{\pi} = \boldsymbol{\pi}$. That is $\boldsymbol{\pi}$ is an eigenvector of $\boldsymbol{W}$ associated with eigenvalue 1. It turns out such a stationary distribution always exists.

Lemma 6.2.1. *Every graph G has a stationary distribution.*

Proof. Let $\boldsymbol{\pi} = \frac{\boldsymbol{d}}{\mathbf{1}^\top \boldsymbol{d}}$. Clearly, we have that $\|\boldsymbol{\pi}\|_1 = \sum_{v \in V} \boldsymbol{d}(v)/\mathbf{1}^\top \boldsymbol{d} = \frac{1}{\mathbf{1}^\top \boldsymbol{d}} \sum_{v \in V} \boldsymbol{d}(v) = 1$,

so $\boldsymbol{\pi}$ is indeed a distribution. Further note that

$$\boldsymbol{W}\boldsymbol{\pi} = \boldsymbol{A}\boldsymbol{D}^{-1} \cdot \frac{\boldsymbol{d}}{\mathbf{1}^\top \boldsymbol{d}} = \frac{\boldsymbol{A}\mathbf{1}}{\mathbf{1}^\top \boldsymbol{d}} = \frac{\boldsymbol{d}}{\mathbf{1}^\top \boldsymbol{d}} = \boldsymbol{\pi}.$$

□

For many graphs one can show that for $t \to \infty$, we have that $\boldsymbol{p}_t \to \boldsymbol{\pi}$, i.e. that independent of the starting distribution $\boldsymbol{p}_0$, the random walk always converges to distribution $\boldsymbol{\pi}$.

Unfortunately, this is not true for all graphs: take the graph of two vertices connected by a single edge with $\boldsymbol{p}_0$ being 1 at one vertex and 0 at the other.

6.2.1 Making Random Walks Lazy

Lazy Random Walks. Luckily, we can overcome this issue by using a *lazy random walk*. A lazy random walk behaves just like a random walk, however, at each time step, with probability $\frac{1}{2}$ instead of transitioning to a neighbor, it simply stays put. We give the lazy random walk matrix by

$$\tilde{\mathbf{W}} = \frac{1}{2}\boldsymbol{I} + \frac{1}{2}\boldsymbol{W} = \frac{1}{2}\left(\boldsymbol{I} + \boldsymbol{A}\boldsymbol{D}^{-1}\right).$$

It is not hard to see that the stationary distribution $\boldsymbol{\pi}$ for $\boldsymbol{W}$, is also a stationary distribution for $\tilde{\mathbf{W}}$.

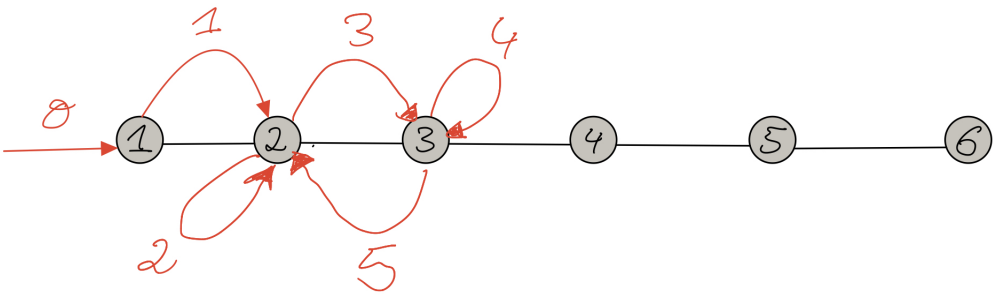


Figure 6.2: A lazy random walk where the red edges indicate the edges that the particle moves along. Here the lazy walk visits the vertices $v_0 = 1, v_1 = 2, v_2 = 2, v_3 = 3, v_4 = 3, v_5 = 2$.

Lazy Random Walks and the Normalized Laplacian. Recall that we defined $\boldsymbol{N} = \boldsymbol{D}^{-1/2}\boldsymbol{L}\boldsymbol{D}^{-1/2} = \boldsymbol{I} - \boldsymbol{D}^{-1/2}\boldsymbol{A}\boldsymbol{D}^{-1/2} \iff \boldsymbol{D}^{-1/2}\boldsymbol{A}\boldsymbol{D}^{-1/2} = \boldsymbol{I} - \boldsymbol{N}$. We can therefore derive

$$\begin{aligned}
\tilde{\mathbf{W}} &= \frac{1}{2}\boldsymbol{I} + \frac{1}{2}\boldsymbol{A}\boldsymbol{D}^{-1} \\
&= \frac{1}{2}\boldsymbol{I} + \frac{1}{2}\boldsymbol{D}^{1/2}\boldsymbol{D}^{-1/2}\boldsymbol{A}\boldsymbol{D}^{-1/2}\boldsymbol{D}^{-1/2} \\
&= \frac{1}{2}\boldsymbol{I} + \frac{1}{2}\boldsymbol{D}^{1/2}(\boldsymbol{I} - \boldsymbol{N})\boldsymbol{D}^{-1/2} \\
&= \frac{1}{2}\boldsymbol{I} + \frac{1}{2}\boldsymbol{D}^{1/2}\boldsymbol{I}\boldsymbol{D}^{-1/2} - \frac{1}{2}\boldsymbol{D}^{1/2}\boldsymbol{N}\boldsymbol{D}^{-1/2} \\
&= \boldsymbol{I} - \frac{1}{2}\boldsymbol{D}^{1/2}\boldsymbol{N}\boldsymbol{D}^{-1/2}
\end{aligned}$$

We will now start to reason about the eigenvalues and eigenvectors of $\tilde{\mathbf{W}}$ in terms of the normalized laplacian $\boldsymbol{N}$ that we are already familiar with.

For the rest of the lecture, we let $\nu_1 \leq \nu_2 \leq \cdots \leq \nu_n$ be the eigenvalues of $\boldsymbol{N}$ associated with the orthogonal eigenvectors $\boldsymbol{\psi}_1, \boldsymbol{\psi}_2, \ldots, \boldsymbol{\psi}_n$ where we know that such eigenvectors exist by the Spectral Theorem. We note in particular that from the last lecture, we have that $\boldsymbol{\psi}_1 = \frac{\boldsymbol{d}^{1/2}}{(\mathbf{1}^\top \boldsymbol{d})^{1/2}}$ (see Equation 5.2 where we added a normalization such that $\boldsymbol{\psi}_1^\top \boldsymbol{\psi}_1 = 1$).

Lemma 6.2.2. *For the i^{th} eigenvalue ν_i of $\boldsymbol{N}$ associated with eigenvector $\boldsymbol{\psi}_i$, we have that $\tilde{\mathbf{W}}$ has an eigenvalue of $(1 - \frac{1}{2}\nu_i)$ associated with eigenvector $\boldsymbol{D}^{1/2}\boldsymbol{\psi}_i$.*

Proof. The proof is by straight-forward calculations

$$\begin{aligned}
\tilde{\mathbf{W}}\boldsymbol{D}^{1/2}\boldsymbol{\psi}_i &= (\boldsymbol{I} - \frac{1}{2}\boldsymbol{D}^{1/2}\boldsymbol{N}\boldsymbol{D}^{-1/2})\boldsymbol{D}^{1/2}\boldsymbol{\psi}_i \\
&= \boldsymbol{D}^{1/2}\boldsymbol{\psi}_i - \frac{1}{2}\boldsymbol{D}^{1/2}\boldsymbol{N}\boldsymbol{\psi}_i \\
&= \boldsymbol{D}^{1/2}\boldsymbol{\psi}_i - \frac{1}{2}\boldsymbol{D}^{1/2}\boldsymbol{\psi}_i\nu_i = \boldsymbol{D}^{1/2}\boldsymbol{\psi}_i(1 - \frac{1}{2}\nu_i).
\end{aligned}$$

□

Corollary 6.2.3. *Every eigenvalue of $\tilde{\mathbf{W}}$ is in $[0, 1]$.*

Proof. Recall that $\boldsymbol{L} \preccurlyeq 2\boldsymbol{D}$ which implies that $\boldsymbol{N} \preccurlyeq 2\boldsymbol{I}$. But this implies that every eigenvalue of $\boldsymbol{N}$ is in $[0, 2]$. Thus, using Lemma 6.2.2, the corollary follows. □

6.2.2 Convergence of Lazy Random Walks

We have now done enough work to obtain an interesting result. We can derive an alternative characterization of $\boldsymbol{p}_t$ by expanding $\boldsymbol{p}_0$ along an orthogonal eigenvectors basis and then we can repeatedly apply $\tilde{\mathbf{W}}$ by taking powers of the eigenvalues.

Unfortunately, $\tilde{\mathbf{W}}$ is not symmetric so its eigenvectors are not necessarily orthogonal. Instead, we use a simple trick that allows to expand along the eigenvectors of $\boldsymbol{N}$

$$\forall i, \boldsymbol{\psi}_i^\top \boldsymbol{D}^{-1/2}\boldsymbol{p}_0 = \alpha_i \iff \boldsymbol{D}^{-1/2}\boldsymbol{p}_0 = \sum_{i=1}^n \alpha_i \boldsymbol{\psi}_i \iff \boldsymbol{p}_0 = \sum_{i=1}^n \alpha_i \boldsymbol{D}^{1/2}\boldsymbol{\psi}_i. \tag{6.1}$$

The above equivalences are best understood if you start from the middle. To get to the left side, you need to observe that multiplying both sides by $\boldsymbol{\psi}_i^\top$ cancels all terms $\boldsymbol{\psi}_j$ with $j \neq i$ in the sum by orthogonality. To get the right hand side expression, one can simply left-multiply by $\boldsymbol{D}^{1/2}$. Technically, we have to show that $\boldsymbol{D}^{-1/2}\boldsymbol{p}_0$ lives in the eigenspace of $\boldsymbol{N}$ but we leave this as an exercise.

This allows us to express a right multiplication by $\tilde{\mathbf{W}}$ as

$$\boldsymbol{p}_1 = \tilde{\mathbf{W}}\boldsymbol{p}_0 = \sum_{i=1}^n \alpha_i \tilde{\mathbf{W}}\boldsymbol{D}^{1/2}\boldsymbol{\psi}_i = \sum_{i=1}^n \alpha_i \left(1 - \frac{\nu_i}{2}\right) \boldsymbol{D}^{1/2}\boldsymbol{\psi}_i.$$

And as promised, if we apply $\tilde{\mathbf{W}}$, the lazy random walk operator, t times, we now obtain

$$\boldsymbol{p}_t = \sum_{i=1}^n \alpha_i \left(1 - \frac{\nu_i}{2}\right)^t \boldsymbol{D}^{1/2}\boldsymbol{\psi}_i = \alpha_1 \boldsymbol{D}^{1/2}\boldsymbol{\psi}_1 + \sum_{i=2}^n \alpha_i \left(1 - \frac{\nu_i}{2}\right)^t \boldsymbol{D}^{1/2}\boldsymbol{\psi}_i. \tag{6.2}$$

where we use in the last equality that $\nu_1 = 0$. Using this simple characterization, we immediately get that $\boldsymbol{p}_t \to \boldsymbol{\pi}$ if $\nu_i > 0$ for all $i \geq 2$ (which is exactly when the graph is connected as you will prove in an exercise). To see this, observe that as t grows sum vanishes. We have that

$$\lim_{t\to\infty} \boldsymbol{p}_t = \alpha_1 \boldsymbol{D}^{1/2}\boldsymbol{\psi}_1 = \boldsymbol{\pi}.$$

where we used in the equality that $\boldsymbol{D}^{1/2}\boldsymbol{\psi}_1 = \frac{\boldsymbol{d}}{(\mathbf{1}^\top \boldsymbol{d})^{1/2}}$ and the value of α_1 (from 6.1).

Theorem 6.2.4. *For any connected graph G, we have that the lazy random walk converges to the stationary distribution of G.*

6.2.3 The Rate of Convergence

Let us now come to the main result that we want to prove in this lecture.

Theorem 6.2.5. *In any unweighted (a.k.a. unit weight) connected graph G, for any $\boldsymbol{p}_0$, at any time step t, we have for $\boldsymbol{p}_t = \tilde{\mathbf{W}}^t\boldsymbol{p}_0$ that*

$$\|\boldsymbol{p}_t - \boldsymbol{\pi}\|_\infty \leq e^{-\nu_2 \cdot t/2}\sqrt{n}$$

Instead of proving the theorem above, we prove the lemma below which gives point-wise convergence. This makes it more convenient to derive a proof and it is not hard to deduce the theorem above as a corollary.

Lemma 6.2.6. *In any weighted connected graph G, for all $a, b \in V$, and any time step t, we have for $\boldsymbol{p}_0 = \mathbf{1}_a$ and $\boldsymbol{p}_t = \tilde{\mathbf{W}}^t \boldsymbol{p}_0$ that*

$$|\boldsymbol{p}_t(b) - \boldsymbol{\pi}(b)| \leq e^{-\nu_2 \cdot t/2} \sqrt{\boldsymbol{d}_b / \boldsymbol{d}_a}$$

From Equation 6.2, we obtain that

$$\boldsymbol{p}_t(b) - \boldsymbol{\pi}(b) = \mathbf{1}_b^\top (\boldsymbol{p}_t - \boldsymbol{\pi}) = \mathbf{1}_b^\top \left(\sum_{i=2}^{n} \alpha_i \left(1 - \frac{\nu_i}{2}\right)^t \boldsymbol{D}^{1/2} \boldsymbol{\psi}_i \right) \tag{6.3}$$

$$= \sum_{i=2}^{n} \alpha_i \left(1 - \frac{\nu_i}{2}\right)^t \mathbf{1}_b^\top \boldsymbol{D}^{1/2} \boldsymbol{\psi}_i \leq \left(1 - \frac{\nu_2}{2}\right)^t \cdot \sum_{i=2}^{n} \alpha_i \mathbf{1}_b^\top \boldsymbol{D}^{1/2} \boldsymbol{\psi}_i \tag{6.4}$$

Taking the absolute value on both sides, we obtain that

$$|\boldsymbol{p}_t(b) - \boldsymbol{\pi}(b)| \leq \left(1 - \frac{\nu_2}{2}\right)^t \sum_{i=2}^{n} \left| \alpha_i \mathbf{1}_b^\top \boldsymbol{D}^{1/2} \boldsymbol{\psi}_i \right| \leq \left(1 - \frac{\nu_2}{2}\right)^t \sqrt{\left(\sum_{i=2}^{n} \alpha_i^2 \right) \left(\sum_{i=2}^{n} \left(\mathbf{1}_b^\top \boldsymbol{D}^{1/2} \boldsymbol{\psi}_i \right)^2 \right)}$$

where we use Cauchy-Schwarz in the last inequality, i.e. $|\langle \boldsymbol{u}, \boldsymbol{v} \rangle|^2 \leq \langle \boldsymbol{u}, \boldsymbol{u} \rangle \cdot \langle \boldsymbol{v}, \boldsymbol{v} \rangle$. Let us finally bound the two sums:

- By 6.1, $\sum_{i=2}^{n} \alpha_i^2 = \sum_{i=2}^{n} \left(\boldsymbol{\psi}_i^\top \boldsymbol{D}^{-1/2} \boldsymbol{p}_0 \right)^2 \leq \| \boldsymbol{D}^{-1/2} \boldsymbol{p}_0 \|_2^2 = \| \boldsymbol{D}^{-1/2} \mathbf{1}_a \|_2^2 = 1/\boldsymbol{d}_a$.
- Finally, we show that $\sum_{i=2}^{n} \left(\mathbf{1}_b^\top \boldsymbol{D}^{1/2} \boldsymbol{\psi}_i \right)^2 \leq \sum_{i=1}^{n} \left(\mathbf{1}_b^\top \boldsymbol{D}^{1/2} \boldsymbol{\psi}_i \right)^2 = \| \boldsymbol{D}^{1/2} \mathbf{1}_b \|_2^2 = \boldsymbol{d}_b$ (we only show the first equality, the other inequalities are straight-forward). We first expand the vector $\boldsymbol{D}^{1/2} \mathbf{1}_b$ along the eigenvectors using some values β_i defined

  $$\boldsymbol{D}^{1/2} \mathbf{1}_b = \sum_{i=1}^{n} \beta_i \boldsymbol{\psi}_i \iff \boldsymbol{\psi}_i^\top \boldsymbol{D}^{1/2} \mathbf{1}_b = \beta_i \iff \mathbf{1}_b^\top \boldsymbol{D}^{1/2} \boldsymbol{\psi}_i = \beta_i$$

  We used orthogonality to get the first equivalence, and then just take the transpose to get the second. We can now write

  $$\| \boldsymbol{D}^{1/2} \mathbf{1}_b \|_2^2 = (\boldsymbol{D}^{1/2} \mathbf{1}_b)^\top (\boldsymbol{D}^{1/2} \mathbf{1}_b) = \left(\sum_{i=1}^{n} \beta_i \boldsymbol{\psi}_i^\top \right) \left(\sum_{i=1}^{n} \beta_i \boldsymbol{\psi}_i \right) = \sum_{i=2}^{n} \beta_i^2$$

  where we again used orthogonality of $\boldsymbol{\psi}_i$. The equality then follows by definition of β_i.

Putting everything together (and using $1 + x \leq e^x, \forall x \in \mathbb{R}$), we obtain

$$|\boldsymbol{p}_t(b) - \boldsymbol{\pi}(b)| \leq \left(1 - \frac{\nu_2}{2}\right)^t \sqrt{\boldsymbol{d}_b / \boldsymbol{d}_a} \leq e^{-\nu_2 \cdot t/2} \sqrt{\boldsymbol{d}_b / \boldsymbol{d}_a}$$

6.3 Properties of Random Walks

We now shift our focus away from convergence of random walks and consider some interesting properties of random walks[1]. Here, we are no longer interested in lazy random walks, although all proofs can be straight-forwardly adapted. While in the previous section, we relied on computing the second eigenvalue of the Normalized Laplacian efficiently, here, we will discover that solving Laplacian systems, that is finding an $\boldsymbol{x}$ such that $\boldsymbol{L}\boldsymbol{x} = \boldsymbol{b}$ can solve a host of problems in random walks.

6.3.1 Hitting Times

One of the most natural questions one can ask about a random walk starting in a vertex a (i.e. $\boldsymbol{p}_0 = \mathbf{1}_a$) is how many steps it takes to get to a special vertex s. This quantity is called the *hitting time* from a to s and we denote it by $H_{a,s} = \inf\{t \mid \boldsymbol{v}_t = s\}$. For the rest of this section, we are concerned with computing the expected hitting time, i.e. $\mathbb{E}[H_{a,s}]$.

It turns out, that it is more convenient to compute *all* expected hitting times $H_{a,s}$ for vertices $a \in V$ to a fixed s. We denote by $\boldsymbol{h} \in \mathbf{R}^V$, the vector with $\boldsymbol{h}(a) = \mathbb{E}[H_{a,s}]$. We now show that we can compute $\boldsymbol{h}$ by solving a Laplacian system $\boldsymbol{L}\boldsymbol{h} = \boldsymbol{b}$. We will see later in the course that such systems (spoiler alert!) can be solved in time $\tilde{O}(m)$, so this will imply a near-linear time algorithm to compute the hitting times.

Hitting Time and the Random Walk Matrix. Let us first observe that if $s = a$, then the answer becomes trivially 0, i.e. $\boldsymbol{h}(s) = 0$.

We compute the rest of the vector by writing down a system of equations that recursively characterizes $\boldsymbol{h}$. Observe therefore first that for any $a \neq s$, we have that the random walks starting at a will next visit a neighbor b of a. If the selected neighbor $b = s$, the random walks stops; otherwise, the random walks needs in expectation $\mathbb{E}[H_{b,s}]$ time to move to s.

We can express this algebraically by

$$\boldsymbol{h}_a = 1 + \sum_{a \sim b} \mathbb{P}[v_{t+1} = b \mid v_t = a] \cdot \boldsymbol{h}(b) = 1 + \sum_{a \sim b} \frac{\boldsymbol{w}(a,b)}{\boldsymbol{d}(a)} \cdot \boldsymbol{h}(b) = 1 + (\boldsymbol{W}\mathbf{1}_a)^\top \boldsymbol{h} = 1 + \mathbf{1}_a^\top \boldsymbol{W}^\top \boldsymbol{h}.$$

Using that $\boldsymbol{h}(a) = \mathbf{1}_a^\top \boldsymbol{h} = \mathbf{1}_a^\top \boldsymbol{I}\boldsymbol{h}$, we can rewrite this as

$$1 = \mathbf{1}_a^\top (\boldsymbol{I} - \boldsymbol{W}^\top)\boldsymbol{h}.$$

This gives a system of (linear) equations, that can be neatly summarized by

$$\mathbf{1} - \alpha \cdot \mathbf{1}_s = (\boldsymbol{I} - \boldsymbol{W}^\top)\boldsymbol{h}$$

[1]Note that this part of the script is in large part inspired by Aaron Sidford's lecture notes on the same subject, in his really interesting course Discrete Mathematics and Algorithms.

where we have an extra degree of freedom in choosing α in formulating a constraint $1-\alpha = \mathbf{1}_s^\top(\boldsymbol{I}-\boldsymbol{W}^\top)\boldsymbol{h}$. This extra degree of freedom stems from the fact that $n-1$ equations suffice for us to enforce that the returned vector $\boldsymbol{x}$ from the system is indeed the hitting times (possibly shifted by the value assigned to coordinate t).

Finding Hitting Times via Laplacian System Solve. Since we assume G connected, we have that multiplying with $\boldsymbol{D} = \boldsymbol{D}^\top$ preserves equality. Further since $\boldsymbol{W} = \boldsymbol{A}\boldsymbol{D}^{-1}$, we obtain

$$\boldsymbol{d} - \alpha \cdot \boldsymbol{d}(s) \cdot \mathbf{1}_s = (\boldsymbol{D}-\boldsymbol{A})\boldsymbol{h}.$$

Defining $\boldsymbol{b} = \boldsymbol{d} - \alpha \cdot \boldsymbol{d}(s) \cdot \mathbf{1}_s$, and observing $\boldsymbol{L} = \boldsymbol{D} - \boldsymbol{A}$, we have $\boldsymbol{L}\boldsymbol{h} = \boldsymbol{b}$.

Finally, we observe that we only have a solution to the above system if and only if $\boldsymbol{b} \in \ker(\boldsymbol{L})^\perp = \operatorname{span}(\mathbf{1})^\perp$. We thus have to set α such that

$$\mathbf{1}^\top(\boldsymbol{d} - \alpha \cdot \boldsymbol{d}(s) \cdot \mathbf{1}_s) = \|\boldsymbol{d}\|_1 - \alpha \cdot \boldsymbol{d}(s) \iff \alpha = \|\boldsymbol{d}\|_1 / \boldsymbol{d}(s).$$

We have now formalized $\boldsymbol{L}$ and $\boldsymbol{b}$ completely. A last detail that we should not forget about is that any solution $\boldsymbol{x}$ to such system $\boldsymbol{L}\boldsymbol{x} = \boldsymbol{b}$ is not necessarily equal $\boldsymbol{h}$ but has the property that it is shifted from $\boldsymbol{h}$ by the all-ones vector. Since we require $\boldsymbol{h}(s) = 0$, we can reconstruct $\boldsymbol{h}$ from $\boldsymbol{x}$ straight-forwardly by subtracting $\boldsymbol{x}(s)\mathbf{1}$.

Theorem 6.3.1. *Given a connected graph G, a special vertex $s \in V$. Then, we can formalize a Laplacian system $\boldsymbol{L}\boldsymbol{x} = \boldsymbol{b}$ (where $\boldsymbol{L}$ is the Laplacian of G) such that the expected hitting times to s are given by $\boldsymbol{h} = \boldsymbol{x} - \boldsymbol{x}(s)\mathbf{1}$. We can reconstruct $\boldsymbol{h}$ from $\boldsymbol{x}$ in time $O(n)$.*

Hitting Times and Electrical Networks. Seeing that hitting times can be computed by formulating a Laplacian system $\boldsymbol{L}\boldsymbol{x} = \boldsymbol{b}$. You might remember that in the first lecture, we argued that a system $\boldsymbol{L}\boldsymbol{x} = \boldsymbol{b}$ also solves the problem of routing a demand $\boldsymbol{b}$ via an electrical flow with voltages $\boldsymbol{x}$.

Indeed, we can interpret computing expected hitting times $\boldsymbol{h}$ to a special vertex s as the problem of computing the electrical voltages $\boldsymbol{x}$ where we insert (or more technically correct apply) $\boldsymbol{d}(a)$ units of current at every vertex $a \neq s$ and where we remove $\mathbf{1}^\top\boldsymbol{d} - \boldsymbol{d}(s)$ units of current at the vertex s. Then, we can express expected hitting time to some vertex a as the voltage difference to s: $\mathbb{E}[H_{a,s}] = \boldsymbol{h}(a) = \boldsymbol{x}(a) - \boldsymbol{x}(s)$.

6.3.2 Commute Time

A topic very related to hitting times are *commute times*. That is for two vertices a, b, the commute time is the time in a random walk starting in a to visit b and then to return to a again. Thus, it can be defined $C_{a,b} = H_{a,b} + H_{b,a}$.

Commute Times via Electric Flows. Recall that expected hitting times have an electric flow interpretation.

Now, let us denote by $\boldsymbol{x}$ a solution to the Laplacian system $\boldsymbol{L}\boldsymbol{x} = \boldsymbol{b}_b$ where the demand is $\boldsymbol{b}_b = \boldsymbol{d} - \boldsymbol{d}^\top \mathbf{1} \cdot \mathbf{1}_b \in \ker(\mathbf{1})^\perp$. Recall that we have $\mathbb{E}[H_{z,b}] = \boldsymbol{x}(z) - \boldsymbol{x}(b)$ for all z. Similarly, we can compute voltages $\boldsymbol{y}$ to the Laplacian system $\boldsymbol{L}\boldsymbol{y} = \boldsymbol{b}_a$ where $\boldsymbol{b}_a = \boldsymbol{d} - \boldsymbol{d}^\top \mathbf{1} \cdot \mathbf{1}_a \in \ker(\mathbf{1})^\perp$. Again, $\mathbb{E}[H_{z,a}] = \boldsymbol{y}(z) - \boldsymbol{y}(a)$ for all z.

But observe that this allows us to argue by linearity that $\mathbb{E}[C_{a,b}] = \mathbb{E}[H_{a,b} + H_{b,a}] = \mathbb{E}[H_{a,b}] + \mathbb{E}[H_{b,a}] = \boldsymbol{x}(a) - \boldsymbol{x}(b) + \boldsymbol{y}(b) - \boldsymbol{y}(a) = (\mathbf{1}_a - \mathbf{1}_b)^\top (\boldsymbol{x} - \boldsymbol{y})$. But using linearity again, we can also argue at the same time that we obtain the vector $\boldsymbol{z} = (\boldsymbol{x} - \boldsymbol{y})$ as a solution to the problem $\boldsymbol{L}\boldsymbol{z} = \boldsymbol{b}_b - \boldsymbol{b}_a = \boldsymbol{d}^\top \mathbf{1}(\mathbf{1}_a - \mathbf{1}_b)$. That is the flow that routes $\|\boldsymbol{d}\|_1$ units of flow from b to a.

Theorem 6.3.2. *Given a graph $G = (V, E)$, for any two fixed vertices $a, b \in V$, the expected commute time $C_{a,b}$ is given by the voltage difference between a and b for any solution $\boldsymbol{z}$ to the Laplacian system $\boldsymbol{L}\boldsymbol{z} = \|\boldsymbol{d}\|_1 \cdot (\mathbf{1}_b - \mathbf{1}_a)$.*

We note that the voltage difference between a and b in an electrical flow routing demand $\mathbf{1}_b - \mathbf{1}_a$ is also called the *effective resistance* $R_{\text{eff}}(a, b)$. This quantity will play a crucial role in the next roles. In the next lecture, we introduce $R_{\text{eff}}(a, b)$ slightly differently as the energy required by the electrical flow that routes $\mathbf{1}_b - \mathbf{1}_a$, however, it is not hard to show that these two definitions are equivalent.

Our theorem can now be restated as saying that the expected commute time $\mathbb{E}[C_{a,b}] = \|\boldsymbol{d}\|_1 \cdot R_{\text{eff}}(a, b)$. This is a classic result.

Chapter 7

Pseudo-inverses and Effective Resistance

7.1 What is a (Moore-Penrose) Pseudoinverse?

Recall that for a connected graph G with Laplacian $\boldsymbol{L}$, we have $\ker(\boldsymbol{L}) = \text{span}\{\mathbf{1}\}$, which means $\boldsymbol{L}$ is not invertible. However, we still want some matrix which behaves like a real inverse. To be more specific, given a Laplacian $\boldsymbol{L} \in \mathbb{R}^{V \times V}$, we want some matrix $\boldsymbol{L}^+ \in \mathbb{R}^{V \times V}$ s.t.

1) $(\boldsymbol{L}^+)^\top = \boldsymbol{L}^+$ (symmetric)

2) $\boldsymbol{L}^+\mathbf{1} = \mathbf{0}$, or more generally, $\boldsymbol{L}^+\boldsymbol{v} = \mathbf{0}$ for $\boldsymbol{v} \in \ker(\boldsymbol{L})$

3) $\boldsymbol{L}^+\boldsymbol{L}\boldsymbol{v} = \boldsymbol{L}\boldsymbol{L}^+\boldsymbol{v} = \boldsymbol{v}$ for $\boldsymbol{v} \perp \mathbf{1}$, or more generally, for $\boldsymbol{v} \in \ker(\boldsymbol{L})^\perp$

Under the above conditions, $\boldsymbol{L}^+$ is uniquely defined and we call it the pseudoinverse of $\boldsymbol{L}$. Note that there are many other equivalent definitions of the pseudoinverse of some matrix $\boldsymbol{A}$, and we can also generalize the concept to matrices that aren't symmetric or even square.

Let $\lambda_i, \boldsymbol{v}_i$ be the i-th pair of eigenvalue and eigenvector of $\boldsymbol{L}$, with $\{\boldsymbol{v}_i\}_{i=1}^n$ forming a orthogonal basis. Then by the spectral theorem,

$$\boldsymbol{L} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^\top = \sum_i \lambda_i \boldsymbol{v}_i \boldsymbol{v}_i^\top,$$

where $\boldsymbol{V} = \begin{bmatrix} \boldsymbol{v}_1 & \cdots & \boldsymbol{v}_n \end{bmatrix}$ and $\boldsymbol{\Lambda} = \text{diag}\{\lambda_1, ..., \lambda_n\}$. And we can show that its pseudoinverse is exactly

$$\boldsymbol{L}^+ = \sum_{i, \lambda_i \neq 0} \lambda_i^{-1} \boldsymbol{v}_i \boldsymbol{v}_i^\top.$$

Checking conditions 1), 2), 3) is immediate. We can also prove uniqueness, but this takes slightly more work.

7.2 Electrical Flows Again

Recall the incidence matrix $\boldsymbol{B} \in \mathbb{R}^{V \times E}$ of a graph $G = (V, E)$.

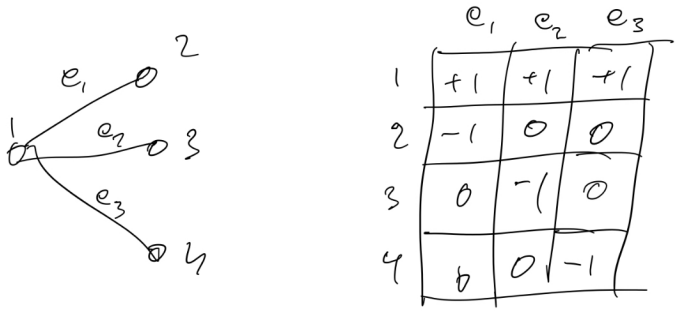


Figure 7.1: An example of a graph and its incidence matrix B.

In Chapter 1, we introduced the electrical flow routing demand $\boldsymbol{d} \in \mathbb{R}^V$. Let's call the electrical flow $\tilde{\boldsymbol{f}} \in \mathbb{R}^E$. The net flow constraint requires $\boldsymbol{B}\tilde{\boldsymbol{f}} = \boldsymbol{d}$. By Ohm's Law, $\tilde{\boldsymbol{f}} = \boldsymbol{R}^{-1}\boldsymbol{B}^\top \boldsymbol{x}$ for some voltage $x \in \mathbb{R}^V$ where $\boldsymbol{R} = \mathrm{diag}(\boldsymbol{r})$ and $\boldsymbol{r}(e) =$ resistance of edge e. We showed (in the exercises) that when $\boldsymbol{d} \perp \mathbf{1}$, there exists an voltage $\tilde{\boldsymbol{x}} \perp \mathbf{1}$ s.t. $\tilde{\boldsymbol{f}} = \boldsymbol{R}^{-1}\boldsymbol{B}^\top \tilde{\boldsymbol{x}}$ and $\boldsymbol{B}\tilde{\boldsymbol{f}} = \boldsymbol{d}$. This $\tilde{\boldsymbol{x}}$ solves $\boldsymbol{L}\boldsymbol{x} = \boldsymbol{d}$ where $\boldsymbol{L} = \boldsymbol{B}\boldsymbol{R}^{-1}\boldsymbol{B}^\top$.

And we also made the following claim.

Claim 7.2.1.

$$\tilde{\boldsymbol{f}} = \operatorname*{arg\,min}_{\boldsymbol{B}\boldsymbol{f}=\boldsymbol{d}} \boldsymbol{f}^\top \boldsymbol{R}\boldsymbol{f} \text{ where } \boldsymbol{f}^\top \boldsymbol{R}\boldsymbol{f} = \sum_e \boldsymbol{r}(e)\boldsymbol{f}(e)^2, \tag{7.1}$$

You proved this in the exercises for Week 1. Let's recap the proof briefly, just to get back into thinking about electrical flows.

Proof. Consider any $\boldsymbol{f} \in \mathbb{R}^E$ s.t. $\boldsymbol{B}\boldsymbol{f} = \boldsymbol{d}$. For any $\boldsymbol{x} \in \mathbb{R}^V$, we have

$$\begin{aligned}
\frac{1}{2}\boldsymbol{f}^\top \boldsymbol{R}\boldsymbol{f} &= \frac{1}{2}\boldsymbol{f}^\top \boldsymbol{R}\boldsymbol{f} - \boldsymbol{x}^\top (\underbrace{\boldsymbol{B}\boldsymbol{f} - \boldsymbol{d}}_{\mathbf{0}}) \\
&\geq \min_{\boldsymbol{f} \in \mathbb{R}^E} \underbrace{\frac{1}{2}\boldsymbol{f}^\top \boldsymbol{R}\boldsymbol{f} - \boldsymbol{x}^\top \boldsymbol{B}\boldsymbol{f} + \boldsymbol{d}^\top \boldsymbol{x}}_{g(\boldsymbol{f})} \\
&= \boldsymbol{d}^\top \boldsymbol{x} - \frac{1}{2}\boldsymbol{x}^\top \boldsymbol{L}\boldsymbol{x}
\end{aligned}$$

since $\nabla_{\boldsymbol{f}} g(\boldsymbol{f}) = \mathbf{0}$ gives us $\boldsymbol{f} = \boldsymbol{R}^{-1}\boldsymbol{B}^\top \boldsymbol{x}$. Thus, for all $\boldsymbol{f} \in \mathbb{R}^E$ s.t. $\boldsymbol{B}\boldsymbol{f} = \boldsymbol{d}$ and all $\boldsymbol{x} \in \mathbb{R}^V$,

$$\frac{1}{2}\boldsymbol{f}^\top \boldsymbol{R}\boldsymbol{f} \geq \boldsymbol{d}^\top \boldsymbol{x} - \frac{1}{2}\boldsymbol{x}^\top \boldsymbol{L}\boldsymbol{x}. \tag{7.2}$$

But for the electrical flow $\tilde{\boldsymbol{f}}$ and electrical voltage $\tilde{\boldsymbol{x}}$, we have $\tilde{\boldsymbol{f}} = \boldsymbol{R}^{-1}\boldsymbol{B}^\top\tilde{\boldsymbol{x}}$ and $\boldsymbol{L}\tilde{\boldsymbol{x}} = \boldsymbol{d}$. So

$$\tilde{\boldsymbol{f}}^\top\boldsymbol{R}\tilde{\boldsymbol{f}} = \left(\boldsymbol{R}^{-1}\boldsymbol{B}^\top\tilde{\boldsymbol{x}}\right)^\top\boldsymbol{R}\left(\boldsymbol{R}^{-1}\boldsymbol{B}^\top\tilde{\boldsymbol{x}}\right) = \tilde{\boldsymbol{x}}^\top\boldsymbol{B}\boldsymbol{R}^{-1}\boldsymbol{B}^\top\tilde{\boldsymbol{x}} = \tilde{\boldsymbol{x}}^\top\boldsymbol{L}\tilde{\boldsymbol{x}} = \tilde{\boldsymbol{x}}^\top\boldsymbol{d}.$$

Therefore,

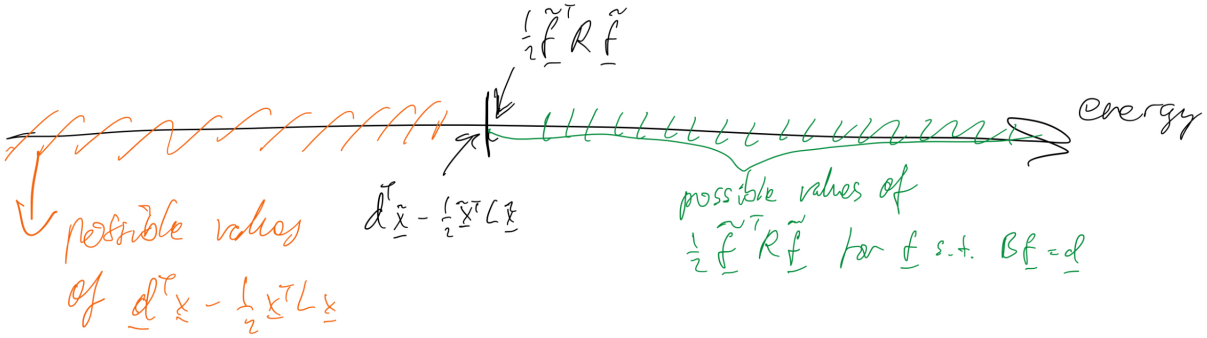
$$\frac{1}{2}\tilde{\boldsymbol{f}}^\top\boldsymbol{R}\tilde{\boldsymbol{f}} = \boldsymbol{d}^\top\tilde{\boldsymbol{x}} - \frac{1}{2}\tilde{\boldsymbol{x}}^\top\boldsymbol{L}\tilde{\boldsymbol{x}}. \tag{7.3}$$

By combining Equation (7.2) and Equation (7.3), we see that for all $\boldsymbol{f}$ s.t. $\boldsymbol{B}\boldsymbol{f} = \boldsymbol{d}$,

$$\frac{1}{2}\boldsymbol{f}^\top\boldsymbol{R}\boldsymbol{f} \geq \boldsymbol{d}^\top\tilde{\boldsymbol{x}} - \frac{1}{2}\tilde{\boldsymbol{x}}^\top\boldsymbol{L}\tilde{\boldsymbol{x}} = \frac{1}{2}\tilde{\boldsymbol{f}}^\top\boldsymbol{R}\tilde{\boldsymbol{f}}.$$

Thus $\tilde{\boldsymbol{f}}$ is the minimum electrical energy flow among all flows that route demand $\boldsymbol{d}$, proving Equation (7.1) holds.

The drawing below shows how the quantities line up:



□

7.3 Effective Resistance

Given a graph $G = (V, E)$, for any pair of vertices $(a, b) \in V$, we want to compute the cost (or energy) of routing 1 unit of current from a to b. We call such cost the effective resistance between a and b, denoted by $R_{\text{eff}}(a, b)$. Recall for a single resistor $r(a, b)$,

$$\text{energy} = r(a, b)f^2(a, b) = r(a, b).$$

So when we have a graph consisting of just one edge (a, b), the effective resistance is just $R_{\text{eff}}(a, b) = r(a, b)$.

In a general graph, we can also consider the energy required to route one unit of current between two vertices. For any pair $a, b \in V$, we have

$$R_{\text{eff}}(a, b) = \min_{\boldsymbol{B}\boldsymbol{f}=\boldsymbol{e}_b-\boldsymbol{e}_a} \boldsymbol{f}^\top\boldsymbol{R}\boldsymbol{f},$$

where $\boldsymbol{e}_v \in \mathbb{R}^V$ is the indicator vector of v. Note that the cost of routing F units of flow from a to b will be $R_{\text{eff}}(a,b) \cdot F^2$.

Since $(\boldsymbol{e}_b - \boldsymbol{e}_a)^\top \mathbf{1} = 0$, we know from the previous section that $R_{\text{eff}}(a,b) = \tilde{\boldsymbol{f}}^\top \boldsymbol{R}\tilde{\boldsymbol{f}}$ where $\tilde{\boldsymbol{f}}$ is the electrical flow. Now we can write $\boldsymbol{L}\tilde{\boldsymbol{x}} = \boldsymbol{e}_b - \boldsymbol{e}_a$ and $\tilde{\boldsymbol{x}} = \boldsymbol{L}^+(\boldsymbol{e}_b - \boldsymbol{e}_a)$ for the electrical voltages routing 1 unit of current from a to b. Now the energy of routing 1 unit of current from a to b is

$$R_{\text{eff}}(a,b) = \tilde{\boldsymbol{f}}^\top \boldsymbol{R}\tilde{\boldsymbol{f}} = \tilde{\boldsymbol{x}}^\top \boldsymbol{L}\tilde{\boldsymbol{x}} = (\boldsymbol{e}_b - \boldsymbol{e}_a)^\top \boldsymbol{L}^+\boldsymbol{L}\boldsymbol{L}^+(\boldsymbol{e}_b - \boldsymbol{e}_a) = (\boldsymbol{e}_b - \boldsymbol{e}_a)^\top \boldsymbol{L}^+(\boldsymbol{e}_b - \boldsymbol{e}_a),$$

where the last equality is due to $\boldsymbol{L}^+\boldsymbol{L}\boldsymbol{L}^+ = \boldsymbol{L}^+$.

Remark 7.3.1. We have now seen several different expressions that all take on the same value: the energy of the electrical flow. It's useful to remind yourself what these are. Consider an electrical flow $\tilde{\boldsymbol{f}}$ routes demand $\boldsymbol{d}$, and associated electrical voltages $\tilde{\boldsymbol{x}}$. We know that $\boldsymbol{B}\tilde{\boldsymbol{f}} = \boldsymbol{d}$, and $\boldsymbol{f} = \boldsymbol{R}^{-1}\boldsymbol{B}^\top\tilde{\boldsymbol{x}}$, and $\boldsymbol{L}\tilde{\boldsymbol{x}} = \boldsymbol{d}$, where $\boldsymbol{L} = \boldsymbol{B}\boldsymbol{R}^{-1}\boldsymbol{B}^\top$. And we have seen how to express the electrical energy using many different quantities:

$$\tilde{\boldsymbol{f}}^\top \boldsymbol{R}\tilde{\boldsymbol{f}} = \tilde{\boldsymbol{x}}^\top \boldsymbol{L}\tilde{\boldsymbol{x}} = \boldsymbol{d}^\top \boldsymbol{L}^+\boldsymbol{d} = \boldsymbol{d}^\top\tilde{\boldsymbol{x}} = \tilde{\boldsymbol{f}}^\top \boldsymbol{B}^\top\tilde{\boldsymbol{x}}$$

Claim 7.3.2. *Any PSD matrix $\boldsymbol{A}$ has a PSD square root $\boldsymbol{A}^{1/2}$ s.t. $\boldsymbol{A}^{1/2}\boldsymbol{A}^{1/2} = \boldsymbol{A}$.*

Proof. By the spectral theorem, $\boldsymbol{A} = \sum_i \lambda_i \boldsymbol{v}_i\boldsymbol{v}_i^\top$ where $\{\boldsymbol{v}_i\}$ are orthonormal. Let $\boldsymbol{A}^{1/2} = \sum_i \lambda_i^{1/2}\boldsymbol{v}_i\boldsymbol{v}_i^\top$. Then

$$\begin{aligned}
\boldsymbol{A}^{1/2}\boldsymbol{A}^{1/2} &= \left(\sum_i \lambda_i^{1/2}\boldsymbol{v}_i\boldsymbol{v}_i^\top\right)^2 \\
&= \sum_i \lambda_i \boldsymbol{v}_i\boldsymbol{v}_i^\top\boldsymbol{v}_i\boldsymbol{v}_i^\top + \sum_{i\neq j} \lambda_i \boldsymbol{v}_i\boldsymbol{v}_i^\top\boldsymbol{v}_j\boldsymbol{v}_j^\top \\
&= \sum_i \lambda_i \boldsymbol{v}_i\boldsymbol{v}_i^\top
\end{aligned}$$

where the last equality is due to $\boldsymbol{v}_i^\top\boldsymbol{v}_j = \delta_{ij}$. It's easy to see that $\boldsymbol{A}^{1/2}$ is also PSD. □

Let $\boldsymbol{L}^{+/2}$ be the square root of $\boldsymbol{L}^+$. So

$$R_{\text{eff}}(a,b) = (\boldsymbol{e}_b - \boldsymbol{e}_a)^\top \boldsymbol{L}^+(\boldsymbol{e}_b - \boldsymbol{e}_a) = \|\boldsymbol{L}^{+/2}(\boldsymbol{e}_b - \boldsymbol{e}_a)\|^2.$$

Example: Effective resistance in a path. Consider a path graph on vertices $V = \{1, 2, 3, \ldots, k+1\}$, with with resistances $\boldsymbol{r}(1), \boldsymbol{r}(2), \ldots, \boldsymbol{r}(k)$ on the edges of the path.

Figure 7.2: A path graph with k edges.

The effective resistance between the endpoints is

$$R_{\text{eff}}(1, k+1) = \sum_{i=1}^{k} \boldsymbol{r}(i)$$

To see this, observe that to have 1 unit of flow going from vertex 1 to vertex $k+1$, we must have one unit flowing across each edge i. Let $\boldsymbol{\Delta}(i)$ be the voltage difference across edge i, and $\boldsymbol{f}(i)$ the flow on the edge. Then $1 = \boldsymbol{f}(i) = \frac{\boldsymbol{\Delta}(i)}{\boldsymbol{r}(i)}$, so that $\boldsymbol{\Delta}(i) = \boldsymbol{r}(i)$. The electrical voltages are then $\tilde{\boldsymbol{x}} \in \mathbb{R}^V$ where $\tilde{\boldsymbol{x}}(i) = \tilde{\boldsymbol{x}}(1) + \sum_{j<i} \boldsymbol{\Delta}(j)$. Hence the effective resistance is

$$R_{\text{eff}}(1, k+1) = \boldsymbol{d}^\top \tilde{\boldsymbol{x}} = (\boldsymbol{e}_{k+1} - \boldsymbol{e}_1)^\top \tilde{\boldsymbol{x}} = \tilde{\boldsymbol{x}}(k+1) - \tilde{\boldsymbol{x}}(1) = \sum_{i=1}^{k} \boldsymbol{r}(i).$$

This behavior is sometimes known as the fact that the resistance of resistors adds up when they are connected in series.

Example: Effective resistance of parallel edges. So far, we have only considered graphs with at most one edge between any two vertices. But that math also works if we allow a pair of vertices to have multiple distinct edges connecting them. We refer to this as *multi-edges*. Suppose we have a graph on just two vertices, $V = \{1, 2\}$, and these are connected by k parallel multi-edges with resistances $\boldsymbol{r}(1), \boldsymbol{r}(2), \ldots, \boldsymbol{r}(k)$.

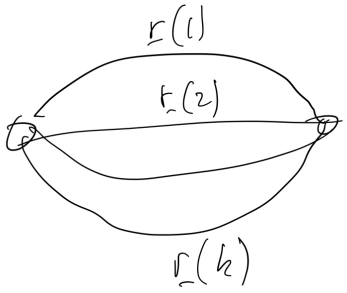


Figure 7.3: A graph on just two vertices with k parallel multiedges.

The effective resistance between the endpoints is

$$R_{\text{eff}}(1, 2) = \frac{1}{\sum_{i=1}^{k} 1/\boldsymbol{r}(i)}.$$

Let's see why. Our electrical voltages $\tilde{\boldsymbol{x}} \in \mathbb{R}^V$ can be described by just the voltage difference $\Delta \in \mathbb{R}$ between vertex 1 and vertex 2, i.e. $\tilde{\boldsymbol{x}}(2) - \tilde{\boldsymbol{x}}(1) = \Delta$. which creates a flow on edge i of $\tilde{\boldsymbol{f}}(i) = \Delta/\boldsymbol{r}(i)$. Thus the total flow from vertex 1 to vertex 2 is $1 = \sum_i \Delta/\boldsymbol{r}(i)$, so that $\Delta = \frac{1}{\sum_{i=1}^k 1/\boldsymbol{r}(i)}$. Meanwhile, the effective resistance is also

$$R_{\text{eff}}(1,2) = (\boldsymbol{e}_2 - \boldsymbol{e}_1)^\top \tilde{\boldsymbol{x}} = \Delta = \frac{1}{\sum_{i=1}^k 1/\boldsymbol{r}(i)}$$

7.3.1 Effective Resistance is a Distance

Definition 7.3.3. Consider a weighted undirected graph G with vertex set V. We say function $d : V \times V \to \mathbb{R}$, which takes a pair of vertices and returns a real number, is a *distance* if it satisfies

1. $d(a,a) = 0$ for all $a \in V$
2. $d(a,b) \geq 0$ for all $a, b \in V$.
3. $d(a,b) = d(b,a)$ for all $a, b \in V$.
4. $d(a,b) \leq d(a,c) + d(c,b)$ for all $a, b, c \in V$.

Lemma 7.3.4. *R_{eff} is a distance.*

Before proving this lemma, let's see a claim that will help us finish the proof.

Claim 7.3.5. *Let $\boldsymbol{L}\tilde{\boldsymbol{x}} = \boldsymbol{e}_b - \boldsymbol{e}_a$. Then for all $\boldsymbol{c} \in V$, we have $\tilde{\boldsymbol{x}}(b) \geq \tilde{\boldsymbol{x}}(c) \geq \tilde{\boldsymbol{x}}(a)$.*

We only sketch a proof of this claim:

Proof sketch. Consider any $c \in V$, where $c \neq a, b$. Now $(\boldsymbol{L}\tilde{\boldsymbol{x}})(c) = 0$, i.e.

$$\left(\sum_{(u,c)} \boldsymbol{w}(u,c)\right) \tilde{\boldsymbol{x}}(c) - \left(\sum_{(u,c)} \boldsymbol{w}(u,c)\tilde{\boldsymbol{x}}(u)\right) = 0$$

Rearranging $\tilde{\boldsymbol{x}}(c) = \frac{\sum_{(u,c)} \boldsymbol{w}(u,c)\tilde{\boldsymbol{x}}(u)}{\sum_{(u,c)} \boldsymbol{w}(u,c)}$. This tells us that $\tilde{\boldsymbol{x}}(c)$ is a weighted average of the voltages of its neighbors. From this, we can show that $\tilde{\boldsymbol{x}}(a)$ and $\tilde{\boldsymbol{x}}(b)$ are the extreme values. □

Proof. It is easy to check that conditions 1, 2, and 3 of Definition 7.3.3 are satisfied by R_{eff}. Let us confirm condition 4.

For any u, v, let $\tilde{\boldsymbol{x}}_{u,v} = \boldsymbol{L}^+(-\boldsymbol{e}_u + \boldsymbol{e}_v)$. Then

$$\tilde{\boldsymbol{x}}_{a,b} = \boldsymbol{L}^+(-\boldsymbol{e}_a + \boldsymbol{e}_b) = \boldsymbol{L}^+(-\boldsymbol{e}_a + \boldsymbol{e}_c - \boldsymbol{e}_c + \boldsymbol{e}_b) = \tilde{\boldsymbol{x}}_{a,c} + \tilde{\boldsymbol{x}}_{c,b}.$$

Thus,

$$\begin{aligned} R_{\text{eff}}(a,b) = (-\boldsymbol{e}_a + \boldsymbol{e}_b)^\top \tilde{\boldsymbol{x}}_{a,b} &= (-\boldsymbol{e}_a + \boldsymbol{e}_b)^\top (\tilde{\boldsymbol{x}}_{a,c} + \tilde{\boldsymbol{x}}_{c,b}) \\ &= -\tilde{\boldsymbol{x}}_{a,c}(a) + \tilde{\boldsymbol{x}}_{a,c}(b) - \tilde{\boldsymbol{x}}_{c,b}(a) + \tilde{\boldsymbol{x}}_{c,b}(b) \\ &\leq -\tilde{\boldsymbol{x}}_{a,c}(a) + \tilde{\boldsymbol{x}}_{a,c}(c) - \tilde{\boldsymbol{x}}_{c,b}(c) + \tilde{\boldsymbol{x}}_{c,b}(b). \end{aligned}$$

where in the last line we applied Claim 7.3.5 to show that $\tilde{\boldsymbol{x}}_{a,c}(b) \leq \tilde{\boldsymbol{x}}_{a,c}(c)$ and $-\tilde{\boldsymbol{x}}_{c,b}(a) \leq -\tilde{\boldsymbol{x}}_{c,b}(c)$. □

Chapter 8

Different Perspectives on Gaussian Elimination

8.1 An Optimization View of Gaussian Elimination for Laplacians

In this section, we will explore how to exactly minimize a Laplacian quadratic form by minimizing over one variable at a time. It turns out that this is in fact Gaussian Elimination in disguise – or, more precisely, the variant of Gaussian elimination that we tend to use on symmetric matrices, which is called Cholesky factorization.

Consider a Laplacian $\boldsymbol{L}$ of a connected graph $G = (V, E, \boldsymbol{w})$, where $\boldsymbol{w} \in \mathbb{R}^E$ is a vector of positive edge weights. Let $\boldsymbol{W} \in \mathbb{R}^{E \times E}$ be the diagonal matrix with the edge weights on the diagonal, i.e. $\boldsymbol{W} = \mathrm{diag}(\boldsymbol{w})$ and $\boldsymbol{L} = \boldsymbol{B}\,\boldsymbol{W}\,\boldsymbol{B}^\top$. Let $\boldsymbol{d} \in \mathbb{R}^V$ be a demand vector s.t. $\boldsymbol{d} \perp \mathbf{1}$.

Let us define an energy

$$\mathcal{E}(\boldsymbol{x}) = -\boldsymbol{d}^\top \boldsymbol{x} + \frac{1}{2}\boldsymbol{x}^\top \boldsymbol{L}\boldsymbol{x}$$

Note that this function is convex and is minimized at $\boldsymbol{x}$ s.t. $\boldsymbol{L}\boldsymbol{x} = \boldsymbol{d}$.

We will now explore an approach to solving the minimization problem

$$\min_{\boldsymbol{x} \in \mathbb{R}^V} \mathcal{E}(\boldsymbol{x})$$

Let $\boldsymbol{x} = \begin{pmatrix} y \\ \boldsymbol{z} \end{pmatrix}$ where $y \in \mathbb{R}$ and $\boldsymbol{z} \in \mathbb{R}^{V \setminus \{1\}}$.

We will now explore how to minimize over y, given any $\boldsymbol{z}$. Once we find an expression for y in terms of $\boldsymbol{z}$, we will be able to reduce it to a new quadratic minimization problem in $\boldsymbol{z}$,

$$\mathcal{E}'(\boldsymbol{z}) = -\boldsymbol{d}'^\top \boldsymbol{z} + \frac{1}{2}\boldsymbol{z}^\top \boldsymbol{L}'\boldsymbol{z}$$

where $\boldsymbol{d}'$ is a demand vector on the remaining vertices, with $\boldsymbol{d} \perp \mathbf{1}$ and $\boldsymbol{L}'$ is a Laplacian of a graph on the remaining vertices $V' = V \setminus \{1\}$. We can then repeat the procedure to eliminate another variable and so on. Eventually, we can then find all the solution to our original minimization problem.

To help us understand how to minimize over the first variable, we introduce some notation for the first row and column of the Laplacian:

$$\boldsymbol{L} = \begin{pmatrix} W & -\boldsymbol{a}^\top \\ -\boldsymbol{a} & \operatorname{diag}(\boldsymbol{a}) + \boldsymbol{L}_{-1} \end{pmatrix}. \tag{8.1}$$

Note that W is the weighted degree of vertex 1, and that

$$\begin{pmatrix} W & -\boldsymbol{a}^\top \\ -\boldsymbol{a} & \operatorname{diag}(\boldsymbol{a}) \end{pmatrix} \tag{8.2}$$

is the Laplacian of the subgraph of G containing only the edges incident on vertex 1, while $\boldsymbol{L}_{-1}$ is the Laplacian of the subgraph of G containing all edges *not* incident on vertex 1.

Let us also write $\boldsymbol{d} = \begin{pmatrix} b \\ \boldsymbol{c} \end{pmatrix}$ where $b \in \mathbb{R}$ and $\boldsymbol{c} \in \mathbb{R}^{V \setminus \{1\}}$.

Now,

$$\begin{aligned} \mathcal{E}(\boldsymbol{x}) &= -\boldsymbol{d}^\top \boldsymbol{x} + \frac{1}{2}\boldsymbol{x}^\top \boldsymbol{L}\boldsymbol{x} = -\begin{pmatrix} b \\ \boldsymbol{c} \end{pmatrix}^\top \begin{pmatrix} y \\ \boldsymbol{z} \end{pmatrix} + \frac{1}{2}\begin{pmatrix} y \\ \boldsymbol{z} \end{pmatrix}^\top \begin{pmatrix} W & -\boldsymbol{a}^\top \\ -\boldsymbol{a} & \operatorname{diag}(\boldsymbol{a}) + \boldsymbol{L}_{-1} \end{pmatrix} \begin{pmatrix} y \\ \boldsymbol{z} \end{pmatrix} \\ &= -by - \boldsymbol{c}^\top \boldsymbol{z} + \frac{1}{2}\left(y^2 W - 2y\boldsymbol{a}^\top \boldsymbol{z} + \boldsymbol{z}^\top \operatorname{diag}(\boldsymbol{a})\boldsymbol{z} + \boldsymbol{z}^\top \boldsymbol{L}_{-1}\boldsymbol{z}\right). \end{aligned}$$

Now, to minimize over y, we set $\frac{\partial}{\partial y}\mathcal{E}(\boldsymbol{x}) = 0$ and get

$$-b + yW - \boldsymbol{a}^\top \boldsymbol{z} = 0.$$

Solving for y, we get that the minimizing y is

$$y = \frac{1}{W}(b + \boldsymbol{a}^\top \boldsymbol{z}). \tag{8.3}$$

Observe that

$$\begin{aligned} \mathcal{E}(\boldsymbol{x}) &= -by - \boldsymbol{c}^\top \boldsymbol{z} + \frac{1}{2}\left(y^2 W - 2y\boldsymbol{a}^\top \boldsymbol{z} + \boldsymbol{z}^\top \operatorname{diag}(\boldsymbol{a})\boldsymbol{z} + \boldsymbol{z}^\top \boldsymbol{L}_{-1}\boldsymbol{z}\right) \\ &= -by - \boldsymbol{c}^\top \boldsymbol{z} + \frac{1}{2}\left(\frac{1}{W}(yW - \boldsymbol{a}^\top \boldsymbol{z})^2 \underbrace{-\frac{1}{W}\boldsymbol{z}^\top \boldsymbol{a}\boldsymbol{a}^\top \boldsymbol{z} + \boldsymbol{z}^\top \operatorname{diag}(\boldsymbol{a})\boldsymbol{z} + \boldsymbol{z}^\top \boldsymbol{L}_{-1}\boldsymbol{z}}_{\text{Let } \boldsymbol{S} = \operatorname{diag}(\boldsymbol{a}) - \frac{1}{W}\boldsymbol{a}\boldsymbol{a}^\top + \boldsymbol{L}_{-1}}\right) \\ &= -by - \boldsymbol{c}^\top \boldsymbol{z} + \frac{1}{2}\left(\frac{1}{W}(yW - \boldsymbol{a}^\top \boldsymbol{z})^2 + \boldsymbol{z}^\top \boldsymbol{S}\boldsymbol{z}\right), \end{aligned}$$

where we simplified the expression by defining $\boldsymbol{S} = \operatorname{diag}(\boldsymbol{a}) - \frac{1}{W}\boldsymbol{a}\boldsymbol{a}^\top + \boldsymbol{L}_{-1}$. Plugging in $y = \frac{1}{W}(b + \boldsymbol{a}^\top \boldsymbol{z})$, we get

$$\min_y \mathcal{E}\begin{pmatrix} y \\ \boldsymbol{z} \end{pmatrix} = -\left(\boldsymbol{c} + b\frac{1}{W}\boldsymbol{a}\right)^\top \boldsymbol{z} - \frac{b^2}{2W} + \frac{1}{2}\boldsymbol{z}^\top \boldsymbol{S}\boldsymbol{z}.$$

Now, we define $\boldsymbol{d}' = \boldsymbol{c} + b\frac{1}{W}\boldsymbol{a}$ and $\mathcal{E}'(\boldsymbol{z}) = -\boldsymbol{d}'^\top \boldsymbol{z} + \frac{1}{2}\boldsymbol{z}^\top \boldsymbol{S}\boldsymbol{z}$. And, we can see that

$$\arg\min_{\boldsymbol{z}} \min_y \mathcal{E}\begin{pmatrix} y \\ \boldsymbol{z} \end{pmatrix} = \arg\min_{\boldsymbol{z}} \mathcal{E}'(\boldsymbol{z}),$$

since dropping the constant term $-\frac{b^2}{2W}$ does not change what the minimizing $\boldsymbol{z}$ values are.

Claim 8.1.1.

1. $\boldsymbol{d}' \perp \mathbf{1}$
2. $\boldsymbol{S} = \operatorname{diag}(\boldsymbol{a}) - \frac{1}{W}\boldsymbol{a}\boldsymbol{a}^\top + \boldsymbol{L}_{-1}$ *is a Laplacian of a graph on the vertex set* $V \setminus \{1\}$.

We will prove Claim 8.1.1 in a moment. From the Claim, we see that the problem of finding $\arg\min_{\boldsymbol{z}} \mathcal{E}'(\boldsymbol{z})$, is exactly of the same form as finding $\arg\min_{\boldsymbol{x}} \mathcal{E}(\boldsymbol{x})$, but with one fewer variables.

We can get a minimizing $\boldsymbol{x}$ that solves $\arg\min_{\boldsymbol{x}} \mathcal{E}(\boldsymbol{x})$ by repeating the variable elimination procedure until we get down to a single variable and finding its value. We then have to work back up to getting a solution for $\boldsymbol{z}$, and then substitute that into Equation (8.3) to get the value for y.

Remark 8.1.2. In fact, this perspective on Gaussian elimination also makes sense for any positive definite matrix. In this setting, minimizing over one variable will leave us with another positive definite quadratic minimization problem.

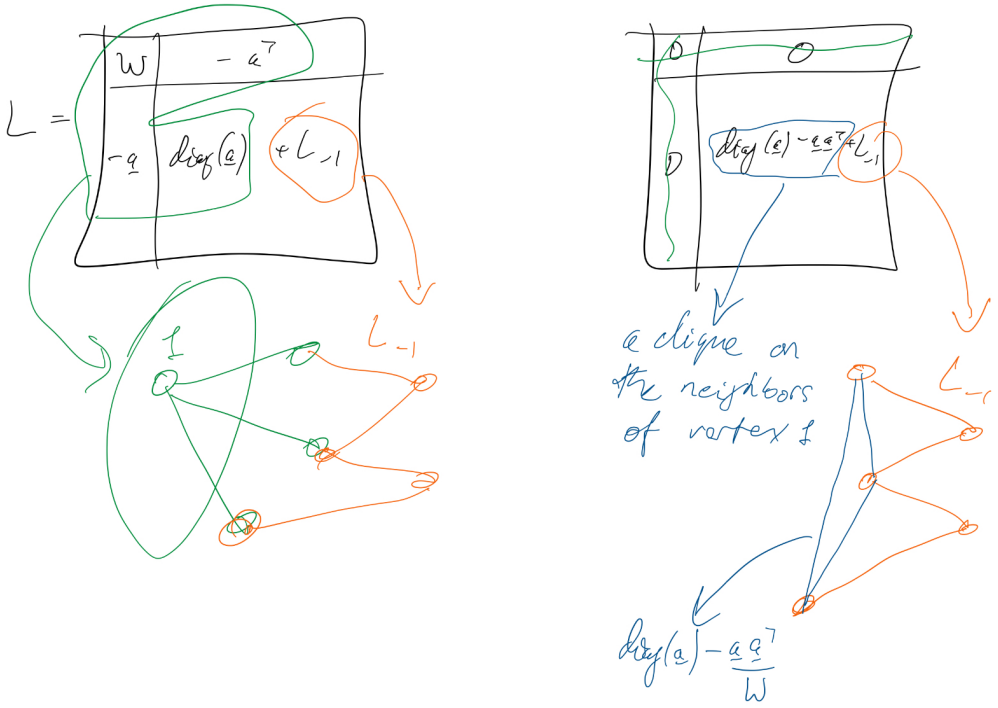
Proof of Claim 8.1.1. To establish the first part, we note that $\mathbf{1}^\top \boldsymbol{d}' = \mathbf{1}^\top \boldsymbol{c} + b\frac{\mathbf{1}^\top \boldsymbol{a}}{W} = \mathbf{1}^\top \boldsymbol{c} + b = \mathbf{1}^\top \boldsymbol{d} = 0$. To establish the second part, we notice that $\boldsymbol{L}_{-1}$ is a graph Laplacian by definition. Since the sum of two graph Laplacians is another graph Laplacian, it now suffices to show that $\boldsymbol{S}$ is a graph Laplacian.

Claim 8.1.3. *A matrix* $\boldsymbol{M}$ *is a graph Laplacian if and only it satisfies the following conditions:*

- $\boldsymbol{M}^\top = \boldsymbol{M}$.
- *The diagonal entries of* $\boldsymbol{M}$ *are non-negative, and the off-diagonal entries of* $\boldsymbol{M}$ *are non-positive.*
- $\boldsymbol{M}\mathbf{1} = \mathbf{0}$.

Let's see that Claim 8.1.3 is true. Firstly, when the conditions hold we can write $\boldsymbol{M} = \boldsymbol{D} - \boldsymbol{A}$ where $\boldsymbol{D}$ is diagonal and non-negative, and $\boldsymbol{A}$ is non-negative, symmetric, and zero on the diagonal, and from the last condition $\boldsymbol{D}(i,i) = \sum_{j \neq i} \boldsymbol{A}(i,j)$. Thus we can view $\boldsymbol{A}$ as a graph adjacency matrix and $\boldsymbol{D}$ as the corresponding diagonal matrix of weighted degrees. Secondly, it is easy to check that the conditions hold for any graph Laplacian, so the conditions indeed hold if and only if. Now we have to check that the claim applies to $\boldsymbol{S}$. We leave this as an exercise for the reader.

Finally, we want to argue that the graph corresponding to $\boldsymbol{S}$ is connected. Consider any $i, j \in V \setminus \{1\}$. Since G, the graph of $\boldsymbol{L}$, is connected, there exists a simple path in G connecting i and j. If this path does not use vertex 1, it is a path in the graph of $\boldsymbol{L}_{-1}$ and hence in the graph of $\boldsymbol{S}$. If the path does use vertex 1, it must do so by reaching the vertex on some edge $(v, 1)$ and leaving on a different edge $(1, u)$. Replace this pair of edges with edge (u, v), which appears in the graph of $\boldsymbol{S}$ because $\boldsymbol{S}(u, v) < 0$. Now we have a path in the graph of $\boldsymbol{S}$. □



8.2 An Additive View of Gaussian Elimination

Cholesky decomposition basics. Again we consider a graph Laplacian $\boldsymbol{L} \in \mathbb{R}^{n \times n}$ of a conected graph $G = (V, E, \boldsymbol{w})$, where as usual $|V| = n$ and $|E| = m$.

In this Section, we'll study how to decompose a graph Laplacian as $\boldsymbol{L} = \boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{L}}^\top$, where $\boldsymbol{\mathcal{L}} \in \mathbb{R}^{n\times n}$ is a lower triangular matrix, i.e. $\boldsymbol{\mathcal{L}}(i,j) = 0$ for $i < j$. Such a factorization is called a Cholesky decomposition. It is essentially the result of Gaussian elimination with a slight twist to ensure the matrices maintained at intermediate steps of the algorithm remain symmetric.

We use $\mathrm{nnz}(\boldsymbol{A})$ to denote the number of non-zero entries of matrix $\boldsymbol{A}$.

Lemma 8.2.1. *Given an* invertible *square lower triangular matrix $\boldsymbol{\mathcal{L}}$, we can solve the linear equation $\boldsymbol{\mathcal{L}}\boldsymbol{y} = \boldsymbol{b}$ in time $O(\mathrm{nnz}(\boldsymbol{\mathcal{L}}))$. Similarly, given an upper triangular matrix $\boldsymbol{\mathcal{U}}$, we can solve linear equations $\boldsymbol{\mathcal{U}}\boldsymbol{z} = \boldsymbol{c}$ in time $O(\mathrm{nnz}(\boldsymbol{\mathcal{U}}))$.*

We omit the proof, which is a straight-forward exercise. The algorithms for solving linear equations in upper and lower triangular matrices are known as forward and back substitution respectively.

Remark 8.2.2. Strictly speaking, the lemma requires us to have access an adjacency list representation of $\boldsymbol{\mathcal{L}}$ so that we can quickly tell where the non-zero entries are.

Using forward and back substitution, if we have a decomposition of an invertible matrix $\boldsymbol{M}$ into $\boldsymbol{M} = \boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{L}}^\top$, we can now solve linear equations in $\boldsymbol{M}$ in time $O(\mathrm{nnz}(\boldsymbol{\mathcal{L}}))$.

Remark 8.2.3. We have learned about decompositions using a lower triangular matrix, and later we will see an algorithm for computing these. In fact, we can have more flexibility than that. From an algorithmic perspective, it is sufficient that there exists a permutation matrix $\boldsymbol{P}$ s.t. $\boldsymbol{P}\boldsymbol{\mathcal{L}}\boldsymbol{P}^\top$ is lower triangular. If we know the ordering under which the matrix becomes lower triangular, we can perform substitution according to that order to solve linear equations in the matrix without having to explicitly apply a permutation to the matrix.

Dealing with pseudoinverses. But how can we solve a linear equation in $\boldsymbol{L} = \boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{L}}^\top$, where $\boldsymbol{L}$ is not invertible? For graph Laplacians we have a simple characterization of the kernel, and because of this, dealing with the lack of invertibility turns out to be fairly easy.

We can use the following lemma which you will prove in an exercise next week.

Lemma 8.2.4. *Consider a real symmetric matrix $\boldsymbol{M} = \boldsymbol{X}\boldsymbol{Y}\boldsymbol{X}^\top$, where $\boldsymbol{X}$ is real and invertible and $\boldsymbol{Y}$ is real symmetric. Let $\boldsymbol{\Pi}_{\boldsymbol{M}}$ denote the orthogonal projection to the image of $\boldsymbol{M}$. Then $\boldsymbol{M}^+ = \boldsymbol{\Pi}_{\boldsymbol{M}}(\boldsymbol{X}^\top)^{-1}\boldsymbol{Y}^+\boldsymbol{X}^{-1}\boldsymbol{\Pi}_{\boldsymbol{M}}$.*

The factorizations $\boldsymbol{L} = \boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{L}}^\top$ that we produce will have the property that all diagonal entries of $\boldsymbol{\mathcal{L}}$ are strictly non-zero, except that $\boldsymbol{\mathcal{L}}(n,n) = 0$. Let $\widehat{\boldsymbol{\mathcal{L}}}$ be the matrix whose entries agree with $\boldsymbol{\mathcal{L}}$, except that $\widehat{\boldsymbol{\mathcal{L}}}(n,n) = 1$. Let $\boldsymbol{\mathcal{D}}$ be the diagonal matrix with $\boldsymbol{\mathcal{D}}(i,i) = 1$ for $i < n$ and $\boldsymbol{\mathcal{D}}(n,n) = 0$. Then $\boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{L}}^\top = \widehat{\boldsymbol{\mathcal{L}}}\boldsymbol{\mathcal{D}}\widehat{\boldsymbol{\mathcal{L}}}^\top$, and $\widehat{\boldsymbol{\mathcal{L}}}$ is invertible, and $\boldsymbol{\mathcal{D}}^+ = \boldsymbol{\mathcal{D}}$. Finally, $\boldsymbol{\Pi}_{\boldsymbol{L}} = \boldsymbol{I} - \frac{1}{n}\boldsymbol{1}\boldsymbol{1}^\top$, because this matrix is acts like identity on vectors orthogonal to $\boldsymbol{1}$ and ensures $\boldsymbol{\Pi}_{\boldsymbol{L}}\boldsymbol{1} = \boldsymbol{0}$, and this matrix can be applied to a vector in $O(n)$ time. Thus $\boldsymbol{L}^+ = \boldsymbol{\Pi}_{\boldsymbol{L}}(\widehat{\boldsymbol{\mathcal{L}}}^\top)^{-1}\boldsymbol{\mathcal{D}}\widehat{\boldsymbol{\mathcal{L}}}^{-1}\boldsymbol{\Pi}_{\boldsymbol{L}}$, and this matrix can be applied in time $O(\mathrm{nnz}(\boldsymbol{\mathcal{L}}))$.

An additive view of Gaussian Elimination. The following theorem describes Gaussian Elimination / Cholesky decompostion of a graph Laplacian.

Theorem 8.2.5 (Cholesky Decomposition on graph Laplacians)**.** *Let $\boldsymbol{L} \in \mathbb{R}^{n\times n}$ be a graph Laplacian of a connected graph $G = (V, E, \boldsymbol{w})$, where $|V| = n$. Using Gaussian Elimination, we can compute in $O(n^3)$ time a factorization $\boldsymbol{L} = \boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{L}}^\top$ where $\boldsymbol{\mathcal{L}}$ is lower triangular, and has positive diagonal entries except $\boldsymbol{\mathcal{L}}(n, n) = 0$.*

Proof. Let $\boldsymbol{L}^{(0)} = \boldsymbol{L}$. We will use $\boldsymbol{A}(:, i)$ to denote the the ith column of a matrix $\boldsymbol{A}$. Now, for $i = 1$ to $i = n - 1$ we define

$$\boldsymbol{l}_i = \frac{1}{\sqrt{\boldsymbol{L}^{(i-1)}(i,i)}}\boldsymbol{L}^{(i-1)}(:, i) \text{ and } \boldsymbol{L}^{(i)} = \boldsymbol{L}^{(i-1)} - \boldsymbol{l}_i\boldsymbol{l}_i^\top$$

Finally, we let $\boldsymbol{l}_n = \boldsymbol{0}_{n\times 1}$. We will show later that

$$\boldsymbol{L}^{(n-1)} = \boldsymbol{0}_{n\times n}. \tag{8.4}$$

It follows that $\boldsymbol{L} = \sum_i \boldsymbol{l}_i\boldsymbol{l}_i^\top$, provided this procedure is well-defined, i.e. $\boldsymbol{L}^{(i-1)}(i, i) \neq 0$ for all $i < n$. We will sketch a proof of this later, while also establishing several other properties of the procedure.

Given a matrix $\boldsymbol{A} \in \mathbb{R}^{n\times n}$ and $U \subseteq [n]$, we will use $\boldsymbol{A}(U, U)$ to denote the principal submatrix of $\boldsymbol{A}$ obtained by restricting to the rows and columns with index in U, i.e. all entries $\boldsymbol{A}(i, j)$ where $i, j \in U$.

Claim 8.2.6. *Fix some $i < n$. Let $U = \{i + 1, \ldots, n\}$. Then $\boldsymbol{L}^{(i)}(i, j) = 0$ if $i \notin U$ or $j \notin U$. And $\boldsymbol{L}^{(i)}(U, U)$ is a graph Laplacian of a connected graph on the vertex set U.*

From this claim, it follows that $\boldsymbol{L}^{(i-1)}(i, i) \neq 0$ for $i < n$, since a connected graph Laplacian on a graph with $|U| > 1$ vertices cannot have a zero on the diagonal, and it follows that $\boldsymbol{L}^{(n-1)}(i, i) = 0$, because the only graph we allow on one vertex is the empty graph. This shows Equation (8.4) holds. □

Sketch of proof of Claim 8.2.6. We will focus on the first elimination, as the remaining are similar. Adopting the same notation as in Equation (8.1), we write

$$\boldsymbol{L}^{(0)} = \boldsymbol{L} = \begin{pmatrix} W & -\boldsymbol{a}^\top \\ -\boldsymbol{a} & \operatorname{diag}(\boldsymbol{a}) + \boldsymbol{L}_{-1} \end{pmatrix}$$

and, noting that

$$\boldsymbol{l}_1\boldsymbol{l}_1^\top = \begin{pmatrix} W & -\boldsymbol{a}^\top \\ -\boldsymbol{a} & \frac{1}{W}\boldsymbol{a}\boldsymbol{a}^\top \end{pmatrix}$$

we see that

$$\boldsymbol{L}^{(1)} = \boldsymbol{L}^{(0)} - \boldsymbol{l}_1\boldsymbol{l}_1^\top = \begin{pmatrix} 0 & \boldsymbol{0} \\ \boldsymbol{0} & \operatorname{diag}(\boldsymbol{a}) - \frac{1}{W}\boldsymbol{a}\boldsymbol{a}^\top + \boldsymbol{L}_{-1} \end{pmatrix}.$$

Thus the first row and column of $\boldsymbol{L}^{(1)}$ are zero claimed. It also follows by Claim 8.1.1 that $\boldsymbol{L}^{(1)}(\{2,\ldots,n\},\{2,\ldots,n\})$ is the Laplacian of a connected graph. This proves Claim 8.2.6 for the case $i = 1$. An induction following the same pattern can be used to prove the claim for all $i < n$. □

Chapter 9

Random Matrix Concentration and Spectral Graph Sparsification

9.1 Matrix Sampling and Approximation

We want to begin understanding how sums of random matrices behave, in particular, whether they exhibit a tendency to concentrate in the same way that sum of scalar random variables do under various conditions.

First, let's recall a scalar Chernoff bound, which shows that a sum of bounded, non-negative random variables tend to concentrate around their mean.

Theorem 9.1.1 (A Chernoff Concentration Bound)**.** *Suppose $X_1, \ldots, X_k \in \mathbb{R}$ are independent, non-negative, random variables with $X_i \leq R$ always. Let $X = \sum_i X_i$, and $\mu = \mathbb{E}[X]$, then for $0 < \epsilon \leq 1$*

$$\Pr[X \geq (1+\epsilon)\mu] \leq \exp\left(\frac{-\epsilon^2\mu}{4R}\right) \text{ and } \Pr[X \leq (1-\epsilon)\mu] \leq \exp\left(\frac{-\epsilon^2\mu}{4R}\right).$$

The Chernoff bound should be familiar to most of you, but you may not have seen the following very similar bound. The Bernstein bound, which we will state in terms of zero-mean variables, is much like the Chernoff bound. It also requires bounded variables. But, when the variables have small variance, the Bernstein bound is sometimes stronger.

Theorem 9.1.2 (A Bernstein Concentration Bound)**.** *Suppose $X_1, \ldots, X_k \in \mathbb{R}$ are independent, zero-mean, random variables with $|X_i| \leq R$ always. Let $X = \sum_i X_i$, and $\sigma^2 = Var[X] = \sum_i \mathbb{E}[X_i^2]$, then for $\epsilon > 0$*

$$\Pr[|X| \geq t] \leq 2\exp\left(\frac{-t^2}{2Rt + 4\sigma^2}\right).$$

We will now prove the Bernstein concentration bound for scalar random variables, as a warm-up to the next section, where we will prove a version of it for matrix-valued random variables.

To help us prove Bernstein's bound, first let's recall Markov's inequality. This is a very weak concentration inequality, but also very versatile, because it requires few assumptions.

Lemma 9.1.3 (Markov's Inequality)**.** *Suppose $\boldsymbol{X} \in \mathbb{R}$ is a non-negative random variable, with a finite expectation. Then for any $t > 0$,*

$$\Pr[X \geq t] \leq \frac{\mathbb{E}[X]}{t}.$$

Proof.

$$\begin{aligned}
\mathbb{E}[X] &= \Pr[X \geq t]\,\mathbb{E}[X \mid X \geq t] + \Pr[X < t]\,\mathbb{E}[X \mid X < t] \\
&\geq \Pr[X \geq t]\,\mathbb{E}[X \mid X \geq t] \\
&\geq Pr[X \geq t] \cdot t.
\end{aligned}$$

We can rearrange this to get the desired statement. □

Now, we are ready to prove Bernstein's bound.

Proof of Theorem 9.1.2. We will focus on bounding the probability that $\Pr[X \geq t]$. The proof that $\Pr[-X \geq t]$ is small proceeds in the same way.

First we observe that

$$\begin{aligned}
\Pr[X \geq t] &= \Pr[\exp(\theta X) \geq \exp(\theta t)] \\
&\qquad \text{for any } \theta > 0, \text{ because } x \mapsto \exp(\theta x) \text{ is strictly increasing.} \\
&\leq \exp(-\theta t)\,\mathbb{E}[\exp(\theta X)] \qquad \text{by Lemma 9.1.3 (Markov's Inequality).}
\end{aligned}$$

Now, let's require that $\theta \leq 1/R$ This will allow us to use the following bound: For all $|z| \leq 1$,

$$\exp(z) \leq 1 + z + z^2. \tag{9.1}$$

We omit a proof of this, but the plots in Figure 9.1 suggest that this upper bound holds. The reader should consider how to prove this. With this in mind, we see that

$$\begin{aligned}
\mathbb{E}[\exp(\theta X)] &= \mathbb{E}\left[\exp\left(\theta \sum_i X_i\right)\right] \\
&= \mathbb{E}[\Pi_i \exp(\theta X_i)] \\
&= \Pi_i\,\mathbb{E}[\exp(\theta X_i)] \quad \text{because } \mathbb{E}[YZ] = \mathbb{E}[Y]\,\mathbb{E}[Z] \text{ for independent } Y \text{ and } Z. \\
&\leq \Pi_i\,\mathbb{E}\left[1 + \theta X_i + (\theta X_i)^2\right] \\
&= \Pi_i(1 + \theta^2\,\mathbb{E}\left[X_i^2\right]) \qquad \text{because } X_i \text{ are zero-mean.} \\
&\leq \Pi_i \exp(\theta^2\,\mathbb{E}\left[X_i^2\right]) \qquad \text{because } 1 + z \leq \exp(z) \text{ for all } z \in R. \\
&= \exp\left(\sum_i \theta^2\,\mathbb{E}\left[X_i^2\right]\right) = \exp(\theta^2\sigma^2).
\end{aligned}$$

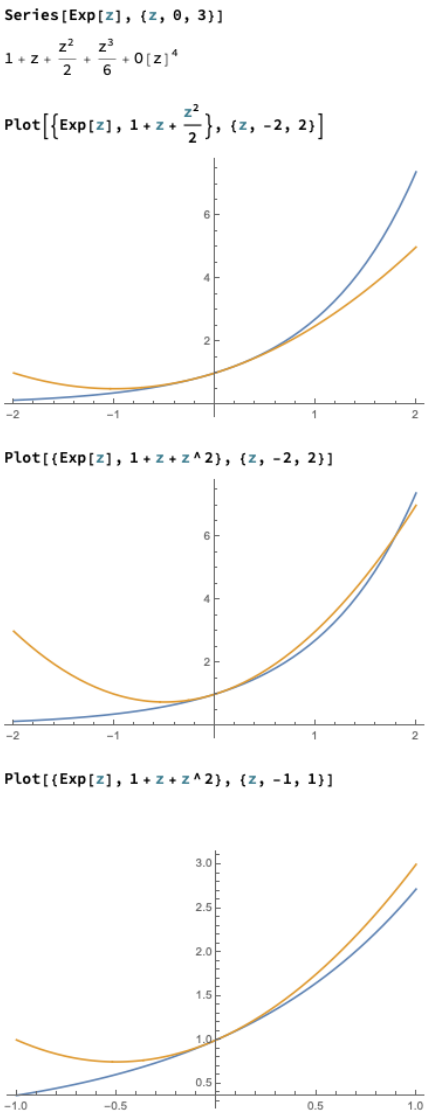


Figure 9.1: Plotting $\exp(z)$ compared to $1 + z + z^2$.

Thus $\Pr[X \geq t] \leq \exp(-\theta t)\,\mathbb{E}\left[\exp(\theta X)\right] \leq \exp(-\theta t + \theta^2\sigma^2)$. Now, to get the best possible bound, we'd like to minimize $-\theta t + \theta^2\sigma^2$ subject to the constraint $0 < \theta \leq 1/R$. Setting

$$\frac{\partial}{\partial\theta}\left(-\theta t + \theta^2\sigma^2\right) = -t + 2\theta\sigma^2.$$

Setting this derivative to zero gives $\theta = \frac{t}{2\sigma^2}$, and plugging that in gives

$$-\theta t + \theta^2\sigma^2 = -\frac{t^2}{4\sigma^2}$$

This choice only satisfies our constraints on θ if $\frac{t}{2\sigma^2} \leq 1/R$. Otherwise, we let $\theta = 1/R$ and note that in this case

$$-\theta t + \theta^2\sigma^2 = -\frac{t}{R} + \frac{\sigma^2}{R^2} \leq -\frac{t}{R} + \frac{t}{2R} = -\frac{t}{2R}$$

where we got the inequality from $t > 2\sigma^2/R$. Altogether, we can conclude that there always is a choice of θ s.t.

$$-\theta t + \theta^2\sigma^2 \leq -\min\left(\frac{t}{2R}, \frac{t^2}{4\sigma^2}\right) \leq -\frac{t^2}{2Rt + 4\sigma^2}.$$

In fact, with the benefit of hindsight, and a little algebra, we arrive at the same conclusion in another way: One can check that the following choice of θ is always valid and achives the same bound: $\theta = \frac{1}{2\sigma^2}\left(t - \frac{\sqrt{R}\cdot t^{3/2}}{\sqrt{2\sigma^2 + Rt}}\right)$. □

We use $\|\cdot\|$ to denote the spectral norm on matrices. Let's take a look at a version of Bernstein's bound that applies to sums of random matrices.

Theorem 9.1.4 (A Bernstein Matrix Concentration Bound (Tropp 2011))**.** *Suppose $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_k \in \mathbb{R}^{n\times n}$ are independent, symmetric matrix-valued random variables. Assume each $\boldsymbol{X}_i$ is zero-mean, i.e. $\mathbb{E}[\boldsymbol{X}_i] = \mathbf{0}_{n\times n}$, and that $\|\boldsymbol{X}_i\| \leq R$ always. Let $\boldsymbol{X} = \sum_i \boldsymbol{X}_i$, and $\sigma^2 = Var[\boldsymbol{X}] = \sum_i \mathbb{E}\left[\boldsymbol{X}_i^2\right]$, then for $\epsilon > 0$*

$$\Pr[\|\boldsymbol{X}\| \geq t] \leq 2n \exp\left(\frac{-t^2}{2Rt + 4\sigma^2}\right).$$

This basically says that probability of $\boldsymbol{X}$ being large in spectral norm behaves like the scalar case, except the bound is larger by a factor n, where the matrices are $n \times n$. We can get a feeling for why this might be a reasonable bound by considering the case of random diagonal matrices. Now $\|\boldsymbol{X}\| = \max_j |\boldsymbol{X}(j,j)| = \max_j |\sum_i \boldsymbol{X}_i(j,j)|$. In this case, we need to bound the largest of the n diagonal entries: We can do this by a union bound over n instances of the scalar problem – and this also turns out to be essentially tight in some cases, meaning we can't expect a better bound in general.

9.2 Matrix Concentration

In this section we will prove the Bernstein matrix concentration bound (Tropp 2011) that we saw in the previous section.

Theorem 9.2.1. *Suppose $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_k \in \mathbb{R}^{n\times n}$ are independent, symmetric matrix-valued random variables. Assume each $\boldsymbol{X}_i$ is zero-mean, i.e. $\mathbb{E}[\boldsymbol{X}_i] = \mathbf{0}_{n\times n}$, and that $\|\boldsymbol{X}_i\| \leq R$ always. Let $\boldsymbol{X} = \sum_i \boldsymbol{X}_i$, and $\sigma^2 = \|\, Var[\boldsymbol{X}]\,\| = \|\sum_i \mathbb{E}\left[\boldsymbol{X}_i^2\right]\|$, then for $t > 0$*

$$\Pr[\|\boldsymbol{X}\| \geq t] \leq 2n \exp\left(\frac{-t^2}{2Rt + 4\sigma^2}\right).$$

But let's collect some useful tools for the proof first.

Definition 9.2.2 (trace)**.** The trace of a square matrix $\boldsymbol{A}$ is defined as

$$\operatorname{Tr}(\boldsymbol{A}) := \sum_i \boldsymbol{A}(i,i)$$

Claim 9.2.3 (cyclic property of trace)**.** $\operatorname{Tr}(\boldsymbol{A}\boldsymbol{B}) = \operatorname{Tr}(\boldsymbol{B}\boldsymbol{A})$

Let S^n denote the set of all $n \times n$ real symmetric matrices, S^n_+ the set of all $n \times n$ positive semidefinite matrices, and S^n_{++} the set of all $n \times n$ positive definite matrices. Their relation is clear, $S^n_{++} \subset S^n_+ \subset S^n$. For any $\boldsymbol{A} \in S^n$ with eigenvalues $\lambda_1(\boldsymbol{A}) \leq \cdots \leq \lambda_n(\boldsymbol{A})$, by spectral decomposition theorem, $\boldsymbol{A} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^\top$ where $\boldsymbol{\Lambda} = \operatorname{diag}_i\{\lambda_i(\boldsymbol{A})\}$ and $\boldsymbol{V}^\top\boldsymbol{V} = \boldsymbol{V}\boldsymbol{V}^\top = \boldsymbol{I}$, we'll use this property without specifying in the sequel.

Claim 9.2.4. *Given a symmetric and real matrix* $\boldsymbol{A}$, $\operatorname{Tr}(\boldsymbol{A}) = \sum_i \lambda_i$, *where* $\{\lambda_i\}$ *are eigenvalues of* A.

Proof.

$$\operatorname{Tr}(\boldsymbol{A}) = \operatorname{Tr}\left(\boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^\top\right) = \operatorname{Tr}\left(\boldsymbol{\Lambda}\underbrace{\boldsymbol{V}^\top\boldsymbol{V}}_{\boldsymbol{I}}\right) = \operatorname{Tr}(\boldsymbol{\Lambda}) = \sum_i \lambda_i.$$

□

9.2.1 Matrix Functions

Definition 9.2.5 (Matrix function)**.** Given a real-valued function $f : \mathbb{R} \to \mathbb{R}$, we extend it to a matrix function $f : S^n \to S^n$. For $\boldsymbol{A} \in S^n$ with spectral decomposition $\boldsymbol{A} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^\top$, let

$$f(\boldsymbol{A}) = \boldsymbol{V} \operatorname*{diag}_i \{f(\lambda_i)\}\, \boldsymbol{V}^\top.$$

Example. Recall that every PSD matrix $\boldsymbol{A}$ has a square root $\boldsymbol{A}^{1/2}$. If $f(x) = x^{1/2}$ for $x \in \mathbb{R}_+$, then $f(\boldsymbol{A}) = \boldsymbol{A}^{1/2}$ for $\boldsymbol{A} \in S^n_+$.

Example. If $f(x) = \exp(x)$ for $x \in \mathbb{R}$, then $f(\boldsymbol{A}) = \exp(\boldsymbol{A}) = \boldsymbol{V}\exp(\boldsymbol{\Lambda})\boldsymbol{V}^\top$ for $\boldsymbol{A} \in S^n$. Note that $\exp(\boldsymbol{A})$ is positive definite for any $\boldsymbol{A} \in S^n$.

9.2.2 Monotonicity and Operator Monotonicity

Cosider a function $f : \mathcal{D} \to \mathcal{C}$. If we have a partial order $\leq_{\mathcal{D}}$ defined on $\mathcal{D}$ and a partial order $\leq_{\mathcal{C}}$ defined on $\mathcal{C}$, then we say that the function is monotone increasing (resp. decreasing) w.r.t. this pair of orderings if for all $d_1, d_2 \in \mathcal{D}$ s.t. $d_1 \leq_{\mathcal{D}} d_2$ we have $f(d_1) \leq_{\mathcal{C}} f(d_2)$ (resp. decreasing if $f(d_2) \leq_{\mathcal{C}} f(d_1)$).

Let's introduce some terminonology for important special cases of this idea. We say that a function $f : \mathcal{S} \to \mathbb{R}$, where $\mathcal{S} \subseteq S^n$, is monotone increasing if $\boldsymbol{A} \preceq \boldsymbol{B}$ implies $f(\boldsymbol{A}) \leq f(\boldsymbol{B})$.

Meanwhile, a function $f : \mathcal{S} \to \mathcal{T}$ where $\mathcal{S}, \mathcal{T} \subseteq S^n$ is said to be operator monotone increasing if $\boldsymbol{A} \preceq \boldsymbol{B}$ implies $f(\boldsymbol{A}) \preceq f(\boldsymbol{B})$.

Lemma 9.2.6. *Let $T \subseteq \mathbb{R}$. If the scalar function $f : T \to \mathbb{R}$ is monotone increasing, the matrix function $\boldsymbol{X} \mapsto \operatorname{Tr}(f(\boldsymbol{X}))$ is monotone increasing.*

Proof. From previous chapters, we know if $\boldsymbol{A} \preceq \boldsymbol{B}$ then $\lambda_i(\boldsymbol{A}) \leq \lambda_i(\boldsymbol{B})$ for all i. As $x \mapsto f(x)$ is monotone, then $\lambda_i(f(\boldsymbol{A})) \leq \lambda_i(f(\boldsymbol{B}))$ for all i. By Claim 9.2.4, $\operatorname{Tr}(f(\boldsymbol{A})) \leq \operatorname{Tr}(f(\boldsymbol{B}))$. □

From this, and the fact that $x \mapsto \exp(x)$ is a monotone function on the reals, we get the following corollary.

Corollary 9.2.7. *If $\boldsymbol{A} \preceq \boldsymbol{B}$, then $\operatorname{Tr}(\exp(\boldsymbol{A})) \leq \operatorname{Tr}(\exp(\boldsymbol{B}))$, i.e. $\boldsymbol{X} \mapsto \operatorname{Tr}(\exp(\boldsymbol{X}))$ is monotone increasing.*

Lemma 9.2.8. *If $\boldsymbol{0} \prec \boldsymbol{A} \preceq \boldsymbol{B}$, then $\boldsymbol{B}^{-1} \preceq \boldsymbol{A}^{-1}$, i.e. $\boldsymbol{X} \mapsto \boldsymbol{X}^{-1}$ is operator monotone decreasing on S^n_{++}.*

You will prove the above lemma in this week's exercises.

Lemma 9.2.9. *If $0 \prec \boldsymbol{A} \preceq \boldsymbol{B}$, then $\log(\boldsymbol{A}) \preceq \log(\boldsymbol{B})$.*

To prove this lemma, we first recall an integral representation of the logarithm.

Lemma 9.2.10.

$$\log a = \int_0^\infty \left(\frac{1}{1+t} - \frac{1}{a+t} \right) \mathrm{d}t$$

Proof.

$$\begin{aligned}
\int_0^\infty \left(\frac{1}{1+t} - \frac{1}{a+t} \right) \mathrm{d}t &= \lim_{T \to \infty} \int_0^T \left(\frac{1}{1+t} - \frac{1}{a+t} \right) \mathrm{d}t \\
&= \lim_{T \to \infty} \left[\log(1+t) - \log(a+t) \right]_0^T \\
&= \log(a) + \lim_{T \to \infty} \log \left(\frac{1+T}{a+T} \right) \\
&= \log(a)
\end{aligned}$$

□

Proof sketch of Lemma 9.2.9. Because all the matrices involved are diagonalized by the same orthogonal transformation, we can conclude from Lemma 9.2.10 that for a matrix $\boldsymbol{A} \succ \boldsymbol{0}$,

$$\log(\boldsymbol{A}) = \int_0^\infty \left(\frac{1}{1+t} \boldsymbol{I} - (t\boldsymbol{I} + \boldsymbol{A})^{-1} \right) \mathrm{d}t$$

This integration can be expressesd as the limit of a sum with positive coefficients, and from this we can show that is the integrand (the term inside the integration symbol) is operator monotone increasing in $\boldsymbol{A}$ by Lemma 9.2.8, the result of the integral, i.e. $\log(\boldsymbol{A})$ must also be operator monotone increasing. □

The following is a more general version of Lemma 1.6.

Lemma 9.2.11. *Let $T \subset \mathbb{R}$. If the scalar function $f : T \to \mathbb{R}$ is monotone, the matrix function $\boldsymbol{X} \mapsto \operatorname{Tr}(f(\boldsymbol{X}))$ is monotone.*

Remark 9.2.12. It is not always true that when $f : \mathbb{R} \to \mathbb{R}$ is monotone, $f : S^n \to S^n$ is operator monotone. For example, $\boldsymbol{X} \mapsto \boldsymbol{X}^2$ and $\boldsymbol{X} \mapsto \exp(\boldsymbol{X})$ are *not* operator monotone.

9.2.3 Some Useful Facts

Lemma 9.2.13. $\exp(\boldsymbol{A}) \preceq \boldsymbol{I} + \boldsymbol{A} + \boldsymbol{A}^2$ *for* $\|\boldsymbol{A}\| \leq 1$.

Proof.

$$\begin{aligned}\boldsymbol{I} + \boldsymbol{A} + \boldsymbol{A}^2 - \exp(\boldsymbol{A}) &= \boldsymbol{V}\boldsymbol{I}\boldsymbol{V}^\top + \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^\top + \boldsymbol{V}\boldsymbol{\Lambda}^2\boldsymbol{V}^\top - \boldsymbol{V}\exp(\boldsymbol{\Lambda})\boldsymbol{V}^\top \\ &= \boldsymbol{V}\left(\boldsymbol{I} + \boldsymbol{\Lambda} + \boldsymbol{\Lambda}^2 - \exp(\boldsymbol{\Lambda})\right)\boldsymbol{V}^\top \\ &= \boldsymbol{V}\operatorname*{diag}_i\{1 + \lambda_i + \lambda_i^2 - \exp(\lambda_i)\}\boldsymbol{V}^\top\end{aligned}$$

Recall $\exp(x) \leq 1 + x + x^2$ for all $|x| \leq 1$. Since $\|A\| \leq 1$ i.e. $|\lambda_i| \leq 1$ for all i, thus $1 + \lambda_i + \lambda_i^2 - \exp(\lambda_i) \geq 0$ for all i, meaning $\boldsymbol{I} + \boldsymbol{A} + \boldsymbol{A}^2 - \exp(\boldsymbol{A}) \succeq 0$. □

Lemma 9.2.14. $\log(\boldsymbol{I} + \boldsymbol{A}) \preceq \boldsymbol{A}$ *for* $A \succ -\boldsymbol{I}$.

Proof.

$$\begin{aligned}\boldsymbol{A} - \log(\boldsymbol{I} + \boldsymbol{A}) &= \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^\top - \boldsymbol{V}\log(\boldsymbol{\Lambda} + \boldsymbol{I})\boldsymbol{V}^\top \\ &= \boldsymbol{V}\left(\boldsymbol{\Lambda} - \log(\boldsymbol{\Lambda} + \boldsymbol{I})\right)\boldsymbol{V}^\top \\ &= \boldsymbol{V}\operatorname*{diag}_i\{\lambda_i - \log(1 + \lambda_i)\}\boldsymbol{V}^\top\end{aligned}$$

Recall $x \geq \log(1 + x)$ for all $x > -1$. Since $\|A\| \succ -\boldsymbol{I}$ i.e. $\lambda_i > -1$ for all i, thus $\lambda_i - \log(1 + \lambda_i) \geq 0$ for all i, meaning $\boldsymbol{A} - \log(\boldsymbol{I} + \boldsymbol{A}) \succeq 0$. □

Theorem 9.2.15 (Lieb)**.** *Let $f : S^n_{++} \to \mathbb{R}$ be a matrix function given by*

$$f(\boldsymbol{A}) = \operatorname{Tr}\left(\exp\left(\boldsymbol{H} + \log(\boldsymbol{A})\right)\right)$$

for some $\boldsymbol{H} \in S^n$. Then $-f$ is convex (i.e. f is concave).

The Lieb's theorem will be crucial in our proof of Theorem 9.2.1, but it is also highly non-trivial and we will omit its proof here. The interested reader can find a proof in Chapter 8 of [T+15].

Lemma 9.2.16 (Jensen's inequality)**.** $\mathbb{E}[f(X)] \geq f(\mathbb{E}[X])$ *when f is convex;* $\mathbb{E}[f(X)] \leq f(\mathbb{E}[X])$ *when f is concave.*

9.2.4 Proof of Matrix Bernstein Concentration Bound

Now, we are ready to prove the Bernstein matrix concentration bound.

Proof of Theorem 9.2.1. For any $\boldsymbol{A} \in S^n$, its spectral norm $\|\boldsymbol{A}\| = \max\{|\lambda_n(\boldsymbol{A})|, |\lambda_1(\boldsymbol{A})|\} = \max\{\lambda_n(\boldsymbol{A}), -\lambda_1(\boldsymbol{A})\}$. Let $\lambda_1 \leq \cdots \leq \lambda_n$ be the eigenvalues of $\boldsymbol{X}$. Then,

$$\Pr[\|\boldsymbol{X}\| \geq t] = \Pr\left[(\lambda_n \geq t) \bigvee (-\lambda_1 \geq t)\right] \leq \Pr[\lambda_n \geq t] + \Pr[-\lambda_1 \geq t].$$

Let $\boldsymbol{Y} := \sum_i -\boldsymbol{X}_i$. It's easy to see that $-\lambda_n \leq \cdots \leq -\lambda_1$ are eigenvalues of $\boldsymbol{Y}$, implying $\lambda_n(\boldsymbol{Y}) = -\lambda_1(\boldsymbol{X})$. Since $\mathbb{E}[-\boldsymbol{X}_i] = \mathbb{E}[\boldsymbol{X}_i] = 0$ and $\|-\boldsymbol{X}_i\| = \|\boldsymbol{X}_i\| \leq R$ for all i, if we can bound $\Pr[\lambda_n(\boldsymbol{X}) \geq t]$, then applying to $\boldsymbol{Y}$, we can bound $\Pr[\lambda_n(\boldsymbol{Y}) \geq t]$. As

$$\Pr[-\lambda_1(\boldsymbol{X}) \geq t] = \Pr[\lambda_n(\boldsymbol{Y}) \geq t],$$

it suffices to bound $\Pr[\lambda_n \geq t]$.

For any $\theta > 0$, $\lambda_n \geq t \iff \exp(\theta\lambda_n) \geq \exp(\theta t)$ and $\operatorname{Tr}(\exp(\theta\boldsymbol{X})) = \sum_i \exp(\theta\lambda_i)$ by Claim 9.2.4, thus $\lambda_n \geq t \Rightarrow \operatorname{Tr}(\exp(\theta\boldsymbol{X})) \geq \exp(\theta t)$. Then, using Markov's inequality,

$$\begin{aligned}\Pr[\lambda_n \geq t] &\leq \Pr[\operatorname{Tr}(\exp(\theta\boldsymbol{X})) \geq \exp(\theta t)] \\ &\leq \exp(-\theta t)\,\mathbb{E}[\operatorname{Tr}(\exp(\theta\boldsymbol{X}))]\end{aligned}$$

For two independent random variables $\boldsymbol{U}$ and $\boldsymbol{V}$, we have

$$\mathop{\mathbb{E}}_{\boldsymbol{U},\boldsymbol{V}} f(\boldsymbol{U}, \boldsymbol{V}) = \mathop{\mathbb{E}}_{\boldsymbol{U}} \mathop{\mathbb{E}}_{\boldsymbol{V}} [f(\boldsymbol{U}, \boldsymbol{V}) | \boldsymbol{U}] = \mathop{\mathbb{E}}_{\boldsymbol{U}} \mathop{\mathbb{E}}_{\boldsymbol{V}} [f(\boldsymbol{U}, \boldsymbol{V})].$$

Define $\boldsymbol{X}_{<i} = \sum_{j<i} \boldsymbol{X}_j$. Let $0 < \theta \le 1/R$,

$$
\begin{aligned}
\mathbb{E}\operatorname{Tr}\left(\exp(\theta \boldsymbol{X})\right) &= \mathop{\mathbb{E}}_{\boldsymbol{X}_1,\ldots,\boldsymbol{X}_{k-1}} \mathop{\mathbb{E}}_{\boldsymbol{X}_k} \operatorname{Tr}\exp\left(\underbrace{\theta \boldsymbol{X}_{<k}}_{\boldsymbol{H}} + \underbrace{\theta \boldsymbol{X}_k}_{=\log\exp(\theta \boldsymbol{X}_k)}\right), \quad \{\boldsymbol{X}_i\} \text{ are independent} \\
&\le \mathop{\mathbb{E}}_{\boldsymbol{X}_1,\ldots,\boldsymbol{X}_{k-1}} \operatorname{Tr}\exp\left(\theta \boldsymbol{X}_{<k} + \log \mathbb{E}\exp(\theta \boldsymbol{X}_k)\right), \quad \text{by 10.4.9 and 9.2.16} \\
&\le \mathop{\mathbb{E}}_{\boldsymbol{X}_1,\ldots,\boldsymbol{X}_{k-1}} \operatorname{Tr}\exp\left(\theta \boldsymbol{X}_{<k} + \log \mathbb{E}\left[\boldsymbol{I} + \theta \boldsymbol{X}_k + \theta^2 \boldsymbol{X}_k^2\right]\right), \quad \text{by 10.4.14, 9.2.7, and 9.2.9} \\
&\le \mathop{\mathbb{E}}_{\boldsymbol{X}_1,\ldots,\boldsymbol{X}_{k-1}} \operatorname{Tr}\exp\left(\theta \boldsymbol{X}_{<k} + \theta^2 \mathbb{E}\,\boldsymbol{X}_k^2\right), \quad \text{by 10.4.12 and 9.2.7} \\
&= \mathop{\mathbb{E}}_{\boldsymbol{X}_1,\ldots,\boldsymbol{X}_{k-2}} \mathop{\mathbb{E}}_{\boldsymbol{X}_{k-1}} \operatorname{Tr}\exp\left(\underbrace{\theta^2 \mathbb{E}\,\boldsymbol{X}_k^2 + \theta \boldsymbol{X}_{<k-1}}_{\boldsymbol{H}} + \theta \boldsymbol{X}_{k-1}\right), \\
&\;\;\vdots \\
&\le \operatorname{Tr}\exp\left(\theta^2 \sum_i \mathbb{E}\left[\boldsymbol{X}_i^2\right]\right), \\
&\le \operatorname{Tr}\exp\left(\theta^2\sigma^2 \boldsymbol{I}\right), \quad \text{by 9.2.7 and } \sum_i \mathbb{E}\left[\boldsymbol{X}_i^2\right] \preceq \sigma^2 \boldsymbol{I} \\
&= n \cdot \exp(\theta^2\sigma^2).
\end{aligned}
$$

Then,

$$\Pr[\lambda_n \ge t] \le n \cdot \exp(-\theta t + \theta^2\sigma^2),$$

and

$$\Pr[\|\boldsymbol{X}\| \ge t] \le 2n \cdot \exp(-\theta t + \theta^2\sigma^2).$$

Similar to the proof of Bernstein concentration bound for one-dimension random variable, minimize the RHS over $0 < \theta \le 1/R$ yields

$$\Pr[\|\boldsymbol{X}\| \ge t] \le 2n \cdot \exp\left(\frac{-t^2}{2Rt + 4\sigma^2}\right).$$

□

9.3 Spectral Graph Sparsification

In this section, we will see that for any dense graph, we can find another sparser graph whose graph Laplacian is approximately the same as measured by their quadratic forms. This turns out to be a very useful tool for designing algorithms.

Definition 9.3.1. Given $\boldsymbol{A}, \boldsymbol{B} \in S_+^n$ and $\epsilon > 0$, we say

$$\boldsymbol{A} \approx_\epsilon \boldsymbol{B} \text{ if and only if } \frac{1}{1+\epsilon}\boldsymbol{A} \preceq \boldsymbol{B} \preceq (1+\epsilon)\boldsymbol{A}.$$

Suppose we start with a connected graph $G = (V, E, \boldsymbol{w})$, where as usual we say that $|V| = n$ and $|E| = m$. We want to produce another graph $\tilde{G} = (V, \tilde{E}, \tilde{\boldsymbol{w}})$ s.t $\left|\tilde{E}\right| \ll |E|$ and at the same time $\boldsymbol{L}_G \approx_\epsilon \boldsymbol{L}_{\tilde{G}}$. We call $\tilde{G}$ a *spectral sparsifier* of G. Our construction will also ensure that $\tilde{E} \subseteq E$, although this is not important in most applications. Figure 9.2 shows an example of a graph G and spectral sparsifier $\tilde{G}$.

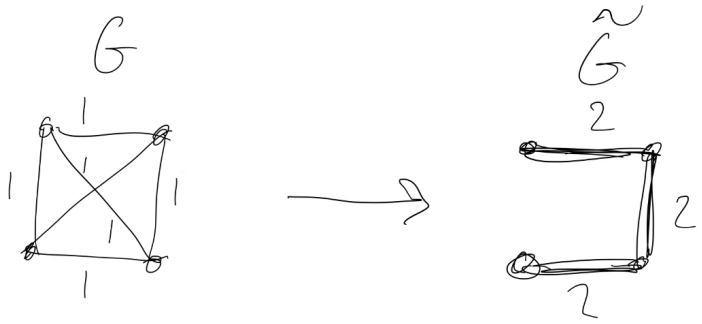


Figure 9.2: A graph G and a spectral sparsifier $\tilde{G}$, satisfisying $\boldsymbol{L}_G \approx_\epsilon \boldsymbol{L}_{\tilde{G}}$ for $\epsilon = 2.42$.

We are going to construct $\tilde{G}$ by sampling some of the edges of G according to a suitable probability distribution and scaling up their weight to make up for the fact that we pick fewer of them.

To get a better understanding for the notion of approximation given in 9.3.1 means, let's observe a simple consequence of it.

Given a vertex subset $T \subseteq V$, we say that $(T, V \setminus T)$ is a *cut* in G and that the value of the cut is

$$c_G(T) = \sum_{e \in E \cap (T \times V \setminus T)} \boldsymbol{w}(e).$$

Figure 9.3 shows the $c_G(T)$ in a graph G.

Theorem 9.3.2. *If $\boldsymbol{L}_G \approx_\epsilon \boldsymbol{L}_{\tilde{G}}$, then for all $T \subseteq V$,*

$$\frac{1}{1+\epsilon} c_G(T) \leq c_{\tilde{G}}(T) \leq (1+\epsilon) c_G(T).$$

Proof. Let $\mathbf{1}_T \in \mathbb{R}^V$ be the indicator of the set T, i.e. $\mathbf{1}_T(u) = 1$ for $u \in V$ and $\mathbf{1}_T(u) = 0$ otherwise. We can see that $\mathbf{1}_T^\top \boldsymbol{L}_G \mathbf{1}_T = c_G(T)$, and hence the theorem follows by comparing the quadratic forms. □

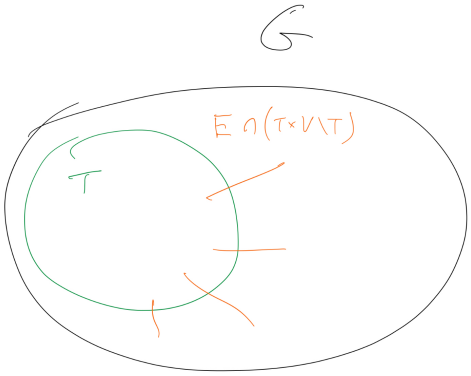


Figure 9.3: The cut $c_G(T)$ in G.

But how well can we spectrally approximate a graph with a sparse graph? The next theorem gives us a nearly optimal answer to this question.

Theorem 9.3.3 (Spectral Graph Approximation by Sampling, (Spielman-Srivastava 2008))**.** *Consider a connected graph $G = (V, E, \boldsymbol{w})$, with $n = |V|$. For any $0 < \epsilon < 1$ and $0 < \delta < 1$, there exist sampling probabilities p_e for each edge $e \in E$ s.t. if we include each edge e in $\tilde{E}$ independently with probabilty p_e and set its weight $\tilde{\boldsymbol{w}}(e) = \frac{1}{p_e}\boldsymbol{w}(e)$, then with probability at least $1 - \delta$ the graph $\tilde{G} = (V, \tilde{E}, \tilde{\boldsymbol{w}})$ satisfies*

$$\boldsymbol{L}_G \approx_\epsilon \boldsymbol{L}_{\tilde{G}} \text{ and } \left|\tilde{E}\right| \leq O(n\epsilon^{-2}\log(n/\delta)).$$

The original proof can be found in [SS11].

Remark 9.3.4. For convenience, we will abbreviate $\boldsymbol{L}_G$ as $\boldsymbol{L}$ and $\boldsymbol{L}_{\tilde{G}}$ as $\tilde{\boldsymbol{L}}$ in the rest of this section.

We are going to analyze a sampling procedure by turning our goal into a problem of matrix concentration. Recall that

Fact 9.3.5. *$\boldsymbol{A} \preceq \boldsymbol{B}$ implies $\boldsymbol{C}\boldsymbol{A}\boldsymbol{C}^\top \preceq \boldsymbol{C}\boldsymbol{B}\boldsymbol{C}^\top$ for any $\boldsymbol{C} \in \mathbb{R}^{n\times n}$.*

By letting $\boldsymbol{C} = \boldsymbol{L}^{+/2}$, we can see that

$$\boldsymbol{L} \approx_\epsilon \tilde{\boldsymbol{L}} \text{ implies } \boldsymbol{\Pi}_{\boldsymbol{L}} \approx_\epsilon \boldsymbol{L}^{+/2}\tilde{\boldsymbol{L}}\boldsymbol{L}^{+/2}, \tag{9.2}$$

where $\boldsymbol{\Pi}_{\boldsymbol{L}} = \boldsymbol{L}^{+/2}\boldsymbol{L}\boldsymbol{L}^{+/2}$ is the orthogonal projection to the complement of the kernel of $\boldsymbol{L}$.

Definition 9.3.6. Given a matrix $\boldsymbol{A}$, we define $\boldsymbol{\Pi}_{\boldsymbol{A}}$ to be the orthogonal projection to the complement of the kernel of $\boldsymbol{A}$, i.e. $\boldsymbol{\Pi}_{\boldsymbol{A}}\boldsymbol{v} = \boldsymbol{0}$ for $\boldsymbol{v} \in \ker(\boldsymbol{A})$ and $\boldsymbol{\Pi}_{\boldsymbol{A}}\boldsymbol{v} = \boldsymbol{v}$ for $\boldsymbol{v} \in \ker(\boldsymbol{A})^\perp$. Recall that $\ker(\boldsymbol{A})^\perp = \mathrm{im}(\boldsymbol{A}^\top)$.

Claim 9.3.7. *For a matrix $\boldsymbol{A} \in S^n$ with spectral decomposition $\boldsymbol{A} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^\top = \sum_i \lambda_i \boldsymbol{v}_i\boldsymbol{v}_i^\top$ s.t. $\boldsymbol{V}^\top\boldsymbol{V} = \boldsymbol{I}$, we have $\boldsymbol{\Pi}_{\boldsymbol{A}} = \sum_{i:\lambda_i\neq 0} \boldsymbol{v}_i\boldsymbol{v}_i^\top$, and $\boldsymbol{\Pi}_{\boldsymbol{A}} = \boldsymbol{A}^{+/2}\boldsymbol{A}\boldsymbol{A}^{+/2} = \boldsymbol{A}\boldsymbol{A}^+ = \boldsymbol{A}^+\boldsymbol{A}$.*

From the definition, we can see that $\boldsymbol{\Pi_L} = \boldsymbol{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^\top$.

Now that we understand the projection $\boldsymbol{\Pi_L}$, it is not hard to show the following claim.

Claim 9.3.8.

1. $\boldsymbol{\Pi_L} \approx_\epsilon \boldsymbol{L}^{+/2}\tilde{\boldsymbol{L}}\boldsymbol{L}^{+/2}$ *implies* $\boldsymbol{L} \approx_\epsilon \tilde{\boldsymbol{L}}$.
2. *For* $\epsilon \leq 1$, *we have that* $\left\|\boldsymbol{\Pi_L} - \boldsymbol{L}^{+/2}\tilde{\boldsymbol{L}}\boldsymbol{L}^{+/2}\right\| \leq \epsilon/2$ *implies* $\boldsymbol{\Pi_L} \approx_\epsilon \boldsymbol{L}^{+/2}\tilde{\boldsymbol{L}}\boldsymbol{L}^{+/2}$.

Really, the only idea needed here is that when comparing quadratic forms in matrices with the same kernel, we necessarily can't have the quadratic forms disagree on vectors in the kernel. Simple! But we are going to write it out carefully, since we're still getting used to these types of calculations.

Proof of Claim 9.3.8. To prove Part 1, we assume $\boldsymbol{\Pi_L} \approx_\epsilon \boldsymbol{L}^{+/2}\tilde{\boldsymbol{L}}\boldsymbol{L}^{+/2}$. Recall that G is a connected graph, so $\ker(\boldsymbol{L}) = \operatorname{span}\{\mathbf{1}\}$, while $\tilde{\boldsymbol{L}}$ is the Laplacian of a graph which may or may not be connected, so $\ker(\tilde{\boldsymbol{L}}) \supseteq \ker(\boldsymbol{L})$, and equivalently $\operatorname{im}(\tilde{\boldsymbol{L}}) \subseteq \operatorname{im}(\boldsymbol{L})$. Now, for any $\boldsymbol{v} \in \ker(\boldsymbol{L})$ we have $\boldsymbol{v}^\top\tilde{\boldsymbol{L}}\boldsymbol{v} = 0 = \boldsymbol{v}^\top\boldsymbol{L}\boldsymbol{v}$. For any $\boldsymbol{v} \in \ker(\boldsymbol{L})^\perp$ we have $\boldsymbol{v} = \boldsymbol{L}^{+/2}\boldsymbol{z}$ for some $\boldsymbol{z}$, as $\ker(\boldsymbol{L})^\perp = \operatorname{im}(\boldsymbol{L}) = \operatorname{im}(\boldsymbol{L}^{+/2})$. Hence

$$\boldsymbol{v}^\top\tilde{\boldsymbol{L}}\boldsymbol{v} = \boldsymbol{z}^\top\boldsymbol{L}^{+/2}\tilde{\boldsymbol{L}}\boldsymbol{L}^{+/2}\boldsymbol{z} \geq \frac{1}{1+\epsilon}\boldsymbol{z}^\top\boldsymbol{L}^{+/2}\boldsymbol{L}\boldsymbol{L}^{+/2}\boldsymbol{z} = \frac{1}{1+\epsilon}\boldsymbol{v}^\top\boldsymbol{L}\boldsymbol{v}$$

and similarly

$$\boldsymbol{v}^\top\tilde{\boldsymbol{L}}\boldsymbol{v} = \boldsymbol{z}^\top\boldsymbol{L}^{+/2}\tilde{\boldsymbol{L}}\boldsymbol{L}^{+/2}\boldsymbol{z} \leq (1+\epsilon)\boldsymbol{z}^\top\boldsymbol{L}^{+/2}\boldsymbol{L}\boldsymbol{L}^{+/2}\boldsymbol{z} = (1+\epsilon)\boldsymbol{v}^\top\boldsymbol{L}\boldsymbol{v}.$$

Thus we have established $\boldsymbol{L} \approx_\epsilon \tilde{\boldsymbol{L}}$.

To prove Part 2, we assume $\left\|\boldsymbol{\Pi_L} - \boldsymbol{L}^{+/2}\tilde{\boldsymbol{L}}\boldsymbol{L}^{+/2}\right\| \leq \epsilon/2$. This is equivalent to

$$-\frac{\epsilon}{2}\boldsymbol{I} \preceq \boldsymbol{L}^{+/2}\tilde{\boldsymbol{L}}\boldsymbol{L}^{+/2} - \boldsymbol{\Pi_L} \preceq \frac{\epsilon}{2}\boldsymbol{I}$$

But since

$$\mathbf{1}^\top(\boldsymbol{L}^{+/2}\tilde{\boldsymbol{L}}\boldsymbol{L}^{+/2} - \boldsymbol{\Pi_L})\mathbf{1} = 0,$$

we can in fact sharpen this to

$$-\frac{\epsilon}{2}\boldsymbol{\Pi_L} \preceq \boldsymbol{L}^{+/2}\tilde{\boldsymbol{L}}\boldsymbol{L}^{+/2} - \boldsymbol{\Pi_L} \preceq \frac{\epsilon}{2}\boldsymbol{\Pi_L}.$$

Rearranging, we then conclude

$$(1-\frac{\epsilon}{2})\boldsymbol{\Pi_L} \preceq \boldsymbol{L}^{+/2}\tilde{\boldsymbol{L}}\boldsymbol{L}^{+/2} \preceq (1+\frac{\epsilon}{2})\boldsymbol{\Pi_L}.$$

Finally, we note that $1/(1+\epsilon) \leq (1-\frac{\epsilon}{2})$ to reach our conclusion, $\boldsymbol{\Pi_L} \approx_\epsilon \boldsymbol{L}^{+/2}\tilde{\boldsymbol{L}}\boldsymbol{L}^{+/2}$. □

We now have most of the tools to prove Theorem 9.3.3, but to help us, we are going to establish one small piece of helpful notation: We define a matrix function $\Phi : \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$ by

$$\Phi(\boldsymbol{A}) = \boldsymbol{L}^{+/2}\boldsymbol{A}\boldsymbol{L}^{+/2}.$$

We sometimes call this a "normalizing map", because it transforms a matrix to the space where spectral norm bounds can be translated into relative error guarantees compare to the $\boldsymbol{L}$ quadratic form.

Proof of Theorem 9.3.3. By Claim 9.3.8, it suffices to show

$$\left\|\boldsymbol{\Pi}_{\boldsymbol{L}} - \boldsymbol{L}^{+/2}\tilde{\boldsymbol{L}}\boldsymbol{L}^{+/2}\right\| \leq \epsilon/2. \tag{9.3}$$

We introduce a set of independent random variables, one for each edge e, with a probability p_e associated with the edge which we will fix later. We then let

$$\boldsymbol{Y}_e = \begin{cases} \frac{\boldsymbol{w}(e)}{p_e}\boldsymbol{b}_e\boldsymbol{b}_e^\top & \text{with probability } p_e \\ \boldsymbol{0} & \text{otherwise.} \end{cases}$$

This way, $\tilde{\boldsymbol{L}} = \sum_e \boldsymbol{Y}_e$. Note that $\mathbb{E}[\boldsymbol{Y}_e] = p_e\frac{\boldsymbol{w}(e)}{p_e}\boldsymbol{b}_e\boldsymbol{b}_e^\top = \boldsymbol{w}(e)\boldsymbol{b}_e\boldsymbol{b}_e^\top$, and so

$$\mathbb{E}\left[\tilde{\boldsymbol{L}}\right] = \sum_e \mathbb{E}[\boldsymbol{Y}_e] = \boldsymbol{L}.$$

By linearity of Φ,

$$\mathbb{E}\left[\Phi(\tilde{\boldsymbol{L}})\right] = \Phi(\mathbb{E}\left[\tilde{\boldsymbol{L}}\right]) = \boldsymbol{\Pi}_{\boldsymbol{L}}.$$

Let us also define

$$\boldsymbol{X}_e = \Phi(\boldsymbol{Y}_e) - \mathbb{E}[\Phi(\boldsymbol{Y}_e)] \text{ and } \boldsymbol{X} = \sum_e \boldsymbol{X}_e$$

Note that this ensures $\mathbb{E}[\boldsymbol{X}_e] = \boldsymbol{0}$. We are now going to fix the edge sampling probabilities, in a way that depends on some overall scaling parameter $\alpha > 0$. We let

$$p_e = \min\left(\alpha\left\|\Phi\left(\boldsymbol{w}(e)\boldsymbol{b}_e\boldsymbol{b}_e^\top\right)\right\|, 1\right)$$

then we see from the definition of $\boldsymbol{Y}_e$ that whenever $p_e < 1$

$$\|\Phi(\boldsymbol{Y}_e)\| \leq \frac{1}{\alpha}$$

from this, we can conclude, with a bit of work, that for all e

$$\|\boldsymbol{X}_e\| \leq \frac{1}{\alpha}. \tag{9.4}$$

We can also show that

$$\left\|\sum_e \mathbb{E}\left[\boldsymbol{X}_e^2\right]\right\| \leq \frac{1}{\alpha}. \tag{9.5}$$

In the exercises for this chapter, we will ask you to show that Equations (9.4) and (9.5) hold.

This means that we can apply Theorem 9.2.1 to our $\boldsymbol{X} = \sum_e \boldsymbol{X}_e$, with $R = \frac{1}{\alpha}$ and $\sigma^2 = \frac{1}{\alpha}$, to get

$$\Pr\left[\left\|\boldsymbol{\Pi}_{\boldsymbol{L}} - \boldsymbol{L}^{+/2}\tilde{\boldsymbol{L}}\boldsymbol{L}^{+/2}\right\| \geq \epsilon/2\right] \leq 2n \exp\left(\frac{-0.25\epsilon^2}{(\epsilon+4)/\alpha}\right)$$

Since $0 < \epsilon < 1$, this means that if $\alpha = 40\epsilon^{-2}\log(n/\delta)$, then

$$Pr\left[\left\|\boldsymbol{\Pi}_{\boldsymbol{L}} - \boldsymbol{L}^{+/2}\tilde{\boldsymbol{L}}\boldsymbol{L}^{+/2}\right\| \geq \epsilon/2\right] \leq \frac{2n\delta^2}{n^2} \leq \delta/2.$$

In the last step, we assumed $n \geq 4$.

Lastly, we'd like to know that the graph $\tilde{G}$ is sparse. The number of edges in $\tilde{G}$ is equal to the number of $\boldsymbol{Y}_e$ that come out nonzero. Thus, the expected value of $\left|\tilde{E}\right|$ is

$$\mathbb{E}\left[\left|\tilde{E}\right|\right] = \sum_e p_e \leq \alpha \sum_e \boldsymbol{w}(e)\left\|\boldsymbol{L}^{+/2}\boldsymbol{b}_e\boldsymbol{b}_e^\top\boldsymbol{L}^{+/2}\right\|$$

We can bound the sum of the norms with a neat trick relating it to the trace of $\boldsymbol{\Pi}_{\boldsymbol{L}}$. Note that in general for a vector $\boldsymbol{a} \in \mathbb{R}^n$, we have $\left\|\boldsymbol{a}\boldsymbol{a}^\top\right\| = \boldsymbol{a}^\top\boldsymbol{a} = \mathrm{Tr}\left(\boldsymbol{a}\boldsymbol{a}^\top\right)$. And hence

$$\begin{aligned}\sum_e \boldsymbol{w}(e)\left\|\boldsymbol{L}^{+/2}\boldsymbol{b}_e\boldsymbol{b}_e^\top\boldsymbol{L}^{+/2}\right\| &= \sum_e \boldsymbol{w}(e)\mathrm{Tr}\left(\boldsymbol{L}^{+/2}\boldsymbol{b}_e\boldsymbol{b}_e^\top\boldsymbol{L}^{+/2}\right)\\ &= \mathrm{Tr}\left(\boldsymbol{L}^{+/2}\left(\sum_e \boldsymbol{w}(e)\boldsymbol{b}_e\boldsymbol{b}_e^\top\right)\boldsymbol{L}^{+/2}\right)\\ &= \mathrm{Tr}\left(\boldsymbol{\Pi}_{\boldsymbol{L}}\right) = n-1.\end{aligned}$$

Thus with our choice of α,

$$\mathbb{E}\left[\left|\tilde{E}\right|\right] \leq 40\epsilon^{-2}\log(n/\delta)n.$$

With a scalar Chernoff bound, can show that $\left|\tilde{E}\right| \leq O(\epsilon^{-2}\log(n/\delta)n)$ with probability at least $1-\delta/2$. Thus by a union bound, the this condition and Equation (9.3) are both satisfied with probability at least $1-\delta$. □

Remark 9.3.9. Note that

$$\left\|\Phi\left(\boldsymbol{w}(e)\boldsymbol{b}_e\boldsymbol{b}_e^\top\right)\right\| = \boldsymbol{w}(e)\left\|\boldsymbol{L}^{+/2}\boldsymbol{b}_e\boldsymbol{b}_e^\top\boldsymbol{L}^{+/2}\right\| \leq \boldsymbol{w}(e)\left\|\boldsymbol{L}^{+/2}\boldsymbol{b}_e\right\|_2^2.$$

Recall that in Chapter 7, we saw that the effective resistance between vertex v and vertex u is given by $\left\|\boldsymbol{L}^{+/2}(\boldsymbol{e}_u - \boldsymbol{e}_v)\right\|_2^2$, and for an edge e connecting vertex u and v, we have $\boldsymbol{b}_e = \boldsymbol{e}_u - \boldsymbol{e}_v$. That means the norm of the "baby Laplacian" $\boldsymbol{w}(e)\boldsymbol{b}_e\boldsymbol{b}_e^\top$ of a single edge with weight $\boldsymbol{w}(e)$ is exactly $\boldsymbol{w}(e)$ times the effective resistance between the two endpoints of the edge.

We haven't shown how to compute the sampling probabilities efficiently, so right now, it isn't clear whether we can efficiently find $\tilde{G}$. It turns out that if we have access to a fast algorithm for solving Laplacian linear equations, then we can find sufficiently good approximations to the effective resistances quickly, and use these to compute $\tilde{G}$. An algorithm for this is described in [SS11].

Chapter 10

Solving Laplacian Linear Equations

10.1 Solving Linear Equations Approximately

Given a Laplacian $\boldsymbol{L}$ of a connected graph and a demand vector $\boldsymbol{d} \perp \mathbf{1}$, we want to find $\boldsymbol{x}^*$ solving the linear equation $\boldsymbol{L}\boldsymbol{x}^* = \boldsymbol{d}$. We are going to focus on fast algorithms for finding approximate (but highly accurate) solutions.

This means we need a notion of an approximate solution. Since our definition is not special to Laplacians, we state it more generally for positive semi-definite matrices.

Definition 10.1.1. Given PSD matrix $\boldsymbol{M}$ and $\boldsymbol{d} \in \ker(\boldsymbol{M})^\perp$, let $\boldsymbol{M}\boldsymbol{x}^* = \boldsymbol{d}$. We say that $\tilde{\boldsymbol{x}}$ is an ϵ-approximate solution to the linear equation $\boldsymbol{M}\boldsymbol{x} = \boldsymbol{d}$ if

$$\|\tilde{\boldsymbol{x}} - \boldsymbol{x}^*\|_{\boldsymbol{M}}^2 \leq \epsilon \|\boldsymbol{x}^*\|_{\boldsymbol{M}}^2 .$$

Remark 10.1.2. The requirement $\boldsymbol{d} \in \ker(\boldsymbol{M})^\perp$ can be removed, but this is not important for us.

Theorem 10.1.3 (Spielman and Teng (2004) [ST04])**.** *Given a Laplacian $\boldsymbol{L}$ of a weighted undirected graph $G = (V, E, \boldsymbol{w})$ with $|E| = m$ and $|V| = n$ and a demand vector $\boldsymbol{d} \in \mathbb{R}^V$, we can find $\tilde{\boldsymbol{x}}$ that is an ϵ-approximate solution to $\boldsymbol{L}\boldsymbol{x} = \boldsymbol{d}$, using an algorithm that takes time $O(m \log^c n \log(1/\epsilon))$ for some fixed constant c and succeeds with probability $1 - 1/n^{10}$.*

In the original algorithm of Spielman and Teng, the exponent on the log in the running time was $c \approx 70$.

Today, we are going to see a simpler algorithm. But first, we'll look at one of the key tools behind all algorithms for solving Laplacian linear equations quickly.

10.2 Preconditioning and Approximate Gaussian Elimination

Recall our definition of two positive semi-definite matrices being approximately equal.

Definition 10.2.1 (Spectral approximation)**.** Given $\boldsymbol{A}, \boldsymbol{B} \in S_+^n$, we say that

$$\boldsymbol{A} \approx_K \boldsymbol{B} \text{ if and only if } \frac{1}{1+K}\boldsymbol{A} \preceq \boldsymbol{B} \preceq (1+K)\boldsymbol{A}.$$

Suppose we have a positive definite matrix $\boldsymbol{M} \in S_{++}^n$ and want to solve a linear equation $\boldsymbol{M}\boldsymbol{x} = \boldsymbol{d}$. We can do this using gradient descent or accelerated gradient descent, as we covered in Graded Homework 1. But if we have access to an easy-to-invert matrix that happens to also be a good spectral approximation of $\boldsymbol{M}$, then we can use this to speed up the (accelerated) gradient descent algorithm. An example of this would be that we have a factorization $\boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{L}}^\top \approx_K \boldsymbol{M}$, where $\boldsymbol{\mathcal{L}}$ is lower triangular and sparse, which means we can invert it quickly.

The following lemma, which you will prove in Problem Set 6, makes this preconditioning precise.

Lemma 10.2.2. *Given a matrix $\boldsymbol{M} \in S_{++}^n$, a vector $\boldsymbol{d}$ and a decomposition $\boldsymbol{M} \approx_K \boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{L}}^\top$, we can find $\tilde{\boldsymbol{x}}$ that ϵ-approximately solves $\boldsymbol{M}\boldsymbol{x} = \boldsymbol{d}$, using $O((1+K)\log(K/\epsilon)(T_{matvec}+T_{sol}+n))$ time.*

- *T_{matvec} denotes the time required to compute $\boldsymbol{M}\boldsymbol{z}$ given a vector $\boldsymbol{z}$, i.e. a "matrix-vector multiplication".*
- *T_{sol} denotes the time required to compute $\boldsymbol{\mathcal{L}}^{-1}\boldsymbol{z}$ or $(\boldsymbol{\mathcal{L}}^\top)^{-1}\boldsymbol{z}$ given a vector $\boldsymbol{z}$.*

Dealing with pseudo-inverses. When our matrices have a null space, preconditioning becomes slightly more complicated, but as long as it is easy to project to the complement of the null space, there's no real issue. The following describes precisely what we need (but you can ignore the null-space issue when first reading these notes without losing anything significant).

Lemma 10.2.3. *Given a matrix $\boldsymbol{M} \in S_+^n$, a vector $\boldsymbol{d} \in \ker(\boldsymbol{M})^\perp$ and a decomposition $\boldsymbol{M} \approx_K \boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{D}}\boldsymbol{\mathcal{L}}^\top$, where $\boldsymbol{\mathcal{L}}$ is invertible, we can find $\tilde{\boldsymbol{x}}$ that ϵ-approximately solves $\boldsymbol{M}\boldsymbol{x} = \boldsymbol{d}$, using $O((1+K)\log(K/\epsilon)(T_{matvec}+T_{sol}+T_{proj}+n))$ time.*

- *T_{matvec} denotes the time required to compute $\boldsymbol{M}\boldsymbol{z}$ given a vector $\boldsymbol{z}$, i.e. a "matrix-vector multiplication".*
- *T_{sol} denotes the time required to compute $\boldsymbol{\mathcal{L}}^{-1}\boldsymbol{z}$ and $(\boldsymbol{\mathcal{L}}^\top)^{-1}\boldsymbol{z}$ and $\boldsymbol{\mathcal{D}}^+\boldsymbol{z}$ given a vector $\boldsymbol{z}$.*

- T_{proj} *denotes the time required to compute* $\mathbf{\Pi}_{\boldsymbol{M}}\boldsymbol{z}$ *given a vector* $\boldsymbol{z}$.

Theorem 10.2.4 (Kyng and Sachdeva (2015) [KS16])**.** *Given a Laplacian* $\boldsymbol{L}$ *of a weighted undirected graph* $G = (V, E, \boldsymbol{w})$ *with* $|E| = M$ *and* $|V| = n$*, we can find a decomposition* $\boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{L}}^\top \approx_{0.5} \boldsymbol{L}$*, such that* $\boldsymbol{\mathcal{L}}$ *has number of non-zeroes* $\mathrm{nnz}(\boldsymbol{\mathcal{L}}) = O(m \log^3 n)$*, with probability at least* $1 - 3/n^5$*. in time* $O(m \log^3 n)$*.*

We can combine Theorem 10.2.4 with Lemma 10.2.3 to get a fast algorithm for solving Laplacian linear equations.

Corollary 10.2.5. *Given a Laplacian* $\boldsymbol{L}$ *of a weighted undirected graph* $G = (V, E, \boldsymbol{w})$ *with* $|E| = m$ *and* $|V| = n$ *and a demand vector* $\boldsymbol{d} \in \mathbb{R}^V$*, we can find* $\tilde{\boldsymbol{x}}$ *that is an* ϵ*-approximate solution to* $\boldsymbol{L}\boldsymbol{x} = \boldsymbol{d}$*, using an algorithm that takes time* $O(m \log^3 n \log(1/\epsilon))$ *and succeeds with probability* $1 - 1/n^{10}$*.*

Proof sketch. First we need to get a factorization that confirms to Lemma 10.2.3. The decomposition $\boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{L}}^\top$ provided by Theorem 10.2.4 can be rewritten as $\boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{L}}^\top = \widetilde{\boldsymbol{\mathcal{L}}}\boldsymbol{\mathcal{D}}(\widetilde{\boldsymbol{\mathcal{L}}})^\top$ where $\widetilde{\boldsymbol{\mathcal{L}}}$ is equal to $\boldsymbol{\mathcal{L}}$ except $\boldsymbol{\mathcal{L}}(n, n) = 1$ and we let $\boldsymbol{\mathcal{D}}$ be the identity matrix, except $\boldsymbol{\mathcal{D}}(n, n) = 0$. This ensures $\boldsymbol{\mathcal{D}}^+ = \boldsymbol{\mathcal{D}}$ and that $\widetilde{\boldsymbol{\mathcal{L}}}$ is invertible and lower triagular with $O(m \log^3 n)$ non-zeros. We note that the inverse of an invertible lower or upper triangular matrix with N non-zeros can be applied in time $O(N)$ given an adjacency list representation of the matrix. Finally, as $\ker(\boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{L}}^\top) = \mathrm{span}\{\mathbf{1}\}$, we have $\mathbf{\Pi}_{\widetilde{\boldsymbol{\mathcal{L}}}\boldsymbol{\mathcal{D}}(\widetilde{\boldsymbol{\mathcal{L}}})^\top} = \boldsymbol{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^\top$, and this projection matrix can be applied in $O(n)$ time. Altogether, this means that $T_{\text{matvec}} + T_{\text{sol}} + T_{\text{proj}} = O(n)$, which suffices to complete the proof. □

10.3 Approximate Gaussian Elimination Algorithm

Recall *Gaussian Elimination / Cholesky decomposition* of a graph Laplacian $\boldsymbol{L}$. We will use $\boldsymbol{A}(:, i)$ to denote the the ith column of a matrix $\boldsymbol{A}$. We can write the algorithm as

Algorithm 1: Gaussian Elimination / Cholesky Decomposition

Input: Graph Laplacian $\boldsymbol{L}$
Output: Lower triangular $\boldsymbol{\mathcal{L}}$ s.t. $\boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{L}}^\top = \boldsymbol{L}$
Let $\boldsymbol{S}_0 = \boldsymbol{L}$;
for $i = 1$ *to* $i = n - 1$ **do**
  $\boldsymbol{l}_i = \frac{1}{\sqrt{\boldsymbol{S}_{i-1}(i,i)}}\boldsymbol{S}_{i-1}(:, i)$;
  $\boldsymbol{S}_i = \boldsymbol{S}_{i-1} - \boldsymbol{l}_i\boldsymbol{l}_i^\top$.
$\boldsymbol{l}_n = \mathbf{0}_{n\times 1}$;
return $\boldsymbol{\mathcal{L}} = \begin{bmatrix}\boldsymbol{l}_1 \cdots \boldsymbol{l}_n\end{bmatrix}$;

We want to introduce some notation that will help us describe and analyze a faster version of Gaussian elimination – one that uses sampling to create a sparse approximation of the decomposition.

Consider a Laplacian $\boldsymbol{S}$ of a graph H and a vertex v of H. We define $\textsc{Star}(v, \boldsymbol{S})$ to be the Laplacian of the subgraph of H consisting of edges incident on v. We define

$$\textsc{Clique}(v, \boldsymbol{S}) = \textsc{Star}(v, \boldsymbol{S}) - \frac{1}{\boldsymbol{S}(v,v)} \boldsymbol{S}(:, v)\boldsymbol{S}(:, v)^\top$$

For example, suppose

$$\boldsymbol{L} = \begin{pmatrix} W & -\boldsymbol{a}^\top \\ -\boldsymbol{a} & \mathrm{diag}(\boldsymbol{a}) + \boldsymbol{L}_{-1} \end{pmatrix}$$

Then

$$\textsc{Star}(1, \boldsymbol{L}) = \begin{pmatrix} W & -\boldsymbol{a}^\top \\ -\boldsymbol{a} & \mathrm{diag}(\boldsymbol{a}) \end{pmatrix} \text{ and } \textsc{Clique}(1, \boldsymbol{L}) = \begin{pmatrix} 0 & \mathbf{0} \\ \mathbf{0} & \mathrm{diag}(\boldsymbol{a}) - \frac{1}{W}\boldsymbol{a}\boldsymbol{a}^\top \end{pmatrix}$$

which is illustrated in Figure 10.1.

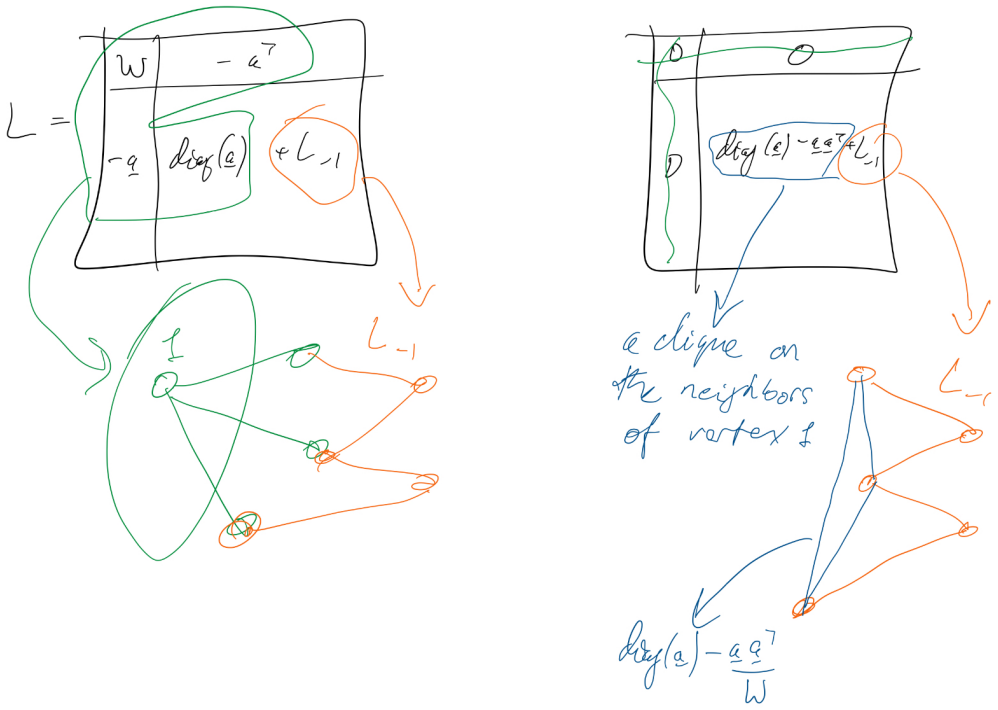


Figure 10.1: Gaussian Elimination: $\textsc{Clique}(1, \boldsymbol{L}) = \textsc{Star}(1, \boldsymbol{L}) - \frac{1}{\boldsymbol{L}(1,1)} \boldsymbol{L}(:, 1)\boldsymbol{L}(:, 1)^\top$.

In Chapter 8, we proved that $\textsc{Clique}(v, \boldsymbol{S})$ is a graph Laplacian – it follows from the proof of Claim 8.1.1 in that chapter. Thus we have that following.

Claim 10.3.1. *If $\boldsymbol{S}$ is the Laplacian of a connected graph, then $\textsc{Clique}(v, \boldsymbol{S})$ is a graph Laplacian.*

Note that in Algorithm 1, we have $\boldsymbol{l}_i \boldsymbol{l}_i^\top = \textsc{Star}(v_i, \boldsymbol{S}_{i-1}) - \textsc{Clique}(v_i, \boldsymbol{S}_{i-1})$. The update rule can be rewritten as

$$\boldsymbol{S}_i = \boldsymbol{S}_{i-1} - \textsc{Star}(v_i, \boldsymbol{S}_{i-1}) + \textsc{Clique}(v_i, \boldsymbol{S}_{i-1}),$$

This also provides way to understand why Gaussian Elimination is slow in some cases. At each step, one vertex is eliminated, but a clique is added to the subgraph on the remaining vertices, making the graph denser. And at the ith step, computing $\textsc{Star}(v_i, \boldsymbol{S}_{i-1})$ takes around $\deg(v_i)$ time, but computing $\textsc{Clique}(v_i, \boldsymbol{S}_{i-1})$ requires around $\deg(v_i)^2$ time. In order to speed up Gaussian Elimination, the algorithmic idea of [KS16] is to plug in a sparser appproximate of the intended clique instead of the entire one.

The following procedure $\textsc{CliqueSample}(v, \boldsymbol{S})$ produces a sparse approximation of $\textsc{clique}(v, \boldsymbol{S})$. Let V be the vertex set of the graph associated with $\boldsymbol{S}$ and E the edge set. We define $\boldsymbol{b}_{i,j} \in \mathbb{R}^V$ to be the vector with

$$\boldsymbol{b}_{i,j}(i) = 1 \text{ and } \boldsymbol{b}_{i,j}(j) = -1 \text{ and } \boldsymbol{b}_{i,j}(k) = 0 \text{ for } k \neq i, j.$$

Given weights $\boldsymbol{w} \in \mathbb{R}^E$ and a vertex $v \in V$, we let

$$\boldsymbol{w}_v = \sum_{(u,v)\in E} \boldsymbol{w}(u, v).$$

Algorithm 2: $\textsc{CliqueSample}(v, \boldsymbol{S})$

Input: Graph Laplacian $\boldsymbol{S} \in \mathbb{R}^{V\times V}$, of a graph with edge weights $\boldsymbol{w}$, and vertex $v \in V$
Output: $\boldsymbol{Y}_v \in \mathbb{R}^{V\times V}$ sparse approximation of $\textsc{clique}(v, \boldsymbol{S})$
$\boldsymbol{Y}_v \leftarrow \boldsymbol{0}_{n\times n}$;
foreach *Multiedge* $e = (v, i)$ *from* v *to a neighbor* i **do**
  Randomly pick a neighbor j of v with probability $\frac{\boldsymbol{w}(j,v)}{\boldsymbol{w}_v}$;
  If $i \neq j$, let $\boldsymbol{Y}_v \leftarrow \boldsymbol{Y}_v + \frac{\boldsymbol{w}(i,v)\boldsymbol{w}(j,v)}{\boldsymbol{w}(i,v)+\boldsymbol{w}(j,v)} \boldsymbol{b}_{i,j}\boldsymbol{b}_{i,j}^\top$;
return $\boldsymbol{Y}_v$;

Remark 10.3.2. We can implement each sampling of a neighbor j in $O(1)$ time using a classical algorithm known as Walker's method (also known as the Alias method or Vose's method). This algorithm requires an additional $O(\deg_{\boldsymbol{S}}(v))$ time to initialize a data structure used for sampling. Overall, this means the total time for $O(\deg_{\boldsymbol{S}}(v))$ samples is still $O(\deg_{\boldsymbol{S}}(v))$.

Lemma 10.3.3. $\mathbb{E}[\boldsymbol{Y}_v] = \textsc{Clique}(v, \boldsymbol{S})$.

Proof. Let $\boldsymbol{C} = \textsc{Clique}(v, \boldsymbol{S})$. Observe that both $\mathbb{E}[\boldsymbol{Y}_v]$ and $\boldsymbol{C}$ are Laplacians. Thus it suffices to verify $\mathbb{E}_{\boldsymbol{Y}_v(i,j)} = \boldsymbol{C}(i, j)$ for $i \neq j$.

$$\boldsymbol{C}(i, j) = -\frac{\boldsymbol{w}(i, v)\boldsymbol{w}(j, v)}{\boldsymbol{w}_v},$$

$$\mathop{\mathbb{E}}_{\boldsymbol{Y}_v(i,j)} = -\frac{\boldsymbol{w}(i, v)\boldsymbol{w}(j, v)}{\boldsymbol{w}(i, v) + \boldsymbol{w}(j, v)}\left(\frac{\boldsymbol{w}(j, v)}{\boldsymbol{w}_v} + \frac{\boldsymbol{w}(i, v)}{\boldsymbol{w}_v}\right) = -\frac{\boldsymbol{w}(i, v)\boldsymbol{w}(j, v)}{\boldsymbol{w}_v} = \boldsymbol{C}(i, j).$$

□

Remark 10.3.4. Lemma 10.3.3 shows that CliqueSample$(v, \boldsymbol{L})$ produces the original Clique$(v, \boldsymbol{L})$ in expectation.

Now, we define *Approximate Gaussian Elimination*.

Algorithm 3: Approximate Gaussian Elimination / Cholesky Decomposition

Input: Graph Laplacian $\boldsymbol{L}$
Output: Lower triangular[a] $\boldsymbol{\mathcal{L}}$ as given in Theorem 10.2.4
Let $\boldsymbol{S}_0 = \boldsymbol{L}$;
Generate a random permutation π on $[n]$;
for $i = 1$ *to* $i = n - 1$ **do**
  $\boldsymbol{l}_i = \frac{1}{\sqrt{\boldsymbol{S}_{i-1}(\pi(i),\pi(i))}} \boldsymbol{S}_{i-1}(:, \pi(i))$;
  $\boldsymbol{S}_i = \boldsymbol{S}_{i-1} - \text{Star}(\pi(i), \boldsymbol{S}_{i-1}) + \text{CliqueSample}(\pi(i), \boldsymbol{S}_{i-1})$
$\boldsymbol{l}_n = \boldsymbol{0}_{n\times 1}$;
return $\boldsymbol{\mathcal{L}} = \begin{bmatrix} \boldsymbol{l}_1 \cdots \boldsymbol{l}_n \end{bmatrix}$ *and* π;

[a] $\boldsymbol{\mathcal{L}}$ is not actually lower triangular. However, if we let $\boldsymbol{P}_\pi$ be the permutation matrix corresponding to π, then $\boldsymbol{P}_\pi \boldsymbol{\mathcal{L}}$ is lower triangular. Knowing the ordering that achieves this is enough to let us implement forward and backward substitution for solving linear equations in $\boldsymbol{\mathcal{L}}$ and $\boldsymbol{\mathcal{L}}^\top$.

Note that if we replace CliqueSample$(\pi(i), \boldsymbol{S}_{i-1})$ by Clique$(\pi(i), \boldsymbol{S}_{i-1})$ at each step, then we can recover Gaussian Elimination, but with a random elimination order.

10.4 Analyzing Approximate Gaussian Elimination

In this Section, we're going to analyze Approximate Gaussian Elimination, and see why it works.

Ultimately, the main challenge in proving Theorem 10.2.4 will be to prove for the output $\boldsymbol{\mathcal{L}}$ of Algorithm 3 that with high probability

$$0.5\boldsymbol{L} \preceq \boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{L}}^\top \preceq 1.5\boldsymbol{L}. \tag{10.1}$$

We can reduce this to proving that with high probability

$$\left\| \boldsymbol{L}^{+/2}(\boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{L}}^\top - \boldsymbol{L})\boldsymbol{L}^{+/2} \right\| \leq 0.5 \tag{10.2}$$

Ultimately, the proof is going to have a lot in common with our proof of Matrix Bernstein in Chapter 9. Overall, the lesson there was that when we have a sum of independent, zero-mean random matrices, we can show that the sum is likely to have small spectral norm if the spectral norm of each random matrix is small, and the matrix-valued variance is also small.

Thus, to replicate the proof, we need control over

1. The *sample norms*.

2. The *sample variance*.

But, there is seemlingly another major obstacle: We are trying to analyze a process where the samples are far from independent. Each time we sample edges, we add new edges to the remaining graph, which we will the later sample again. This creates a lot of dependencies between the samples, which we have to handle.

However, it turns out that independence is more than what is needed to prove concentration. Instead, it suffices to have a sequence of random variables such that each is mean-zero in expectation, conditional on the previous ones. This is called a martingale difference sequence. We'll now learn about those.

10.4.1 Normalization, a.k.a. Isotropic Position

Since our analysis requires frequently measuring matrices after right and left-multiplication by $\boldsymbol{L}^{+/2}$, we reintroduce the "normalizing map" $\Phi : \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$ defined by

$$\Phi(\boldsymbol{A}) = \boldsymbol{L}^{+/2}\boldsymbol{A}\boldsymbol{L}^{+/2}.$$

We previously saw this in Chapter 9.

10.4.2 Martingales

A scalar martingale is a sequence of random variables $Z_0, \ldots, Z_k$, such that

$$\mathbb{E}\left[Z_i \mid Z_0, \ldots, Z_{i-1}\right] = Z_{i-1}. \tag{10.3}$$

That is, conditional on the outcome of all the previous random variables, the expectation of Z_i equals Z_{i-1}. If we unravel the sequence of conditional expectations, we get that *without conditioning* $\mathbb{E}\left[Z_k\right] = \mathbb{E}\left[Z_0\right]$.

Typically, we use martingales to show a statement along like "Z_k is concentrated around $\mathbb{E}\left[Z_k\right]$".

We can also think of a martingale in terms of the sequence of changes in the Z_i variables. Let $X_i = Z_i - Z_{i-1}$. The sequence of X_is is called a martingale difference sequence. We can now state the martingale condition as

$$\mathbb{E}\left[X_i \mid Z_0, \ldots, Z_{i-1}\right] = 0.$$

And because Z_0 and $X_1, \ldots, X_{i-1}$ completely determine $Z_1, \ldots, Z_{i-1}$, we could also write the martingale condition equivalently as

$$\mathbb{E}\left[X_i \mid Z_0, X_1, \ldots, X_{i-1}\right] = 0.$$

Crucially, we can write

$$Z_k = Z_0 + \sum_{i=1}^{k} Z_i - Z_{i-1} = Z_0 + \sum_{i=1}^{k} X_i$$

and when we are trying to prove concentration, the martingale difference property of the X_i's is often "as good as" independence, meaning that $\sum_{i=1}^{k} X_i$ concentrates similarly to a sum of independent random variables.

Matrix-valued martingales. We can also define matrix-valued martingales. In this case, we replace the martingalue condition of Equation (10.3), with the condition that the whole matrix stays the same in expectation. For example, we could have a sequence of random matrices $\boldsymbol{Z}_0, \ldots, \boldsymbol{Z}_k \in \mathbb{R}^{n \times n}$, such that

$$\mathbb{E}\left[\boldsymbol{Z}_i \mid \boldsymbol{Z}_0, \ldots, \boldsymbol{Z}_{i-1}\right] = \boldsymbol{Z}_{i-1}. \tag{10.4}$$

Lemma 10.4.1. *Let $\boldsymbol{L}_i = \boldsymbol{S}_i + \sum_{j=1}^{i} \boldsymbol{l}_j \boldsymbol{l}_j^\top$ for $i = 1, ..., n$ and $\boldsymbol{L}_0 = \boldsymbol{S}_0 = \boldsymbol{L}$. Then*

$$\mathbb{E}\left[\boldsymbol{L}_i | \textit{all random variables before } \textsc{CliqueSample}(\pi(i), \boldsymbol{S}_{i-1})\right] = \boldsymbol{L}_{i-1}.$$

Proof. Let's only consider $i = 1$ here as other cases are similar.

$$\boldsymbol{L}_0 = \boldsymbol{L} = \boldsymbol{l}_1 \boldsymbol{l}_1^\top + \textsc{Clique}(v, \boldsymbol{L}) + \boldsymbol{L}_{-1}$$

$$\begin{aligned}
\boldsymbol{L}_1 &= \boldsymbol{l}_1 \boldsymbol{l}_1^\top + \textsc{CliqueSample}(v, \boldsymbol{L}) + \boldsymbol{L}_{-1} \\
\mathbb{E}\left[\boldsymbol{L}_1 | \pi(1)\right] &= \boldsymbol{l}_1 \boldsymbol{l}_1^\top + \mathbb{E}\left[\textsc{CliqueSample}(v, \boldsymbol{L}) \,|\pi(1)\right] + \boldsymbol{L}_{-1} \\
&= \boldsymbol{l}_1 \boldsymbol{l}_1^\top + \textsc{Clique}(v, \boldsymbol{L}) + \boldsymbol{L}_{-1} \\
&= \boldsymbol{L}_0
\end{aligned}$$

where we used Lemma 10.3.3 to get $\mathbb{E}\left[\textsc{CliqueSample}(v, \boldsymbol{L}) \,|\pi(1)\right] = \textsc{Clique}(v, \boldsymbol{L})$. □

Remark 10.4.2. $\sum_{j=1}^{i} \boldsymbol{l}_j \boldsymbol{l}_j^\top$ can be treated as what has already been eliminated by (Approximate) Gaussian Elimination, while $\boldsymbol{S}_i$ is what still left or going to be eliminated. In Approximate Gaussian Elimination, $\boldsymbol{L}_n = \sum_{i=1}^{n} \boldsymbol{l}_i \boldsymbol{l}_i^\top$ and our goal is to show that $\boldsymbol{L}_n \approx_K \boldsymbol{L}$. Note that $\boldsymbol{L}_i$ is always equal to the original Laplacian $\boldsymbol{L}$ for all i in Gaussian Elimination. Lemma 10.4.1 demonstrates that $\boldsymbol{L}_0, \boldsymbol{L}_1, ..., \boldsymbol{L}_n$ forms a matrix martingale.

Ultimately, our plan is to use this matrix martingale structure to show that "$\boldsymbol{L}_n$ is concentrated around $\boldsymbol{L}$" in some appropriate sense. More precisely, the spectral approximation we would like to show can be established by showing that "$\Phi(\boldsymbol{L}_n)$ is concentrated around $\Phi(\boldsymbol{L})$"

10.4.3 Martingale Difference Sequence as Edge-Samples

We start by taking a slightly different view of the observations we used to prove Lemma 10.4.1. Recall that $\boldsymbol{L}_i = \boldsymbol{S}_i + \sum_{j=1}^{i} \boldsymbol{l}_j \boldsymbol{l}_j^\top$, and $\boldsymbol{L}_{i-1} = \boldsymbol{S}_{i-1} + \sum_{j=1}^{i-1} \boldsymbol{l}_j \boldsymbol{l}_j^\top$ and

$$\boldsymbol{S}_i = \boldsymbol{S}_{i-1} - \textsc{Star}(\pi(i), \boldsymbol{S}_{i-1}) + \textsc{CliqueSample}(\pi(i), \boldsymbol{S}_{i-1})\,.$$

Putting these together, we get

$$\begin{aligned}\boldsymbol{L}_i - \boldsymbol{L}_{i-1} &= \boldsymbol{l}_i \boldsymbol{l}_i^\top + \textsc{CliqueSample}(\pi(i), \boldsymbol{S}_{i-1}) - \textsc{Star}(\pi(i), \boldsymbol{S}_{i-1}) \\ &= \textsc{CliqueSample}(\pi(i), \boldsymbol{S}_{i-1}) - \textsc{Clique}(\pi(i), \boldsymbol{S}_{i-1}) \qquad (10.5) \\ &= \textsc{CliqueSample}(\pi(i), \boldsymbol{S}_{i-1}) - \mathbb{E}\left[\textsc{CliqueSample}(\pi(i), \boldsymbol{S}_{i-1}) \mid \text{preceding samples}\right] \\ &\qquad\qquad \text{by Lemma 10.3.3.}\end{aligned}$$

In particular, recall that by Lemma 10.3.3, conditional on the randomness before the call to $\textsc{CliqueSample}(\pi(i), \boldsymbol{S}_{i-1})$, we have

$$\mathbb{E}\left[\textsc{CliqueSample}(\pi(i), \boldsymbol{S}_{i-1}) \mid \text{preceding samples}\right] = \textsc{Clique}(\pi(i), \boldsymbol{S}_{i-1})$$

Adopting the notation of Lemma 10.3.3 we write

$$\boldsymbol{Y}_{\pi(i)} = \textsc{CliqueSample}(\pi(i), \boldsymbol{S}_{i-1})$$

and we further introduce notation each multi-edge sample for $e \in \textsc{Star}(\pi(i), \boldsymbol{S}_{i-1})$, as $\boldsymbol{Y}_{\pi(i),e}$, denoting the random edge Laplacian sampled when the algorithm is processing multi-edge e. Thus, conditional on preceding samples, we have

$$\boldsymbol{Y}_{\pi(i)} = \sum_{e \in \textsc{Star}(\pi(i), \boldsymbol{S}_{i-1})} \boldsymbol{Y}_{\pi(i),e} \qquad (10.6)$$

Note that even the number of multi-edges in $\textsc{Star}(\pi(i), \boldsymbol{S}_{i-1})$ depends on the preceding samples. We also want to associate zero-mean variables with each edge. Conditional on preceding samples, we also define

$$\boldsymbol{X}_{i,e} = \Phi\left(\boldsymbol{Y}_{\pi(i),e} - \mathbb{E}\left[\boldsymbol{Y}_{\pi(i),e}\right]\right) \text{ and } \boldsymbol{X}_i = \sum_{e \in \textsc{Star}(\pi(i), \boldsymbol{S}_{i-1})} \boldsymbol{X}_{i,e}$$

and combining this with Equations (10.5) and (10.6)

$$\boldsymbol{X}_i = \Phi(\boldsymbol{Y}_{\pi(i)} - \mathbb{E}\left[\boldsymbol{Y}_{\pi(i)}\right]) = \Phi(\boldsymbol{L}_i - \boldsymbol{L}_{i-1})$$

Altogether, we can write

$$\Phi\left(\boldsymbol{L}_n - \boldsymbol{L}\right) = \sum_{i=1}^{n} \Phi(\boldsymbol{L}_i - \boldsymbol{L}_{i-1}) = \sum_{i=1}^{n} \boldsymbol{X}_i = \sum_{i=1}^{n} \sum_{e \in \textsc{Star}(\pi(i), \boldsymbol{S}_{i-1})} \boldsymbol{X}_{i,e}$$

Note that the $\boldsymbol{X}_{i,e}$ variables form a martingale difference sequence, because the linearity of Φ ensures they are zero-mean conditional on preceding randomness.

10.4.4 Stopped Martingales

Unfortunately, directly analyzing the concentration properties of the $\boldsymbol{L}_i$ martingale that we just introduced turns out to be difficult. The reason is that we're trying to prove some very delicate multiplicative error guarantees. And, if we analyze $\boldsymbol{L}_i$, we find that the multiplicative error is not easy to control, *after it's already gotten big*. But that's not really what we care about anyway: We want to say it never gets big in the first place, with high probability. So we need to introduce another martingale, that lets us ignore the bad case when the error has already gotten too big. At the same time, we also need to make sure that statements about our new martingale can help us prove guarantees about $\boldsymbol{L}_i$. Fortunately, we can achieve both at once. The technique we use is related to the much broader topic of martingale *stopping times*, which we only scratch the surface of here. We're also going to be quite informal about it, in the interest of brevity. Lecture notes by Tropp [Tro19] give a more formal introduction for those who are interested.

We define the stopped martingale sequence $\tilde{\boldsymbol{L}}_i$ by

$$\tilde{\boldsymbol{L}}_i = \begin{cases} \boldsymbol{L}_i & \text{if for all } j < i \text{ we have } \boldsymbol{L}_i \preceq 1.5\boldsymbol{L} \\ \boldsymbol{L}_{j^*} & \text{for } j^* \text{ being the least } j \text{ such that } \boldsymbol{L}_j \not\preceq 1.5\boldsymbol{L} \end{cases} \tag{10.7}$$

Figure 10.2 shows the $\tilde{\boldsymbol{L}}_i$ martingale getting stuck at the first time $\boldsymbol{L}_{j^*} \not\preceq 1.5\boldsymbol{L}$.

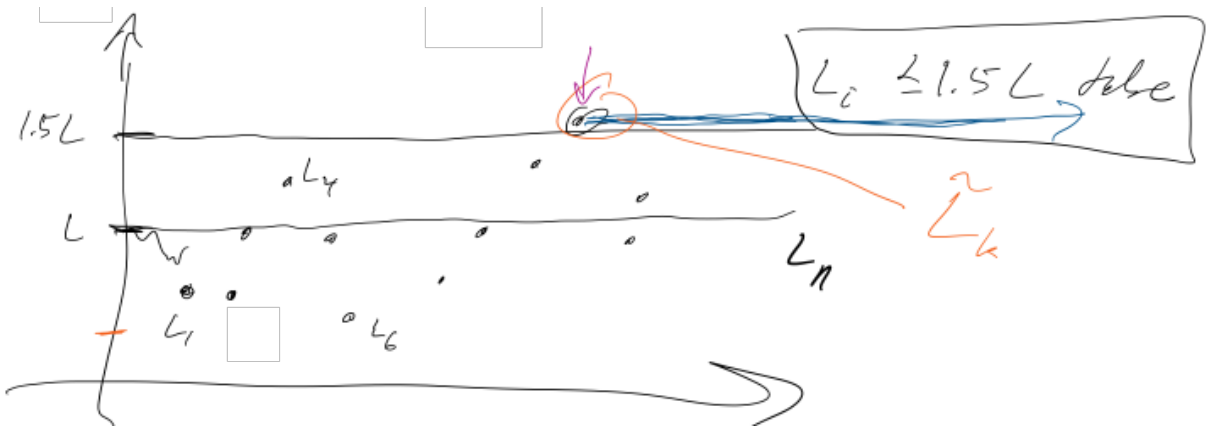


Figure 10.2: Gaussian Elimination : $\textsc{Clique}(1, \boldsymbol{L}) = \textsc{Star}(1, \boldsymbol{L}) - \frac{1}{\boldsymbol{L}(1,1)}\boldsymbol{L}(:,1)\boldsymbol{L}(:,1)^\top$.

We state the following without proof:

Claim 10.4.3.

1. *The sequence* $\left\{\tilde{\boldsymbol{L}}_i\right\}$ *for* $i = 0, \ldots, n$ *is a martingale.*
2. $\left\|\boldsymbol{L}^{+/2}(\tilde{\boldsymbol{L}}_i - \boldsymbol{L})\boldsymbol{L}^{+/2}\right\| \leq 0.5$ *implies* $\left\|\boldsymbol{L}^{+/2}(\boldsymbol{L}_i - \boldsymbol{L})\boldsymbol{L}^{+/2}\right\| \leq 0.5$

The martingale property also implies that the unconditional expectation satisfies $\mathbb{E}\left[\tilde{\boldsymbol{L}}_n\right] = \boldsymbol{L}$. The proof of the claim is easy to sketch: For Part 1, each difference is zero-mean if the condition has not been violated, and is identically zero (and hence zero-mean) if it has been violated. For Part 2, if the martingale $\left\{\tilde{\boldsymbol{L}}_i\right\}$ has stopped, then $\left\|\boldsymbol{L}^{+/2}(\tilde{\boldsymbol{L}}_i - \boldsymbol{L})\boldsymbol{L}^{+/2}\right\| \leq 0.5$ is false, and the implication is vacuosly true. If, on the other hand, the martingale has not stopped, the quantities are equal, because $\tilde{\boldsymbol{L}}_i = \boldsymbol{L}_i$, and again it's easy to see the implication holds.

Thus, ultimately, our strategy is goin to be to show that $\left\|\boldsymbol{L}^{+/2}(\tilde{\boldsymbol{L}}_i - \boldsymbol{L})\boldsymbol{L}^{+/2}\right\| \leq 0.5$ with high probability. Expressed using the normalizing map $\Phi(\cdot)$, our goal is to show that with high probability

$$\left\|\Phi(\tilde{\boldsymbol{L}}_n - \boldsymbol{L})\right\| \leq 0.5.$$

Stopped martingale difference sequence. In order to prove the spectral norm bound, we want to express the $\left\{\tilde{\boldsymbol{L}}_i\right\}$ martingale in terms of a sequence of martingale differences. To this end, we define $\tilde{\boldsymbol{X}}_i = \Phi(\tilde{\boldsymbol{L}}_i - \tilde{\boldsymbol{L}}_{i-1})$. This ensures that

$$\tilde{\boldsymbol{X}}_i = \begin{cases} \boldsymbol{X}_i & \text{if for all } j < i \text{ we have } \boldsymbol{L}_i \preceq 1.5\boldsymbol{L} \\ \boldsymbol{0} & \text{otherwise} \end{cases} \tag{10.8}$$

Whenever the modified martingale $\tilde{\boldsymbol{X}}_i$ has not yet stopped, we also introduce individual modified edge samples $\tilde{\boldsymbol{X}}_{i,e} = \boldsymbol{X}_{i,e}$. If the martingale *has* stopped, i.e. $\tilde{\boldsymbol{X}}_i = \boldsymbol{0}$, then we can take these edge samples $\tilde{\boldsymbol{X}}_{i,e}$ to be zero. We can now write

$$\Phi\left(\tilde{\boldsymbol{L}}_n - \boldsymbol{L}\right) = \sum_{i=1}^{n} \Phi(\tilde{\boldsymbol{L}}_i - \tilde{\boldsymbol{L}}_{i-1}) = \sum_{i=1}^{n} \tilde{\boldsymbol{X}}_i = \sum_{i=1}^{n} \sum_{e \in \textsc{Star}(\pi(i), \boldsymbol{S}_{i-1})} \tilde{\boldsymbol{X}}_{i,e}.$$

Thus, we can see that Equation (10.2) is implied by

$$\left\|\sum_{i=1}^{n} \tilde{\boldsymbol{X}}_i\right\| \leq 0.5. \tag{10.9}$$

10.4.5 Sample Norm Control

In this Subsection, we're going to see that the norms of each multi-edge sample is controlled throughout the algorithm.

Lemma 10.4.4. *Given two Laplacians $\boldsymbol{L}$ and $\boldsymbol{S}$ on the same vertex set.*[1] *If each multiedge e of* $\textsc{Star}(v, \boldsymbol{S})$ *has bounded norm in the following sense,*

$$\left\|\boldsymbol{L}^{+/2}\boldsymbol{w}_{\boldsymbol{S}}(e)\boldsymbol{b}_e\boldsymbol{b}_e^\top\boldsymbol{L}^{+/2}\right\| \leq R,$$

[1] $\boldsymbol{L}$ can be regarded as the original Laplacian we care about, while $\boldsymbol{S}$ can be regarded as some intermediate Laplacian appearing during Approximate Gaussian Elimination.

then each possible sampled multiedge e' of CliqueSample$(v, \boldsymbol{S})$ *also satisfies*

$$\left\| \boldsymbol{L}^{+/2} \boldsymbol{w}_{\text{new}}(e') \boldsymbol{b}_{e'} \boldsymbol{b}_{e'}^\top \boldsymbol{L}^{+/2} \right\| \leq R.$$

Proof. Let $\boldsymbol{w} = \boldsymbol{w}_{\boldsymbol{S}}$ for simplicity. Consider a sampled edge between i and j with weight $\boldsymbol{w}_{\text{new}}(i,j) = \boldsymbol{w}(i,v)\boldsymbol{w}(j,v)/(\boldsymbol{w}(i,v) + \boldsymbol{w}(j,v))$.

$$\begin{aligned}
\left\| \boldsymbol{L}^{+/2} \boldsymbol{w}_{\text{new}}(i,j) \boldsymbol{b}_{ij} \boldsymbol{b}_{ij}^\top \boldsymbol{L}^{+/2} \right\| &= \boldsymbol{w}_{\text{new}}(i,j) \left\| \boldsymbol{L}^{+/2} \boldsymbol{b}_{ij} \boldsymbol{b}_{ij}^\top \boldsymbol{L}^{+/2} \right\| \\
&= \boldsymbol{w}_{\text{new}}(i,j) \left\| \boldsymbol{L}^{+/2} \boldsymbol{b}_{ij} \right\|^2 \\
&\leq \boldsymbol{w}_{\text{new}}(i,j) \left(\left\| \boldsymbol{L}^{+/2} \boldsymbol{b}_{iv} \right\|^2 + \left\| \boldsymbol{L}^{+/2} \boldsymbol{b}_{jv} \right\|^2 \right) \\
&= \frac{\boldsymbol{w}(j,v)}{\boldsymbol{w}(i,v) + \boldsymbol{w}(j,v)} \left\| \boldsymbol{L}^{+/2} \boldsymbol{w}(i,v) \boldsymbol{b}_{iv} \boldsymbol{b}_{iv}^\top \boldsymbol{L}^{+/2} \right\| + \\
&\quad \frac{\boldsymbol{w}(i,v)}{\boldsymbol{w}(i,v) + \boldsymbol{w}(j,v)} \left\| \boldsymbol{L}^{+/2} \boldsymbol{w}(j,v) \boldsymbol{b}_{jv} \boldsymbol{b}_{jv}^\top \boldsymbol{L}^{+/2} \right\| \\
&\leq \frac{\boldsymbol{w}(j,v)}{\boldsymbol{w}(i,v) + \boldsymbol{w}(j,v)} R + \frac{\boldsymbol{w}(i,v)}{\boldsymbol{w}(i,v) + \boldsymbol{w}(j,v)} R \\
&= R
\end{aligned}$$

The first inequality uses the triangle inequality of effective resistance in $\boldsymbol{L}$, in that effective resistance is a distance as we proved in Chapter 7. The second inequality just uses the conditions of this lemma. □

Remark 10.4.5. Lemma 10.4.4 only requires that each single multiedge has small norm instead of that the sum of all edges between a pair of vertices have small norm. And this lemma tells us, after sampling, each multiedge in the new graph still satisfies the bounded norm condition.

From the Lemma, we can conclude that each edge sample $\boldsymbol{Y}_{\pi(i),e}$ satisfies $\left\| \Phi(\boldsymbol{Y}_{\pi(i),e}) \right\| \leq R$ provided the assumptions of the Lemma hold. Let's record this observation as a Lemma.

Lemma 10.4.6. *If for all $e \in$ Star$(v, \boldsymbol{S}_i)$,*

$$\left\| \Phi(\boldsymbol{w}_{\boldsymbol{S}_i}(e) \boldsymbol{b}_e \boldsymbol{b}_e^\top) \right\| \leq R.$$

then all $e \in$ Star$(\pi(i), \boldsymbol{S}_i)$,

$$\left\| \Phi(\boldsymbol{Y}_{\pi(i),e}) \right\| \leq R.$$

Preprocessing by multi-edge splitting. In the original graph of Laplacian $\boldsymbol{L}$ of graph $G = (V, E, \boldsymbol{w})$, we have for each edge $\hat{e}$ that

$$\boldsymbol{w}(\hat{e}) \boldsymbol{b}_{\hat{e}} \boldsymbol{b}_{\hat{e}}^\top \preceq \sum_e \boldsymbol{w}(e) \boldsymbol{b}_e \boldsymbol{b}_e^\top = \boldsymbol{L}$$

This also implies that

$$\left\| \boldsymbol{L}^{+/2} \boldsymbol{w}(\hat{e}) \boldsymbol{b}_{\hat{e}} \boldsymbol{b}_{\hat{e}}^\top \boldsymbol{L}^{+/2} \right\| \leq 1.$$

Now, that means that if we split every original edge e of the graph into K multi-edges $e_1, \ldots e_K$, with a fraction $1/K$ of the weight, we get a new graph $G' = (V, E', \boldsymbol{w}')$ such that

Claim 10.4.7.

1. *G' and G have the same graph Laplacian.*
2. *$|E'| = K\,|E|$*
3. *For every multi-edge in G'*

$$\left\| \boldsymbol{L}^{+/2} \boldsymbol{w}'(e) \boldsymbol{b}_e \boldsymbol{b}_e^\top \boldsymbol{L}^{+/2} \right\| \leq 1/K.$$

Before we run Approximate Gaussian Elimination, we are going to do this multi-edge splitting to ensure we have control over multi-edge sample norms. Combined with Lemma 10.4.4 immediately establishes the next lemma, because we start off with all multi-edges having bounded norm and only produce multi-edges with bounded norm.

Lemma 10.4.8. *When Algorithm 3 is run on the (multi-edge) Laplacian of G', arising from splitting edges of G into K multi-edges, the every edge sample $\boldsymbol{Y}_{\pi(i),e}$ satisfies*

$$\left\| \Phi(\boldsymbol{Y}_{\pi(i),e}) \right\| \leq 1/K.$$

As we will see later $K = 200 \log^2 n$ suffices.

10.4.6 Random Matrix Concentration from Trace Exponentials

Let us recall how matrix-valued variances come into the picture when proving concentration following the strategy from Matrix Bernstein in Chapter 9.

For some matrix-valued random variable $\boldsymbol{X} \in S^n$, we'd like to show $\Pr[\|\boldsymbol{X}\| \leq 0.5]$. Using Markov's inequality, and some observations about matrix exponentials and traces, we saw that for all $\theta > 0$,

$$\Pr[\|\boldsymbol{X}\| \geq 0.5] \leq \exp(-0.5\theta) \left(\mathbb{E}\left[\mathrm{Tr}\left(\exp\left(\theta \boldsymbol{X}\right)\right)\right] + \mathbb{E}\left[\mathrm{Tr}\left(\exp\left(-\theta \boldsymbol{X}\right)\right)\right] \right). \tag{10.10}$$

We then want to bound $\mathbb{E}\left[\mathrm{Tr}\left(\exp\left(\theta \boldsymbol{X}\right)\right)\right]$ using Lieb's theorem. We can handle $\mathbb{E}\left[\mathrm{Tr}\left(\exp\left(-\theta \boldsymbol{X}\right)\right)\right]$ similarly.

Theorem 10.4.9 (Lieb)**.** *Let $f : S^n_{++} \to \mathbb{R}$ be a matrix function given by*

$$f(\boldsymbol{A}) = \mathrm{Tr}\left(\exp\left(\boldsymbol{H} + \log(\boldsymbol{A})\right)\right)$$

for some $\boldsymbol{H} \in S^n$. Then $-f$ is convex (i.e. f is concave).

As observed by Tropp, this is useful for proving matrix concentration statements. Combined with Jensen's inequality, it gives that for a random matrix $\boldsymbol{X} \in S^n$ and a fixed $\boldsymbol{H} \in S^n$

$$\mathbb{E}\left[\operatorname{Tr}\left(\exp\left(\boldsymbol{H}+\boldsymbol{X}\right)\right)\right] \leq \operatorname{Tr}\left(\exp\left(\boldsymbol{H}+\log(\mathbb{E}\left[\exp(\boldsymbol{X})\right])\right)\right).$$

The next crucial step was to show that it suffices to obtain an upper bound on the matrix $\mathbb{E}\left[\exp(\boldsymbol{X})\right]$ w.r.t the Loewner order. Using the following three lemmas, this conclusion is an immediate corollary.

Lemma 10.4.10. *If $\boldsymbol{A} \preceq \boldsymbol{B}$, then $\operatorname{Tr}\left(\exp(\boldsymbol{A})\right) \leq \operatorname{Tr}\left(\exp(\boldsymbol{B})\right)$.*

Lemma 10.4.11. *If $0 \prec \boldsymbol{A} \preceq \boldsymbol{B}$, then $\log(\boldsymbol{A}) \preceq \log(\boldsymbol{B})$.*

Lemma 10.4.12. *$\log(\boldsymbol{I}+\boldsymbol{A}) \preceq \boldsymbol{A}$ for $\boldsymbol{A} \succ -\boldsymbol{I}$.*

Corollary 10.4.13. *For a random matrix $\boldsymbol{X} \in S^n$ and a fixed $\boldsymbol{H} \in S^n$, if $\mathbb{E}\left[\exp(\boldsymbol{X})\right] \preceq \boldsymbol{I}+\boldsymbol{U}$ where $\boldsymbol{U} \succ -\boldsymbol{I}$, then*

$$\mathbb{E}\left[\operatorname{Tr}\left(\exp\left(\boldsymbol{H}+\boldsymbol{X}\right)\right)\right] \leq \operatorname{Tr}\left(\exp\left(\boldsymbol{H}+\boldsymbol{U}\right)\right).$$

10.4.7 Mean-Exponential Bounds from Variance Bounds

To use Corollary 10.4.13, we need to construct useful upper bounds on $\mathbb{E}\left[\exp(\boldsymbol{X})\right]$. This can be done, starting from the following lemma.

Lemma 10.4.14. *$\exp(\boldsymbol{A}) \preceq \boldsymbol{I}+\boldsymbol{A}+\boldsymbol{A}^2$ for $\|\boldsymbol{A}\| \leq 1$.*

If $\boldsymbol{X}$ is zero-mean and $\|\boldsymbol{X}\| \leq 1$, this means that $\mathbb{E}\left[\exp(\boldsymbol{X})\right] \preceq \boldsymbol{I}+\mathbb{E}\left[\boldsymbol{X}^2\right]$, which is how we end up wanting to bound the matrix-valued variance $\mathbb{E}\left[\boldsymbol{X}^2\right]$. In the rest of this Subsection, we're going to see the matrix-valued variance of the stopped martingale is bounded throughout the algorithm.

Firstly, we note that for a single edge sample $\tilde{\boldsymbol{X}}_{i,e}$, by Lemma 10.4.8, we have that

$$\left\|\tilde{\boldsymbol{X}}_{i,e}\right\| \leq \left\|\Phi\left(\boldsymbol{Y}_{\pi(i),e}-\mathbb{E}\left[\boldsymbol{Y}_{\pi(i),e}\right]\right)\right\| \leq 1/K,$$

using that $\|\boldsymbol{A}-\boldsymbol{B}\| \leq \max(\|\boldsymbol{A}\|,\|\boldsymbol{B}\|)$, for $\boldsymbol{A},\boldsymbol{B} \succeq \boldsymbol{0}$, and $\|\mathbb{E}\left[\boldsymbol{A}\right]\| \leq \mathbb{E}\left[\|\boldsymbol{A}\|\right]$ by Jensen's inequality.

Thus, if $0 < \theta \leq K$, we have that

$$\begin{aligned}\mathbb{E}\left[\exp(\theta\tilde{\boldsymbol{X}}_{i,e}) \mid \text{preceding samples}\right] &\preceq \boldsymbol{I}+\mathbb{E}\left[(\theta\tilde{\boldsymbol{X}}_{i,e})^2 \mid \text{preceding samples}\right] \\ &\preceq \boldsymbol{I}+\frac{1}{K}\theta^2\cdot\mathbb{E}\left[\Phi(\boldsymbol{Y}_{\pi(i),e}) \mid \text{preceding samples}\right]\end{aligned} \tag{10.11}$$

10.4.8 The Overall Mean-Trace-Exponential Bound

We will use $\mathbb{E}_{(<i)}$ to denote expectation over variables preceding the ith elimination step. We are going to refrain from explicitly writing out conditioning in our expectations, but any *inner* expectation that appears inside another *outer* expectation should be taken as conditional on the outer expectation. We are going to use d_i to denote the multi-edge degree of vertex $\pi(i)$ in $\boldsymbol{S}_{i-1}$. This is exactly the number of edge samples in the ith elimination. Note that there is no elimination at step n (the algorithm is already finished). As a notational convenience, let's write $\hat{n} = n - 1$. With all that in mind, we bound the mean-trace-exponential for some parameter $0 < \theta \leq 0.5/\sqrt{K}$

$$\mathbb{E}\operatorname{Tr}\left(\exp(\theta\sum_{i=1}^{\hat{n}}\tilde{\boldsymbol{X}}_i)\right) \tag{10.12}$$

$$= \mathop{\mathbb{E}}_{(<\hat{n})}\mathop{\mathbb{E}}_{\pi(\hat{n})}\mathop{\mathbb{E}}_{\tilde{\boldsymbol{X}}_{\hat{n},1}}\cdots\mathop{\mathbb{E}}_{\tilde{\boldsymbol{X}}_{\hat{n},d_{\hat{n}}-1}}\mathop{\mathbb{E}}_{\tilde{\boldsymbol{X}}_{\hat{n},d_{\hat{n}}}}\operatorname{Tr}\exp\left(\underbrace{\sum_{i=1}^{\hat{n}-1}\theta\tilde{\boldsymbol{X}}_i + \sum_{e=1}^{d_{\hat{n}}-1}\theta\tilde{\boldsymbol{X}}_{\hat{n},e}}_{\boldsymbol{H}} + \theta\tilde{\boldsymbol{X}}_{\hat{n},d_{\hat{n}}}\right)$$

$\tilde{\boldsymbol{X}}_{\hat{n},1}\ldots,\tilde{\boldsymbol{X}}_{\hat{n},d_{\hat{n}}}$ are independent conditional on $(<\hat{n}),\pi(\hat{n})$

$$\leq \mathop{\mathbb{E}}_{(<\hat{n})}\mathop{\mathbb{E}}_{\pi(\hat{n})}\mathop{\mathbb{E}}_{\tilde{\boldsymbol{X}}_{\hat{n},1}}\cdots\mathop{\mathbb{E}}_{\tilde{\boldsymbol{X}}_{\hat{n},d_{\hat{n}}-1}}\operatorname{Tr}\exp\left(\sum_{i=1}^{\hat{n}-1}\theta\tilde{\boldsymbol{X}}_i + \sum_{e=1}^{d_{\hat{n}}-1}\theta\tilde{\boldsymbol{X}}_{\hat{n},e} + \frac{1}{K}\theta^2\cdot\mathop{\mathbb{E}}_{\tilde{\boldsymbol{X}}_{\hat{n},d_{\hat{n}}}}\Phi(\boldsymbol{Y}_{\pi(\hat{n}),d_{\hat{n}}})\right)$$

By Equation (10.11) and Corollary 10.4.13 .

$\vdots$ Repeat for each multi-edge sample $\tilde{\boldsymbol{X}}_{\hat{n},1}\ldots,\tilde{\boldsymbol{X}}_{\hat{n},d_{\hat{n}}-1}$

$$\leq \mathop{\mathbb{E}}_{(<\hat{n})}\mathop{\mathbb{E}}_{\pi(\hat{n})}\operatorname{Tr}\exp\left(\sum_{i=1}^{\hat{n}-1}\theta\tilde{\boldsymbol{X}}_i + \sum_{e=1}^{d_{\hat{n}}}\frac{1}{K}\theta^2\cdot\mathop{\mathbb{E}}_{\tilde{\boldsymbol{X}}_{\hat{n},e}}\Phi(\boldsymbol{Y}_{\pi(\hat{n}),e})\right)$$

$$= \mathop{\mathbb{E}}_{(<\hat{n})}\mathop{\mathbb{E}}_{\pi(\hat{n})}\operatorname{Tr}\exp\left(\sum_{i=1}^{\hat{n}-1}\theta\tilde{\boldsymbol{X}}_i + \frac{1}{K}\theta^2\Phi(\textsc{Clique}(\pi(\hat{n}),\boldsymbol{S}_{\hat{n}-1}))\right)$$

To further bound the this quantity, we now need to deal with the random choice of $\pi(\hat{n})$. We'll be able to use this to bound the trace-exponential in a very strong way. From a random matrix perspective, it's the following few steps that give the analysis it's surprising strength.

We can treat $\frac{1}{K}\theta^2\Phi(\textsc{Clique}(\pi(\hat{n}),\boldsymbol{S}_{\hat{n}-1}))$ as a random matrix. It is not zero-mean, but we can still bound the trace-exponential using Corollary 10.4.13.

We can also bound the expected matrix exponential in that case, using a simple corollary of Lemma 10.4.14.

Corollary 10.4.15. $\exp(\boldsymbol{A}) \preceq \boldsymbol{I} + (1+R)\boldsymbol{A}$ *for* $\boldsymbol{0} \preceq \boldsymbol{A}$ *with* $\|\boldsymbol{A}\| \leq R \leq 1$.

Proof. The conclusion follows after observing that for $\boldsymbol{0} \preceq \boldsymbol{A}$ with $\|\boldsymbol{A}\| \leq R$, we have $\boldsymbol{A}^2 \preceq R\boldsymbol{A}$. We can see this by considering the spectral decomposition of $\boldsymbol{A}$ and dealing with each eigenvalue separately. □

Next, we need a simple structural observation about the cliques created by elimination:

Claim 10.4.16.

$$\textsc{Clique}(\pi(i), \boldsymbol{S}_i) \preceq \textsc{Star}(\pi(i), \boldsymbol{S}_i) \preceq \boldsymbol{S}_i$$

Proof. The first inequality is immediate from $\textsc{Clique}(\pi(i), \boldsymbol{S}_i) \preceq \textsc{Clique}(\pi(i), \boldsymbol{S}_i) + \boldsymbol{l}_i \boldsymbol{l}_i^\top = \textsc{Star}(\pi(i), \boldsymbol{S}_i)$. The latter inequality $\textsc{Star}(\pi(i), \boldsymbol{S}_i) \preceq \boldsymbol{S}_i$ follows from the star being a subgraph of the whole Laplacian $\boldsymbol{S}_i$. □

Next we make use of the fact that $\tilde{\boldsymbol{X}}_i$ is from the difference sequence of the *stopped* martingale. This means we can assume

$$\boldsymbol{S}_i \preceq 1.5\boldsymbol{L},$$

since otherwise $\tilde{\boldsymbol{X}}_i = \boldsymbol{0}$ and we get an even better bound on the trace-exponential. To make this formal, in Equation (10.12), we ought to do a case analysis that also includes the case $\tilde{\boldsymbol{X}}_i = \boldsymbol{0}$ when the martingale has stopped, but we omit this.

Thus we can conclude by Claim 10.4.16 that

$$\|\Phi(\textsc{Clique}(\pi(i), \boldsymbol{S}_i))\| \leq 1.5.$$

By our assumption $0 < \theta \leq 0.5/\sqrt{K}$, we have $\left\| \frac{1}{K}\theta^2 \Phi(\textsc{Clique}(\pi(i), \boldsymbol{S}_{i-1})) \right\| \leq 1$, so that by Corollary 10.4.15,

$$\begin{aligned} \mathop{\mathbb{E}}_{\pi(i)} \exp\left(\frac{1}{K}\theta^2 \Phi(\textsc{Clique}(\pi(i), \boldsymbol{S}_{i-1})) \right) &\preceq \boldsymbol{I} + \frac{2}{K}\theta^2 \mathop{\mathbb{E}}_{\pi(i)} \Phi(\textsc{Clique}(\pi(i), \boldsymbol{S}_{i-1})) \qquad (10.13) \\ &\preceq \boldsymbol{I} + \frac{2}{K}\theta^2 \mathop{\mathbb{E}}_{\pi(i)} \Phi(\textsc{Star}(\pi(i), \boldsymbol{S}_{i-1})) \end{aligned}$$

by Claim 10.4.16.

Next we observe that, because every multi-edge appears in exactly two stars, and $\pi(i)$ is chosen uniformly at random among the $n+1-i$ vertices that $\boldsymbol{S}_{i-1}$ is supported on, we have

$$\mathop{\mathbb{E}}_{\pi(i)} \textsc{Star}(\pi(i), \boldsymbol{S}_{i-1}) = 2\frac{1}{n+1-i}\boldsymbol{S}_{i-1}.$$

And, since we assume $\boldsymbol{S}_i \preceq 1.5\boldsymbol{L}$, we further get

$$\mathop{\mathbb{E}}_{\pi(i)} \exp\left(\frac{1}{K}\theta^2 \Phi(\textsc{Clique}(\pi(i), \boldsymbol{S}_{i-1})) \right) \preceq \boldsymbol{I} + \frac{6\theta^2}{K(n+1-i)}\boldsymbol{I}.$$

We can combine this with Equation (10.12) and Corollary 10.4.13 to get

$$\begin{aligned} &\mathbb{E}\,\mathrm{Tr}\left(\exp(\theta \sum_{i=1}^{\hat{n}} \tilde{\boldsymbol{X}}_i) \right) \\ &\leq \mathop{\mathbb{E}}_{(<\hat{n})} \mathop{\mathbb{E}}_{\pi(\hat{n})} \mathrm{Tr}\exp\left(\sum_{i=1}^{\hat{n}-1} \theta\tilde{\boldsymbol{X}}_i + \frac{1}{K}\theta^2 \Phi(\textsc{Clique}(\pi(\hat{n}), \boldsymbol{S}_{\hat{n}-1})) \right) \\ &\leq \mathop{\mathbb{E}}_{(<\hat{n})} \mathrm{Tr}\exp\left(\sum_{i=1}^{\hat{n}-1} \theta\tilde{\boldsymbol{X}}_i + \frac{6\theta^2}{K(n+1-i)}\boldsymbol{I} \right) \end{aligned}$$

And by repeating this analysis for each term $\tilde{\boldsymbol{X}}_i$, we get

$$\begin{aligned}\mathbb{E}\,\mathrm{Tr}\left(\exp(\theta\sum_{i=1}^{\hat{n}}\tilde{\boldsymbol{X}}_i)\right) &\leq \mathrm{Tr}\exp\left(\sum_{i=1}^{\hat{n}}\frac{6\theta^2}{K(n+1-i)}\boldsymbol{I}\right)\\ &\leq \mathrm{Tr}\exp\left(\frac{7\theta^2\log(n)}{K}\boldsymbol{I}\right)\\ &= n\exp\left(\frac{7\theta^2\log(n)}{K}\right)\end{aligned}$$

Then, by choosing $K = 200\log^2 n$ and $\theta = 0.5\sqrt{K}$, we get

$$\exp(-0.5\theta)\,\mathbb{E}\,\mathrm{Tr}\left(\exp(\theta\sum_{i=1}^{\hat{n}}\tilde{\boldsymbol{X}}_i)\right) \leq \exp(-0.5\theta)n\exp\left(\frac{7\theta^2\log(n)}{K}\right) \leq 1/n^5.$$

$\mathbb{E}\,\mathrm{Tr}\left(\exp(-\theta\sum_{i=1}^{\hat{n}}\tilde{\boldsymbol{X}}_i)\right)$ can be bounded by an identical argument, so that Equation (10.10) gives

$$\Pr\left[\left\|\sum_{i=1}^{\hat{n}}\tilde{\boldsymbol{X}}_i\right\| \geq 0.5\right] \leq 2/n^5.$$

Thus we have established $\left\|\sum_{i=1}^{\hat{n}}\tilde{\boldsymbol{X}}_i\right\| \leq 0.5$ with high probability (Equation (10.9)), and this in turn implies Equation (10.2), and finally Equation (10.1):

$$0.5\boldsymbol{L} \preceq \boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{L}}^\top \preceq 1.5\boldsymbol{L}.$$

Now, all that's left to note is that the running time is linear in the multi-edge degree of the vertex being eliminated in each iteration (and this also bounds the number of non-zero entries being created in $\boldsymbol{\mathcal{L}}$). The total number of multi-edges left in the remaining graph stays constant at $Km = O(m\log^2 n)$. Thus the expected degree in the ith elimination is $Km/(n+i-1)$, because the remaining number of vertices is $n+i-1$. Hence the total running time and total number of non-zero entries created can both be bounded as

$$Km\sum_i 1/(n+i-1) = O(m\log^3 n).$$

We can further prove that the bound $O(m\log^3 n)$ on running time and number of non-zeros in $\boldsymbol{L}$ holds with high probability (e.g. $1-1/n^5$). To show this, we essentially need a scalar Chernoff bound, in except the degrees are in fact not independent, and so we need a scalar martingale concentration result, e.g. Azuma's Inequality. This way, we complete the proof of Theorem 10.2.4.

Part III

Combinatorial Graph Algorithms

Chapter 11

Classical Algorithms for Maximum Flow I

11.1 Maximum Flow

In this chapter, we will study the *Maximum Flow Problem* and discuss some classical algorithms for finding solutions to it.

Setup. Consider a directed graph $G = (V, E, \boldsymbol{c})$, where V denotes vertices, E denotes edges and $\boldsymbol{c} \in \mathbb{R}^E, \boldsymbol{c} \geq 0$ denotes edge capacities. In contrast to earlier chapters, the direction of each edge will be important, and not just as a book keeping tool (which is how we previously used it in undirected graphs). We consider an edge $(u, v) \in E$ to be *from* u and *to* v. Edge capacities are associated with directed edges, and we allow both edge (u, v) and (v, u) to exist, and they may have different capacities.

A *flow* is any vector $\boldsymbol{f} \in \mathbb{R}^E$.

We say that a flow is feasible when $\mathbf{0} \leq \boldsymbol{f} \leq \boldsymbol{c}$. The constraint $\mathbf{0} \leq \boldsymbol{f}$ ensures that the flow respects edge directions, while the constraint $\boldsymbol{f} \leq \boldsymbol{c}$ ensures that the flow does not exceed capacity on any edge.

We still define the edge-vertex incidence matrix $\boldsymbol{B} \in \mathbb{R}^{V \times E}$ of G by

$$\boldsymbol{B}(v, e) = \begin{cases} 1 & \text{if } e = (u, v) \\ -1 & \text{if } e = (v, u) \\ 0 & \text{o.w.} \end{cases}$$

As in the undirected case, a *demand vector* is a vector $\boldsymbol{d} \in \mathbb{R}^V$. And as in the undirected case, we can express the net flow constraint that $\boldsymbol{f}$ routes the demand $\boldsymbol{d}$ by

$$\boldsymbol{B}\boldsymbol{f} = \boldsymbol{d}.$$

We will focus on the case:

$$\boldsymbol{B}\boldsymbol{f} = F(-\boldsymbol{e}_s + \boldsymbol{e}_t) = F\boldsymbol{b}_{st}.$$

Flows that satisfy the above equation for some scalar F are called s-t flows where $s, t \in V$. The vertex s is called the source, t is called the sink and $\boldsymbol{e}_s$, $\boldsymbol{e}_t$ are indicator vectors for source and sink nodes respectively. The vector $\boldsymbol{b}_{st}$ has -1 at source and 1 at sink. The maximum flow can be expressed as a linear program as follows

$$\begin{aligned} \max_{\boldsymbol{f} \in \mathbb{R}^E, F} \quad & F \\ \text{s.t.} \quad & \boldsymbol{B}\boldsymbol{f} = F\boldsymbol{b}_{st} \\ & 0 \leq \boldsymbol{f} \leq \boldsymbol{c} \end{aligned} \tag{11.1}$$

We use $\text{val}(\boldsymbol{f})$ to denote F when $\boldsymbol{B}\boldsymbol{f} = F\boldsymbol{b}_{st}$.

11.2 Flow Decomposition

We now look at a way of simplifying flows

Definition 11.2.1. A s-t path flow is a flow $\boldsymbol{f} \geq \boldsymbol{0}$ that can be written as

$$\boldsymbol{f} = \alpha \sum_{e \in p} \boldsymbol{e}_e$$

where p is a simple path from s to t.

Definition 11.2.2. A cycle flow is a flow $\boldsymbol{f} \geq \boldsymbol{0}$ that can be written as a cycle i.e.

$$\boldsymbol{f} = \alpha \sum_{e \in c} \boldsymbol{e}_e$$

where c is a simple cycle.

Lemma 11.2.3 (The path-cycle decomposition lemma)**.** *Any s-t flow $\boldsymbol{f}$ can be decomposed into a sum of s-t path flows and cycle flows such that the sum contains at most* $\text{nnz}(\boldsymbol{f})$ *terms. Note* $\text{nnz}(\boldsymbol{f}) \leq |E|$.

Proof. We perform induction on the number of edges with non-zero flow, which we denote by $\text{nnz}(\boldsymbol{f})$. Note that by "the support of $\boldsymbol{f}$", we mean the set $\{e \in E : \boldsymbol{f}(e) \neq 0\}$.

Base case: $\boldsymbol{f} = 0$: nothing to do.

Inductive step: Try to find a path from s to t OR a cycle in the support of $\boldsymbol{f}$.
"Path" case. If there exists such a s-t path, let α be the minimum flow value along the edges of the path, i.e.

$$\alpha = \min_{(a,b)\in p} \boldsymbol{f}(a,b)$$

$$\boldsymbol{f}' = \alpha \sum_{e\in p} \boldsymbol{e}_e$$

Update the flow $\boldsymbol{f}$ by

$$\boldsymbol{f} \leftarrow \boldsymbol{f} - \boldsymbol{f}'$$

The value of the flow will still be non-negative after this update as we subtracted the minimum entry along any positive edge on the path. The number of non-zeros, $\text{nnz}(\boldsymbol{f})$, went down by at least one. Note that the updated $\boldsymbol{f}$ must again be an s-t flow, as it is the difference of two s-t flows.

"Cycle" case. Suppose we find a cycle c in the support of $\boldsymbol{f}$. Let α be the minimum flow value along the edges of the cycle, i.e.

$$\alpha = \min_{(a,b)\in c} \boldsymbol{f}(a,b)$$

$$\boldsymbol{f}' = \alpha \sum_{e\in c} \boldsymbol{e}_e$$

Update the flow $\boldsymbol{f}$ by

$$\boldsymbol{f} \leftarrow \boldsymbol{f} - \boldsymbol{f}'$$

As in the path case, $\boldsymbol{f}$ stays non-negative, and number of non-zeros, $\text{nnz}(\boldsymbol{f})$, goes down by at least one. Note that the updated $\boldsymbol{f}$ must again be an s-t flow, as it is the difference of two s-t flows.

"No path or cycle" case. Suppose we can find neither a path nor a cycle, and $\boldsymbol{f} \neq \boldsymbol{0}$. Then there must be an edge (u,v) with non-zero flow leading into a vertex $v \neq s,t$ and with no outgoing edge from v in the support of $\boldsymbol{f}$. In that case, we must have $(\boldsymbol{B}\boldsymbol{f})(v) \geq 0$. But since $v \neq t$, this contradicts $\boldsymbol{B}\boldsymbol{f} = F\boldsymbol{b}_{st}$. So this case cannot occur. □

Lemma 11.2.4. *In any s-t max flow problem instance, there is an optimal flow $\boldsymbol{f}^*$ with a path-cycle decomposition that has only paths and no cycles.*

Proof. Let $\tilde{\boldsymbol{f}}$ be an optimal flow. Let $\boldsymbol{f}^*$ be the sum of path flows in the path cycle decomposition of $\tilde{\boldsymbol{f}}$. They route the same flow (as cycles contribute to no net flow from s to t). Thus

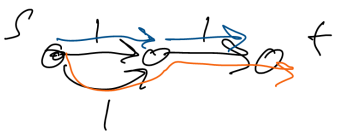
$$\boldsymbol{B}\boldsymbol{f}^* = \boldsymbol{B}\tilde{\boldsymbol{f}}$$

and hence $\text{val}(\boldsymbol{f}^*) = \text{val}(\tilde{\boldsymbol{f}})$. Furthermore

$$\boldsymbol{0} \leq \boldsymbol{f}^* \leq \tilde{\boldsymbol{f}} \leq \boldsymbol{c}$$

The first inequality follows from $\boldsymbol{f}^*$ being a sum of positive path flow. The second inequality holds as $\boldsymbol{f}^*$ is upper bounded in every single entry by $\tilde{\boldsymbol{f}}$, because we reduced it by positive entry cycles. The third inequality holds because $\tilde{\boldsymbol{f}}$ is a feasible flow, so it is upper bounded by the capacities. □

An optimal flow solving the maximum flow problem may not be unique. For example, consider the graph below with source s and sink t:



There are two optimal paths in this example. Maximum flow is a convex optimization problem but not a strongly convex problem as the solutions are not unique, and this is part of what makes it hard to solve.

11.3 Cuts and Minimum Cuts

The decomposition shown earlier provides a way to show that the maximum flow in a graph is upper bounded by constructing graph cuts.

Given a vertex subset $S \subseteq V$, we say that $(S, V \setminus S)$ is a *cut* in G and that the value of the cut is

$$c_G(S) = \sum_{e \in E \cap (S \times V \setminus S)} \boldsymbol{w}(e).$$

Note that in a directed graph, only edges crossing the cut going *from* S and *to* $V \setminus S$ count toward the cut.

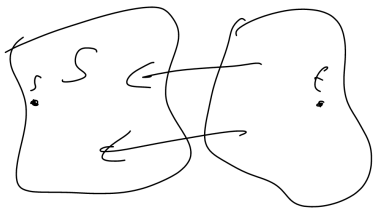


Figure 11.1: Example of a cut: No edges go from S to $(S, V \setminus S)$, and so the value of this cut is zero.

Definition. (s-t cuts). We define an s-t cut to be a subset $S \subset V$, where $s \in S$ and $t \in V \setminus S$.

A decision problem: *"Given an instance of the Maximum Flow problem, is there a flow from s to t such that $\boldsymbol{f} \neq \mathbf{0}$?"*

If YES: We can decompose this flow into s-t path flows and cycle flows.

If NO: There is no flow path from s to t. Let S be the set of vertices reachable from source s. Then $(S, V \setminus S)$ is a cut in the graph, with no edges crossing from S to $V \setminus S$. Figure 11.1 gives an example.

Upper bounding the maximum possible flow value. How can we recognize a maximum flow? Is there a way to confirm that a flow is of maximum value?

We can now introduce the *Minimum Cut* problem.

$$\begin{aligned} &\min_{S \subseteq V} c_G(S) \\ &\text{s.t. } s \in V \text{ and } t \notin V \end{aligned} \tag{11.2}$$

The Minimum Cut problem can also be phrased as a linear program, although we won't see that today.

We'd like to obtain a tight connection between flows and cuts in the graph. As a first step, we won't get that, but we can at least observe that the value of any s-t cut provides an upper bound to the maximum possible s-t flow value.

Theorem 11.3.1 (Max Flow $\leq$ Min Cut)**.** *The maximum s-t flow value in a directed graph G (Program* (17.1)*) is upper bounded by the minimum value of any s-t cut (Program* (11.2)*). I.e. if S is an s-t cut, and $\boldsymbol{f}$ a feasible s-t flow then*

$$\text{val}(\boldsymbol{f}) \leq c_G(S)$$

And in particular this holds for any minimum cut S^* and maximum flow $\boldsymbol{f}^*$, i.e. $\text{val}(\boldsymbol{f}^*) \leq c_G(S^*)$.

Proof. Consider any feasible flow $0 \leq \boldsymbol{f} \leq \boldsymbol{c}$ and a cut $S, T = V \setminus S$. Consider a path-cycle decomposition of $\boldsymbol{f}$, where each s-t path must cross the cut going forward from S to T at least once. We pick a cut S, T with source on one side and sink on the other side as shown in the Figure (11.2). Every time the path flow passes through the cut, it has to use one of the edges that connect S and T. Total amount of flow crossing the cut is bounded above by total amount of capacity of the cut, otherwise the capacities would be violated, thus $\text{val}(\boldsymbol{f}) \leq c_G(S, T) = \sum_{e \in E \cap S \times T} \boldsymbol{c}(e)$.

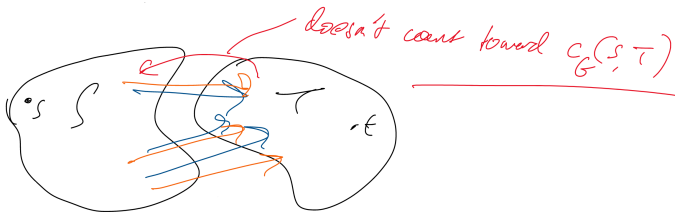


Figure 11.2: s-t Cut

Note that the edges from T to S do not count towards the cut. The above equation holds for all flows with all s-t cuts. This implies that **max flow** $\leq$ **min cut**. □

This theorem is an instance of a general pattern, known as *weak duality*. Weak duality is a relationship between two optimization programs, a maximization problem and a minimization problem, where any solution to the former has its value upper bounded by the value of any solution to the latter.

11.4 Algorithms for Max flow

How can we find a good flow?

Algorithm 4: A first attempt – bad idea?

$\boldsymbol{f} \leftarrow \mathbf{0}$;
repeat
  Find an s-t path flow $\tilde{\boldsymbol{f}}$ that is feasible with respect to $\boldsymbol{c} - \boldsymbol{f}$.
  $\boldsymbol{f} \leftarrow \boldsymbol{f} + \tilde{\boldsymbol{f}}$

Does Algorithm 1 work? Consider the graph below with directed edges with capacities 1 at every edge. If we make a single path update as shown by the orange lines in Figure 11.3, then afterwards, using the remaining capacity, there's no path flow we can route, as shown in Figure 11.3. But the max flow is 2, as shown by the flow on orange edges in Figure 11.5. So, the above algorithm does not always find a maximum flow: It can get stuck at a point where it cannot make progress despite not having reached the maximum value.

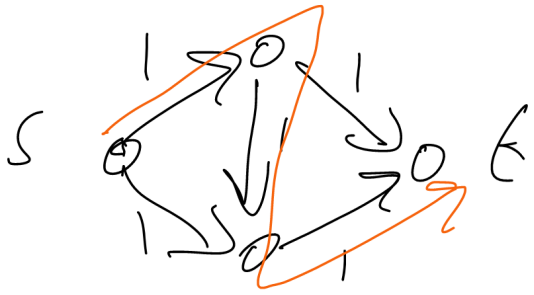


Figure 11.3: Sending a unit s-t path flow through the graph.

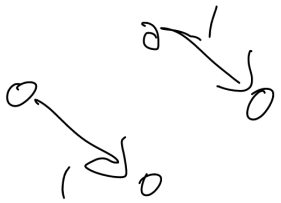


Figure 11.4: Remaining edge capacities after sending a path flow through the graph as depicted in Figure 11.3.

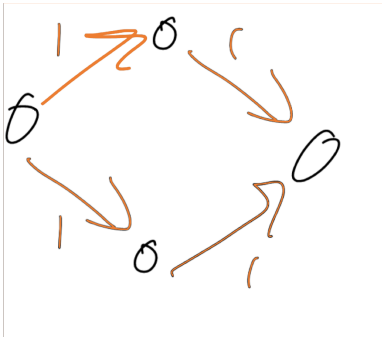


Figure 11.5: The flow depicted routes two units from s to t.

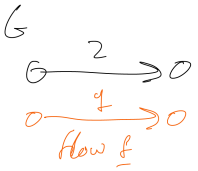
A better approach. It turns out we can fix the problem with the previous algorithm using a simple fix. This idea is known as *residual graphs*.

Algorithm 5: Better Idea (Residual Graph)

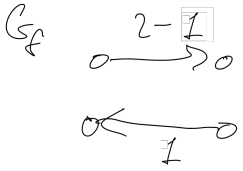
$\boldsymbol{f} \leftarrow \mathbf{0}$;
repeat
  Find an s-t path flow $\tilde{\boldsymbol{f}}$ that is feasible with respect to $-\boldsymbol{f} \leq \tilde{\boldsymbol{f}} \leq \boldsymbol{c} - \boldsymbol{f}$.
  $\boldsymbol{f} \leftarrow \boldsymbol{f} + \tilde{\boldsymbol{f}}$

The $-\boldsymbol{f}(e)$ can be treated as an edge going in the other direction with capacity $\boldsymbol{f}(e)$. By convention, an edge in G with $\boldsymbol{f}(e) = \boldsymbol{c}(e)$ is called *saturated*, and we do not include the edge in G_f. The graph defined above with such capacities is called **the residual graph of $\boldsymbol{f}$**, $G_{\boldsymbol{f}}$. $G_{\boldsymbol{f}}$ is only defined for feasible $\boldsymbol{f}$, since otherwise the constraint $\tilde{\boldsymbol{f}} \leq \boldsymbol{c} - \boldsymbol{f}$ gives trouble.

Suppose we start with a graph having a single edge with capacity 2 and we introduce a flow of 1 unit.



The residual graph $G_{\boldsymbol{f}}$ has an edge with capacity 1 going forward and -1 capacity going forward, but we can treat the latter as $+1$ capacity going backwards. So it is an edge that allows you to undo the choice made to send flow along that direction.



Let us consider the same example with its residual graph. The original graph is shown in Figure 11.6.

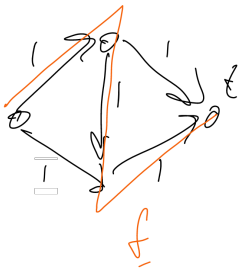


Figure 11.6: Original graph G and an s-t path flow in G shown in orange.

The residual graph for the same is shown in Figure 11.7.

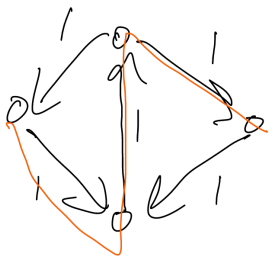


Figure 11.7: The residual graph w.r.t. the flow from Figure 11.6, and new s-t path flow which is feasible in the residual graph.

Adding both flows together, we get the paths as shown in Figure 11.8 with value 2, which is the optimum.

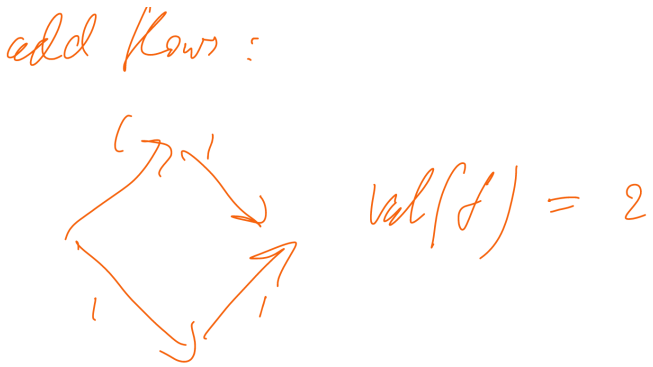


Figure 11.8: Maximum flow in the graph.

Let's prove some important properties of residual graphs.

Lemma 11.4.1. *Suppose $\boldsymbol{f}$, $\hat{\boldsymbol{f}}$ are feasible in G. Then this implies that $\hat{\boldsymbol{f}} - \boldsymbol{f}$ (where negative entries count as flow in opposite direction) is feasible in $G_{\boldsymbol{f}}$.*

Proof. $\mathbf{0} \leq \boldsymbol{f} \leq \boldsymbol{c}$ and $\mathbf{0} \leq \tilde{\boldsymbol{f}} \leq \boldsymbol{c}$, this implies $-\boldsymbol{f} \leq \tilde{\boldsymbol{f}} - \boldsymbol{f} \leq \boldsymbol{c} - \boldsymbol{f}$. Hence, proved. □

Lemma 11.4.2. *Suppose that $\boldsymbol{f}$ is feasible in G and $\hat{\boldsymbol{f}}$ is feasible in $G_{\boldsymbol{f}}$. Then, $\boldsymbol{f} + \hat{\boldsymbol{f}}$ is feasible in G.*

Proof. $\mathbf{0} \leq \boldsymbol{f} \leq \boldsymbol{c}$ and $-\boldsymbol{f} \leq \tilde{\boldsymbol{f}} \leq \boldsymbol{c} - \boldsymbol{f}$, this implies $\mathbf{0} \leq \tilde{\boldsymbol{f}} + \boldsymbol{f} \leq \boldsymbol{c}$. □

Lemma 11.4.3. *A feasible $\boldsymbol{f}$ is optimal if and only if t is not reachable from s in $G_{\boldsymbol{f}}$.*

Proof. Let $\boldsymbol{f}$ be optimal, and suppose t is reachable from s in $G_{\boldsymbol{f}}$ then, we can find a s-t path flow $\tilde{\boldsymbol{f}}$ that is feasible in $G_{\boldsymbol{f}}$, and $\text{val}(\boldsymbol{f} + \tilde{\boldsymbol{f}}) > \text{val}(\boldsymbol{f})$. $\boldsymbol{f} + \tilde{\boldsymbol{f}}$ is feasible in G by Lemma 11.4.2. This is a contradiction, as we assumed $\boldsymbol{f}$ was supposed to be optimal.

Suppose t is not reachable from s in $G_{\boldsymbol{f}}$, and $\boldsymbol{f}$ is feasible, but not optimal. Let $\boldsymbol{f}^*$ be optimal, then by Lemma 11.4.1, the flow $\boldsymbol{f}^* - \boldsymbol{f}$ is feasible in $G_{\boldsymbol{f}}$ and $\text{val}(\boldsymbol{f}^* - \boldsymbol{f}) > 0$. So there exists a s-t path flow from s to t in $G_{\boldsymbol{f}}$ (as we can do a path decomposition of $\boldsymbol{f}^* - \boldsymbol{f}$). But, this is a contradiction as t is not reachable from s in $G_{\boldsymbol{f}}$. □

Theorem 11.4.4 (Max Flow = Min Cut theorem)**.** *The maximum flow in a directed graph G equals the minimum cut.*

Proof. Consider the set $S = \{\text{vertices reachable from } s \text{ in } G_{\boldsymbol{f}}\}$. Note that $\boldsymbol{f}$ saturates the edge capacities in cut $S, V \setminus S$ in G: Consider any edge from S to $T := V \setminus S$ in G. Since this edge does not exist in the residual graph, we must have $\boldsymbol{f}(e) = \boldsymbol{c}(e)$.

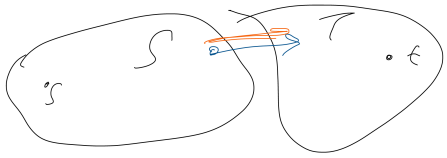


Figure 11.9: The cut between vertices reachable from S and everything else in G_f must have all outgoing edges saturated by $\boldsymbol{f}$.

This means that

$$\text{val}(\boldsymbol{f}) \geq c_G(S, V \setminus S).$$

Since we already know the opposite inequality by weak duality, we have shown that

$$\text{val}(\boldsymbol{f}) = c_G(S, V \setminus S)$$

which proves the **Max Flow = Min Cut** theorem; also called strong duality. □

Remark 11.4.5. Note that this proof also gives an algorithm to compute an s,t-min cut given an s,t maximum flow $\boldsymbol{f}^*$: Take one side of the cut to be the set S of nodes reachable from s in the residual graph w.r.t. $\boldsymbol{f}^*$.

Ford-Fulkerson Algorithm.

Algorithm 6: Ford-Fulkerson Algorithm

repeat
| Add update by arbitrary s-t path flow in $G_{\boldsymbol{f}}$ (augment the flow $\boldsymbol{f}$ by the path flow)

Convergence properties and analysis of runtime of Ford-Fulkerson algorithm

- **Does this algorithm terminate?**
  The algorithm terminates if the capacities are integers. However for irrational capacities the algorithm may not terminate.

- **Does it converge towards the max flow value?**
  No, it does not converge to max flow value if the updates are poor and the capacities are irrational.

Lemma 11.4.6. *Consider Ford-Fulkerson algorithm with integer capacities. The algorithm terminates in* $\text{val}(\boldsymbol{f}^*)$ *augmentations i.e.* $O(m \, \text{val}(\boldsymbol{f}^*))$ *time.*

Proof. Each iteration increases the flow by at least one unit as the capacities in $G_{\boldsymbol{f}}$ are integral and each iteration can be computed in $O(m)$ time. □

Can we do better than this? Suppose we pick the maximum bottleneck capacity (minimum capacity along path) augmenting path. This gives an algorithm that is better in some regimes.

How to pick the maximum bottleneck capacity augmenting path? We are going to perform a binary search on the capacities in $G_{\boldsymbol{f}}$, to find a path with maximum bottleneck capacity. Each time our binary search has picked a threshold capacity, we then try to find an s-t path flow in $G_{\boldsymbol{f}}$ using only edges with capacity above that threshold. If we find a path, the binary search tries a higher capacity next. If we don't find a path, the binary search tries a lower capacity next.

Using this approach, the time to find a single path is $O(m \log(n))$ where m is number of edges in the graph. This path must carry at least a $\frac{1}{m}$ fraction of the total amount of flow left in $G_{\boldsymbol{f}}$. For instance, if $\hat{F}$ is the amount of flow left in $G_{\boldsymbol{f}}$, then the path must carry $\frac{\hat{F}}{m}$ flow (from the path decomposition lemma, we know that there exists a decomposition into at most m paths, and the one carrying the most flow must carry at least the average amount).

So if the flow is integral, the algorithms completes when

$$\left(1 - \frac{1}{m}\right)^T \text{val}(\boldsymbol{f}^*) < 1$$

where T is the number of augmentations.

This means

$$T = m \log F$$

$$\begin{aligned}
\text{Total time} &= O(m \log nT) \\
&= O(m^2 \log n \log F) \\
&\leq O(m^2 \log n \log mU) \text{ as } F \leq mU \text{ where U is the maximum capacity}
\end{aligned}$$

Current state-of-the-art approaches for Max Flow. For the interested reader, we'll briefly mention the current state-of-the-art for Maximum Flow algorithms, which is a very active area of research.

- Strongly polynomial time algorithm:
  - has to work with real valued capacities, then the best time $O(mn)$ by Orlin.
- General integer capacities: For a long time, the state-of-the-art was a result by Goldberg and Rao achieving a runtime of $O(m \min(\sqrt{m}, n^{2/3}) \log(n) \log(U))$ where U is the maximum capacity. Very recently, $m^{1+o(1)} \log(U)$ has been claimed (not yet published in a peer-reviewed venue), see `https://arxiv.org/abs/2203.00671`. There are many other recent results prior to this work that we don't have time to cover here.

Chapter 12

Classical Algorithms for Maximum Flow II

12.1 Overview

In this chapter we continue looking at classical max flow algorithms. We derive Dinic's algorithm which (unlike Ford-Fulkerson) converges in a polynomial number of iterations. We will also show faster convergence on unit capacity graphs. The setting is the same as last chapter: we have a directed graph $G = (V, E, \boldsymbol{c})$ with positive capacities on the edges. Our goal is to solve the maximum flow problem on this graph for a given source s and sink $t \neq s$:

$$\begin{aligned} \max_{F>0, \boldsymbol{f}} \ F \qquad \text{s.t.} \quad & \boldsymbol{B}\boldsymbol{f} = F\boldsymbol{b}_{s,t} \\ & \boldsymbol{0} \leq \boldsymbol{f} \leq \boldsymbol{c} \end{aligned} \tag{12.1}$$

12.2 Blocking Flows

Let $\boldsymbol{f}$ be any feasible flow in G and let $G_{\boldsymbol{f}}$ be its residual graph. Observe that we can partition the vertices of $G_{\boldsymbol{f}}$ into 'layers': first s itself, then all vertices reachable from s in one hop, then all vertices reachable in two hops, etc. For each vertex $v \in V$ define its **level** in $G_{\boldsymbol{f}}$ as the length of the shortest path in $G_{\boldsymbol{f}}$ from s to v, denoted by $\ell_{G_{\boldsymbol{f}}}(v)$ (or just $\ell(v)$ if the graph is clear from context). An edge $(u, v) \in E$ can only take you up 'one level': if $\ell(v) \geq 2 + \ell(u)$ this would imply we can find a shorter s-v path by appending (u, v) to the shortest s-u path. However, edges can 'drop down' multiple levels (or be contained in the same level).

A key strategy in Dinic's algorithm will be to focus on 'short' augmenting paths. We can use the levels we defined above to isolate a subgraph of $G_{\boldsymbol{f}}$ containing all information we

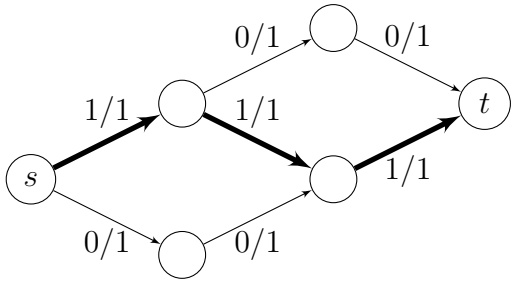


Figure 12.1: A blocking flow is not a maximum flow.

need to find shortest paths.

Definition 12.2.1. Call an edge (u, v) **admissible** if $\ell(u) + 1 = \ell(v)$. Let L be the set of admissible edges in $G_{\boldsymbol{f}}$ and define the **level graph** of $G_{\boldsymbol{f}}$ to be the subgraph induced by these edges.

Definition 12.2.2. Define a **blocking flow** in a residual graph $G_{\boldsymbol{f}}$ to be a flow $\hat{\boldsymbol{f}}$ feasible in $G_{\boldsymbol{f}}$, such that $\hat{\boldsymbol{f}}$ only uses admissible edges. Furthermore we require that for any s-t path in the level graph of $G_{\boldsymbol{f}}$, $\hat{\boldsymbol{f}}$ saturates at least one edge on this path.

The last condition makes a blocking flow 'blocking': it blocks any shortest augmenting path in $G_{\boldsymbol{f}}$ by saturating one of its edges. Note however that a blocking flow is not necessarily a maximum flow in the level graph.

12.3 Dinic's Algorithm

We can now formulate Dinic[1]'s algorithm: start with $\boldsymbol{f} = \boldsymbol{0}$, and then repeatedly add to $\boldsymbol{f}$ a blocking flow $\hat{\boldsymbol{f}}$ in $G_{\boldsymbol{f}}$, until no more s-t paths exist in $G_{\boldsymbol{f}}$.

Note that by doing a path decomposition on $\hat{\boldsymbol{f}}$ and adding these paths to $\boldsymbol{f}$ one by one, we see that our algorithm is a 'special case' of Ford-Fulkerson (with a particular augmenting path strategy) and hence inherits all the behaviors/bounds we proved in the last chapter.

Lemma 12.3.1. *Let $\boldsymbol{f}$ be a feasible flow, $\hat{\boldsymbol{f}}$ a blocking flow in $G_{\boldsymbol{f}}$ and define $\boldsymbol{f}' = \boldsymbol{f} + \hat{\boldsymbol{f}}$ (think of $\boldsymbol{f}$ and $\boldsymbol{f}'$ to be the flows at some steps k and $k+1$ in the algorithm). Then $\ell_{G_{\boldsymbol{f}'}}(t) \geq \ell_{G_{\boldsymbol{f}}}(t) + 1$.*

Proof. Let L, L' be the edge sets of the level graphs of $G_{\boldsymbol{f}}, G_{\boldsymbol{f}'}$ respectively. We would now like to show that $d_{L'}(s,t) \geq 1 + d_L(s,t)$. Let's first assume that in fact $d_{L'}(s,t) < d_L(s,t)$. Now take a shortest s-t path in the level graph of $G_{\boldsymbol{f}'}$, say $s = v_0, v_1, \ldots, v_{d_{L'}(s,t)} = t$. Let v_j be the first vertex along the path such that $d_{L'}(s, v_j) < d_L(s, v_j)$. As $d_{L'}(s,t) < d_L(s,t)$, such a v_j must exist.

[1]Sometimes also transliterated as Dinitz.

We'd like to understand the edges in the level graph L'. Let $E(G_{\boldsymbol{f}})$ denote the edges of the $G_{\boldsymbol{f}}$, and let $\text{rev}(L)$ denote the set of reversed edges of L. The level graph edges of $G_{\boldsymbol{f}'}$ must satisfy $L' \subseteq L \cup \text{rev}(L) \cup (E(G_{\boldsymbol{f}}) \setminus L)$.

In our s-t path in L', the vertex v_j is reached by an edge from v_{j-1}, and the level of v_{j-1} in $G_{\boldsymbol{f}}$ and $G_{\boldsymbol{f}'}$ are the same, so the edge $(v_{j-1}, v_j) \in L$ skips at least one level forward in $G_{\boldsymbol{f}}$. But, edges in L do not skip a level in $G_{\boldsymbol{f}}$, and edges in $\text{rev}(L)$ or $E(G_{\boldsymbol{f}}) \setminus L$ do not move from a lower level to higher level in $G_{\boldsymbol{f}}$. So this edge cannot exist and we have reached a contradiction.

Now suppose that $d_{L'}(s,t) = d_L(s,t)$. This means there is an s-t path in L' using edges in L – but such a path must contain an edge saturated by the blocking flow $\hat{\boldsymbol{f}}$.

(Note: the reason this path must use only edges in L is similar to the previous case: the other possible types of edges do not move to higher levels in $G_{\boldsymbol{f}}$ at all, making the path too long if we use any of them.)

So we must have $d_{L'}(s,t) \geq 1 + d_L(s,t)$. □

An immediate corollary of this lemma is the convergence of Dinic's algorithm:

Theorem 12.3.2. *Dinic's algorithm terminates in $O(n)$ iterations.*

Proof. By the previous lemma, the level of t increases by at least one each iteration. A shortest path can only contain each vertex once (otherwise it would contain a cycle) so the level of any vertex is never more than n. □

For graphs with unit capacities ($c = 1$) we can prove even better bounds on the number of iterations.

Theorem 12.3.3. *On unit capacity graphs, Dinic's algorithm terminates in*

$$O\left(\min\{m^{1/2}, n^{2/3}\}\right)$$

iterations.

Proof. We prove the two bounds separately.

1. Suppose we run Dinic's algorithm for k iterations, obtaining a flow $\boldsymbol{f}$ that is feasible but not necessarily yet optimal. Let $\tilde{\boldsymbol{f}}$ be an optimal flow in $G_{\boldsymbol{f}}$ (i.e. $\boldsymbol{f} + \tilde{\boldsymbol{f}}$ is a maximum flow for the whole graph), and consider a path decomposition of $\tilde{\boldsymbol{f}}$. Since after k iterations any s-t path has length k or more, we use up a total capacity of at least $\text{val}(\tilde{\boldsymbol{f}})k$ across all edges. But the edges in $G_{\boldsymbol{f}}$ are either edges from the original graph G or their reversals (but never both) meaning the total capacity of $G_{\boldsymbol{f}}$ is at most m, hence $\text{val}(\tilde{\boldsymbol{f}}) \leq m/k$.

   Recalling our earlier observation that our algorithm is a special case of Ford-Fulkerson, this implies that our algorithm will terminate after at most another m/k iterations.

Hence the number of iterations is bounded by $k + m/k$ for any $k > 0$. Substituting $k = \sqrt{m}$ gives the first desired bound.

2. Suppose again that we run Dinic's algorithm for k iterations obtaining a flow $\boldsymbol{f}$. The level graph of $G_{\boldsymbol{f}}$ partitions the vertices into sets $D_i = \{u \mid \ell(u) = i\}$ for $i \geq 0$. As shown before, the sink t must be at a level of at least k, meaning we have at least this many non-empty levels starting from $D_0 = \{s\}$. To simplify, discard all vertices and levels beyond $D_{\ell(t)}$.

   Now, consider choosing a level I uniformly at random from $\{1, \ldots, k\}$. Since there are at most $n-1$ vertices in total across these levels, $\mathbb{E}[|D_I|] \leq (n-1)/k$, and by Markov's inequality

$$\Pr[|D_I| \geq 2n/k] \leq \frac{(n-1)/k}{2n/k} < \frac{1}{2}.$$

   Thus strictly more than $k/2$ of the levels $i \in \{1, \ldots, k\}$ have $|D_i| < 2n/k$ and so there must be two adjacent levels j, $j+1$ for which this upper bound on the size holds. There can be at most $|D_j| \cdot |D_{j+1}| \leq 4n^2/k^2$ edges between these levels, and by the min-cost max-flow theorem we saw in the previous chapter, this is an upper bound on the flow in $G_{\boldsymbol{f}}$, and hence on the number of iterations still needed for our algorithm to terminate.

   This means the number of iterations is bounded by $k + 4n^2/k^2$ for any $k > 0$, which is $O(n^{2/3})$ at $k = 2n^{2/3}$.

□

12.4 Finding Blocking Flows

What has been missing from our discussion so far is the process of actually finding a blocking flow. We can achieve this using repeated depth-first search. We repeatedly do a search in the level graph (so only using edges L) for s-t paths and augment these. We erase edges whose subtrees have been exhausted and do not contain any augmenting paths to t. Pseudocode

for the algorithm is given below.

Algorithm 7: FindBlockingFlow

$\boldsymbol{f} \leftarrow \mathbf{0}$;
$H \leftarrow L$;
repeat
  $P \leftarrow \text{Dfs}(s, H, t)$;
  if $P \neq \emptyset$ **then**
    Let $\hat{\boldsymbol{f}}$ be a flow that saturates path P.
    $\boldsymbol{f} \leftarrow \boldsymbol{f} + \hat{\boldsymbol{f}}$;
    Remove from H all edges saturated by $\hat{\boldsymbol{f}}$.
  else
    return $\boldsymbol{f}$;
  end

Algorithm 8: Dfs(u, H, t)

if $u = t$ **then**
  return the path P on the dfs-stack.
end
for $(u, v) \in H$ **do**
  $P \leftarrow \text{Dfs}(v, H, t)$;
  if $P \neq \emptyset$ **then**
    return P;
  else
    Erase (u, v) from H.
  end
end
return $\emptyset$;

Lemma 12.4.1. *For general graphs,* FindBlockingFlow *returns a blocking flow in $O(nm)$ time. Hence Dinic's algorithm runs in $O(n^2m)$ time on general capacity graphs.*

Proof. First, consider the amount of work spent pushing edges onto the stack which eventually results in augmentation along an s-t path consisting of those edges (i.e. adding flow along that path). Since each augmenting path saturates at least one edge, we do at most m augmentations. Each path has length at most n. Thus the total amount of work pushing these edges to the stack, and removing them from the stack upon augmentation, and deleting saturated edges, can be bounded by $O(mn)$. Now consider the work spent pushing edges onto the stack which are later deleted because we "retreat" after not finding an s-t. An edge can only be pushed onto the stack once in this way, since it is then deleted. So the total amount spent pushing edges to the stack and deleting them this way is $O(m)$. □

Lemma 12.4.2. *For unit capacity graphs,* FindBlockingFlow *returns a blocking flow in $O(m)$ time. Hence Dinic's algorithm runs in $O\left(\min\{m^{3/2}, mn^{2/3}\}\right)$ time on unit capacity graphs.*

Proof. When our depth-first search traverses some edge (u, v), one of two things will happen: either we find no augmenting path in the subtree of v, leading to the erasure of this edge, or we find an augmenting path which will necessarily saturate (u, v), again leading to its erasure. This means each edge will be traversed at most once by the depth-first search. □

Another interesting bound on the runtime, which we will not prove here, is that Dinic's algorithm will run in $O\left(|E|\sqrt{|V|}\right)$ time on bipartite matching graphs.

12.5 Minimum Cut as a Linear Program

Finally we show that minimum cut may be formulated as a linear program. For a subset $S \subseteq V$ write $c_G(S)$ for the sum of $\boldsymbol{c}(e)$ over all edges $e = (u, v)$ that cross the cut, i.e. $u \in S, v \notin S$. Note that 'reverse' edges are not counted in this cut. The minimum cut problem asks us to find some $S \subseteq V$ such that $s \in S$ and $t \notin S$ such that $c_G(S)$ is minimal.

$$\begin{aligned} \min_{S \subseteq V} \quad & c_G(S) \\ s.t. \quad & s \in S \\ & t \notin S \end{aligned} \tag{12.2}$$

We claim this is equivalent to the following minimization problem:

$$\begin{aligned} \min_{\boldsymbol{x} \in \mathbb{R}^V} \quad & \sum_{e \in E} \boldsymbol{c}(e) \max\left\{\boldsymbol{b}_e^\top \boldsymbol{x}, 0\right\} \\ s.t. \quad & \boldsymbol{x}(s) = 0 \\ & \boldsymbol{x}(t) = 1 \\ & \mathbf{0} \leq \boldsymbol{x} \leq \mathbf{1} \end{aligned} \tag{12.3}$$

Recall $\boldsymbol{b}_e^\top \boldsymbol{x} = \boldsymbol{x}(v) - \boldsymbol{x}(u)$ for $e = (u, v)$. We can rewrite this as a proper linear program by introducing extra variables for the maximum:

$$\begin{aligned} \min_{\boldsymbol{x} \in \mathbb{R}^V, \boldsymbol{u} \in \mathbb{R}^E} \quad & \boldsymbol{c}^\top \boldsymbol{u} \\ s.t. \quad & \boldsymbol{b}_{s,t}^\top \boldsymbol{x} = 1 \\ & \mathbf{0} \leq \boldsymbol{x} \leq \mathbf{1} \\ & \boldsymbol{u} \geq \mathbf{0} \\ & \boldsymbol{u} \geq \boldsymbol{B}^\top \boldsymbol{x} \end{aligned} \tag{12.4}$$

And, in fact, we'll also see that we don't need the constraint $\mathbf{0} \leq \boldsymbol{x} \leq \mathbf{1}$, leading to the

following simpler program:

$$\begin{aligned} \min_{\boldsymbol{x}\in\mathbb{R}^V, \boldsymbol{u}\in\mathbb{R}^E} \quad & \boldsymbol{c}^\top \boldsymbol{u} \\ s.t. \quad & \boldsymbol{b}_{s,t}^\top \boldsymbol{x} = 1 \\ & \boldsymbol{u} \geq \boldsymbol{0} \\ & \boldsymbol{u} \geq \boldsymbol{B}^\top \boldsymbol{x} \end{aligned} \tag{12.5}$$

Lemma 12.5.1. *Programs* (12.2), (12.4), *and* (12.5) *have equal optimal values.*

Proof. We start by considering equality between optimal values of Program (12.2) and Program (12.4) Let S be an optimal solution to Program (12.2) and take $\boldsymbol{x} = \mathbf{1}_{V\setminus S}$. Then $\boldsymbol{x}$ is a feasible solution to Program (12.4) with cost equal to $c_G(S)$.

Conversely, suppose $\boldsymbol{x}$ is an optimal solution to Program (12.4). Let α be uniform in $[0, 1]$ and define $S = \{v \in V \mid \boldsymbol{x}(v) \leq \alpha\}$. This is called a threshold cut. We can verify that

$$\Pr[e \text{ is cut by } S] = \max\{\boldsymbol{b}_e^\top \boldsymbol{x}, 0\}.$$

and hence $\mathbb{E}_t[c_G(S)]$ is exactly the optimization function of 12.3 (and hence 12.4). Since at least one outcome must do as well as the average, there is a subset $S \subseteq V$ achieving this value (or less).

We can use the same threshold cut to show that we can round a solution to Program (12.5) to an equal or smaller value cut feasible for Program (12.2). The only difference is that in this case, we get

$$\Pr[e \text{ is cut by } S] \leq \max\{\boldsymbol{b}_e^\top \boldsymbol{x}, 0\}$$

which is still sufficient. □

Chapter 13

Link-Cut Trees

In this chapter, we will learn about a dynamic data structure that allows us to speed-up Dinic's algorithm even more: *Link-Cut Trees*. This chapter is inspired by lecture notes of Richard Peng[1] and the presentation in a very nice book on data structures and network flows by Robert Tarjan [Tar83].

13.1 Overview

Model. We consider a directed graph $G = (V, E)$ that is undergoing *updates* in the form of edge insertions and/or deletions. We number the graph in its different *versions* $G^0, G^1, G^2, \ldots$ such that G^0 is the initial input graph, and G^i is the initial graph after the first i updates were applied. Such a graph is called a *dynamic* graph.

In this lecture, we restrict ourselves to *dynamic rooted forests* that is we assume that every G^i forms a directed forest where in each forest a single root vertex is reached by every other vertex in the tree. For simplicity, we assume that $G^0 = (V, \emptyset)$ is an empty graph.

The Interface. Let us now describe the interface of our data structure that we call a link-cut tree. We want to support the following operations:

- INITIALIZE(G): Creates the data structure initially and returns a pointer to it. Each vertex is initialized to have an associated cost $cost(v)$ equal to 0.
- FINDROOT(v): Returns the root of vertex v.
- ADDCOST(v, Δ): Add Δ to the cost of every vertex on the path from v to the root vertex FINDROOT(v).

[1] CS7510 Graph Algorithms Fall 2019, Lecture 17 at `https://faculty.cc.gatech.edu/~rpeng/CS7510_F19/`

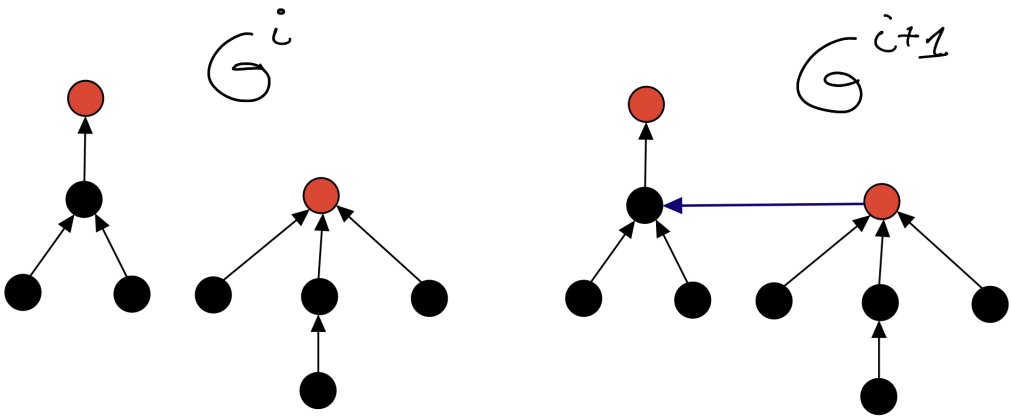


Figure 13.1: The i^{th} version of G is a rooted forest. Here, red vertices are roots and there are two trees. The $(i+1)^{th}$ version of G differs from G^i by a single edge that was inserted (the blue edge). Note that edge insertions are only valid if the tail of the edge was a root. In the right picture, the former root on the right side is turned into a normal node in the tree by the update.

- FindMin(v): Returns tuple $(w, cost(w))$ where w is the (first) vertex on the path from v to FindRoot(v) of lowest cost.
- Link(u, v): Links two trees that contain u and v into a single tree by inserting the edge (u, v). This assumes that u, v are initially in different trees and u was a root vertex.
- Cut(u, v): Cuts the edge (u, v) from the graph which causes the subtree rooted at u to become a tree and u to become a root vertex. Assumes (u, v) is in the current graph.

Main Result. The following theorem is the main result of today's lecture.

Theorem 13.1.1. *We can implement a link-cut tree such that any sequence of m operations takes total expected time $O(m \log^2 n + |V|)$.*

13.2 Balanced Binary Search Trees: A Recap

In Chapter 2 of the course Algorithms, Probability and Computing, we introduced (balanced) binary search trees, and studied *treaps*, which are a simple randomized approach to building a binary search tree with good performance, at least in expectation. If you are not familiar with balanced binary search trees, we encourage you to read this chapter from the APC script. That said, we will quickly recap the important properties of binary search trees and treaps. If you're already familiar with treaps, you can skip ahead to the next section to see how we use them for building Link-Cut trees. A binary search tree $\mathcal{T}$ is a data structure for keeping track of a set of *items* where each item has a *key* associated with it. The data structure stores the items in a rooted binary tree with a node for each item, and maintains

the property for each node v, all items in the *left* subtree of v have keys less than v, and all items in the *right* subtree of v have keys greater than v. This is called the *search property* of the tree, because it makes it simple to search through the tree to determine if it contains an item with a given key.

The binary trees we studied in APC supported the following operations, while maintaining the search property:

insert: We can add an item to the tree with a specified key.

delete: We can remove an item from the tree with a specified key.

find: Determine if the tree contains an item with a specified key.

split: Suppose the tree contains two items v_1 and v_2 with keys k_1 and k_2 where $k_1 < k_2$, and suppose no item in tree has a key k in the interval (k_1, k_2). Then the split operation applied to these two items should split the current tree into two: One tree containing all items with keys in $(-\infty, k_1]$ and the other with all items in $[k_2, \infty)$.

join: Given two binary search trees, one with keys in the interval $(-\infty, k]$, the other with keys in the interval (k, ∞), form a single binary search tree containing the items of both.

Treaps allow us to implement all of these operations, each with expected time $O(\log n)$ for each operation when working over n items.

Tree rotations. A crucial operation when implementing binary search trees in general and treaps in particular is *tree rotation*. A tree rotation makes a local change to the tree by changing only a constant number of pointers around, while preserving the search property. Given two items v_1 and v_2 such that v_1 is a child of v_2, a tree rotation applied to these two nodes will make v_2 the child of v_1, while moving their subtrees around to preserve the search property. This is shown in Figure 13.2. When the rotation makes v_2 the right child of v_1 (because v_2 has the larger key), this is called a *right rotation*, and when it makes v_2 the left child of v_1 (because v_2 has a smaller key), it is called a *left rotation*.

13.3 A Data Structure for Path Graphs

Before we prove Theorem 13.1.1 in its full generality, let us reason about implementing a link-cut tree data structure in a weaker setting: we assume that every version G^i of G is just a collection of rooted vertex-disjoint paths. We will later build on the routines we develop for the path case to construct the data structure for the general tree case. To distinguish the routines we develop for paths from those we develop for the general case, we will prefix the path-case routines with a "P", i.e.

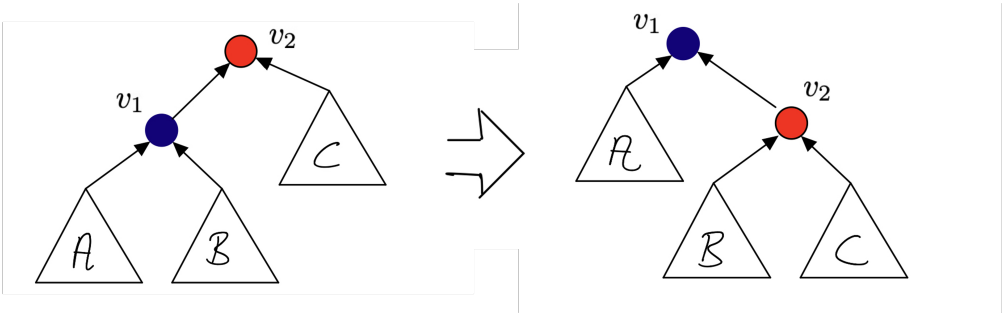


Figure 13.2: Given two items v_1 and v_2 such that v_1 is a child of v_2, a tree rotation applied to these two nodes will make v_2 the child of v_1, while moving their subtrees around to preserve the search property. This figure shows a *right rotation*.

we denote our implementations of FindRoot, AddCost, FindMin, Link, and Cut by PFindRoot, PAddCost, PFindMin, PLink, and PCut.

Representing Paths via Balanced Binary Search Trees. It turns out that paths can be represented rather straight-forwardly via Balanced Binary Search Trees, with an node/item for each vertex of the graph. For the sake of concreteness, we here use *treaps* to represent paths[2]. Most other balanced binary search trees would also work.

Note that we now represent each rooted path with a tree, and this tree as its own root, which is usually *not* the root of othe path. To minimize confusion, we will refer to the root of the path as the *path-root* and the root of the associated tree as the *tree-root* (or *subtree-root* for the root of a subtree).

In our earlier discussion of binary trees, we always assumed each item has a key: Instead we will now let the key of each vertex correspond to its distance to the path-root in the path that contains it. We will make sure the treap respects the search property w.r.t. this set of keys/ordering, but we will not actually explicitly compute these keys or store them. Note one important difference to the scenario of treaps-with-keys: When we have two paths, with path-roots r_1 and r_2, we will allow ourselves to join these paths in two different ways: either so that r_1 or r_2 becomes the overall path-root.

Let us describe how to represent a path P in G. First, we pick for each vertex v, we assign it a *priority* denoted $\text{prio}(v)$, which we choose to be a uniformly random integer sampled from a large universe, say $[1, n^{100})$. We assume henceforth that $\text{prio}(v) \neq \text{prio}(w)$ for all $v \neq w \in V$.

Then, for each path P in G, we store the vertices in P in a binary tree, in particular a treap, $\mathcal{T}_P$ and enforce the following invariants:

- **Search-Property**: for all v, $left_{\mathcal{T}_P}(v)$ precedes v on P and $right_{\mathcal{T}_P}(v)$ appears later

[2]If you have not seen treaps before, don't worry, they are simple enough to understand them from our application here.

on P than v. See the Figure 13.3 below for an illustration.

- **Heap-Order**: for each vertex $v \in P$, its parent $w = parent_{\mathcal{T}_P}(v)$ in $\mathcal{T}_P$ is either $NULL$ (if v is the path-root) or has $\text{prio}(v) > \text{prio}(w)$.

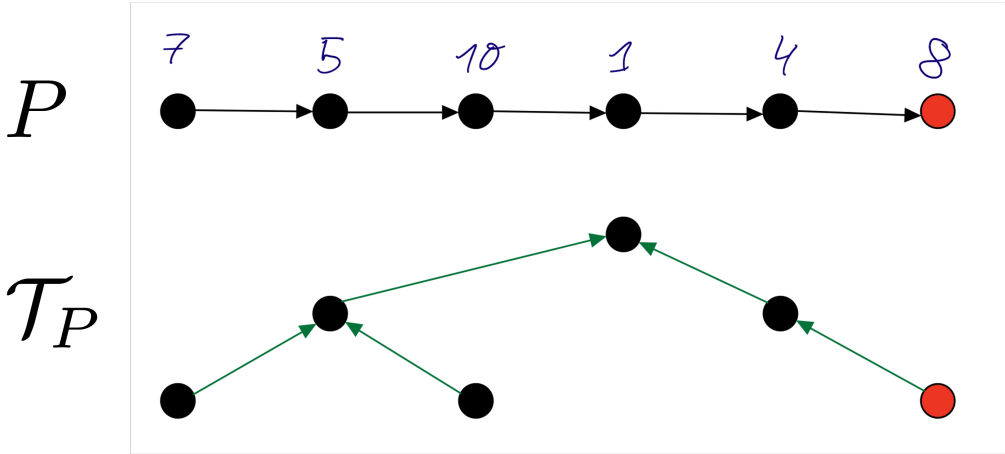


Figure 13.3: In the upper half of the picture, the original path P in G is shown, along with the random numbers $\text{prio}(v)$ for each v. The lower half depicts the resulting treap with vertices on the same vertical line as before.

Depth of Vertex in a Treap. Let us next analyze the expected depth of a vertex v in a treap $\mathcal{T}_P$ representing a path P. Let $P = \langle x_1, x_2, \ldots, x_k = v, \ldots, x_{|P|} \rangle$, i.e. v is the k^{th} vertex on the path P. Observe that a vertex x_i with $i < k$ is an ancestor of v in $\mathcal{T}_P$ if and only if no vertex $\{x_{i+1}, x_{i+2}, \ldots, x_k\}$ has received a smaller random number than $\text{prio}(x_i)$. Since we sample $\text{prio}(w)$ uniformly at random for each w, we have that $\mathbb{P}[x_i \text{ ancestor of } v] = \frac{1}{k-i+1}$. The case where $i > k$ is analogous and has $\mathbb{P}[x_i \text{ ancestor of } v] = \frac{1}{i-k+1}$. Letting X_i be the indicator variable for the event that x_i is an ancestor of v, it is straight-forward to calculate the expected depth of v in $\mathcal{T}_P$:

$$\mathbb{E}[depth(v)] = \sum_{i \neq k} \mathbb{E}[X_i] = \sum_{i=1}^{k-1} \frac{1}{k-i+1} + \sum_{i=k+1}^{|P|} \frac{1}{i-k+1} = H_k + H_{|P|-k+1} - 2 = O(\log |P|)$$

It is straight-forward to see that the operation PFindRoot(v) can thus be implemented to run in expected $O(\log n)$ time by just iteratively following the parent pointers starting in v.

Implementing PFindRoot(v). From any vertex v, we can simply follow the parent pointers in $\mathcal{T}_P$ until we are at the tree-root of $\mathcal{T}_P$. Then, we find the right-most child of $\mathcal{T}_P$ by following the $right_{\mathcal{T}_P}$ pointers. Finally, we return the right-most child which is the path-root.

Extra fields to help with PAddCost(v, Δ) and PFindMin(v). The key trick to do the Link-Cut tree operations efficiently is to store the change to subtrees instead of updating $cost(v)$ for each affected vertex.

To this end, we store two fields $\Delta cost(v)$ and $\Delta min(v)$ for every vertex v. We let $cost(v)$ be the cost of each vertex, and $mincost(v)$ denote the minimum cost of any descendant of v in $\mathcal{T}_P$ (where we let v be a descendant of itself). A warning: the $mincost(v)$ value is the minimum cost in the treap-subtree; *not* the minimum cost on the path between v and the path-root that could be different. Note also that we do not explicitly maintain these fields.

Then, we maintain for each v

$$\Delta cost(v) = cost(v) - mincost(v)$$

$$\Delta min(v) = \begin{cases} mincost(v) & parent_{\mathcal{T}_P}(v) = NULL, \\ mincost(v) - mincost(parent_{\mathcal{T}_P}(v)) & otherwise \end{cases}$$

With a bit of work, we can see that with these definitions, we obtain $mincost(v) = \sum_{w \in \mathcal{T}_P[v]} \Delta min(v)$ where $\mathcal{T}_P[v]$ is the v-to-tree-root path in $\mathcal{T}_P$. We can then recover $cost(v) = mincost(v) + \Delta cost(v)$. We say that $\Delta min(v)$ and $\Delta cost(v)$ are *field-preserving* if we can compute $mincost(v)$ and $cost(v)$ in the above way.

Implementing PAddCost(v, Δ) and PFindMin(v) – the easy way. First, we will discuss ways to implement PAddCost and PFindMin in ways that rely on the fact that PLink and PCut can preserve that $\Delta cost(v)$ and $\Delta mincost(v)$ still satisfy the relations we described above.

Now, PAddCost(v, Δ) is very easy: First, consider the case when v as no precessor on the path. If this is the case, we can simply find the tree-root of the tree $\mathcal{T}_P$ containing v and at this root increase the value of the field *mincost* by Δ. This implicitly increases the cost of all nodes in the tree by Δ. Second, consider the case when v has a precessor u in the path (we can store these explicitly, or we can search for it in the tree). Call PCut(u, v) – now v no longer has a precessor and we can proceed as before. Finally, call PLink(u, v). That's it.

Implemeting PFindMin(v) is also very easy: First, consider the case when v as no precessor on the path. Again, we can find the tree-root r of the tree $\mathcal{T}_P$ containing v. By definition $mincost(r)$ is the minimum cost across the whole tree, and hence across the path between v and the path-root. We can also find the node with the minimum cost: Search in the tree, starting from the tree-root, and, if possible follow the child where $\Delta min(v) = 0$ (going left if both are eligible). Eventually, we get to a node where there is no child with $\Delta min(v) = 0$. This must be a minimizer. Now, to deal with the case where v has a precessor, we do the same we did for PAddCost: Find the precessor u, call PCut(u, v), then find the minimizer, finally call PLink(u, v).

Implementing PAddCost(v, Δ) and PFindMin(v) – the hard way. We can also implement PAddCost(v, Δ) and PFindMin(v) without relying on PLink and PCut,

which is more efficient, but also more unpleasant[3].

To implement the operation PFINDMIN(v) more efficiently, consider the sequence of nodes on the path in the tree $\mathcal{T}_P$ (not the path P) between v and the path-root. First let $v = x_1, x_2, \ldots, x_k = r$ be the nodes leading to the tree-root if v is left of the tree root, and then let $y_1, \ldots, y_l$ be the remaining nodes on the tree path to the path-root. Observe that either the minimizer one of these nodes (which we can check by checking their Δmin), or it is in a right subtree of some x_i, or in any subtree of some y_j. So we just search through these subtrees for their minimizers (looking for $\Delta min(v) = 0$) and pick the best one. There will only be $O(\log n)$ trees in expectation.

Next, let us discuss the implementation of the operation PADDCOST(v, Δ) which is given in pseudo-code above. The first for-loop of this algorithm ensures that the tree is again *field-preserving*. This is ensured by walking down the path from the path-root of v to v and whenever we walk to the left, we make sure to increase all costs in the right subtree by adding Δ to the subtree-root of the right subtree r in the form of adding it to $\Delta min(r)$. On the vertices along the path it updates the costs by using the $\Delta cost(\cdot)$ fields. It is easy to prove from this that thereafter the tree is *field-preserving*.

Algorithm 9: PADDCOST(v, Δ)

Store the vertices on the path in the tree $\mathcal{T}_P$ between v and the path-root, i.e.
$\langle v = x_1, x_2, \ldots, x_k = \text{PFINDROOT}(v) \rangle$.
for $i = k$ *down to* 1 **do**
  $\Delta cost(x_i) = \Delta cost(x_i) + \Delta$.
  if $(r \leftarrow right_{\mathcal{T}_P}(x_i)) \neq NULL$ *AND* $(i = 0$ *OR* $x_{i-1} \neq r)$ **then**
    $\Delta min(r) \leftarrow \Delta min(r) + \Delta$
  end
end
for $i = 1$ *up to* k **do**
  $minval \leftarrow \Delta cost(x_i)$.
  foreach $w \in \{left_{\mathcal{T}_P}(x_i), right_{\mathcal{T}_P}(x_i)\}, w \neq NULL$ **do**
    $minval \leftarrow \min\{minval, \Delta min(w)\}$.
  $\Delta min(x_i) \leftarrow \Delta min(x_i) + minval$.
  $\Delta cost(x_i) \leftarrow \Delta cost(x_i) - minval$.
  foreach $w \in \{left_{\mathcal{T}_P}(x_i), right_{\mathcal{T}_P}(x_i)\}, w \neq NULL$ **do**
    $\Delta min(w) \leftarrow \Delta min(w) - minval$.
end

While after the first for-loop the values can be computed efficiently, we might now be in the situation that $\Delta min(w)$ or/and $\Delta cost(w)$ are negative for some vertices w. We may also violate the invariants we want to preserve on the relationship between the $\Delta min(w)$ or/and $\Delta cost(w)$ fields and the true *cost* and *mincost* values at each node. We recover through the

[3]You don't have to know these more complicated approaches for the exam, but we include them for the interested reader.

second for-loop that at each vertex on the tree path from v to its path-root first computes the correct minimum in the subtree again (using the helper variable *minval*) and then adjusts all values in its left/right subtree and its own fields. Since we argued that v is at expected depth $O(\log(n))$, we can see that this can be done in expected $O(\log n)$ time.

Implementing PCut(u, v). Let us first assume that we have a dummy node d_0 with $\text{prio}(d_0) = 0$ in the vertex set. The trick is to first treat the operation as splitting the edge (u, v) into (u, d_0) and (d_0, v) by inserting the vertex d_0 in between u and v in the tree $\mathcal{T}_P$ as a leaf (this is always possible). Then, we can do standard binary tree rotations to re-establish the heap-order invariant (see Figure 13.4). It is not hard to see that after $O(\log n)$ tree rotations in expectation, the heap-order is re-established and d_0 is at new tree-root of $\mathcal{T}_P$. It remains to remove d_0 and make $left_{\mathcal{T}_P}(d_0)$ and $right_{\mathcal{T}_P}(d_0)$ tree-roots.

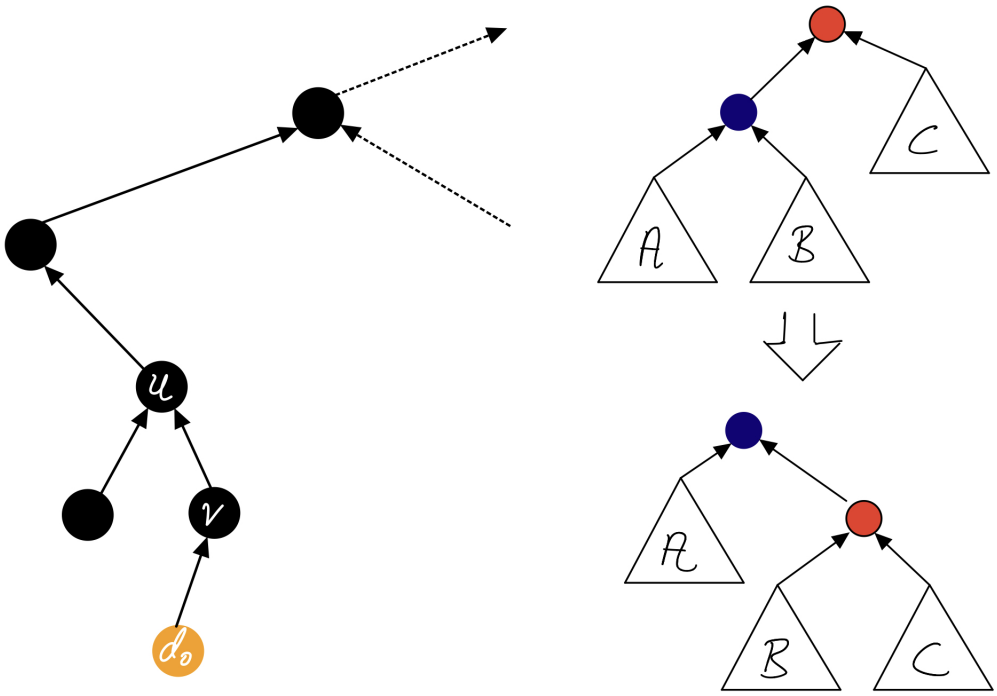


Figure 13.4: For PCut(u, v), we insert a vertex d_0 as a leaf of either u or v to formally split (u, v) into (u, d_0) and (d_0, v) (this is shown on the left). While this preserves that Search-Property, it will violate the Heap-Order. Thus, we need to use tree rotations (shown on the left) to push d_0 to the top of the tree $\mathcal{T}_P$ (the arrow between the tree rotations should point in both ways).

To ensure that the fields are correctly adjusted, we can make the $\Delta min(\cdot)$ values of the two vertices that are rotated equal to zero while ensuring that the tree is still *field-preserving* by changing the $\Delta min(\cdot)$ fields of the (at most 3) subtree-roots of the subtrees to be rotated, and adapting the $\Delta cost(\cdot)$ fields of the two vertices to be rotated. Then, after the rotation, it is not hard to see that the tree is still *field-preserving* and that the procedure applied

in the second for-loop of the operation PAddCost(v, Δ) can then just be applied to the two rotated vertices and the subtree-roots of their subtrees. This ensures that the fields are maintained correctly. All of these operations can be implemented in $O(1)$ time per tree rotation. Note that PCut is basically just the treap split operation. In the exercises for this week, we ask you to come up with the pseudo-code for maintaing that the tree is *field-preserving* during tree rotations.

Implementing PLink(u, v). Implementing PLink(u, v) could be done by reversing the process described above. We choose however a slightly different strategy: we insert a vertex d_∞ with $\text{prio}(d_\infty) = n^{100}$ and make it a right child of u. We then find the tree-root r of the tree over the path containing v (as a tail). Finally, we make r a right child of d_∞. It remains to use tree rotations to make d_∞ a leaf in the tree. Once this is accomplished, one can simply remove d_∞ from the tree entirely (which can be seen as un-splitting two edges into (u, v)). Note that PLink is essentially the treap join operation.

Notes. The operations PLink/PCut can be implemented using almost all Balanced Binary Search Trees (especially the ones you have seen in your first courses on data structures). Thus, it is not hard to get a $O(\log n)$ worst-case time bound for all operations discussed above.

13.4 Implementing Trees via Paths

We now use the result from last section as a black box to obtain Theorem 13.1.1.

Path Decomposition. For each rooted tree T, the idea is to decompose T into paths. In particular, we decompose each T into a collection of vertex-disjoint paths $P_1, P_2, \ldots, P_k$ such that each internal vertex v in T has exactly one incoming edge in some P_i. We call the edges on some P_i *solid* edges and say that the other edges are *dashed*.

We maintain the paths $P_1, P_2, \ldots, P_k$ using the data structure described in the last section. To avoid confusion, we use the prefix P when we invoke operations of the path data structure, for example PFindRoot(v) finds the root of v in the path graph P_i where $v \in P_i$. We no longer need to think about the balanced binary trees that are used internally to represent each P_i. Instead, in this section, we use path-root to refer to the root of a path P_i and we use tree root (or just root) to refer to a root of one of the trees in our given collection of rooted trees.

The Expose(v) Operation. We start by discussing the most important operation of the data structure that will be used by all other operations internally: the operation Expose(v). This operation flips solid/dashed edges such that after the procedure the path from v to its

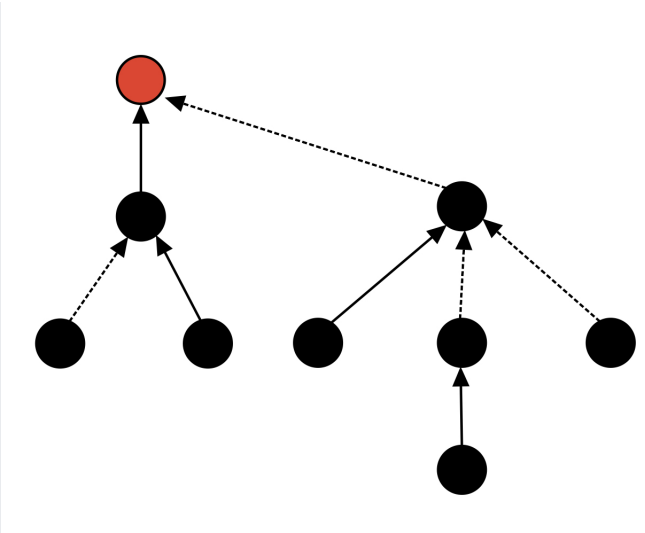


Figure 13.5: The dashed edges are the edges not on any path P_i. The collection of (non-empty) paths $P_1, P_2, \ldots, P_k$ can be seen to be the maximal path segments of solid edges.

tree root in G is solid (possibly as a subpath in the path collection). Below you can find an implementation of the procedure EXPOSE(v).

Algorithm 10: EXPOSE(v)

$w \leftarrow v$.
while $(w' = parent_G(\text{PFINDROOT}(w))) \neq NULL$ **do**
  Invoke PCUT(z, w') for the solid edge (z, w') incoming to w'.
  PLINK(PFINDROOT$(w), w')$.
  $w \leftarrow w'$.
end

Implementing Operations via Expose(v). We can now implement link-cut tree operations by invoking EXPOSE(v) and then forwarding the operation to the path data structure.

Algorithm 11: AddCost(v, Δ)

Expose(v); PAddCost(v, Δ)

Algorithm 12: FindMin(v)

Expose(v); **return** PFindMin(v)

Algorithm 13: Link(u,v)

$parent_G(u) \leftarrow v$;
if *v has an incoming solid edge (z, v)* **then** PCut(z, v) ;
PLink(u, v)

Algorithm 14: Cut(u,v)

Expose(u); $parent_G(u) \leftarrow NULL$; PCut$(u, v)$;
if *v has other incoming edge (z, v)* **then** PLink(z, v);

Analysis. All of the operations above can be implemented using a single Expose$(\cdot)$ operation plus $O(1)$ operations on paths. Since path operations can be executed efficiently, our main task is to bound the run-time of Expose$(\cdot)$. More precisely, since each iteration of Expose$(\cdot)$ also runs in time $O(\log n)$, the total number of while-loop iterations in Expose$(\cdot)$.

To this end, we introduce a dichotomy over the vertices in G. We let $parent_G(v)$ denote the unique parent of v in G and let $size_G(v)$ denote the number of vertices in the subtree rooted at v (including v).

Definition 13.4.1. Then, we say that an edge (u, v) is *heavy* if $size_G(u) > size_G(v)/2$. Otherwise, we say (u, v) is *light*.

It can now be seen that the number of *light* edges on the v-to-root path for any v is at most $\lg n$: every time we follow a light edge (w, w'), i.e. when $size_G(w') > 2size_G(w)$, we double the size of the subtree so after taking more than $\lg n$ such edges, we have $> 2^{\lg n} = n$ vertices in the graph (which is a contradiction).

Thus, when Expose$(\cdot)$ runs for many iterations, it must turn many *heavy* edges *solid* (this is also since each vertex has at most one incoming heavy edge, so when we make a heavy edge solid, we also don't make any other heavy edge solid).

Claim 13.4.2. *Each update can only increase the number of dashed, heavy edges by $O(\log n)$.*

Proof. First observe that every time Expose$(\cdot)$ is invoked, it turns at most $\lg n$ heavy edges from solid to dashed (since it has to visit a light edge to do so).

The only two operations that can cause additional dashed, heavy edges are Link(u, v) and Cut(u, v) by toggling heavy/light. For Link(u, v), we observe that only the vertices on the

v-to-root path increase their sizes. Since there are at most $\lg n$ light edges on this path that can turn heavy, this increases the number of dashed, heavy edges by at most $\lg n$.

The case for $\textsc{Cut}(u, v)$ is almost analogous: only vertices on the v-to-root path decrease their sizes which can cause any heavy edge on such a path to become light, and instead for a sibling of such a vertex might becomes heavy. But there can be at most $\lg n$ such new heavy edges, otherwise the total size of the tree must exceed again n which leads to a contradiction. □

Thus, after m updates, we have created at most $O(m \log n)$ dashed heavy edges. The iterations of $\textsc{Expose}(\cdot)$ either visit a dashed light edge (at most $\ln n$ of them), or consumes a dashed heavy edge, i.e. turning them . We conclude that after m updates, the while-loop in $\textsc{Expose}(\cdot)$ runs for at most $O(m \log n)$ iterations, *in total*, i.e. summed across the updates so far. Each iteration can be implemented in $O(\log n)$ expected time. This dominates the total running time and proves Theorem 13.1.1.

13.5 Fast Blocking Flow via Dynamic Trees

Recall from Section 12.4 that computing blocking flows in a level graph L from a vertex s to t can be done by successively running DFS(s) and routing flow along the s-t path found if one such path exists and otherwise we know that we have found a blocking flow.

We can now speed-up this procedure by storing the DFS-tree explicitly as a dynamic tree. To simplify exposition, we transform L to obtain a graph $\textsc{Transform}(L)$ that has capacities on vertices instead of edges. To obtain $\textsc{Transform}(L)$, we simply split each edge in L and assign the edge capacity to the mid-point vertex while assigning capacity ∞ to all vertices that were already in L. This creates an identical flow problem with at most $O(m)$ vertices and edges.

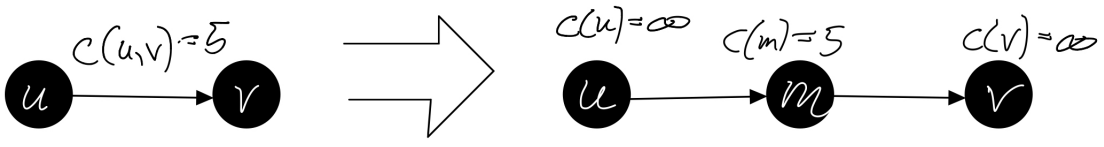


Figure 13.6: Each edge (u, v) with capacity $c(u, v)$ is split into two edges (u, m) and (m, v). The capacity is then on the vertex m.

Finally, we give the new pseudo-code for the blocking flow procedure below.

Algorithm 15: FindBlockingFlow(s, t, L)

```
H ← Transform(L);
LC-Tree ← Initialize(H);
while s ∈ H do
    u ← LC-Tree.FindRoot(s);
    if there is an edge (u, v) ∈ H then
        LC-Tree.Link(u, v);
        if v = t then
            (w, c) ← LC-Tree.FindMin(s);
            LC-Tree.AddCost(s, −c);
            Remove w and all its incident edges from H and LC-Tree (via Cut(·)).
        end
    else
        Remove u and all its incident edges from H and LC-Tree (via Cut(·)).
    end
end
Construct f by setting for each edge (u, v) of L, with mid-point m in Transform(L),
 the flow equal to c(m) minus the cost on m just before it was removed from H.
```

Claim 13.5.1. *The running time of* FindBlockingFlow(s, t, L) *is* $O(m \log^2 n + |V|)$.

Proof. Each edge (u, v) in the graph Transform(L) enters the link-cut tree at most once (we only invoke Cut(u, v) when we delete (u, v) from H).

Next, observe that the first **if**-case requires $O(1 + \#edgesDeletedFromH)$ many tree operations. The *else*-case requires $O(\#edgesDeletedFromH)$ many tree operations.

But each edge is only deleted once from H, thus we have a total of $O(m)$ tree operations over all iterations. Since each link-cut tree operation takes amortized expected time $O(\log^2 n)$, we obtain the bound on the total running time. □

The correctness of this algorithm follows almost immediately using that the level graph L (and therefore Transform(L)) is an acyclic graph.

Chapter 14

The Cut-Matching Game: Expanders via Max Flow

In this chapter, we learn about a new algorithm to compute expanders that employs max flow as a subroutine.

14.1 Introduction

We start with a review of expanders where make a subtle change the notion of an expander in comparison to chapter 5 to ease the exposition.

Definitions. We let $G = (V, E)$ be an unweighted, connected graph in this chapter, and let $\boldsymbol{d}$ be the degree vector, $E(S, V \setminus S)$ denote the set of edges crossing the cut A, B

Given set $\emptyset \subset S \subset V$, then we define the **sparsity** $\psi(S)$ of S by

$$\psi(S) = \frac{|E(S, V \setminus S)|}{\min\{|S|, |V \setminus S|\}}$$

Note that **sparsity** $\psi(S)$ differs from **conductance** $\phi(S) = \frac{|E(S,V\setminus S)|}{\min\{\text{vol}(S),\text{vol}(V\setminus S)\}}$, as defined in 5, in the denominator. It is straight-forward to see that in a connected graph $\psi(S) \geq \phi(S)$ for all S.

Clearly, we again have $\psi(S) = \psi(V \setminus S)$. We define the *sparsity* of a graph G by $\psi(G) = \min_{\emptyset \subset S \subset V} \psi(S)$. For any $\psi \in (0, n]$, we say a graph G is a ψ-expander with regard to sparsity, if $\psi(G) \geq \psi$. When the context is clear, we simply say that G is a ψ-expander.

The Main Result. The main result of this chapter is the following theorem.

Theorem 14.1.1. *There is an algorithm* SparsityCertifyOrCut(G, ψ) *that given a graph* G *and a parameter* $0 < \psi \leq 1$ *either:*

- Certifies *that* G *is a* $\Omega(\psi/\log^2 n)$*-expander with regard to sparsity, or*
- *Presents a* cut S *such that* $\psi(S) \leq O(\psi)$*.*

The algorithm runs in time $O(\log^2 n) \cdot T_{max\_flow}(G) + \tilde{O}(m)$ *where* $T_{max\_flow}(G)$ *is the time it takes to solve a Max Flow problem on* G[1]*.*

The bounds above can further be extended to compute ϕ-expanders (with regard to conductance). Using current state-of-the art Max Flow results, the above problem can be solved in $\tilde{O}(m + n^{3/2+o(1)})$ time [vdBLL+21].

14.2 Embedding Graphs into Expanders

Let us start by exploring the first key idea behind the algorithm. We therefore need a definition of what it means to embed one graph into another.

Definition of Embedding. Given graphs H and G that are defined over the same vertex set, then we say that a function $\textsc{Embed}_{H \to G}$ is an *embedding* if it maps each edge $(u, v) \in H$ to a u-to-v path $P_{u,v} = \textsc{Embed}_{H \to G}(u, v)$ in G.

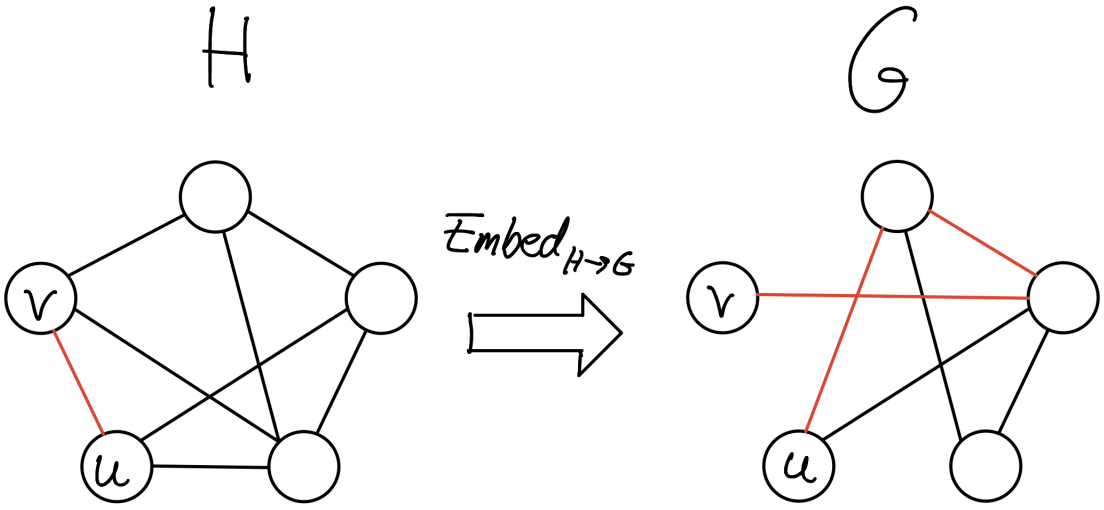


Figure 14.1: In this example the red edge (u, v) in H is mapped to the red u-to-v path in G.

[1]Technically, we will solve problems with two additional vertices and n additional edges but this will not change the run-time of any known max-flow algorithm asymptotically.

We say that the *congestion* of $\textsc{Embed}_{H\to G}$ is the maximum number of times that any edge $e \in E(G)$ appears on any embedding path:

$$cong(\textsc{Embed}_{H\to G}) = \max_{e\in E(G)} |\{e' \in E(H) \mid e \in \textsc{Embed}_{H\to G}(e')\}|.$$

Certifying Expander Graphs via Embeddings. Let us next prove the following lemma that is often consider Folklore.

Lemma 14.2.1. *Given a $\frac{1}{2}$-expander graph H and an embedding of H into G with congestion C, then G must be an $\Omega\left(\frac{1}{C}\right)$-expander.*

Proof. Consider any cut $(S, V \setminus S)$ with $|S| \leq |V \setminus S|$. Since H is a ψ-expander, we have that $|E_H(S, V \setminus S)| \geq |S|/2$. We also know by the embedding of H into G, that for each edge $(u, v) \in E_H(S, V \setminus S)$, we can find path a $P_{u,v}$ in G that also has to cross the cut $(S, V \setminus S)$ at least once. But since each edge in G is on at most C such paths, we can conclude that at least $|E_H(S, V \setminus S)|/C \geq |S|/2C$ edges in G cross the cut $(S, V \setminus S)$. □

Unfortunately, the reverse of the above lemma is not true, i.e. even if there exists no embedding from 1/2-expander H into G of congestion C, then G might still be an $\Omega\left(\frac{1}{C}\right)$-expander.

14.3 The Cut-Matching Algorithm

Although there are still some missing pieces, let us next discuss the algorithm 16. The algorithm runs for T iterations where we will later find that the right value to set T to is in $\Theta(\log^2 n)$.

Algorithm 16: $\textsc{SparsityCertifyOrCut}(G, \psi)$

for $i = 0, 1, 2, \ldots, T$ **do**
  $(S_i, \overline{S}_i) \leftarrow \textsc{FindBiPartition}(G, \{M_1, M_2, \ldots, M_i\})$; `// Assume` $|S| = |\overline{S}| = n/2$
  Solve the flow problem on G where each vertex $e \in E$ receives capacity $\boldsymbol{c}(e) = 1/\psi$ and the demand at each edge $v \in S$ is $+1$ and for each $v \in \overline{S}$ is -1, by introducing a super-source s and super-sink t;
  if *flow procedure returns a flow* $\boldsymbol{f}$ *with* $\text{val}(f) = n/2$ **then**
    Remove s, t to derive S-$\overline{S}$ flow; then decompose flow $\boldsymbol{f}$ into flow paths $P_1, P_2, \ldots, P_{n/2}$;
    Create a matching M_i where for each s-to-$\overline{s}$ flow path P_i, we add $(s, \overline{s})$ to M_i.
  else
    return the minimum cut $(X_S, X_{\overline{S}})$ in the flow problem after removing the super-source s and the super-sink t from the two sets.
return $H = \bigcup_i M_i$

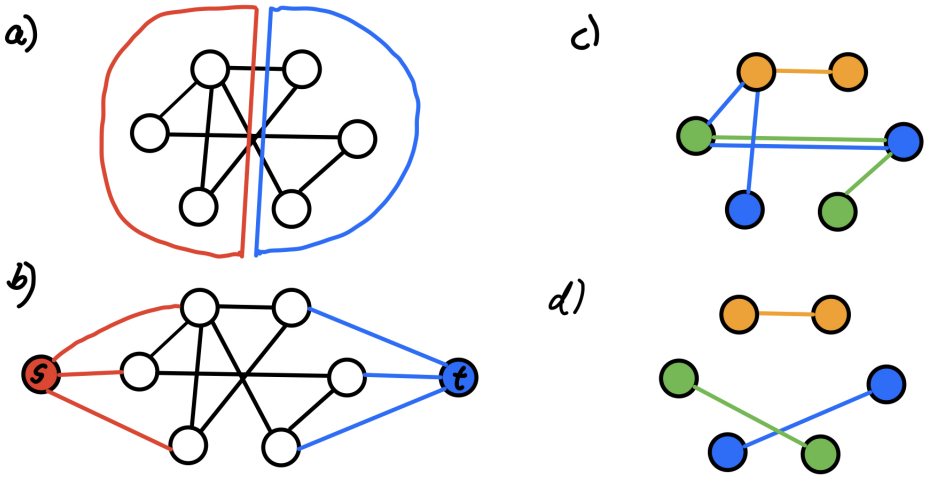


Figure 14.2: Illustration of the steps of the Algorithm. In a), a bi-partition of V is found. In b), the bi-partition is used to obtain a flow problem where we inject one unit of flow to each vertex in S via super-source s and extract one unit via super-sink t. c) A path flow decomposition. For each path, the first vertex is in S and the last vertex in $\overline{S}$. d) We find M_i to be the one-to-one matching between endpoints in S and $\overline{S}$ defined by the path flows.

Beginning of an Iteration. In each iteration of the algorithm, we first invoke a sub-procedure FindBiPartition$(\cdot)$ that returns a cut $(S, \overline{S})$ (where $\overline{S} = V \setminus S$) that partitions the vertex set into two equal-sized sides. Here, we implicitly assume that the number of vertices n is even which is w.l.o.g.

Next, the algorithm creates a flow problem where each vertex $s \in S$ has to send exactly one unit of flow and each vertex $\overline{s} \in S$ has to receive exactly one unit of flow. We therefore introduce dummy nodes s and t, add for each vertex $v \in S$ an edge of capacity 1 between s and v; and for each vertex $v \in \overline{S}$ and edge between t and v of capacity 1. We set the capacity of edges in the original graph G to $1/\psi$ (which we assume wlog to be integer).

The If Statement. If the flow problem can be solved exactly, then we can find a path decomposition of the flow $\boldsymbol{f}$ in $\tilde{O}(m)$ time (for example using a DFS) where each path starts in S ends in $\overline{S}$ and carries one unit of flow[2]. This defines a one-to-one correspondence between the vertices in S and the vertices in $\overline{S}$. We capture this correspondences in the matching M_i. We will later prove the following lemma.

Lemma 14.3.1. *If the algorithm returns after constructing T matchings, for an appropriately chosen $T = \Theta(\log^2 n)$, then the graph H returned by the algorithm is a $\frac{1}{2}$-expander and H can be embedded into G with congestion $O(\log^2 n/\psi)$.*

[2]For simplicity, assume that the returned flow is integral.

The Else Statement. On the other hand, if the flow problem on G could not be solved, then we return the min-cut of the flow problem. Such a cut can be found in $O(m)$ time by using the above reduction to an s-t flow problem on which one can compute maximum flow $\boldsymbol{f}$ from which the s-t min-cut can be constructed by following the construction in the proof of Theorem 11.4.4.

It turns out that this min-cut already is a sparse cut by the way our flow problem is defined.

Lemma 14.3.2. *If the algorithm finds a cut $(X_S, X_{\overline{S}})$, then the returned cut satisfies $|E_G(X_S \setminus \{s\}, X_{\overline{S}} \setminus \{t\})| = O(\psi)$.*

Proof. First observe that since a min-cut was returned, we have that $|E_G(X_S, X_{\overline{S}})| < n/2$ (otherwise we could have routed the demands).

Let n_s be the number of edges incident to the super-source s that cross the cut $(X_S, X_{\overline{S}})$. Let n_t be the number of edges incident to t that cross the cut $(X_S, X_{\overline{S}})$.

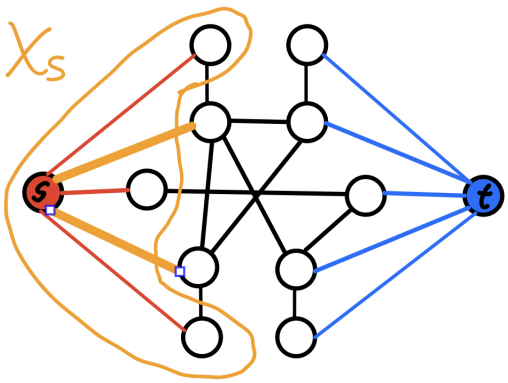


Figure 14.3: Set X_S is enclosed by the orange circle. The thick orange edges are in the cut and incident to super-source s. Thus they count towards n_s. Here $n_s = 2, n_t = 0$. Note that all remaining edges in the cut are black, i.e. were originally in G and therefore have capacity $1/\psi$.

Observe that after taking away the vertices s and t, the cut $(X_S \setminus \{s\}, X_{\overline{S}} \setminus \{t\})$ has less than $n/2 - n_s - n_t$ capacity. But each remaining edge has capacity $1/\psi$, so the total number of edges in the cut can be at most $\psi \cdot (n/2 - n_s - n_t)$. Since $X_S \setminus \{s\}$ is of size at least $n/2 - n_s$, and $X_{\overline{S}} \setminus \{t\}$ is of size at least $n/2 - n_t$, we have that the induced cut in G has

$$\psi(X_S \setminus \{s\}) < \frac{\psi \cdot (n/2 - n_s - n_t)}{\min\{n/2 - n_s, n/2 - n_t\}} \leq \psi.$$

□

14.4 Constructing an Expander via Random Walks

Next, we give the implementation and analysis for the procedure FindBiPartition$(\cdot)$. We start however by giving some more preliminaries.

Random Walk on Matchings. Let $\{M_1, M_2, \ldots, M_{T+1}\}$ be the set of matchings we compute (if we never find a cut). In the i^{th}-step of the lazy random walk, we let the mass at each vertex j stay put with probability $1/2$, and otherwise traverses the edge in matching M_i incident to j with probability $1/2$.

We let $\boldsymbol{p}^t_{j\mapsto i}$ denote the probability that a particle that started at vertex j is at vertex i after a t-step lazy random walk. We let $\boldsymbol{p}^t_i = [\boldsymbol{p}^t_{1\mapsto i}\ \boldsymbol{p}^t_{2\mapsto i}\ \ldots\ \boldsymbol{p}^t_{n\mapsto i}]$. Note that for each edge $(i,j) \in M_{t+1}$, we have that

$$\boldsymbol{p}^{(t+1)}_i = \frac{1}{2}\boldsymbol{p}^t_i + \frac{1}{2}\boldsymbol{p}^t_j = \boldsymbol{p}^{(t+1)}_j.$$

We define the projection matrix $\boldsymbol{\Pi}^t = [\boldsymbol{p}^t_1, \boldsymbol{p}^t_2, \ldots, \boldsymbol{p}^t_n]^\top$ that maps an initial probability distribution $\boldsymbol{d}$ to the probability distribution over the vertices that the random walk visits them at step t. You will prove in the exercises that $\boldsymbol{\Pi}^t$ is *doubly-stochastic*.

We say that a lazy random walk is *mixing* at step t, if for each i, j, $\boldsymbol{p}^t_{j\mapsto i} \geq 1/(2n)$.

Lemma 14.4.1. *If t-step lazy random walk is* mixing, *then $H = \bigcup_{i\leq t} M_i$ is a $\frac{1}{2}$-expander.*

Proof. Consider any cut $(S, \overline{S})$ with $|S| \leq |\overline{S}|$. It is convenient to think about the random walks in terms of probability mass that is moved around. Observe that each vertex $j \in \overline{S}$ has to push at least $1/(2n)$ units of probability from j to i (by definition of mixing).

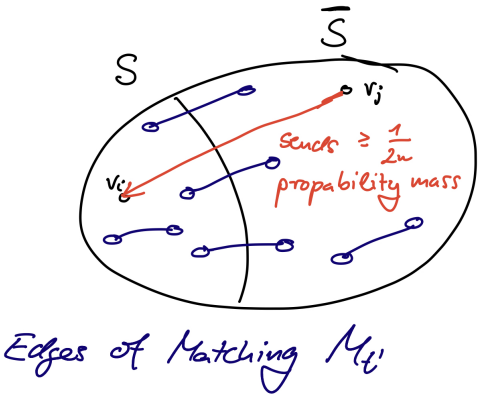


Figure 14.4: Each vertex $j \in \overline{S}$ sends at least $1/(2n)$ probability mass to i (red arrow). But in order to transport it, it does have to push the mass through edges in the matchings $M_1, M_2, \ldots, M_t$ that cross the cut.

Clearly, to move the mass from $\overline{S}$ to S it has to use the matching edges that also cross the cut.

Now observe that since there are $\geq n/2$ vertices in $\overline{S}$, and each of them has to push $\geq 1/(2n)$ mass to i, the total amount of probability mass pushed through the cut for i is $\geq 1/4$. Since there are $|S|$ such vertices i, the total amount of mass that has to cross the cut is $\geq |S|/4$. But note, that after each step of the random walk, the total probability mass at each vertex is exactly 1. Thus, at each step t', each edge in $M_{t'}$ crossing the cut can push at most $1/2$ units of probability mass over the cut (and thereafter the edge is gone).

It follows that there must be at least $|S|/2$ edges in the matchings $M_1, M_2, \ldots M_t$. But this implies that $H = \cup_i M_i$ is a $\frac{1}{2}$-expander.

□

Implementing FindBiPartition$(\cdot)$. We can now give away the implementation of FindBiPartition$(\cdot)$ which you can find below.

Algorithm 17: FindBiPartition$(G, \{M_1, M_2, \ldots, M_t\})$

Choose random n-dimensional vector $\boldsymbol{r}$ orthogonal to $\mathbf{1}$.;
Compute vector $\boldsymbol{u} = \boldsymbol{\Pi}^t \boldsymbol{r}$, i.e. each $\boldsymbol{u}(i) = \boldsymbol{p}_i^t \cdot \boldsymbol{r}$;
Let S be the $n/2$ smallest vertices w.r.t. $\boldsymbol{u}$; and $\overline{S}$ be the $n/2$ largest w.r.t $\boldsymbol{u}$ (ties broken arbitrarily but consistently).;
return $(S, \overline{S})$

The central claim, we want to prove is the following: given a potential function for the random walk at step t

$$\Phi^t = \sum_{i,j} (\boldsymbol{p}_{j \mapsto i}^t - 1/n)^2 = \sum_i \|\boldsymbol{p}_i^t - \mathbf{1}/n\|_2^2.$$

Claim 14.4.2. *In the algorithm* SparsityCertifyOrCut$(\cdot)$*, we have* $\mathbb{E}[\Phi^t - \Phi^{(t+1)}] = \Omega(\Phi^t / \log n) - O(1/n^{-5})$*. Further, we have that* $\Phi^t - \Phi^{(t+1)}$ *is always non-negative. The expectation is over the random vector* $\boldsymbol{r}$ *chosen in the current round.*

Corollary 14.4.3. *For appropriate* $T = \Theta(\log^2 n)$*, the algorithm* SparsityCertifyOrCut$(\cdot)$ *has* $\Phi^{(T+1)} \leq 4/n^2$*.*

To obtain the Corollary, one can simply set up a sequence of random 0-1 variables $X^1, X^2, \ldots, X^{(T+1)}$ where each $X^{(t+1)}$ is 1 if and only if the decrease in potential is at least an $\Omega(1/\log n)$-fraction of the previous potential. Since the expectation is only over the current $\boldsymbol{r}$ in each round and we choose these independently at random, one can then use a Chernoff bound to argue that after T rounds (for an appropriate hidden constant), one has at least $\Omega(T)$ rounds during which the potential is decreased substantially (unless it is already tiny and the $O(n^{-5})$ factor dominates).

We further observe that this implies that $\{M_1, M_2, \ldots, M_{T+1}\}$ is mixing (you can straightforwardly prove it by a proof of contradiction), and thereby we conclude the proof of our main theorem.

Let us now give the prove of Claim 14.4.2:

Interpreting the Potential Drop. Let us start by writing out the amount by which the potential decreases

$$\Phi^t - \Phi^{(t+1)} = \sum_i \|\boldsymbol{p}_i^t - \mathbf{1}/n\|_2^2 - \sum_i \|\boldsymbol{p}_i^{(t+1)} - \mathbf{1}/n\|_2^2$$

Considering now matching M_{t+1}, and an edge $(i,j) \in M_{t+1}$. We can re-write the former sum as $\sum_i \|\boldsymbol{p}_i^t - \mathbf{1}/n\|_2^2 = \sum_{(i,j)\in M_{t+1}} \|\boldsymbol{p}_i^t - \mathbf{1}/n\|_2^2 + \|\boldsymbol{p}_j^t - \mathbf{1}/n\|_2^2$ as each vertex occurs as exactly one endpoint of a matching edge. We can do the same for the $t+1$-step walk probabilities. Further, recall that for $(i,j) \in M_{t+1}$, we have $\boldsymbol{p}_i^{(t+1)} = \boldsymbol{p}_j^{(t+1)} = \frac{\boldsymbol{p}_i^t + \boldsymbol{p}_j^t}{2}$. Thus,

$$\begin{aligned}\Phi^t - \Phi^{(t+1)} &= \sum_{(i,j)\in M_{t+1}} \|\boldsymbol{p}_i^t - \mathbf{1}/n\|_2^2 + \|\boldsymbol{p}_j^t - \mathbf{1}/n\|_2^2 - \|\boldsymbol{p}_i^{(t+1)} - \mathbf{1}/n\|_2^2 - \|\boldsymbol{p}_j^{(t+1)} - \mathbf{1}/n\|_2^2 \\ &= \sum_{(i,j)\in M_{t+1}} \|\boldsymbol{p}_i^t - \mathbf{1}/n\|_2^2 + \|\boldsymbol{p}_j^t - \mathbf{1}/n\|_2^2 - 2\left\|\frac{\boldsymbol{p}_i^t + \boldsymbol{p}_j^t}{2} - \mathbf{1}/n\right\|_2^2.\end{aligned}$$

Finally, we can use the formula $\|\boldsymbol{x}\|^2 + \|\boldsymbol{y}\|^2 - 2\|(\boldsymbol{x}+\boldsymbol{y})/2\|^2 = \frac{1}{2}\|\boldsymbol{x}-\boldsymbol{y}\|^2$ term-wise to derive

$$\Phi^t - \Phi^{(t+1)} = \frac{1}{2}\sum_{(i,j)\in M_{t+1}} \|(\boldsymbol{p}_i^t - \mathbf{1}/n) - (\boldsymbol{p}_j^t - \mathbf{1}/n)\|_2^2 = \frac{1}{2}\sum_{(i,j)\in M_{t+1}} \|\boldsymbol{p}_i^t - \boldsymbol{p}_j^t\|_2^2.$$

The potential thus drops by a lot if vertices i and j are matched where $\boldsymbol{p}_i^t$ and $\boldsymbol{p}_j^t$ differ starkly. Note that this equality implies directly the remark in our claim that $\Phi^t - \Phi^{(t+1)}$ is non-negative.

Understanding the Random Projection. Next, we want to further lower bound the potential drop using the random vector $\boldsymbol{u}$. This intuitively helps a lot in our analysis since we are matching vertices i,j with high value $\boldsymbol{u}(i)$ and low value $\boldsymbol{u}(j)$ (or vice versa). We will show that (w.p. $\geq 1 - n^{-3}$)

$$\Phi^t - \Phi^{(t+1)} = \frac{1}{2}\sum_{(i,j)\in M_{t+1}} \|\boldsymbol{p}_i^t - \boldsymbol{p}_j^t\|_2^2 \geq \frac{n-1}{64\cdot\log n}\sum_{(i,j)\in M_{t+1}} |\boldsymbol{u}(i) - \boldsymbol{u}(j)|^2. \tag{14.1}$$

To prove this claim, we will prove this again term-wise, showing that for each pair of vertices $i,j \in V$, we have $\|\boldsymbol{p}_i^t - \boldsymbol{p}_j^t\|_2^2 \geq \frac{n-1}{16\cdot\log n}|\boldsymbol{u}(i) - \boldsymbol{u}(j)|^2$ w.h.p. It will then suffice to talk a union bound over all pairs i,j.

To this end, let us make the following observations: since $\boldsymbol{u}(i) = \boldsymbol{p}_i^t \cdot \boldsymbol{r}$, we have that $\boldsymbol{u}(i) - \boldsymbol{u}(j) = (\boldsymbol{p}_i^t - \boldsymbol{p}_j^t)\cdot\boldsymbol{r}$ by linearity. Also note that since $\sum_j \boldsymbol{p}_{j\mapsto i}^t = 1$ for all i (since $\boldsymbol{\Pi}^t$ is doubly-stochastic), we further have that the projection $(\boldsymbol{p}_i^t - \boldsymbol{p}_j^t)$ is orthogonal to $\mathbf{1}$.

We can now use the following statement about random vector $\boldsymbol{r}$ to argue about the effect of projecting $(\boldsymbol{p}_i^t - \boldsymbol{p}_j^t)$ onto $\boldsymbol{r}$. Below, we note that we have $d = n - 1$ since $\boldsymbol{r}$ is chosen from the $(n-1)$-dimensional space orthogonal to $\mathbf{1}$.

Theorem 14.4.4. *If $\boldsymbol{y}$ is a vector of length ℓ in $\mathbb{R}^d$, and $\boldsymbol{r}$ a unit random vector in $\mathbb{R}^d$, then*

- $\mathbb{E}[(\boldsymbol{y}^\top \boldsymbol{r})^2] = \frac{\ell^2}{d}$, *and*
- *for $x \leq d/16$, then $\mathbb{P}[(\boldsymbol{y}^\top \boldsymbol{r})^2 \geq x\ell^2/d] \leq e^{-x/4}$*

This allows us to pick $x = 32 \cdot \log n$, and we then we obtain that

$$\mathbb{P}\left[((\boldsymbol{p}_i^t - \boldsymbol{p}_j^t) \cdot \boldsymbol{r})^2 \geq \frac{32 \log n}{n-1} \|\boldsymbol{p}_i^t - \boldsymbol{p}_j^t\|_2^2\right] \leq e^{-4 \log n} = n^{-8}. \tag{14.2}$$

Multiplying both sides of the event by $(n-1)/(64 \log n)$, we derive the claimed Inequality (14.1). We can further union bound over the $n/2$ matching pairs to all satisfy this bound with probability $\geq 1 - n^{-7}$, as desired.

Relating to the Lengths of the Projections. Let $\mu = \max_{i \in S} \boldsymbol{u}(i)$, then we have by definition that $\boldsymbol{u}(i) \leq \mu \leq \boldsymbol{u}(j)$ for all $i \in S, j \in \overline{S}$.

Now we can write

$$\begin{aligned}
\Phi^t - \Phi^{(t+1)} &\geq \frac{n-1}{64 \cdot \log n} \sum_{(i,j) \in M_{t+1}} |\boldsymbol{u}(i) - \boldsymbol{u}(j)|^2 \\
&\geq \frac{n-1}{64 \cdot \log n} \sum_{(i,j) \in M_{t+1}} (\boldsymbol{u}(i) - \mu)^2 + (\boldsymbol{u}(j) - \mu)^2 \\
&= \frac{n-1}{64 \cdot \log n} \sum_{i \in V} (\boldsymbol{u}(i) - \mu)^2 \\
&= \frac{n-1}{64 \cdot \log n} \left(\sum_{i \in V} \boldsymbol{u}(i)^2 - 2\mu \cdot \sum_{i \in V} \boldsymbol{u}(i) + n\mu^2 \right)
\end{aligned}$$

by standard calculations. We then observe that $\sum_i \boldsymbol{u}(i) = \sum_i \boldsymbol{p}_i^t \cdot \boldsymbol{r} = \mathbf{1} \cdot \boldsymbol{r} = 0$ by the fact that $\boldsymbol{\Pi}^t$ is doubly-stochastic and since $\boldsymbol{r}$ is orthogonal to the all-ones vector. We can therefore conclude

$$\frac{n-1}{64 \cdot \log n} \left(\sum_{i \in V} \boldsymbol{u}(i)^2 - 2\mu \cdot \sum_i \boldsymbol{u}(i) + n\mu^2 \right) \geq \frac{n-1}{64 \cdot \log n} \sum_{i \in V} \boldsymbol{u}(i)^2. \tag{14.3}$$

Taking the Expectation. Then, from the second fact of Theorem 14.4.4, we obtain that

$$\mathbb{E}\left[\sum_{i\in V} \boldsymbol{u}(i)^2\right] = \sum_{i\in V} \mathbb{E}[\boldsymbol{u}(i)^2] = \sum_{i\in V} \mathbb{E}[(\boldsymbol{p}_i^t \cdot \boldsymbol{r})^2] = \sum_{i\in V} \mathbb{E}[(\boldsymbol{p}_i^t - \mathbf{1}/n) \cdot \boldsymbol{r})^2] \tag{14.4}$$

$$= \sum_{i\in V} \frac{\|\boldsymbol{p}_i^t - \mathbf{1}/n\|_2^2}{n-1} = \frac{\Phi^t}{n-1} \tag{14.5}$$

where we used again that $\boldsymbol{r}$ is orthogonal to $\mathbf{1}$.

Unfortunately, we cannot directly use this expectation since we already conditioned on the high probability events in Equation (14.2). But a simple trick allows us to recover: Let $\mathcal{E}$ denote the union of all of these events. We have by the law of total expectation

$$\mathbb{E}\left[\sum_{i\in V} \boldsymbol{u}(i)^2\right] = \mathbb{P}[\neg\mathcal{E}] \cdot \mathbb{E}\left[\sum_{i\in V} \boldsymbol{u}(i)^2 | \neg\mathcal{E}\right] + \mathbb{P}[\mathcal{E}] \cdot \mathbb{E}\left[\sum_{i\in V} \boldsymbol{u}(i)^2 | \mathcal{E}\right]$$

But note that $\mathbb{E}\left[\sum_{i\in V} \boldsymbol{u}(i)^2 | \mathcal{E}\right]$ has to be smaller than n because $\sum_{i\in V} \boldsymbol{u}(i)^2 = \sum_{i\in V} (\boldsymbol{p}_i^t \cdot \boldsymbol{r})^2 \leq n$ with probability 1 (because each $\boldsymbol{p}_i^t$ is a unit vector). Recall that we calculated $\mathbb{P}[\mathcal{E}] \leq n^{-7}$. Thus, we can conclude that $\mathbb{E}\left[\sum_{i\in V} \boldsymbol{u}(i)^2 | \neg\mathcal{E}\right] \geq \frac{\Phi^t}{n-1} - n^{-6}$.

It remains to combine our insights to conclude

$$\mathbb{E}[\Phi^t - \Phi^{(t+1)} | \neg\mathcal{E}] \geq \frac{n-1}{64 \cdot \log n} \left(\frac{\Phi^t}{n-1} - n^{-6}\right) = \Omega(\Phi^t / \log n) - O(1/n^{-5}).$$

Since again the event $\mathcal{E}$ occurs with very low probability, and since $\Phi^t - \Phi^{t+1}$ is non-negative always, we can then conclude that in unconditionally, in expectation, the potential decreases by $\Omega(\Phi^t / \log n) - O(1/n^{-5})$.

Part IV

Further Topics

Chapter 15

Separating Hyperplanes, Lagrange Multipliers, KKT Conditions, and Convex Duality

15.1 Overview

First part of this chapter introduces the concept of a separating hyperplane of two sets followed by a proof that for two closed, convex and disjoint sets a separating hyperplane always exists. This is a variant of the more general *separating hyperplane theorem*[1] due to Minkowski. Then *Lagrange multipliers* $\boldsymbol{x}$, $\boldsymbol{s}$ of a convex optimization problem

$$\begin{aligned} \min_{y} \ & \mathcal{E}(\boldsymbol{y}) \\ \text{s.t. } & \boldsymbol{A}\boldsymbol{y} = \boldsymbol{b} \\ & c(\boldsymbol{y}) \leq 0 \end{aligned}$$

are introduced and with that, the *Lagrangian*

$$\boldsymbol{L}(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}) = \mathcal{E}(\boldsymbol{y}) + \boldsymbol{x}^\top(\boldsymbol{b} - \boldsymbol{A}\boldsymbol{y}) + \boldsymbol{s}^\top c(\boldsymbol{y})$$

is defined. Finally, we deal with the dual problem

$$\max_{\boldsymbol{x},\boldsymbol{s},\boldsymbol{s}\geq 0} L(\boldsymbol{x}, \boldsymbol{s}),$$

where $L(\boldsymbol{x}, \boldsymbol{s}) = \min_y L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s})$. We show *weak duality*, i.e. $L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}) \leq \mathcal{E}(\boldsymbol{y})$ and that assuming *Slater's condition* the values of both the primal and dual is equal, which is referred to as *strong duality*.

[1] Wikipedia is good on this: https://en.wikipedia.org/wiki/Hyperplane_separation_theorem

15.2 Separating Hyperplane Theorem

Suppose we have two convex subsets $A, B \subseteq \mathbb{R}^n$ that are disjoint ($A \cup B = \emptyset$). We wish to show that there will always be a (hyper-)plane H that separates these two sets, i.e. A lies on one side, and B on the other side of H.

So what exactly do we mean by Hyperplane? Let's define it.

Definition 15.2.1 (Hyperplane)**.** A *hyperplane* H of dimension n is the subset $H := \{\boldsymbol{x} \in \mathbb{R}^n : \langle \boldsymbol{n}, \boldsymbol{x} \rangle = \mu\}$. We say H has *normal* $\boldsymbol{n} \in \mathbb{R}^n$ and *threshold* μ. It is required that $\boldsymbol{n} \neq \boldsymbol{0}$.

Every hyperplane divides $\mathbb{R}^n$ into two halfspaces $\{\boldsymbol{x} : \langle \boldsymbol{v}, \boldsymbol{x} \rangle \geq \mu\}$ and $\{\boldsymbol{x} : \langle \boldsymbol{v}, \boldsymbol{x} \rangle \leq \mu\}$. It separates two sets, if they lie in different halfspaces. We formally define separating hyperplane as follows.

Definition 15.2.2 (Separating Hyperplane)**.** We say a hyperplane H *separates* two sets A, B iff

$$\forall \boldsymbol{a} \in A : \langle \boldsymbol{n}, \boldsymbol{a} \rangle \geq \mu$$
$$\forall \boldsymbol{b} \in B : \langle \boldsymbol{n}, \boldsymbol{b} \rangle \leq \mu$$

If we replace $\geq$ with $>$ and $\leq$ with $<$ we say H *strictly* separates A and B.

It is easy to see that there exists disjoint non-convex sets that can not be separated by a hyperplane (e.g. a point cannot be separated from a ring around it). But can two disjoint convex sets always be strictly separated by a hyperplane? The answer is no: consider the two-dimensional case depicted in Figure 15.1 with $A = \{(x, y) : x \leq 0\}$ and $B = \{(x, y) : x > 0 \text{ and } y \geq \frac{1}{x}\}$. Clearly they are disjoint; however the only separating hyperplane is $H = \{(x, y) : x = 0\}$ but it intersects A.

One can prove that there exists a non-strictly separating hyperplane for any two disjoint convex sets. We will prove that if we further require A,B to be closed and bounded, then a strictly separating hyperplane always exists. (Note in the example above how our choice of B is not bounded.)

Theorem 15.2.3 (Separating Hyperplane Theorem; closed, bounded sets)**.** *For two closed, bounded, and disjoint convex sets $A, B \in \mathbb{R}^n$ there exists a strictly separating hyperplane H. One such hyperplane is given by normal $\boldsymbol{n} = \boldsymbol{d} - \boldsymbol{c}$ and threshold $\mu = \frac{1}{2}\left(\|\boldsymbol{d}\|_2^2 - \|\boldsymbol{c}\|_2^2\right)$, where $\boldsymbol{c} \in A$, $\boldsymbol{d} \in B$ are the minimizers of the distance between A and B*

$$dist(A, B) = \min_{\boldsymbol{a} \in A, \boldsymbol{b} \in B} \|\boldsymbol{a} - \boldsymbol{b}\|_2 > 0.$$

Proof. We omit the proof that $\text{dist}(A, B) = \min_{\boldsymbol{a} \in A, \boldsymbol{b} \in B} \|\boldsymbol{a} - \boldsymbol{b}\|_2 > 0$, which follows from A, B being disjoint, closed, and bounded. Now, we want to show that $\langle \boldsymbol{n}, \boldsymbol{b} \rangle > \mu$ for all $\boldsymbol{b} \in B$; then $\langle \boldsymbol{n}, \boldsymbol{a} \rangle < \mu$ for all $\boldsymbol{a} \in A$ follows by symmetry. Observe that

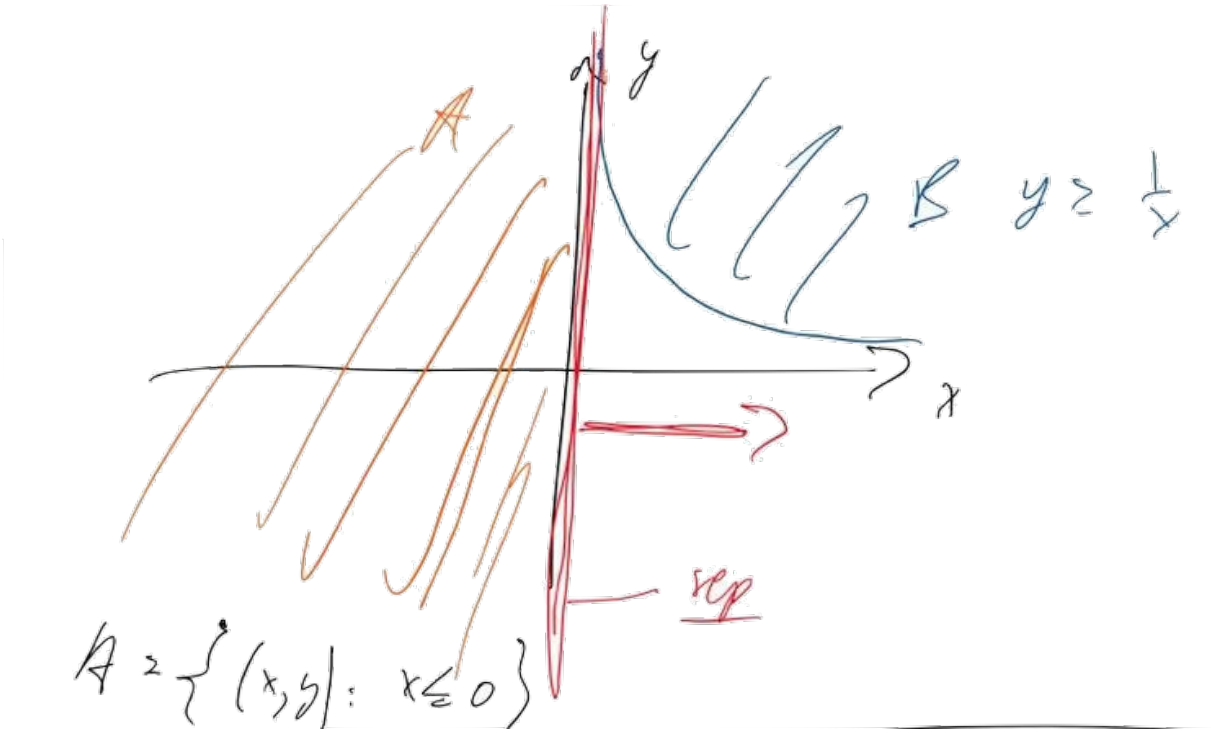


Figure 15.1: The sets $A = \{(x, y) : x \leq 0\}$ and $B = \{(x, y) : x > 0 \text{ and } y \geq \frac{1}{x}\}$ only permit a non-strictly separating hyperplane.

$$\begin{aligned}
\langle \boldsymbol{n}, \boldsymbol{d} \rangle - \mu &= \langle \boldsymbol{d} - \boldsymbol{c}, \boldsymbol{d} \rangle - \frac{1}{2} \left(\|\boldsymbol{d}\|_2^2 - \|\boldsymbol{c}\|_2^2 \right) \\
&= \|\boldsymbol{d}\|_2^2 - \boldsymbol{d}^\top \boldsymbol{c} - \frac{1}{2} \|\boldsymbol{d}\|_2^2 + \frac{1}{2} \|\boldsymbol{c}\|_2^2 \\
&= \frac{1}{2} \|\boldsymbol{d} - \boldsymbol{c}\|_2^2 > 0.
\end{aligned}$$

So suppose there exists $\boldsymbol{u} \in B$ such that $\langle \boldsymbol{n}, \boldsymbol{u} \rangle - \mu \leq 0$. We now look at the line defined by the distance minimizer $\boldsymbol{d}$ and the point on the "wrong side" $\boldsymbol{u}$. Define $\boldsymbol{b}(\lambda) = \boldsymbol{d} + \lambda(\boldsymbol{u} - \boldsymbol{d})$, and take the derivative of the distance between $\boldsymbol{b}(\lambda)$ and $\boldsymbol{c}$. Evaluated at $\lambda = 0$ (which is when $\boldsymbol{b}(\lambda) = \boldsymbol{d}$), this yields

$$\frac{d}{d\lambda} \|\boldsymbol{b}(\lambda) - \boldsymbol{c}\|_2^2 \Big|_{\lambda=0} = 2 \langle \boldsymbol{d} - \lambda \boldsymbol{d} + \lambda \boldsymbol{u} - \boldsymbol{c}, \boldsymbol{u} - \boldsymbol{d} \rangle|_{\lambda=0} = 2 \langle \boldsymbol{d} - \boldsymbol{c}, \boldsymbol{u} - \boldsymbol{d} \rangle .$$

However, this would imply that the gradient is strictly negative since

$$\begin{aligned}
\langle \boldsymbol{n}, \boldsymbol{u} \rangle - \mu &= \langle \boldsymbol{d} - \boldsymbol{c}, \boldsymbol{u} \rangle - \langle \boldsymbol{d} - \boldsymbol{c}, \boldsymbol{d} \rangle + \langle \boldsymbol{d} - \boldsymbol{c}, \boldsymbol{d} \rangle - \mu \\
&= \langle \boldsymbol{d} - \boldsymbol{c}, \boldsymbol{u} - \boldsymbol{d} \rangle + \|\boldsymbol{d}\|_2^2 - \langle \boldsymbol{c}, \boldsymbol{d} \rangle - \frac{1}{2} \|\boldsymbol{d}\|_2^2 + \frac{1}{2} \|\boldsymbol{c}\|_2^2 \\
&= \langle \boldsymbol{d} - \boldsymbol{c}, \boldsymbol{u} - \boldsymbol{d} \rangle + \frac{1}{2} \|\boldsymbol{d} - \boldsymbol{c}\|_2^2 \leq 0.
\end{aligned}$$

This contradicts the minimality of $\boldsymbol{d}$ and thus concludes this proof. □

A more general separating hyperplane theorem holds even when the sets are not closed and bounded:

Theorem 15.2.4 (Separating Hyperplane Theorem)**.** *Given two disjoint convex sets $A, B \in \mathbb{R}^n$ there exists a hyperplane H separating them.*

15.3 Lagrange Multipliers and Duality of Convex Problems

In this Section, we'll learn about *Langrange Multipliers* and how they lead to convex duality. But first, let's see an example to help illustrate where these ideas come from.

Imagine you were to prove that for all $\boldsymbol{x} \in \mathbb{R}^n$ we have $\|\boldsymbol{x}\|_p \leq n^{\frac{1}{2}-\frac{1}{p}} \|\boldsymbol{x}\|_2$ for some $1 \leq p \leq 2$;. We can look at this as optimizing $\max_{\boldsymbol{x}} \|\boldsymbol{x}\|_p$ subject to $\|\boldsymbol{x}\|_2$ being constant, e.g. simply $\|\boldsymbol{x}\|_2 = 1$. Then the statement above follows from a scaling argument.

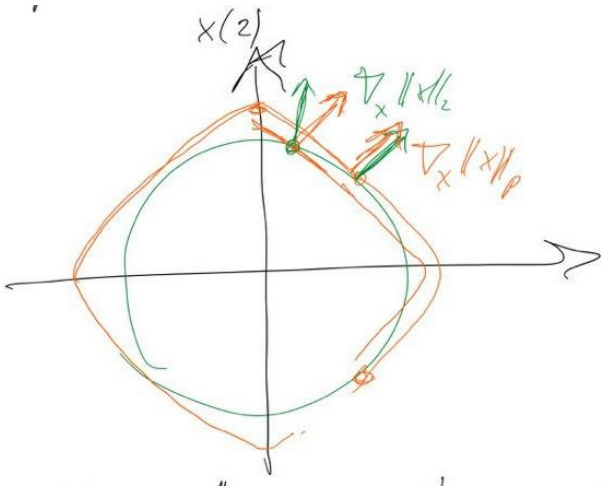


Figure 15.2: Looking at fixed $\|\boldsymbol{x}\|_p = \alpha$ and $\|\boldsymbol{x}\|_2 = 1$. (Here, $p = 1.5$.)

If we move from $\boldsymbol{x}$ to $\boldsymbol{x}+\boldsymbol{\delta}$ with $\boldsymbol{\delta} \perp \boldsymbol{\nabla}_{\boldsymbol{x}} \|\boldsymbol{x}\|_2$ and $\boldsymbol{\delta} \not\perp \boldsymbol{\nabla}_{\boldsymbol{x}} \|\boldsymbol{x}\|_p$ means that for infinitesimally small $\boldsymbol{\delta}$ the 2-norm stays constant but the p-norm changes. That means for either $\boldsymbol{x} - \boldsymbol{\delta}$ or $\boldsymbol{x} + \boldsymbol{\delta}$ the p-norm increases while the 2-norm stays constant. Hence at the maximum of $\|\boldsymbol{x}\|_p$ the gradients of both norms have to be parallel, i.e.

$$\boldsymbol{\nabla}_{\boldsymbol{x}} \left(\|\boldsymbol{x}\|_p - \lambda \|\boldsymbol{x}\|_2 \right) = 0.$$

This insight is the core idea of Lagrange multipliers (in this case λ).

Note that here the problem is not convex, because $\{\boldsymbol{x} : \|\boldsymbol{x}\|_2^2 = 1\}$ is not convex and because we are asking to *maximize* a norm. In the following we will study Lagrange multipliers for general convex problems.

15.3.1 Karush-Kuhn Tucker Optimality Conditions for Convex Problems

A full formal treament of convex duality would require us to be more careful about using inf and sup in place of min and max, as well as considering problems that have no feasible solutions. Today, we'll ignore these concerns.

Let us consider a general convex optimization problem with convex objective, linear equality constraints and convex inequality constraints

$$\begin{aligned} &\min_{y \in S} \mathcal{E}(\boldsymbol{y}) \\ &\text{s.t. } \boldsymbol{A}\boldsymbol{y} = \boldsymbol{b} \\ &\qquad \boldsymbol{c}(\boldsymbol{y}) \leq \boldsymbol{0}, \end{aligned} \tag{15.1}$$

where $\mathcal{E}(\boldsymbol{y}) : S \to \mathbb{R}$ is defined on a convex subset $S \subseteq \mathbb{R}^n$, $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ and $\boldsymbol{c}(\boldsymbol{y})$ is a vector of constraints $\boldsymbol{c}(\boldsymbol{y}) = (c_i(\boldsymbol{y}))_{i \in [k]}$. For every $i \in [k]$ the function $c_i : S \to \mathbb{R}$ should be convex, which implies the sublevel set $\{y : c_i(\boldsymbol{y}) \leq 0\}$ is convex. Given a solution $\boldsymbol{y}$, we say an inequality constraint is *tight* at $\boldsymbol{y}$ if $c_i(\boldsymbol{y}) = 0$. In the following we will denote by $\alpha^* = \mathcal{E}(\boldsymbol{y}^*)$ the optimal value of this program where $\boldsymbol{y}^*$ is a minimizer.

We will call this *the primal program* – and later we will see that we can associate another related convex program with any such convex program – and we will call this second program *the dual program*.

Definition 15.3.1 (Primal feasibility)**.** We say that $\boldsymbol{y} \in S$ is *primal feasible* if all constraints are satisfied, i.e. $\boldsymbol{A}\boldsymbol{y} = \boldsymbol{b}$ and $\boldsymbol{c}(\boldsymbol{y}) \leq \boldsymbol{0}$.

Now, as we did in our example with the 2- and p-norms, we will try to understand the relationship between the gradient of the objective function and of the constraint functions at an optimal solution $\boldsymbol{y}^*$.

An (not quite true!) intuition. Suppose $\boldsymbol{y}^*$ is an optimal solution to the convex program above. Let us additionally suppose that $\boldsymbol{y}^*$ is *not* on the boundary of S. Then, generally speaking, because we are at a constrained minimum of $\mathcal{E}(\boldsymbol{y}^*)$, we must have that for any infinitesimal $\boldsymbol{\delta}$ s.t. $\boldsymbol{y}^* + \boldsymbol{\delta}$ is also feasible, $\boldsymbol{\delta}^\top \boldsymbol{\nabla} \mathcal{E}(\boldsymbol{y}^*) \geq 0$, i.e. the infinitesimal does not decrease the objective. We can also view this as saying that if $\boldsymbol{\delta}^\top \boldsymbol{\nabla} \mathcal{E}(\boldsymbol{y}^*) < 0$, the update must be infeasible. But what kind of updates will make $\boldsymbol{y}^* + \boldsymbol{\delta}$ infeasible? This will be true if $\boldsymbol{a}_j^\top \boldsymbol{\delta} \neq 0$ for some linear constraint j or, roughly speaking, $\boldsymbol{\nabla} c_i(\boldsymbol{y}^*)^\top \boldsymbol{\delta} \neq 0$ for some *tight* inequality constraint. But, if this is true for *all* directions that have a negative inner product with $\boldsymbol{\nabla} \mathcal{E}(\boldsymbol{y}^*)$, then we must have that $-\boldsymbol{\nabla} \mathcal{E}(\boldsymbol{y}^*)$ can be written as a linear combination of $\boldsymbol{a}_j$, i.e. gradients of the linear constraint, and of gradients $\boldsymbol{\nabla} c_i(\boldsymbol{y}^*)$ of tight inequality constraints, and furthermore the cofficients of the gradients of these tight inequality constraints must be *positive*, so that moving along this direction will increase the function value and violate the constraint.

To recap, given cofficients $\boldsymbol{x} \in \mathbb{R}^m$ and $\boldsymbol{s} \in \mathbb{R}^k$ with $\boldsymbol{s}(i) \geq 0$ if $c_i(\boldsymbol{y}^*) = 0$, and $\boldsymbol{s}(i) = 0$ otherwise, we should be able to write

$$-\nabla_{\boldsymbol{y}} \mathcal{E}(\boldsymbol{y}^*) = \sum_j \boldsymbol{x}(j)\boldsymbol{a}_j + \sum_i \boldsymbol{s}(i)\nabla c_i(\boldsymbol{y}^*) \tag{15.2}$$

Note that since $\boldsymbol{y}^*$ is feasible, and hence $\boldsymbol{c}(\boldsymbol{y}^*) \leq 0$, we can write the condition that $\boldsymbol{s}(i) \geq 0$ if $c_i(\boldsymbol{y}^*) = 0$, and $\boldsymbol{s}(i) = 0$ otherwise, in a very slick way: namely as $\boldsymbol{s} \geq \mathbf{0}$ and $\boldsymbol{s}^\top \boldsymbol{c}(\boldsymbol{y}^*) = 0$. Traditionally, the variables in $\boldsymbol{s}$ are called *slack variables*, because of this, i.e. they are non-zero only if there is no *slack* in the constraint. This condition has a fancy name: when $\boldsymbol{s}^\top \boldsymbol{c}(\boldsymbol{y}) = 0$ for some feasible $\boldsymbol{y}$ and $\boldsymbol{s} \geq \mathbf{0}$, we say that $\boldsymbol{y}$ and $\boldsymbol{s}$ satisfy *complementary slackness*. We will think of the vectors $\boldsymbol{s}$ and $\boldsymbol{x}$ as variables that help us prove optimality of a current solution $\boldsymbol{y}$, and we call them *dual variables*.

Definition 15.3.2 (Dual feasibility)**.** We say $(\boldsymbol{x}, \boldsymbol{s})$ is dual feasible if $\boldsymbol{s} \geq 0$. If additionally $\boldsymbol{y}$ is primal feasible, we say $(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s})$ is primal-dual feasible.

Now, we have essentially argued that at any optimal solution $\boldsymbol{y}^*$, we must have that complementary slackness holds, and that Equation (15.2) holds for some $\boldsymbol{x}$ and some $\boldsymbol{s} \geq \mathbf{0}$. However, while this intuitive explanation is largely correct, it turns out that it can fail for technical reasons in some weird situations[2]. Nonetheless, under some mild conditions, it is indeed true that the conditions we argued for above must hold at any optimal solution. These conditions have a name: The Karush-Kuhn-Tucker Conditions. For convenience, we will state the conditions using $\nabla \boldsymbol{c}(\boldsymbol{y})$ to denote the matrix whose ith column is given by $\nabla c_i(\boldsymbol{y})$. This is sometimes called the Jacobian of $\boldsymbol{c}$.

Definition 15.3.3 (The Karush-Kuhn-Tucker (KKT) Conditions)**.** Given a convex optimization problem of form (15.1) where the domain S is *open*. Suppose $\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}$ satisfy the following conditions:

- $\boldsymbol{A}\boldsymbol{y} = \boldsymbol{b}$ and $\boldsymbol{c}(\boldsymbol{y}) \leq 0$ (primal feasibility)
- $\boldsymbol{s} \geq 0$ (dual feasibility)
- $\nabla_{\boldsymbol{y}} \mathcal{E}(\boldsymbol{y}) + \boldsymbol{A}^\top \boldsymbol{x} + \nabla \boldsymbol{c}(\boldsymbol{y})\boldsymbol{s} = \mathbf{0}$ (KKT gradient condition, i.e. Eq. (15.2) restated)
- $\boldsymbol{s}(i) \cdot \boldsymbol{c}_i(\boldsymbol{y}) = 0$ for all i (complementary slackness)

Then we say that $\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}$ satisfy the *Karush-Kuhn-Tucker* (KKT) conditions.

[2]Consider the following single-variable optimization problem

$$\begin{aligned} &\min_{x \in \mathbb{R}} x \\ &\text{s.t. } x^2 = 0. \end{aligned}$$

This has only a single feasible point $x = 0$, which must then be optimal. But at this point, the gradient of the constraint function is zero, while the gradient of the objective is non-zero. Thus our informal reasoning breaks down, because there exists an infeasible direction δ we can move along where the constraint function grows, but at a rate of $O(\delta^2)$.

15.3.2 Slater's Condition

There exists many different mild technical conditions under which the KKT conditions do indeed hold at any optimal solution $\boldsymbol{y}$. The simplest and most useful is probably *Slater's condition*.

Definition 15.3.4 (Slater's condition with full domain)**.** A (primal) problem as defined in (15.1) with $S = \mathbb{R}^n$ fulfills Slater's condition if there exists a *strictly feasible* point, i.e. there exists $\tilde{\boldsymbol{y}}$ s.t. $\boldsymbol{A}\tilde{\boldsymbol{y}} = \boldsymbol{b}$ and $\boldsymbol{c}(\tilde{\boldsymbol{y}}) < \boldsymbol{0}$. This means that the strictly feasible point $\tilde{\boldsymbol{y}}$ lies strictly inside the set $\{\boldsymbol{y} : \boldsymbol{c}(\boldsymbol{y}) \leq \boldsymbol{0}\}$ defined by the inequality constraints.

One way to think about Slater's condition is that your inequality constraints should not restrict the solution space to be lower-dimensional. This is a degenerate case as the sublevel sets of the inequality constraints are generically full-dimenensional and you want to avoid this degenerate case.

We can also extend Slater's condition to the case when the domain S is an open set. To extend Slater's condition to this case, we need the notion of a "relative interior".

Definition 15.3.5 (Relative interior)**.** Given a convex set $S \subset \mathbb{R}^n$, the *relative interior* of S is

$$\text{relint}(S) = \{x \in S : \text{ for all } \boldsymbol{y} \in S \text{ there exists } \epsilon > 0 \text{ such that } \boldsymbol{x} - \epsilon(\boldsymbol{y} - \boldsymbol{x}) \in S\}.$$

In other words, $\boldsymbol{x} \in \text{relint}(S)$ if starting at $\boldsymbol{x} \in S$ we can move "away" from any $\boldsymbol{y} \in S$ by a little and still be in $\boldsymbol{S}$. As an example, suppose $S = \{(s,t) \in \mathbb{R}^2 \text{ such that } s \geq 0 \text{ and } t = 0\}$. Then $(0,0) \in S$ but $(0,0) \notin \text{relint}(S)$, while $(1,0) \in \text{relint}(S)$.

Now, we can state a more general version of Slater's condition.

Definition 15.3.6 (Slater's condition)**.** A (primal) problem as defined in (15.1) fulfills Slater's condition if there exists a *strictly feasible* point $\tilde{\boldsymbol{y}} \in \text{relint}(S)$. We require $\boldsymbol{A}\tilde{\boldsymbol{y}} = \boldsymbol{b}$ and $\boldsymbol{c}(\tilde{\boldsymbol{y}}) < \boldsymbol{0}$. This means that the strictly feasible point $\tilde{\boldsymbol{y}}$ lies strictly inside the set $\{\boldsymbol{y} : \boldsymbol{c}(\boldsymbol{y}) \leq \boldsymbol{0}\}$ defined by the inequality constraints.

Finally, we end with a proposition that tells us that given Slater's condition, the KKT are indeed necessary for optimality of our convex programs.

Proposition 15.3.7 (KKT necessary for optimality when Slater's condition holds)**.** *Consider a convex program in the form* (15.1) *that satisfies Slater's condition and has an open set S as its domain. Suppose $\boldsymbol{y}$ is a primal optimal (feasible) solution, and that $\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}$ satisfy the KKT conditions.*

We will prove this lemma later, after developing some tools we will use in the proof. In fact, we will also see later that assuming Slater's condition, the KKT conditions are sufficient for optimality.

15.3.3 The Lagrangian and The Dual Program

Notice that we can also rewrite the KKT gradient condition as

$$\nabla_{\boldsymbol{y}} \left[\underbrace{\mathcal{E}(\boldsymbol{y}) + \boldsymbol{x}^\top(\boldsymbol{b} - \boldsymbol{A}\boldsymbol{y}) + \boldsymbol{s}^\top \boldsymbol{c}(\boldsymbol{y})}_{(\star)} \right] = \boldsymbol{0}$$

That is, we can write this condition as the gradient of the quantity $(\star)$ is zero. But what is this quantity $(\star)$? We call it *the Lagrangian* of the program.

Definition 15.3.8. Given a convex program (15.1), we define the *Lagrangian* of the program as

$$L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}) = \mathcal{E}(\boldsymbol{y}) + \boldsymbol{x}^\top(\boldsymbol{b} - \boldsymbol{A}\boldsymbol{y}) + \boldsymbol{s}^\top \boldsymbol{c}(\boldsymbol{y}).$$

We also define a Lagrangian only in terms of the dual variables by minimizing over $\boldsymbol{y}$ as

$$L(\boldsymbol{x}, \boldsymbol{s}) = \min_{\boldsymbol{y}} L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}).$$

When $\boldsymbol{s} \geq 0$, we have that $L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s})$ is a convex function of $\boldsymbol{y}$. For each $\boldsymbol{y}$, the Lagrangian $L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s})$ is linear in $(\boldsymbol{x}, \boldsymbol{s})$ and hence also concave in them. Hence $L(\boldsymbol{x}, \boldsymbol{s})$ is a concave function, because it is the pointwise minimum (over $\boldsymbol{y}$), of a collection of concave functions in $(\boldsymbol{x}, \boldsymbol{s})$.

We can think of $\boldsymbol{x}$ as assigning a price to violating the linear constraints, and of $\boldsymbol{s}$ as assigning a price to violating the inequality constraints. The KKT gradient condition tells us that at the given prices, the there is no benefit gained from locally violating the constraints – i.e. changing the primal solution $\boldsymbol{y}$ would not improve the cost.

Notice that if $\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}$ are primal-dual feasible, then

$$\begin{aligned} \mathcal{E}(\boldsymbol{y}) &= \mathcal{E}(\boldsymbol{y}) + \boldsymbol{x}^\top(\boldsymbol{b} - \boldsymbol{A}\boldsymbol{y}) && \text{as } \boldsymbol{b} - \boldsymbol{A}\boldsymbol{y} = \boldsymbol{0}. \\ &\geq \mathcal{E}(\boldsymbol{y}) + \boldsymbol{x}^\top(\boldsymbol{b} - \boldsymbol{A}\boldsymbol{y}) + \boldsymbol{s}^\top \boldsymbol{c}(\boldsymbol{y}) && \text{as } \boldsymbol{c}(\boldsymbol{y}) \leq \boldsymbol{0} \text{ and } \boldsymbol{s} \geq \boldsymbol{0}. \\ &= L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}) && (15.3) \end{aligned}$$

Thus, for primal-dual feasible variables, the Lagrangian is always a lower bound on the objective value.

$L(\boldsymbol{x}, \boldsymbol{s})$ is defined by minizming $L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s})$ over $\boldsymbol{y}$, i.e. what is the worst case value of the lower bound $L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s})$ across all $\boldsymbol{y}$. We can think of this as computing how good the given "prices" are at approximately enforcing the constraints. This naturally leads to a new optimization problem: How can we choose our prices $\boldsymbol{x}, \boldsymbol{s}$ to get the best (highest) possible lower bound?

Definition 15.3.9 (Dual problem)**.** We define the *dual problem* as

$$\max_{\substack{\boldsymbol{x}, \boldsymbol{s} \\ \boldsymbol{s} \geq 0}} \min_{\boldsymbol{y}} L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}) = \max_{\substack{\boldsymbol{x}, \boldsymbol{s} \\ \boldsymbol{s} \geq 0}} L(\boldsymbol{x}, \boldsymbol{s}) \tag{15.4}$$

and denote the optimal dual value by β^*.

The dual problem is really a convex optimization problem in disguise, because we can flip the sign of $-L(\boldsymbol{x}, \boldsymbol{s})$ to get a convex function and minimizing this is equivalent to maximizing $L(\boldsymbol{x}, \boldsymbol{s})$.

$$\max_{\substack{\boldsymbol{x},\boldsymbol{s} \\ \boldsymbol{s}\geq 0}} L(\boldsymbol{x}, \boldsymbol{s}) = -\min_{\substack{\boldsymbol{x},\boldsymbol{s} \\ \boldsymbol{s}\geq 0}} -L(\boldsymbol{x}, \boldsymbol{s})$$

When $\boldsymbol{x}$ and $\boldsymbol{s}$ are optimal for the dual program, we say they are dual optimal. And for convenience, when we also have a primal optimal $\boldsymbol{y}$, altogether, we will say that $(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s})$ are primal-dual optimal.

The primal problem can also be written in terms of the Lagrangian.

$$\alpha^* = \min_{\boldsymbol{y}} \max_{\boldsymbol{x};\boldsymbol{s}\geq \boldsymbol{0}} L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}) \tag{15.5}$$

This is because for a minimizing $\boldsymbol{y}$ all constraints have to be satisfied and the Lagrangian simplifies to $L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}) = \mathcal{E}(\boldsymbol{y})$. If $\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b} = \boldsymbol{0}$ was violated, making $\boldsymbol{x}$ large sends $L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}) \to \infty$. And if $\boldsymbol{c}(\boldsymbol{y}) \leq \boldsymbol{0}$ is violated, we can make $L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}) \to \infty$ by choosing large $\boldsymbol{s}$.

Note that we require $\boldsymbol{s} \geq \boldsymbol{0}$, as we only want to penalize the violation of the inequality constraints in one direction, i.e. when $\boldsymbol{c}(\boldsymbol{y}) > 0$.

For any primal-dual feasible $\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}$ we have $L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}) \leq \mathcal{E}(\boldsymbol{y})$ (see Equation (15.3)) and hence also $L(\boldsymbol{x}, \boldsymbol{s}) = \min_y L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}) \leq \mathcal{E}(\boldsymbol{y})$.

In other words $\max_{\boldsymbol{x};\boldsymbol{s}\geq 0} L(\boldsymbol{x}, \boldsymbol{s}) = \beta^* \leq \alpha^*$. This is referred to as *weak duality*.

Using the forms in Equations (15.4) and (15.5), we can also state this as

Theorem 15.3.10 (The Weak Duality Theorem)**.** *For any convex program* (15.4) *and its dual, we have*

$$\alpha^* = \min_{\boldsymbol{y}} \max_{\boldsymbol{x};\boldsymbol{s}\geq \boldsymbol{0}} L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}) \geq \max_{\boldsymbol{x};\boldsymbol{s}\geq \boldsymbol{0}} \min_{\boldsymbol{y}} L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}) = \beta^*.$$

15.3.4 Strong Duality

So now that we have proved weak duality $\beta^* \leq \alpha^*$, what is strong duality? $\beta^* = \alpha^*$? The answer is yes, but strong duality only holds under some conditions. Again, a simple sufficient condition is Slater's condition (Definition 15.3.6.

Theorem 15.3.11. *For a program* (15.1) *satisfying Slater's condition, strong duality holds, i.e.* $\alpha^* = \beta^*$*. In other words, the optimal value of the primal problem* α^* *is equal to the optimal value of the dual.*

Note that at primal optimal $\boldsymbol{y}^*$ and dual optimal $\boldsymbol{x}^*, \boldsymbol{s}^*$, we have

$$\alpha^* = \mathcal{E}(\boldsymbol{y}^*) \geq L(\boldsymbol{y}^*, \boldsymbol{x}^*, \boldsymbol{s}^*) \geq \beta^* = \alpha^*.$$

Thus, we can conclude that $L(\boldsymbol{y}^*, \boldsymbol{x}^*, \boldsymbol{s}^*) = \alpha^* = \beta^*$.

How are we going to prove this? Before we prove the theorem, let's make a few observations to get us warmed up. If you get bored, skip ahead to the proof.

It is sufficient to prove that $\alpha^* \leq \beta^*$, as the statement then follows in conjunction with weak duality. We define the set

$$G = \{(\mathcal{E}(\boldsymbol{y}), \boldsymbol{A}\boldsymbol{y} - \boldsymbol{b}, \boldsymbol{c}(\boldsymbol{y})) : \boldsymbol{y} \in S\},$$

where $S \subseteq \mathbb{R}^n$ is the domain of $\mathcal{E}$.

Immediately, we observe that we can write the optimal primal value as

$$\alpha^* = \min\{t : (t, \boldsymbol{v}, \boldsymbol{u}) \in G, \boldsymbol{v} = \boldsymbol{0}, \boldsymbol{u} \leq \boldsymbol{0}\}.$$

Similarly, we can write the Lagrangian (after minimizing over $\boldsymbol{y}$)

$$L(\boldsymbol{x}, \boldsymbol{s}) = \min_{(t,\boldsymbol{v},\boldsymbol{u})\in G} (1, \boldsymbol{x}, \boldsymbol{s})^\top (t, \boldsymbol{v}, \boldsymbol{u}).$$

This is equivalent to the inequality, for $(t, \boldsymbol{v}, \boldsymbol{u}) \in G$,

$$(1, \boldsymbol{x}, \boldsymbol{s})^\top (t, \boldsymbol{v}, \boldsymbol{u}) \geq L(\boldsymbol{x}, \boldsymbol{s}).$$

which defines a hyperplane with $\boldsymbol{n} = (1, \boldsymbol{x}, \boldsymbol{s})$ and $\mu = L(\boldsymbol{x}, \boldsymbol{s})$ such that G is on one side.

To establish strong duality, we would like to show the existence of a hyperplane such that for $(t, \boldsymbol{v}, \boldsymbol{u}) \in G$

$$\boldsymbol{n}^\top (t, \boldsymbol{v}, \boldsymbol{u}) \geq \alpha^* \text{ and } \boldsymbol{n} = (1, \widehat{\boldsymbol{x}}, \widehat{\boldsymbol{s}}) \text{ with } \widehat{\boldsymbol{s}} \geq \boldsymbol{0}.$$

Then we would immediately get

$$\beta^* \geq L(\widehat{\boldsymbol{x}}, \widehat{\boldsymbol{s}}) = \min_{(t,\boldsymbol{v},\boldsymbol{u})\in G} (1, \boldsymbol{x}, \boldsymbol{s})^\top (t, \boldsymbol{v}, \boldsymbol{u}) \geq \alpha^*.$$

Perhaps not surprisingly, we will use the Separating Hyperplane Theorem. What are the challenges we need to deal with?

- We need to replace G with a convex set (which we will call A) and separate A from some other convex set (which we will call B).
- We need to make sure the hyperplane normal $\boldsymbol{n}$ has 1 in the first coordinate and $\boldsymbol{s} \geq \boldsymbol{0}$, and the hyperplane threshold is α^*.

Proof of Theorem 15.3.11. For simplicity, our proof will assume that $S = \mathbb{R}^n$, but only a little extra work is required to handle the general case.

Let's move to on finding two convex disjoints sets A, B to enable the use of the separating hyperplane Theorem 15.2.4.

First set we define A, roughly speaking, as a multi-dimensional epigraph of G. More precisely

$$A = \{(t, \boldsymbol{v}, \boldsymbol{u}) : \exists \boldsymbol{y} \in S, t \geq \mathcal{E}(\boldsymbol{y}), \boldsymbol{v} = \boldsymbol{A}\boldsymbol{y} - \boldsymbol{b}, \boldsymbol{u} \geq \boldsymbol{c}(\boldsymbol{y})\}.$$

Note that A is a convex set. The proof is similar to the proof that the epigraph of a convex function is a convex set. The optimal value of the primal program can be now written as

$$\alpha^* = \min_{(t,\mathbf{0},\mathbf{0}) \in A} t.$$

And we define another set B of the same dimensionality as A by

$$B := \{(r \in \mathbb{R}, \mathbf{0} \in \mathbb{R}^m, \mathbf{0} \in \mathbb{R}^k) : r < \alpha^*\}.$$

This set B is convex, as it is a ray. An example of two such sets A, B is illustrated in Figure 15.3.

We show that $A \cap B = \emptyset$ by contradiction. Suppose A, B are not disjoint; then there exists $\boldsymbol{y}$ such that

$$(\mathcal{E}(\boldsymbol{y}), \boldsymbol{A}\boldsymbol{y} - \boldsymbol{b}, \boldsymbol{c}(\boldsymbol{y})) = (r, \mathbf{0}, \boldsymbol{u})$$

with $\boldsymbol{u} \leq \mathbf{0}$. But this means that $\boldsymbol{y}$ is feasible and $\mathcal{E}(\boldsymbol{y}) = r < \alpha^*$; contradicting the optimality of α^*.

To make things simpler, we assume that our linear constraint matrix $\boldsymbol{A} \in \mathbb{R}^{m \times n}$, has full row rank and $m < n$ (but very little extra work is required to deal with the remaining cases, which we omit).

As we just proved, A and B are convex and disjoint sets and hence the separating hyperplane theorem (Theorem 15.2.4) we introduced earlier in this chapter implies the existence a separating hyperplane. This means there exists a normal $\boldsymbol{n} = (\tilde{\rho}, \tilde{\boldsymbol{x}}, \tilde{\boldsymbol{s}})$ and threshold μ and with A on one side, i.e.

$$(t, \boldsymbol{v}, \boldsymbol{u}) \in A \implies (t, \boldsymbol{v}, \boldsymbol{u})^\top (\tilde{\rho}, \tilde{\boldsymbol{x}}, \tilde{\boldsymbol{s}}) \geq \mu \tag{15.6}$$

and the set B on the other side:

$$(t, \boldsymbol{v}, \boldsymbol{u}) \in B \implies (t, \boldsymbol{v}, \boldsymbol{u})^\top (\tilde{\rho}, \tilde{\boldsymbol{x}}, \tilde{\boldsymbol{s}}) \leq \mu. \tag{15.7}$$

Now, we claim that $\tilde{\boldsymbol{s}} \geq 0$. Suppose $\tilde{\boldsymbol{s}}(i) < 0$, then for $\boldsymbol{u}(i) \to \infty$ the threshold would grow unbounded, i.e. $\mu \to -\infty$ contradicting that the threshold μ is finite by the separating hyperplane theorem. Similarly we claim $\tilde{\rho} \geq 0$, as if this were not the case, having $t \to \infty$ implies that $\mu \to -\infty$ again contradicting the finiteness of μ.

From Equation (15.7) it follows that $t\tilde{\rho} \leq \mu$ for all $t < \alpha^*$ which implies that $t\tilde{\rho} \leq \mu$ for $t = \alpha^*$ by taking the limit. Hence we have $\alpha^*\tilde{\rho} \leq \mu$. From $(t, \boldsymbol{v}, \boldsymbol{u}) \in A$ we get from Equation (15.6)

$$(\tilde{\rho}, \tilde{\boldsymbol{x}}, \tilde{\boldsymbol{s}})^\top (t, \boldsymbol{v}, \boldsymbol{u}) \geq \mu \geq \alpha^* \tilde{\rho}$$

and thus

$$(\tilde{\rho}, \tilde{\boldsymbol{x}}, \tilde{\boldsymbol{s}})^\top (\mathcal{E}(\boldsymbol{y}), \boldsymbol{A}\boldsymbol{y} - \boldsymbol{b}, \boldsymbol{c}(\boldsymbol{y})) \geq \alpha^* \tilde{\rho}. \tag{15.8}$$

Now we consider two cases; starting with the "good" case where $\tilde{\rho} > 0$. Dividing Equation (15.8) by $\tilde{\rho}$ gives

$$\mathcal{E}(\boldsymbol{y}) + \frac{\tilde{\boldsymbol{x}}^\top}{\tilde{\rho}} (\boldsymbol{A}\boldsymbol{y} - \boldsymbol{b}) + \frac{\tilde{\boldsymbol{s}}^\top}{\tilde{\rho}} \boldsymbol{c}(\boldsymbol{y}) \geq \alpha^*.$$

Noting that the left hand side above is $L(\boldsymbol{y}, \frac{\tilde{\boldsymbol{x}}}{\tilde{\rho}}, \frac{\tilde{\boldsymbol{s}}}{\tilde{\rho}})$ and that the equation holds for arbitrary $\boldsymbol{y}$; therefore also for the minimum we get

$$\min_{\boldsymbol{y}} L\left(\boldsymbol{y}, \frac{\tilde{\boldsymbol{x}}}{\tilde{\rho}}, \frac{\tilde{\boldsymbol{s}}}{\tilde{\rho}}\right) \geq \alpha^*$$

and hence via definition of β^* finally

$$\beta^* \geq L\left(\frac{\tilde{\boldsymbol{x}}}{\tilde{\rho}}, \frac{\tilde{\boldsymbol{s}}}{\tilde{\rho}}\right) \geq \alpha^*.$$

Next consider the "bad" case $\tilde{\rho} = 0$. As $\alpha^* \tilde{\rho} \leq \mu$, we have $0 \leq \mu$. From Equation (15.6) we get

$$\boldsymbol{c}(\boldsymbol{y})^\top \boldsymbol{s} + \boldsymbol{x}^\top (\boldsymbol{b} - \boldsymbol{A}\boldsymbol{y}) \geq \mu \geq 0.$$

As Slater's condition holds, there is an interior point $\tilde{\boldsymbol{y}}$, i.e. it satisfies $\boldsymbol{b} - \boldsymbol{A}\tilde{\boldsymbol{y}} = \boldsymbol{0}$ and $\boldsymbol{c}(\tilde{\boldsymbol{y}}) < \boldsymbol{0}$. Together with the equation above this yields

$$\boldsymbol{c}(\tilde{\boldsymbol{y}})^\top \tilde{\boldsymbol{s}} + \tilde{\boldsymbol{x}}^\top \boldsymbol{0} \geq 0$$

which implies $\boldsymbol{c}(\tilde{\boldsymbol{y}})^\top \tilde{\boldsymbol{s}} \geq 0$ and as $\boldsymbol{c}(\tilde{\boldsymbol{y}}) < \boldsymbol{0}$ this means $\tilde{\boldsymbol{s}} = \boldsymbol{0}$.

As the normal $(\tilde{\rho}, \tilde{\boldsymbol{s}}, \tilde{\boldsymbol{x}})$ of the hyperplane can not be all zeroes, this means the last "component" $\tilde{\boldsymbol{x}}$ must contain a non-zero entry, i.e. $\tilde{\boldsymbol{x}} \neq \boldsymbol{0}$. Furthermore $\tilde{\boldsymbol{x}}^\top (\boldsymbol{b} - \boldsymbol{A}\tilde{\boldsymbol{y}}) = \boldsymbol{0}$, $\boldsymbol{c}(\tilde{\boldsymbol{y}}) < \boldsymbol{0}$ and $\boldsymbol{A}$ has full row rank, hence there exists $\boldsymbol{\delta}$ such that

$$\tilde{\boldsymbol{x}}^\top (\boldsymbol{b} - \boldsymbol{A}(\tilde{\boldsymbol{y}} + \boldsymbol{\delta})) < \boldsymbol{0} \text{ and } \boldsymbol{c}(\tilde{\boldsymbol{y}} + \boldsymbol{\delta}) < 0.$$

This, however, means that there is a point in A on the wrong side of the hyperplane, as

$$(\tilde{\rho}, \tilde{\boldsymbol{x}}, \tilde{\boldsymbol{s}})^\top (\mathcal{E}(\tilde{\boldsymbol{y}} + \boldsymbol{\delta}), \boldsymbol{b} - \boldsymbol{A}(\tilde{\boldsymbol{y}} + \boldsymbol{\delta}), \boldsymbol{c}(\tilde{\boldsymbol{y}} + \boldsymbol{\delta})) < 0$$

but the threshold is $\mu \geq 0$. □

Remark. Note that our reasoning about why $\boldsymbol{s} \geq \boldsymbol{0}$ in the proof above is very similar to our reasoning for why the primal program can be written as Problem (15.5).

Example. As an example of A and B as they appear in the above proof, consider

$$\min_{\substack{y\in(0,\infty)\\ 1/y-1\leq 0}} y^2$$

This leads to $\alpha^* = 1, y^* = 1$, and $A = \{(t,u) : y \in (0,\infty) \text{ and } t > y^2 \text{ and } u \geq 1/y - 1\}$, and $B = \{(t,0) : t < 1\}$ and the separating hyperplane normal is $\boldsymbol{n} = (1,2)$. These two sets A, B are illustrated in Figure 15.3.

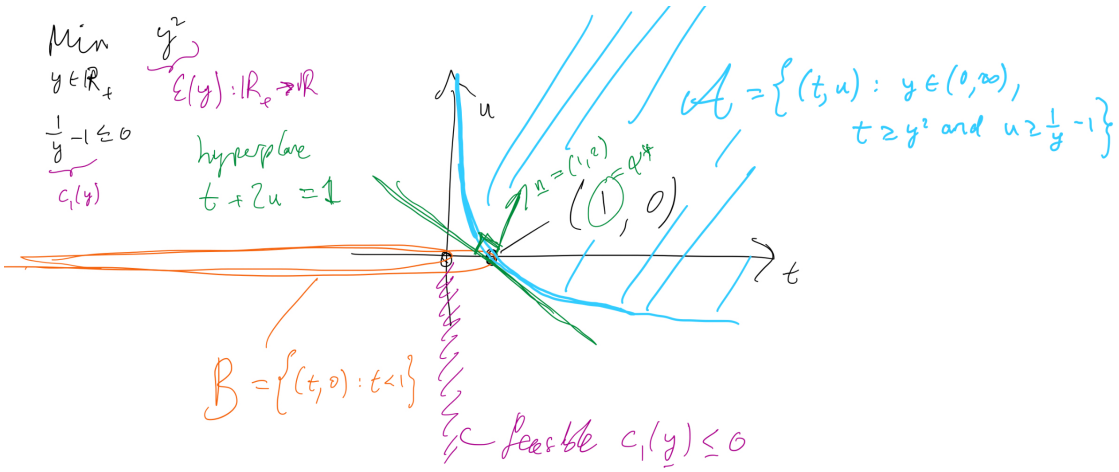


Figure 15.3: Example of the convex sets A and B we wish to separate by hyperplane.

15.3.5 KKT Revisited

Let's come back to our earlier discussion of parallel gradients and the KKT conditions. Consider a convex program (15.1) with an open set S as its domain. Suppose $\boldsymbol{y}^*$ is an optimizer of the primal problem and $\boldsymbol{x}^*, \boldsymbol{s}^*$ for the dual, and suppose that strong duality holds. We thus have

$$L(\boldsymbol{y}^*, \boldsymbol{x}^*, \boldsymbol{s}^*) = \alpha^* = \beta^*.$$

Because $L(\boldsymbol{y}, \boldsymbol{x}^*, \boldsymbol{s}^*)$ is a convex function in $\boldsymbol{y}$, it also follows that as $\mathcal{E} : S \to \mathbb{R}$ and $\boldsymbol{c}$ are differentiable then we must have that the gradient w.r.t. $\boldsymbol{y}$ is zero, i.e.

$$\boldsymbol{\nabla}_{\boldsymbol{y}} L(\boldsymbol{y}, \boldsymbol{x}^*, \boldsymbol{s}^*)|_{\boldsymbol{y}=\boldsymbol{y}^*} = 0 \tag{15.9}$$

This says exactly that the KKT gradient condition holds at $(\boldsymbol{y}^*, \boldsymbol{x}^*, \boldsymbol{s}^*)$.

Complementary slackness. We can also see that

$$\mathcal{E}(\boldsymbol{y}^*) = \alpha^* = \mathcal{E}(\boldsymbol{y}^*) + \boldsymbol{x}^\top(\boldsymbol{b} - \boldsymbol{A}\boldsymbol{y}^*) + \boldsymbol{s}^\top \boldsymbol{c}(\boldsymbol{y}^*) = \mathcal{E}(\boldsymbol{y}^*) + \boldsymbol{s}^\top \boldsymbol{c}(\boldsymbol{y}^*)$$

and hence when the i-th convex constraint is not active, i.e. $c_i(\boldsymbol{y}^*) < 0$ the *slack* must be zero, i.e. $\boldsymbol{s}(i) = 0$. Conversely if the slack is non-zero, that is $\boldsymbol{s}(i) \neq 0$ implies that the

constraint is active, i.e. $c_i(\boldsymbol{y}^*) = 0$. This says precisely that the complementary slackness condition holds at primal-dual optimal $(\boldsymbol{y}^*, \boldsymbol{x}^*, \boldsymbol{s}^*)$. Combined with our previous observation Equation (15.9), we get the following result.

Theorem 15.3.12. *Consider a convex program* (15.1) *with an open domain set S and whose dual satisfies strong duality. Then KKT conditions necessarily hold at primal-dual optimal* $(\boldsymbol{y}^*, \boldsymbol{x}^*, \boldsymbol{s}^*)$.

Theorem 15.3.12 combined with Theorem 15.3.11 immediately imply Proposition 15.3.7.

KKT is sufficient. We've seen that when strong duality holds, the KKT conditions are necessary for optimality. In fact, they're also sufficient for optimality, as the next theorem shows. And in this case, we do not need to assume strong duality, as now it is implied by the KKT conditions.

Theorem 15.3.13. *Consider a convex program* (15.1) *with an open domain set S. Then if the KKT conditions hold at $(\tilde{\boldsymbol{y}}, \tilde{\boldsymbol{x}}, \tilde{\boldsymbol{s}})$, they must be primal-dual optimal, and strong duality must hold.*

Proof. $\tilde{\boldsymbol{y}}$ is global minimizer of $\boldsymbol{y} \mapsto L(\boldsymbol{y}, \tilde{\boldsymbol{x}}, \tilde{\boldsymbol{s}})$, since this function is convex with vanishing gradient at $\tilde{\boldsymbol{y}}$. Hence,

$$L(\tilde{\boldsymbol{y}}, \tilde{\boldsymbol{x}}, \tilde{\boldsymbol{s}}) = \inf_{\boldsymbol{y}} L(\boldsymbol{y}, \tilde{\boldsymbol{x}}, \tilde{\boldsymbol{s}}) = L(\tilde{\boldsymbol{x}}, \tilde{\boldsymbol{s}}) \leq \beta^*.$$

On the other hand, due to primal feasibility and complementary slackness,

$$L(\tilde{\boldsymbol{y}}, \tilde{\boldsymbol{x}}, \tilde{\boldsymbol{s}}) = \mathcal{E}(\tilde{\boldsymbol{y}}) + \tilde{\boldsymbol{x}}^\top(\boldsymbol{b} - \boldsymbol{A}^\top \tilde{\boldsymbol{y}}) + \tilde{\boldsymbol{s}}^\top \boldsymbol{c}(\tilde{\boldsymbol{y}}) = \mathcal{E}(\tilde{\boldsymbol{y}}) \geq \alpha^*.$$

Thus, $\beta^* \geq \alpha^*$. But also $\beta^* \leq \alpha^*$ by weak duality. Therefore, $\beta^* = \alpha^*$ and $\tilde{\boldsymbol{y}}, \tilde{\boldsymbol{x}}, \tilde{\boldsymbol{s}}$ are primal/dual optimal. □

A good reference for basic convex duality theory is Boyd's free online book "Convex optimization" (linked to on the course website). It provides a number of different interpretations of duality. One particularly interesting one comes from economics: economists see the slack variables $\boldsymbol{s}$ as prices for violating the constraints.

Chapter 16

Fenchel Conjugates and Newton's Method

16.1 Lagrange Multipliers and Convex Duality Recap

Recall the convex optimization program we studied last chapter,

$$\begin{aligned} \min \quad & \mathcal{E}(\boldsymbol{y}) \\ \text{s.t.} \quad & \boldsymbol{A}\boldsymbol{y} = \boldsymbol{b} \\ & \boldsymbol{c}(\boldsymbol{y}) \leq \boldsymbol{0}, \end{aligned} \tag{16.1}$$

where $\mathcal{E}(\boldsymbol{y}) : S \to \mathbb{R}$ is defined on a subset $S \subseteq \mathbb{R}^n$, $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ and $\boldsymbol{c}(\boldsymbol{y})$ is a vector of constraints $\boldsymbol{c}(\boldsymbol{y}) = (c_i(\boldsymbol{y}))_{i \in [k]}$. For every $i \in [k]$ the function $c_i : S \to \mathbb{R}$ is convex. We call (16.1) the primal (program) and denote its optimal value by α^*.

The associated Lagrangian is defined by

$$L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}) = \mathcal{E}(\boldsymbol{y}) + \boldsymbol{x}^T(\boldsymbol{b} - \boldsymbol{A}\boldsymbol{y}) + \boldsymbol{s}^T\boldsymbol{c}(\boldsymbol{y}).$$

where $\boldsymbol{x} \in \mathbb{R}^m$, $\boldsymbol{s} \in \mathbb{R}^k$ are dual variables. The dual (program) is given by

$$\max_{\substack{\boldsymbol{x}, \boldsymbol{s} \\ \boldsymbol{s} \geq 0}} \quad L(\boldsymbol{x}, \boldsymbol{s}) \tag{16.2}$$

whose optimal value is denoted by β^*. The dual is always a convex optimization program even though the primal is non-convex. The optimal value of the primal (16.1) can also be written as

$$\alpha^* = \inf_{\boldsymbol{y}} \sup_{\boldsymbol{x}; \boldsymbol{s} \geq \boldsymbol{0}} L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}), \tag{16.3}$$

where no constraint is imposed on the primal variable $\boldsymbol{y}$. The optimal value of the dual (16.2) is

$$\beta^* = \sup_{\boldsymbol{x}; \boldsymbol{s} \geq \boldsymbol{0}} \inf_{\boldsymbol{y}} L(\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{s}). \tag{16.4}$$

Note the only difference between (16.3) and (16.4) is that the positions of "inf" and "sup" are swapped. The weak duality theorem states that the dual optimal value is a lower bound of the primal optimal value, i.e. $\beta^* \leq \alpha^*$.

The Slater's condition for (16.1) open domain S requires the existence of a *strictly feasible* point, i.e. there exists $\tilde{\boldsymbol{y}} \in S$ s.t. $\boldsymbol{A}\tilde{\boldsymbol{y}} = \boldsymbol{b}$ and $\boldsymbol{c}(\tilde{\boldsymbol{y}}) < \boldsymbol{0}$. This means that the strictly feasible point $\tilde{\boldsymbol{y}}$ lies inside the interior of the set $\{\boldsymbol{y} : \boldsymbol{c}(\boldsymbol{y}) \leq \boldsymbol{0}\}$ defined by the inequality constraints. If the domain S is not open, Slater's condition also requires that a strictly feasible point is in the relative interior of S (NB: when S is open, S is equal to its relative interior). The strong duality theorem says that Slater's condition implies strong duality, $\beta^* = \alpha^*$.

We were also introduced to the KKT conditions, and we saw that for our convex programs with continuously differentiable objective and constraints functions, when the domain is open, the conditions are sufficient to imply strong duality and primal-dual optimality of the points that satisfy them. If Slater's condition holds, we also have that KKT necessarily holds at any optimal solution. **In summary:** Slater's condition $\implies$ strong duality $\iff$ KKT

Example. In Chapter 12, we gave a combinatorial proof of the min-cut max-flow theorem, and showed that the min-cut program can be expressed as a linear program. Now, we will use the strong duality theorem to give an alternative proof, and directly find the min-cut linear program is the dual program to our maximum flow linear program.

We will assume that Slater's condition holds for our primal program. Since scaling the flow down enough will always ensure that capacity constraints are strictly satisfied i.e. $\boldsymbol{f} < \boldsymbol{c}$, the only concern is to make sure that non-negativity constraints are satisfied. This means that there is an s-t flow that sends a non-zero flow on every edge. In fact, this may not always be possible, but it is easy to detect such edges and remove them without changing the value of the program: an edge (u, v) should be removed if there is no path s to u or no path v to t. We can identify all such edges using a BFS from s along the directed edges and a BFS along reversed directed edges from t.

Slater's condition holds whenever there is a directed path from s to t with non-zero capacity (and if there is not, the maximum flow and minimum cut are both zero).

$$\min_{\substack{F\in\mathbb{R}\\ \boldsymbol{B}\boldsymbol{f}=F\boldsymbol{b}_{s,t}\\ \boldsymbol{0}\leq\boldsymbol{f}\leq\boldsymbol{c}}} -F = \min_{F;\boldsymbol{f}\geq\boldsymbol{0}} \max_{\boldsymbol{x};\boldsymbol{s}\geq\boldsymbol{0}} -F + \boldsymbol{x}^\top(F\boldsymbol{b}_{s,t} - \boldsymbol{B}\boldsymbol{f}) + (\boldsymbol{f}-\boldsymbol{c})^\top\boldsymbol{s}$$

$$\text{(Slater's condition } \implies \text{ strong duality)}$$

$$-\max_{\substack{F\in\mathbb{R}\\ \boldsymbol{B}\boldsymbol{f}=F\boldsymbol{b}_{s,t}\\ \boldsymbol{0}\leq\boldsymbol{f}\leq\boldsymbol{c}}} F = \max_{\boldsymbol{x};\boldsymbol{s}\geq\boldsymbol{0}} \min_{F;\boldsymbol{f}\geq\boldsymbol{0}} F(\boldsymbol{b}_{s,t}^\top\boldsymbol{x} - 1) + \boldsymbol{f}^\top(\boldsymbol{s} - \boldsymbol{B}^\top\boldsymbol{x}) - \boldsymbol{c}^\top\boldsymbol{s}$$

$$= \max_{\substack{\boldsymbol{x};\,\boldsymbol{s}\geq\boldsymbol{0}\\ \boldsymbol{b}_{s,t}^\top\boldsymbol{x}=1\\ \boldsymbol{s}\geq\boldsymbol{B}^\top\boldsymbol{x}}} -\boldsymbol{c}^\top\boldsymbol{s}$$

Thus switching signs gives us

$$\max_{\substack{F\in\mathbb{R} \\ \boldsymbol{B}\boldsymbol{f}=F\boldsymbol{b}_{s,t} \\ \boldsymbol{0}\le\boldsymbol{f}\le\boldsymbol{c}}} F = \min_{\substack{\boldsymbol{x};\,\boldsymbol{s}\ge\boldsymbol{0} \\ \boldsymbol{b}_{s,t}^\top\boldsymbol{x}=1 \\ \boldsymbol{s}\ge\boldsymbol{B}^\top\boldsymbol{x}}} \boldsymbol{c}^\top\boldsymbol{s} \tag{16.5}$$

The LHS of (16.5) is exactly the LP formulation of max-flow, while the RHS is exactly the LP formulation of min-cut. Note that we treated the "constraint" $\boldsymbol{0} \le \boldsymbol{f}$ as a restriction on the domain of $\boldsymbol{f}$ rather than a constraint with a dual variable associated with it. We always have this kind of flexibility when deciding how to compute a dual, and some choices may lead to a simpler dual program than others.

16.2 Fenchel Conjugates

In this section we will learn about Fenchel conjugates. This is a notion of dual function that is closely related to duality of convex programs, and we will learn more about how dual programs behave by studying these functions.

Definition 16.2.1 (Fenchel conjugate)**.** Given a (convex) function $\mathcal{E} : S \subseteq \mathbb{R}^n \to \mathbb{R}$, its *Fenchel conjugate* is a function $\mathcal{E}^* : \mathbb{R}^n \to \mathbb{R}$ defined as

$$\mathcal{E}^*(\boldsymbol{z}) = \sup_{\boldsymbol{y}\in S} \langle \boldsymbol{z}, \boldsymbol{y}\rangle - \mathcal{E}(\boldsymbol{y}).$$

Remark 16.2.2. $\mathcal{E}^*$ is a convex function whether $\mathcal{E}$ is convex or not, since $\mathcal{E}^*(z)$ is pointwise supremum of a family of convex (here, affine) functions of z.

In this course, we have only considered convex functions that are real-valued and continuous and defined on a convex domain. For any such $\mathcal{E}$, we have $\mathcal{E}^{**} = \mathcal{E}$, i.e. the Fenchel conjugate of the Fenchel conjugate is the original function. This is a consequence of the Fenchel-Moreau theorem, which establishes this under slightly more general conditions. We will not prove this generally, but as part of Theorem 16.2.3 below, we sketch a proof under more restrictive assumptions.

Example. Let $\mathcal{E}(\boldsymbol{y}) = \frac{1}{p}\|\boldsymbol{y}\|_p^p$ $(p > 1)$. We want to evaluate its Fenchel conjugate $\mathcal{E}^*$ at any given point $\boldsymbol{z} \in \mathbb{R}^n$. Since $\mathcal{E}$ is convex and differentiable, the supremum must be achieved at some $\boldsymbol{y}$ with vanishing gradient

$$\boldsymbol{\nabla}_{\boldsymbol{y}}\langle \boldsymbol{z}, \boldsymbol{y}^*\rangle - \boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y}^*) = \boldsymbol{z} - \boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y}^*) = \boldsymbol{0} \iff \boldsymbol{z} = \boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y}^*).$$

It's not difficult to see, for all i,

$$\boldsymbol{z}(i) = \operatorname{sgn}(\boldsymbol{y}(i))|\boldsymbol{y}(i)|^{p-1}.$$

Then,

$$\begin{aligned}\mathcal{E}^*(\boldsymbol{z}) &= \langle \boldsymbol{z}, \boldsymbol{y} \rangle - \mathcal{E}(\boldsymbol{y}) \\ &= \sum_i |\boldsymbol{z}(i)|^{\frac{1}{p-1}+1} - \frac{1}{p}|\boldsymbol{z}(i)|^{\frac{p}{p-1}} \\ &\quad (\text{define } q \text{ s.t. } \frac{1}{q} + \frac{1}{p} = 1) \\ &= \frac{1}{q}\|\boldsymbol{z}\|_q^q.\end{aligned}$$

More generally, given a convex and differentiable function $\mathcal{E} : S \to \mathbb{R}$, if there exists $\boldsymbol{y} \in S$ s.t. $\boldsymbol{z} = \boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y})$, then $\mathcal{E}^*(\boldsymbol{z}) = (\boldsymbol{y}^*)^\top \boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y}^*) - \mathcal{E}(\boldsymbol{y}^*)$. The Fenchel conjugate and Lagrange duality are closely related, which is demonstrated in the following example.

Example. Consider a convex optimization program with only linear constraints,

$$\begin{aligned}\min_{\boldsymbol{y}\in\mathbb{R}^n} \quad & \mathcal{E}(\boldsymbol{y}) \\ \text{s.t.} \quad & \boldsymbol{A}\boldsymbol{y} = \boldsymbol{b}\end{aligned}$$

where $\mathcal{E} : \mathbb{R}^n \to \mathbb{R}$ is a convex function and $\boldsymbol{A} \in \mathbb{R}^{m\times n}$. Then the corresponding dual program is

$$\begin{aligned}\sup_{\boldsymbol{x}\in\mathbb{R}^n} \inf_{\boldsymbol{y}\in\mathbb{R}^n} \mathcal{E}(\boldsymbol{y}) + \boldsymbol{x}^\top(\boldsymbol{b} - \boldsymbol{A}\boldsymbol{y}) &= \sup_{\boldsymbol{x}\in\mathbb{R}^n} \boldsymbol{b}^\top\boldsymbol{x} - \sup_{\boldsymbol{y}\in\mathbb{R}^n} \left(\boldsymbol{x}^\top\boldsymbol{A}\boldsymbol{y} - \mathcal{E}(\boldsymbol{y})\right) \\ &= \sup_{\boldsymbol{x}\in\mathbb{R}^n} \boldsymbol{b}^\top\boldsymbol{x} - \mathcal{E}^*(\boldsymbol{A}^\top\boldsymbol{x})\end{aligned}$$

Theorem 16.2.3 (Properties of the Fenchel conjugate)**.** *Consider a strictly convex function $\mathcal{E} : S \to \mathbb{R}$ where $S \subseteq R^n$ is an open convex set. When $\mathcal{E}$ is differentiable with a Hessian that is positive definite everywhere and its gradient $\boldsymbol{\nabla}\mathcal{E}$ is surjective onto $\mathbb{R}^n$, we have the following three properties:*

1. $\boldsymbol{\nabla}\mathcal{E}(\boldsymbol{\nabla}\mathcal{E}^*(\boldsymbol{z})) = \boldsymbol{z}$ *and* $\boldsymbol{\nabla}\mathcal{E}^*(\boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y})) = \boldsymbol{y}$

2. $(\mathcal{E}^*)^* = \mathcal{E}$*, i.e. the Fenchel conjugate of the Fenchel conjugate is the original function.*

3. $\boldsymbol{H}_{\mathcal{E}^*}(\boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y})) = \boldsymbol{H}_{\mathcal{E}}^{-1}(\boldsymbol{y})$

primal point $\boldsymbol{y}$	$\xrightarrow{\nabla_y \mathcal{E}}$ $\xleftarrow{\nabla_z \mathcal{E}^*}$	dual point $\boldsymbol{z}$
gradient $\nabla_y \mathcal{E}(\boldsymbol{y}) = \boldsymbol{z}$		gradient $\nabla_z \mathcal{E}^*(\boldsymbol{z}) = \boldsymbol{y}$
Hessian $\boldsymbol{H}_{\mathcal{E}}(\boldsymbol{y}) = \boldsymbol{H}^{-1}_{\mathcal{E}^*}(\boldsymbol{z})$		Hessian $\boldsymbol{H}_{\mathcal{E}^*}(\boldsymbol{y}) = \boldsymbol{H}^{-1}_{\mathcal{E}}(\boldsymbol{y})$

Figure 16.1: Properties of Fenchel conjugate

Proof sketch. Part 1. Because the gradient $\nabla_y \mathcal{E}$ is surjective onto $\mathbb{R}^n$, given any $\boldsymbol{z} \in \mathbb{R}^n$, there exists a $\boldsymbol{y}$ such that $\nabla \mathcal{E}(\boldsymbol{y}) = \boldsymbol{z}$. Let $\boldsymbol{y}(\boldsymbol{z})$ be a $\boldsymbol{y}$ s.t. $\nabla \mathcal{E}(\boldsymbol{y}) = \boldsymbol{z}$. It can be shown that because $\mathcal{E}$ is strictly convex, $\boldsymbol{y}(\boldsymbol{z})$ is unique.

The function $\boldsymbol{y} \mapsto \langle \boldsymbol{z}, \boldsymbol{y} \rangle - \mathcal{E}(\boldsymbol{y})$ is concave in $\boldsymbol{y}$ and has gradient $\boldsymbol{z} - \nabla \mathcal{E}(\boldsymbol{y})$ and is hence maximized at $\boldsymbol{y} = \boldsymbol{y}(\boldsymbol{z})$. This follows because we know a differentiable convex function is minimized when its gradient is zero and so a differentiable concave function is maximized when its gradient is zero.

Then, using the product rule and composition rule of derivatives,

$$\begin{aligned}
\nabla \mathcal{E}^*(\boldsymbol{z}) &= \nabla_z \left(\langle \boldsymbol{z}, \boldsymbol{y}(\boldsymbol{z}) \rangle - \mathcal{E}(\boldsymbol{y}(\boldsymbol{z})) \right) \\
&= \boldsymbol{y}(\boldsymbol{z}) + \operatorname{diag}(\boldsymbol{z}) \nabla_z \boldsymbol{y}(\boldsymbol{z}) - \operatorname{diag}(\underbrace{\nabla_y \mathcal{E}(\boldsymbol{y}(\boldsymbol{z}))}_{=\boldsymbol{z}}) \nabla_z \boldsymbol{y}(\boldsymbol{z}) \\
&= \boldsymbol{y}(\boldsymbol{z})
\end{aligned}$$

Thus we have $\nabla_y \mathcal{E}(\boldsymbol{y}(\boldsymbol{z})) = \boldsymbol{z}$ and $\nabla_z \mathcal{E}^*(\boldsymbol{z}) = \boldsymbol{y}(\boldsymbol{z})$. Combining the two, we have $\nabla \mathcal{E}(\nabla \mathcal{E}^*(\boldsymbol{z})) = \boldsymbol{z}$.

We can also see that for any $\boldsymbol{y}$, there exists a $\boldsymbol{z}$ such that $\nabla_z \mathcal{E}^*(\boldsymbol{z}) = \boldsymbol{y}$, namely, this is attained by $\boldsymbol{z} = \nabla_y \mathcal{E}(\boldsymbol{y})$. Thus, $\nabla \mathcal{E}^*(\nabla \mathcal{E}(\boldsymbol{y})) = \boldsymbol{y}$.

Part 2. Observe that

$$\mathcal{E}^{**}(\boldsymbol{u}) = \sup_{\boldsymbol{z} \in \mathbb{R}^n} \langle \boldsymbol{u}, \boldsymbol{z} \rangle - \mathcal{E}^*(\boldsymbol{z})$$

and let $\boldsymbol{z}(\boldsymbol{u})$ denote the $\boldsymbol{z}$ obtaining the supremum, in the above program. We then have $\boldsymbol{u} = \nabla \mathcal{E}^*(\boldsymbol{z}(\boldsymbol{u}))$. Letting $\boldsymbol{y}(\boldsymbol{z})$ be defined as in Part 1, we get $\boldsymbol{y}(\boldsymbol{z}(\boldsymbol{u})) = \nabla_z \mathcal{E}^*(\boldsymbol{z}(\boldsymbol{u})) = \boldsymbol{u}$

$$\mathcal{E}^{**}(\boldsymbol{u}) = \langle \boldsymbol{u}, \boldsymbol{z}(\boldsymbol{u}) \rangle - (\langle \boldsymbol{z}(\boldsymbol{u}), \boldsymbol{y}(\boldsymbol{z}(\boldsymbol{u})) \rangle - \mathcal{E}(\boldsymbol{y}(\boldsymbol{z}(\boldsymbol{u})))) = \mathcal{E}(\boldsymbol{u}).$$

Part 3. Now we add two infinitesimals $\boldsymbol{\tau}$ and $\boldsymbol{\delta}$ to $\boldsymbol{z}$ and $\boldsymbol{y}$ respectively s.t.

$$\nabla_z \mathcal{E}^*(\boldsymbol{z} + \boldsymbol{\tau}) = \boldsymbol{y} + \boldsymbol{\delta}, \quad \nabla_y \mathcal{E}(\boldsymbol{y} + \boldsymbol{\delta}) = \boldsymbol{z} + \boldsymbol{\tau}.$$

Then,

$$\nabla_y \mathcal{E}(\boldsymbol{y} + \boldsymbol{\delta}) - \nabla_y \mathcal{E}(\boldsymbol{y}) = \boldsymbol{\tau}, \quad \nabla_z \mathcal{E}^*(\boldsymbol{z} + \boldsymbol{\tau}) - \nabla_z \mathcal{E}^*(\boldsymbol{z}) = \boldsymbol{\delta}.$$

Since $\boldsymbol{H}_{\mathcal{E}}(\boldsymbol{y})$ measures the change of $\boldsymbol{\nabla}_{\boldsymbol{y}}\mathcal{E}(\boldsymbol{y})$ when $\boldsymbol{y}$ changes by an infinitesimal $\boldsymbol{\delta}$, then

$$\begin{aligned}
&\boldsymbol{\nabla}_{\boldsymbol{y}}\mathcal{E}(\boldsymbol{y}+\boldsymbol{\delta}) - \boldsymbol{\nabla}_{\boldsymbol{y}}\mathcal{E}(\boldsymbol{y}) \approx \boldsymbol{H}_{\mathcal{E}}(\boldsymbol{y})\boldsymbol{\delta} \\
\iff &\boldsymbol{H}_{\mathcal{E}}^{-1}(\boldsymbol{y})\left(\boldsymbol{\nabla}_{\boldsymbol{y}}\mathcal{E}(\boldsymbol{y}+\boldsymbol{\delta}) - \boldsymbol{\nabla}_{\boldsymbol{y}}\mathcal{E}(\boldsymbol{y})\right) \approx \boldsymbol{\delta} \\
\iff &\boldsymbol{H}_{\mathcal{E}}^{-1}(\boldsymbol{y})\boldsymbol{\tau} \approx \boldsymbol{\delta} = \boldsymbol{\nabla}\mathcal{E}^*(\boldsymbol{z}+\boldsymbol{\tau}) - \boldsymbol{\nabla}\mathcal{E}^*(\boldsymbol{z}) \\
\iff &\boldsymbol{H}_{\mathcal{E}}^{-1}(\boldsymbol{y})\boldsymbol{\tau} \approx \boldsymbol{\nabla}\mathcal{E}^*(\boldsymbol{z}+\boldsymbol{\tau}) - \boldsymbol{\nabla}\mathcal{E}^*(\boldsymbol{z}) \qquad (16.6)
\end{aligned}$$

Similarly,

$$\boldsymbol{H}_{\mathcal{E}^*}(\boldsymbol{z})\boldsymbol{\tau} \approx \boldsymbol{\nabla}_{\boldsymbol{z}}\mathcal{E}^*(\boldsymbol{z}+\boldsymbol{\tau}) - \boldsymbol{\nabla}_{\boldsymbol{z}}\mathcal{E}^*(\boldsymbol{z}) \qquad (16.7)$$

Comparing (16.6) and (16.7), it is easy to see

$$\boldsymbol{H}_{\mathcal{E}^*}(\boldsymbol{z}) = \boldsymbol{H}_{\mathcal{E}}^{-1}(\boldsymbol{y}) \iff \boldsymbol{H}_{\mathcal{E}^*}(\boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y})) = \boldsymbol{H}_{\mathcal{E}}^{-1}(\boldsymbol{y}).$$

□

Remark 16.2.4. Theorem 16.2.3 can be generalized to show that the Fenchel conjugate has similar nice properties under much more general conditions, e.g. see [BV04].

16.3 Newton's Method

16.3.1 Warm-up: Quadratic Optimization

First, let us play with a toy example, minimizing a quadratic function

$$\mathcal{E}(\boldsymbol{y}) = \frac{1}{2}\boldsymbol{y}^\top \boldsymbol{A}\boldsymbol{y} + \boldsymbol{b}^\top \boldsymbol{y} + \boldsymbol{c}$$

where $\boldsymbol{A} \in \mathbb{R}^{n\times n}$ is positive definite. By setting the gradient w.r.t. $\boldsymbol{y}$ to zero,

$$\boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y}) = \boldsymbol{A}\boldsymbol{y} + \boldsymbol{b} = \boldsymbol{0},$$

we obtain the global minimizer

$$\boldsymbol{y}^* = -\boldsymbol{A}^{-1}\boldsymbol{b}.$$

To make it more like gradient descent, let us start at some "guess" point $\boldsymbol{y}$ and take a step $\boldsymbol{\delta}$ to move to the new point $\boldsymbol{y}+\boldsymbol{\delta}$. Then we try to minimize $\mathcal{E}(\boldsymbol{y}+\boldsymbol{\delta})$ by setting the gradient w.r.t. $\boldsymbol{\delta}$ to zero,

$$\begin{aligned}
\boldsymbol{\nabla}_{\boldsymbol{\delta}}\mathcal{E}(\boldsymbol{y}+\boldsymbol{\delta}) = \boldsymbol{A}(\boldsymbol{y}+\boldsymbol{\delta}) + \boldsymbol{b} &= \boldsymbol{0} \\
\boldsymbol{\delta} &= -\boldsymbol{y} - \boldsymbol{A}^{-1}\boldsymbol{b} \\
\boldsymbol{y}+\boldsymbol{\delta} &= -\boldsymbol{A}^{-1}\boldsymbol{b}
\end{aligned}$$

This gives us exactly global minimizer in just one step. However, the situation changes when the function is not quadratic anymore and thus we do not have a constant Hessian. But taking a step which tries to set the gradient to zero might still be a good idea.

16.3.2 K-stable Hessian

Next, consider a convex function $\mathcal{E} : \mathbb{R}^n \to \mathbb{R}$ whose Hessian is "nearly constant". Recall the Hessian $\boldsymbol{H}_{\mathcal{E}}(\boldsymbol{y})$ aka $\boldsymbol{\nabla}^2\mathcal{E}(\boldsymbol{y})$ at a point $\boldsymbol{y}$ is just a matrix of pairwise 2nd order partial derivatives $\frac{\partial^2\mathcal{E}(\boldsymbol{y})}{\partial \boldsymbol{y}_i \partial \boldsymbol{y}_j}$. We say $\mathcal{E}$ has a k-stable Hessian if there exists a constant matrix $\boldsymbol{A}$ s.t. for all $\boldsymbol{y}$

$$\boldsymbol{H}_{\mathcal{E}}(\boldsymbol{y}) \approx_K \boldsymbol{A} \iff \frac{1}{1+K}\boldsymbol{A} \preceq \boldsymbol{H}_{\mathcal{E}}(\boldsymbol{y}) \preceq (1+K)\boldsymbol{A}.$$

Note that we just require the existence of $\boldsymbol{A}$ and do not assume we know $\boldsymbol{A}$. Then a natural question is to ask what convergence rate can be achieved if we take a gradient step "guided" by the Hessian, which is called a "Newton step". Such method is also known as the 2nd order method. Note that this is very similar to preconditioning.

Now, let us make our setting precise. We want to minimize a convex function $\mathcal{E}$ with k-stable Hessian $\boldsymbol{A} \succ \boldsymbol{0}$. And $\boldsymbol{y}^*$ is a global minimizer of $\mathcal{E}$. Start from some initial point $\boldsymbol{y}_0$. The update rule is

$$\boldsymbol{y}_{i+1} = \boldsymbol{y}_i - \alpha \cdot \boldsymbol{H}_{\mathcal{E}}^{-1}(\boldsymbol{y}_i)\boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y}_i),$$

where α is the step size and it will be decided later.

Theorem 16.3.1. *$\mathcal{E}(\boldsymbol{y}_k) - \mathcal{E}(\boldsymbol{y}^*) \le \epsilon\,(\mathcal{E}(\boldsymbol{y}_0) - \mathcal{E}(\boldsymbol{y}^*))$ when $k > (K+1)^6 \log(1/\epsilon)$.*

Proof. By Taylor's theorem, there exists $\tilde{\boldsymbol{y}} \in [\boldsymbol{y}, \boldsymbol{y}+\boldsymbol{\delta}]$ s.t.

$$\begin{aligned}\mathcal{E}(\boldsymbol{y}+\boldsymbol{\delta}) &= \mathcal{E}(\boldsymbol{y}) + \boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y})^\top\boldsymbol{\delta} + \frac{1}{2}\boldsymbol{\delta}^\top\boldsymbol{H}_{\mathcal{E}}(\tilde{\boldsymbol{y}})\boldsymbol{\delta} \\ &\le \underbrace{\mathcal{E}(\boldsymbol{y}) + \boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y})^\top\boldsymbol{\delta} + \frac{(K+1)^2}{2}\boldsymbol{\delta}^\top\boldsymbol{H}_{\mathcal{E}}(\boldsymbol{y})\boldsymbol{\delta}}_{=:f(\boldsymbol{\delta})} \qquad (16.8)\end{aligned}$$

where the inequality comes from the K-stability of the Hessian,

$$\boldsymbol{H}_{\mathcal{E}}(\tilde{\boldsymbol{y}}) \preceq (1+K)\boldsymbol{A} \preceq (1+K)^2\boldsymbol{H}_{\mathcal{E}}(\boldsymbol{y}).$$

Observe that $f(\boldsymbol{\delta})$ is a convex quadratic function in $\boldsymbol{\delta}$. By minimizing it, or equivalently setting $\boldsymbol{\nabla}_{\boldsymbol{\delta}} f(\boldsymbol{\delta}^*) = \boldsymbol{0}$, we get

$$\boldsymbol{\delta}^* = -\frac{1}{(K+1)^2}\boldsymbol{H}_{\mathcal{E}}^{-1}(\boldsymbol{y})\boldsymbol{\nabla}_{\boldsymbol{y}}\mathcal{E}(\boldsymbol{y}) \qquad (16.9)$$

Here, the step size α is equal to $(K+1)^{-2}$. Then, plugging (16.9) into (16.8),

$$\begin{aligned}\mathcal{E}(\boldsymbol{y}+\boldsymbol{\delta}^*) &\le \mathcal{E}(\boldsymbol{y}) - \frac{1}{2(K+1)^2}\boldsymbol{\nabla}_{\boldsymbol{y}}\mathcal{E}(\boldsymbol{y})^\top\boldsymbol{H}_{\mathcal{E}}^{-1}(\boldsymbol{y})\boldsymbol{\nabla}_{\boldsymbol{y}}\mathcal{E}(\boldsymbol{y}) \\ &\le \mathcal{E}(\boldsymbol{y}) - \frac{1}{2(K+1)^3}\boldsymbol{\nabla}_{\boldsymbol{y}}\mathcal{E}(\boldsymbol{y})^\top\boldsymbol{A}^{-1}\boldsymbol{\nabla}_{\boldsymbol{y}}\mathcal{E}(\boldsymbol{y}) \\ &\text{(subtract } \mathcal{E}(\boldsymbol{y}^*) \text{ on both sides)} \\ \mathcal{E}(\boldsymbol{y}+\boldsymbol{\delta}^*) - \mathcal{E}(\boldsymbol{y}^*) &\le \mathcal{E}(\boldsymbol{y}) - \mathcal{E}(\boldsymbol{y}^*) - \frac{1}{2(K+1)^3}\underbrace{\boldsymbol{\nabla}_{\boldsymbol{y}}\mathcal{E}(\boldsymbol{y})^\top\boldsymbol{A}^{-1}\boldsymbol{\nabla}_{\boldsymbol{y}}\mathcal{E}(\boldsymbol{y})}_{=:\sigma}\end{aligned}$$

where the second inequality is due to K-stability of the inverse Hessian,

$$\frac{1}{1+K}\boldsymbol{A}^{-1} \preceq \boldsymbol{H}_{\mathcal{E}}(\boldsymbol{y})^{-1} \preceq (1+K)\boldsymbol{A}^{-1}.$$

Meanwhile, using Taylor's theorem and K-stability, for some $\hat{\boldsymbol{y}}$ between $\boldsymbol{y}$ and $\boldsymbol{y}^*$, and noting $\boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y}^*) = \boldsymbol{0}$, we have

$$\begin{aligned}\mathcal{E}(\boldsymbol{y}) &= \mathcal{E}(\boldsymbol{y}^*) + \boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y}^*)^\top(\boldsymbol{y}-\boldsymbol{y}^*) + \frac{1}{2}(\boldsymbol{y}-\boldsymbol{y}^*)^\top \boldsymbol{H}_{\mathcal{E}}(\hat{\boldsymbol{y}})(\boldsymbol{y}-\boldsymbol{y}^*)\\ \mathcal{E}(\boldsymbol{y}) - \mathcal{E}(\boldsymbol{y}^*) &\le \frac{(K+1)}{2}\underbrace{(\boldsymbol{y}-\boldsymbol{y}^*)^\top \boldsymbol{A}(\boldsymbol{y}-\boldsymbol{y}^*)}_{=:\gamma}\end{aligned}$$

Next, our task is reduced to comparing σ and γ. $\boldsymbol{y}_t := \boldsymbol{y}^* + t(\boldsymbol{y}-\boldsymbol{y}^*)$ ($t \in [0,1]$) is a point on the segment connecting $\boldsymbol{y}^*$ and $\boldsymbol{y}$. Since

$$\boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y}) = \boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y}) - \boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y}^*) = \int_0^1 H(\boldsymbol{y}_t)(\boldsymbol{y}-\boldsymbol{y}^*)\mathrm{d}t,$$

then

$$\begin{aligned}(\boldsymbol{y}-\boldsymbol{y}^*)^\top\boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y}) &= \int_0^1 (\boldsymbol{y}-\boldsymbol{y}^*)^\top H(\boldsymbol{y}_t)(\boldsymbol{y}-\boldsymbol{y}^*)\mathrm{d}t\\ &\ge \frac{1}{K+1}\int_0^1 (\boldsymbol{y}-\boldsymbol{y}^*)^\top \boldsymbol{A}(\boldsymbol{y}-\boldsymbol{y}^*)\mathrm{d}t\\ &= \frac{\gamma}{K+1}\end{aligned} \tag{16.10}$$

On the other hand, define $\boldsymbol{z}_s = \boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y}^*) + s(\boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y}) - \boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y}^*))$ and then $\mathrm{d}\boldsymbol{z}_s = \boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y})\mathrm{d}s$. Using *Theorem 16.2.3*, we have

$$\boldsymbol{y}-\boldsymbol{y}^* = \int_0^1 \boldsymbol{H}_{\mathcal{E}^*}(\boldsymbol{z}_s)\boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y})\mathrm{d}s.$$

Then,

$$\begin{aligned}\boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y})^\top(\boldsymbol{y}-\boldsymbol{y}^*) &= \int_0^1 \boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y})^\top \boldsymbol{H}_{\mathcal{E}^*}(\boldsymbol{z}_s)\boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y})\mathrm{d}s\\ &\le (K+1)\int_0^1 \boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y})^\top \boldsymbol{A}^{-1}\boldsymbol{\nabla}\mathcal{E}(\boldsymbol{y})\mathrm{d}s\\ &\le (K+1)\sigma\end{aligned} \tag{16.11}$$

Combining (16.10) and (16.11) yields

$$\gamma \le (K+1)^2\sigma.$$

Therefore,

$$\mathcal{E}(\boldsymbol{y}+\boldsymbol{\delta}^*) - \mathcal{E}(\boldsymbol{y}^*) \le (\mathcal{E}(\boldsymbol{y}) - \mathcal{E}(\boldsymbol{y}^*))\left(1 - \frac{1}{(K+1)^6}\right).$$

□

Remark 16.3.2. The basic idea of relating σ and γ in the above proof is writing the same quantity, $\nabla\mathcal{E}(\boldsymbol{y})^\top(\boldsymbol{y}-\boldsymbol{y}^*)$, as two integrations along different lines. $(K+1)^6$ can be reduced to $(K+1)^2$ and even to $(K+1)$ with more care. In some settings, Newton's method converges in $\log\log(1/\epsilon)$ steps.

16.3.3 Linearly Constrained Newton's Method

Let us apply Newton's method to convex optimization programs with only linear constraints,

$$\begin{aligned}\min_{\boldsymbol{f}\in\mathbb{R}^m} \quad & \mathcal{E}(\boldsymbol{f})\\ \text{s.t.} \quad & \boldsymbol{B}\boldsymbol{f}=\boldsymbol{d}\end{aligned}$$

where $\mathcal{E}:\mathbb{R}^m\to\mathbb{R}$ is a convex function and $\boldsymbol{B}\in\mathbb{R}^{n\times m}$. Wlog, let $\boldsymbol{d}=\boldsymbol{0}$, since otherwise we can equivalently deal the following program with $\boldsymbol{B}\boldsymbol{f}_0=\boldsymbol{d}$,

$$\begin{aligned}\min_{\boldsymbol{\rho}\in\mathbb{R}^m} \quad & \mathcal{E}(\boldsymbol{f}_0+\boldsymbol{\rho})\\ \text{s.t.} \quad & \boldsymbol{B}\boldsymbol{\rho}=\boldsymbol{0}\end{aligned}$$

It is useful to think of the variable $\boldsymbol{f}\in\mathbb{R}^m$ as a flow in a graph. Define $C:=\{\boldsymbol{f}:\boldsymbol{B}\boldsymbol{f}=\boldsymbol{0}\}$ which is the kernel space of $\boldsymbol{B}$. C is also called the "cycle space" as it is the set of cycle flows when treating $\boldsymbol{f}$ as flows.

Analyzing the convergence of Newton's method with linear constraints. It is not immediately obvious, but our analysis of Newton step's and their convergence on objectives with a K-stable Hessian carries over directly to linearly constrained convex optimization problems. We will only sketch a proof of this. Firstly, we should notice that instead of thinking of our objective function $\mathcal{E}$ as defined on $\mathbb{R}^m$ and then constrained to inputs $\boldsymbol{f}\in C$, we can think of a new function $\hat{\mathcal{E}}:C\to\mathbb{R}$ defined such that for $\boldsymbol{f}\in C$ we have $\hat{\mathcal{E}}(\boldsymbol{f})=\mathcal{E}(\boldsymbol{f})$. But, C is a linear subspace and is isomorphic[1] to $\mathbb{R}^{\dim(C)}$. This means that our previous analysis can be directly applied, if we can compute the gradient and Hessian of the function viewed as an *unconstrained* function on C (or equivalently $\mathbb{R}^{\dim(C)}$). We now have two important questions to answer:

1. What does the gradient and Hessian, and hence Newton steps, of $\hat{\mathcal{E}}(\boldsymbol{f})$ look like?
2. Does the K-stability of the Hessian of $\mathcal{E}$ carry over to the function $\hat{\mathcal{E}}$?

The gradient and Hessian of $\hat{\mathcal{E}}$ should live in $\mathbb{R}^{\dim(C)}$ and $\mathbb{R}^{\dim(C)\times\dim(C)}$ respectively. Let Π_C be the orthogonal projection matrix onto $\boldsymbol{C}$, meaning Π_C is symmetric and $\Pi_C\boldsymbol{\delta}=\boldsymbol{\delta}$ for

[1]You don't need to know the formal definition of isomorphism on vector spaces. In this context, it means equivalent up to a transformation by an invertible matrix. In fact in our case, the isomorphism is given by an orthonormal matrix.

any $\boldsymbol{\delta} \in C$. Given any $\boldsymbol{f} \in C$, add to it an infinitesimal $\boldsymbol{\delta} \in C$, then

$$\begin{aligned}\hat{\mathcal{E}}(\boldsymbol{f}+\boldsymbol{\delta}) = \mathcal{E}(\boldsymbol{f}+\boldsymbol{\delta}) &\approx \mathcal{E}(\boldsymbol{f}) + \langle \boldsymbol{\nabla}\mathcal{E}(\boldsymbol{f}), \boldsymbol{\delta}\rangle \\ &= \mathcal{E}(\boldsymbol{f}) + \langle \boldsymbol{\nabla}\mathcal{E}(\boldsymbol{f}), \Pi_C\boldsymbol{\delta}\rangle \\ &= \mathcal{E}(\boldsymbol{f}) + \langle \Pi_C\boldsymbol{\nabla}\mathcal{E}(\boldsymbol{f}), \boldsymbol{\delta}\rangle\end{aligned}$$

From this, we can deduce that the gradient of $\hat{\mathcal{E}}$ at a point $\boldsymbol{f} \in C$ is essentially equal (up to a fixed linear transformation independent of $\boldsymbol{f}$) to the projection of gradient of $\boldsymbol{\nabla}\mathcal{E}$ at $\boldsymbol{f}$ onto the subspace C. Similarly,

$$\hat{\mathcal{E}}(\boldsymbol{f}+\boldsymbol{\delta}) = \mathcal{E}(\boldsymbol{f}+\boldsymbol{\delta}) \approx \mathcal{E}(\boldsymbol{f}) + \langle \Pi_C\boldsymbol{\nabla}\mathcal{E}(\boldsymbol{f}), \boldsymbol{\delta}\rangle + \frac{1}{2}\langle \boldsymbol{\delta}, \Pi_C\boldsymbol{H}_{\mathcal{E}}(\boldsymbol{f})\Pi_C\boldsymbol{\delta}\rangle$$

Again from this, we can deduce that the Hessian of $\hat{\mathcal{E}}$ at a point $\boldsymbol{f} \in C$ is essentially equal (again up to a fixed linear transformation independent of $\boldsymbol{f}$) to the matrix $\Pi_C\boldsymbol{H}_{\mathcal{E}}(\boldsymbol{f})\Pi_C$. Note that $\boldsymbol{X} \preceq \boldsymbol{Y}$ implies $\Pi_C\boldsymbol{X}\Pi_C \preceq \Pi_C\boldsymbol{Y}\Pi_C$, and from this we can see that the Hessian of $\hat{\mathcal{E}}$ is K-stable if the Hessian of $\mathcal{E}$ is. Also note that we were not terribly formal in the discussion above. We can be more precise by replacing Π_C with a linear map from $\mathbb{R}^{\dim(C)}$ to $\mathbb{R}^m$ which maps any vector in $\mathbb{R}^{\dim(C)}$ to a vector in C and then going through a similar chain of reasoning.

What is a Newton step $\boldsymbol{\delta}^*$ w.r.t. $\hat{\mathcal{E}}$? It turns out that for actually computing the Newton step, it is easier to think again of $\mathcal{E}$ with a constraint that the Newton step must lie in the subspace C. One can show that this is equivalent to the Newton step of $\hat{\mathcal{E}}$, but we omit this.

In the constrained view, $\boldsymbol{\delta}^*$ should be a minimizer of

$$\begin{aligned}&\min_{\substack{\boldsymbol{\delta}\in\mathbb{R}^m \\ \boldsymbol{B}\boldsymbol{\delta}=\boldsymbol{0}}} \langle \underbrace{\boldsymbol{\nabla}\mathcal{E}(\boldsymbol{f})}_{=:\boldsymbol{g}}, \boldsymbol{\delta}\rangle + \frac{1}{2}\langle \boldsymbol{\delta}, \underbrace{\boldsymbol{H}_{\mathcal{E}}(\boldsymbol{f})}_{=:\boldsymbol{H}}\boldsymbol{\delta}\rangle \\ &\quad \text{(Lagrange duality)} \\ \iff &\max_{\boldsymbol{x}\in\mathbb{R}^n}\min_{\boldsymbol{\delta}\in\mathbb{R}^m} \underbrace{\langle \boldsymbol{g}, \boldsymbol{\delta}\rangle + \frac{1}{2}\langle \boldsymbol{\delta}, \boldsymbol{H}\boldsymbol{\delta}\rangle - \boldsymbol{x}^\top\boldsymbol{B}\boldsymbol{\delta}}_{\text{Lagrangian } L(\boldsymbol{\delta},\boldsymbol{x})} \qquad (16.12)\end{aligned}$$

Applying the KKT optimality conditions, one has

$$\begin{aligned}\boldsymbol{B}\boldsymbol{\delta} &= \boldsymbol{0}, \\ \boldsymbol{\nabla}_{\boldsymbol{\delta}} L(\boldsymbol{\delta}, \boldsymbol{x}) = \boldsymbol{g} + \boldsymbol{H}\boldsymbol{\delta} - \boldsymbol{B}^\top\boldsymbol{x} &= \boldsymbol{0},\end{aligned}$$

from which we get

$$\begin{aligned}\boldsymbol{\delta} + \boldsymbol{H}^{-1}\boldsymbol{g} &= \boldsymbol{H}^{-1}\boldsymbol{B}^\top\boldsymbol{x} \\ \underbrace{\boldsymbol{B}\boldsymbol{\delta}}_{=\boldsymbol{0}} + \boldsymbol{B}\boldsymbol{H}^{-1}\boldsymbol{g} &= \boldsymbol{B}\boldsymbol{H}^{-1}\boldsymbol{B}^\top\boldsymbol{x} \\ \boldsymbol{B}\boldsymbol{H}^{-1}\boldsymbol{g} &= \underbrace{\boldsymbol{B}\boldsymbol{H}^{-1}\boldsymbol{B}^\top}_{=:\boldsymbol{L}}\boldsymbol{x}\end{aligned}$$

Finally, the solutions to (16.12) are

$$\begin{cases} \boldsymbol{x}^* & = \boldsymbol{L}^{-1}\boldsymbol{B}\boldsymbol{H}^{-1}\boldsymbol{g} \\ \boldsymbol{\delta}^* & = -\boldsymbol{H}^{-1}\boldsymbol{g} + \boldsymbol{H}^{-1}\boldsymbol{B}^\top \boldsymbol{x}^* \end{cases}$$

It is easy to verify that $\boldsymbol{B}\boldsymbol{\delta}^* = \boldsymbol{0}$. Thus, our update rule is $\boldsymbol{f}_{i+1} = \boldsymbol{f}_i + \boldsymbol{\delta}^*$. And we have the following convergence result.

Theorem 16.3.3. $\hat{\mathcal{E}}(\boldsymbol{f}_k) - \hat{\mathcal{E}}(\boldsymbol{f}^*) \leq \epsilon \cdot \left(\hat{\mathcal{E}}(\boldsymbol{f}_0) - \hat{\mathcal{E}}(\boldsymbol{f}^*)\right)$ *when* $k > (K+1)^6 \log(1/\epsilon)$.

Remark 16.3.4. Note if $\mathcal{E}(\boldsymbol{f}) = \sum_{i=1}^m \mathcal{E}_i(\boldsymbol{f}(i))$, then $\boldsymbol{H}_{\mathcal{E}}(\boldsymbol{f})$ is diagonal. Thus, $\boldsymbol{L} = \boldsymbol{B}\boldsymbol{H}^{-1}\boldsymbol{B}^\top$ is indeed a Laplacian provided that $\boldsymbol{B}$ is an incidence matrix. Therefore, the linear equations we need to solve to apply Newton's method in a network flow setting are Laplacians, which means we can solve them very quickly.

Chapter 17

Interior Point Methods for Maximum Flow

Background and Notation

In this chapter, we'll learn about interior point methods for solving maximum flow, which is a rich and active area of research [DS08, Mad13, LS20b, LS20a].

We're going to frequently need to refer to vectors arising from elementwise operations combining other vectors.

To that end, given two vector $\boldsymbol{a} \in \mathbb{R}^m$, and $\boldsymbol{b} \in \mathbb{R}^m$, we will use $\overrightarrow{(\boldsymbol{a}(i)\boldsymbol{b}(i))}$ to denote the vector $\boldsymbol{z}$ with $\boldsymbol{z}(i) = \boldsymbol{a}(i)\boldsymbol{b}(i)$ and so on.

Throughout this chapter, when we are working in the context of some given graph G with vertices V and edges E, we will let $m = |E|$ and $n = |V|$.

The plots in this chapter were made using Mathematica, which is available to ETH students for download through the ETH IT Shop.

17.1 An Interior Point Method

The Maximum Flow problem in undirected graphs.

$$\begin{aligned} \max_{\boldsymbol{f} \in \mathbb{R}^E} \quad & F \\ \text{s.t. } & \boldsymbol{B}\boldsymbol{f} = F\boldsymbol{b}_{st} \\ & -\boldsymbol{c} \leq \boldsymbol{f} \leq \boldsymbol{c} \end{aligned} \tag{17.1}$$

"The Undirected Maximum Flow Problem"

We use $\text{val}(\boldsymbol{f})$ to denote F when $B\boldsymbol{f} = F\boldsymbol{b}_{st}$.

As we develop algorithms for this problem, we will assume that we know the maximum flow value F^*. Let $\boldsymbol{f}^*$ denote some maximum flow, i.e. a flow with $-\boldsymbol{c} \leq \boldsymbol{f} \leq \boldsymbol{c}$ can $\text{val}(\boldsymbol{f}^*) = F^*$.

In general, an a lower bound $F \leq F^*$ will allow us to find a flow with value F, and because of this, we can use a binary search to approximate F^*.

17.1.1 A Barrier Function and an Algorithm

$$V(\boldsymbol{f}) = \sum_e -\log(\boldsymbol{c}(e) - \boldsymbol{f}(e)) - \log(\boldsymbol{c}(e) + \boldsymbol{f}(e))$$

We assume the optimal value of Program (17.1) is F^*. Then for a given $0 \leq \alpha < 1$ we define a program

$$\begin{aligned} \min_{\boldsymbol{f} \in \mathbb{R}^E} \quad & V(\boldsymbol{f}) \\ \text{s.t. } & \boldsymbol{B}\boldsymbol{f} = \alpha F^* \boldsymbol{b}_{st} \end{aligned} \tag{17.2}$$

"The Barrier Problem"

This problem makes sense for any $0 \leq \alpha < 1$. When $\alpha = 0$, we are not routing any flow yet. This will be our starting point. For any $0 \leq \alpha < 1$, the scaled-down maximum flow $\alpha \boldsymbol{f}^*$ strictly satisfies the capacities $-\boldsymbol{c} < \alpha \boldsymbol{f}^* < \boldsymbol{c}$, and $\boldsymbol{B}\alpha\boldsymbol{f}^* = \alpha F^* \boldsymbol{b}_{st}$. Hence $\alpha \boldsymbol{f}^*$ is a feasible flow for this value of α and hence $V(\alpha \boldsymbol{f}^*) < \infty$ and so the optimal flow for the Barrier Problem at this α must also have objective value strictly below ∞, and hence in turn strictly satisfy the capacity constraints. Thus, if we can find the optimal flow for Program (17.2) for $\alpha = 1 - \epsilon$, we will have a feasible flow with Program (17.1), the Undirected Maximum Flow Problem, routing $(1 - \epsilon)F^*$. This is how we will develop an algorithm for computing the maximum flow.

Program (17.2) has the Lagrangian

$$\mathcal{L}(\boldsymbol{f}, \boldsymbol{x}) = V(\boldsymbol{f}) + \boldsymbol{x}^\top (\alpha F^* \boldsymbol{b}_{st} - \boldsymbol{B}\boldsymbol{f})$$

And we have optimality when

$$\boldsymbol{B}\boldsymbol{f} = \alpha F^* \boldsymbol{b}_{st} \text{ and } -\boldsymbol{c} \leq \boldsymbol{f} \leq \boldsymbol{c} \tag{17.3}$$

"Barrier feasibility"

and $\boldsymbol{\nabla}_{\boldsymbol{f}} \mathcal{L}(\boldsymbol{f}, \boldsymbol{x}) = \boldsymbol{0}$, i.e.

$$\boldsymbol{\nabla} V(\boldsymbol{f}) = \boldsymbol{B}^\top \boldsymbol{x} \tag{17.4}$$

"Barrier Lagrangian gradient optimality"

Let $\boldsymbol{f}^*_\alpha$ denote the optimal solution to Problem 17.2 for a given $0 \leq \alpha < 1$, and let $\boldsymbol{x}^*_\alpha$ be optimal dual voltages such that $\boldsymbol{\nabla} V(\boldsymbol{f}^*_\alpha) = \boldsymbol{B}^\top \boldsymbol{x}^*_\alpha$.

It turns out that, if we have a solution $\boldsymbol{f}^*_\alpha$ to this problem for some $\alpha < 1$, then we can find a solution $\boldsymbol{f}_{\alpha+\alpha'}$ for some $\alpha' < 1 - \alpha$. And, we can compute $\boldsymbol{f}_{\alpha+\alpha'}$ using a small number of Newton steps, each of which will only require a Laplacian linear equation solve, and hence is computable in $\widetilde{O}(m)$ time. Concretely, for any $0 \leq \alpha < 1$, given the optimal flow at this α, we will be able to compute the optimal flow at $\alpha_{\text{new}} = \alpha + (1-\alpha)\frac{1}{150\sqrt{m}}$. This means that after $T = 150\sqrt{m}\log(1/\epsilon)$ updates, we have a solution for $\alpha \geq 1 - \epsilon$.

We can state the update problem as

$$\begin{aligned} \min_{\boldsymbol{\delta} \in \mathbb{R}^E} \quad & V(\boldsymbol{\delta} + \boldsymbol{f}) \\ \text{s.t. } \boldsymbol{B}\boldsymbol{\delta} &= \alpha' F^* \boldsymbol{b}_{st} \end{aligned} \tag{17.5}$$

"The Update Problem"

17.1.2 Updates using Divergence

It turns out that for the purposes of analysis, it will be useful to ensure that our "Update Problem" uses an objective function that is minimized at $\boldsymbol{\delta} = \mathbf{0}$.

This leads to a variant of the Update Problem, which we call the "Divergence Update Problem". We obtain our new problem by switching from $V(\boldsymbol{\delta} + \boldsymbol{f})$ as our objective to $V(\boldsymbol{\delta}+\boldsymbol{f}) - (V(\boldsymbol{f}) + \langle \boldsymbol{\nabla} V(\boldsymbol{f}), \boldsymbol{\delta} \rangle)$ as our objective, and this is called the *divergece* of V w.r.t. $\boldsymbol{\delta}$ *based* at $\boldsymbol{f}$.

$$\begin{aligned} \min_{\boldsymbol{\delta} \in \mathbb{R}^E} \quad & V(\boldsymbol{\delta} + \boldsymbol{f}) - (V(\boldsymbol{f}) + \langle \boldsymbol{\nabla} V(\boldsymbol{f}), \boldsymbol{\delta} \rangle) \\ \text{s.t. } \boldsymbol{B}\boldsymbol{\delta} &= \alpha' F^* \boldsymbol{b}_{st} \end{aligned} \tag{17.6}$$

"The Divergence Update Problem"

Now, for any flow $\boldsymbol{\delta}$ such that $\boldsymbol{B}\boldsymbol{\delta} = \alpha' F^* \boldsymbol{b}_{st}$, using the Lagrangian gradient condition (17.4), we have $\langle \boldsymbol{\nabla} V(\boldsymbol{f}^*_\alpha), \boldsymbol{\delta} \rangle = \langle \boldsymbol{x}^*_\alpha, \alpha' F^* \boldsymbol{b}_{st} \rangle$. Hence, for such $\boldsymbol{\delta}$, we have

$$V(\boldsymbol{\delta} + \boldsymbol{f}^*_\alpha) - (V(\boldsymbol{f}^*_\alpha) + \langle \boldsymbol{\nabla} V(\boldsymbol{f}^*_\alpha), \boldsymbol{\delta} \rangle) = V(\boldsymbol{\delta} + \boldsymbol{f}^*_\alpha) - (V(\boldsymbol{f}^*_\alpha) + \langle \boldsymbol{x}^*_\alpha, \alpha' F^* \boldsymbol{b}_{st} \rangle)$$

We conclude that the objectives of the Update Problem (17.5) and the Divergence Update Problem (17.6) have the same minimizer, which we denote $\boldsymbol{\delta}^*_{\alpha'}$, although, to be precise, it is also a function of α.

Thus $\boldsymbol{f}^*_\alpha + \boldsymbol{\delta}^*_{\alpha'}$ is optimal for the optimization problem

$$\begin{aligned} \min_{\boldsymbol{f} \in \mathbb{R}^E} \quad & V(\boldsymbol{f}) \\ \text{s.t. } \boldsymbol{B}\boldsymbol{f} &= (\alpha + \alpha') F^* \boldsymbol{b}_{st} \end{aligned} \tag{17.7}$$

Lemma 17.1.1. *Suppose $\boldsymbol{f}^*_\alpha$ is the minimizer of Problem* (17.2) *(the Barrier Problem with parameter α) and $\boldsymbol{\delta}^*_{\alpha'}$ is the minimizer of Problem* (17.6) *(the Update Problem with parameters $\boldsymbol{f}^*_\alpha$ and α'), then $\boldsymbol{f}^*_\alpha + \boldsymbol{\delta}^*_{\alpha'}$ is optimal for Problem* (17.2) *with parameter $\alpha + \alpha'$ (i.e. a new instance of the Barrier problem).*

Algorithm 18: Interior Point Method

$\boldsymbol{f} \leftarrow \mathbf{0}$;
$\alpha \leftarrow 0$;
while $\alpha < 1 - \epsilon$ **do**
  $a' \leftarrow \frac{1-\alpha}{20\sqrt{m}}$;
  Compute $\boldsymbol{\delta}$, the minimizer of Problem (17.6);
  Let $\boldsymbol{f} \leftarrow \boldsymbol{f} + \boldsymbol{\delta}$ and $\alpha \leftarrow \alpha + \alpha'$;
end
return $\boldsymbol{f}$

Pseudotheorem 17.1.1. *Let $\boldsymbol{f}$ be the minimizer of Problem* (17.2)*. Then, when $a' \leq \frac{1-\alpha}{20\sqrt{m}}$, the minimizer $\boldsymbol{\delta}$ of Problem* (17.7) *can be computed in $\widetilde{O}(m)$ time.*

The key insight in this type of interior point method is that when the update α' is small enough,

Theorem 17.1.2. *Algorithm 18 returns a flow $\boldsymbol{f}$ that is feasible for Problem* (17.1) *in time $\widetilde{O}(m^{1.5}\log(1/\epsilon))$.*

Proof Sketch. First note that for $\alpha = 0$, the minimizer of Problem (17.2) is $\boldsymbol{f} = \mathbf{0}$. The proof now essentially follows by Lemma (17.1.1), and Pseudotheorem 17.1.1. Note that $1-\alpha$ shrinks by a factor $(1 - \frac{1}{20\sqrt{m}})$ in each iteration of the while-loop, and so after $20\sqrt{m}\log(1/\epsilon)$ iterations, we have $1 - \alpha \leq \epsilon$, at which point the loop terminates. To turn this into a formal proof, we need to take care of the fact the proper theorem corresponding to Pseudotheorem 17.1.1 only gives a highly accurate but not exact solution δ to the "Update Problem". But it's possible to show that this is good enough (even though both $\boldsymbol{f}$ and $\boldsymbol{\delta}$ end up not being exactly optimal in each iteration). □

Remark 17.1.3. For the maximum flow problem, when capacities are integral and polynomially bounded, if we choose $\epsilon = m^{-c}$ for some large enough constant c, given a feasible flow with $\text{val}(\boldsymbol{f}) = 1 - \epsilon$, is it possible to compute an exact maximum flow in nearly linear time. Thus Theorem 17.1.2 can also be used to compute an exact maximum flow in $\widetilde{O}(m)$ time, but we omit the proof. The idea is to first round to an almost optimal, feasible integral flow (which requires a non-trivial combinatorial algorithm), and then to recover the exact flow using Ford-Fulkerson. See [Mad13] for details.

Remark 17.1.4. It is possible to reduce an instance of directed maximum flow to an instance of undirected maximum flow in nearly-linear time, in such a way that if we can *exactly* solve the undirected instance, then in nearly-linear time we can recover an exact solution to the directed maximum flow problem. Thus Theorem (17.1.2) can also be used to solve directed maximum flow. We will ask you to develop this reduction in Graded Homework 2.

Remark 17.1.5. For sparse graphs with $m = \widetilde{O}(n)$ and large capacities, this running time is the best known, and improving it is major open problem.

17.1.3 Understanding the Divergence Objective

Note that if $V(x) = -\log(1-x)$, then $D(x) = V(x) - (V(0) + V'(0)x)$.

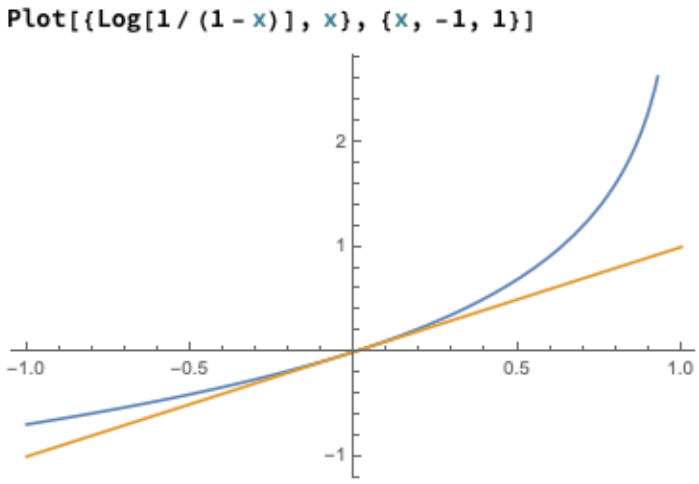


Figure 17.1: Plot showing $V(x) = -\log(1-x)$ and then linear approximation $V(0) + V'(0)x$.

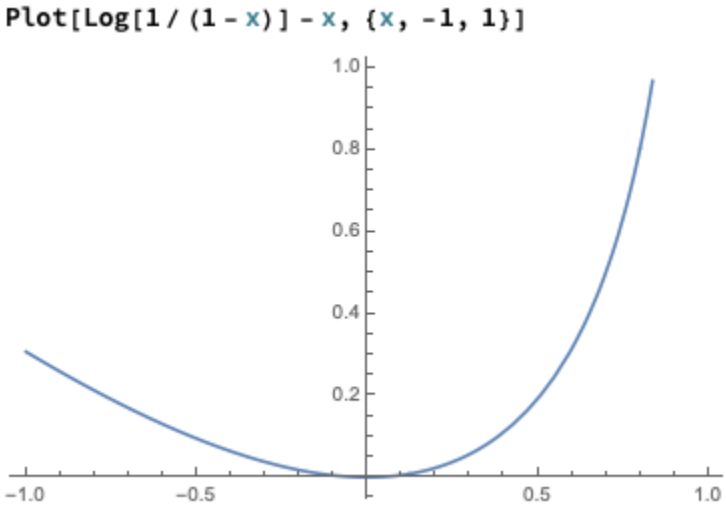


Figure 17.2: Plot showing $D(x) = V(x) - (V(0) + V'(0)x)$.

We let

$$\boldsymbol{c}_+(e) = \boldsymbol{c}(e) - \boldsymbol{f}(e) \text{ and } \boldsymbol{c}_-(e) = \boldsymbol{c}(e) + \boldsymbol{f}(e)$$

So then

$$\begin{aligned} D_V(\boldsymbol{\delta}) &= V(\boldsymbol{\delta}+\boldsymbol{f}) - (V(\boldsymbol{f}) + \langle \boldsymbol{\nabla} V(\boldsymbol{f}), \boldsymbol{\delta}\rangle) \\ &= \sum_e -\log\left(\frac{\boldsymbol{c}(e) - (\boldsymbol{\delta}(e)+\boldsymbol{f}(e))}{\boldsymbol{c}(e)-\boldsymbol{f}(e)}\right) - \frac{\boldsymbol{\delta}(e)}{\boldsymbol{c}(e)-\boldsymbol{f}(e)} \\ &\qquad -\log\left(\frac{\boldsymbol{c}(e) + (\boldsymbol{\delta}(e)+\boldsymbol{f}(e))}{\boldsymbol{c}(e)+\boldsymbol{f}(e)}\right) + \frac{\boldsymbol{\delta}(e)}{\boldsymbol{c}(e)+\boldsymbol{f}(e)} \\ &= \sum_e D\left(\frac{\boldsymbol{\delta}(e)}{\boldsymbol{c}(e)-\boldsymbol{f}(e)}\right) + D\left(-\frac{\boldsymbol{\delta}(e)}{\boldsymbol{c}(e)+\boldsymbol{f}(e)}\right) \\ &= \sum_e D\left(\frac{\boldsymbol{\delta}(e)}{\boldsymbol{c}_+(e)}\right) + D\left(-\frac{\boldsymbol{\delta}(e)}{\boldsymbol{c}_-(e)}\right) \end{aligned}$$

Note that we can express Problem (17.6) as

$$\begin{aligned} &\min_{\boldsymbol{\delta}\in\mathbb{R}^E} \quad D_V(\boldsymbol{\delta}) && (17.8) \\ &\text{s.t. } \boldsymbol{B}\boldsymbol{\delta} = \alpha' F^* \boldsymbol{b}_{st} && \text{The Update Problem, restated} \end{aligned}$$

Note that $D_V(\boldsymbol{\delta})$ is strictly convex of over the feasible set, so the argmin is unique.

17.1.4 Quadratically Smoothing Divergence and Local Agreement

$$\tilde{D}_\epsilon(x) = \begin{cases} -\log(1-x) - x & \text{if } |x| \le \epsilon \\ D(\epsilon) + D'(\epsilon)(x-\epsilon) + \frac{D''(\epsilon)}{2}(x-\epsilon)^2 & \text{if } x > \epsilon \\ D(-\epsilon) + D'(-\epsilon)(x+\epsilon) + \frac{D''(-\epsilon)}{2}(x+\epsilon)^2 & \text{if } x < -\epsilon \end{cases}$$

For brevity, we define

$$\tilde{D}(x) = \tilde{D}_{0.1}(x)$$

Lemma 17.1.6.

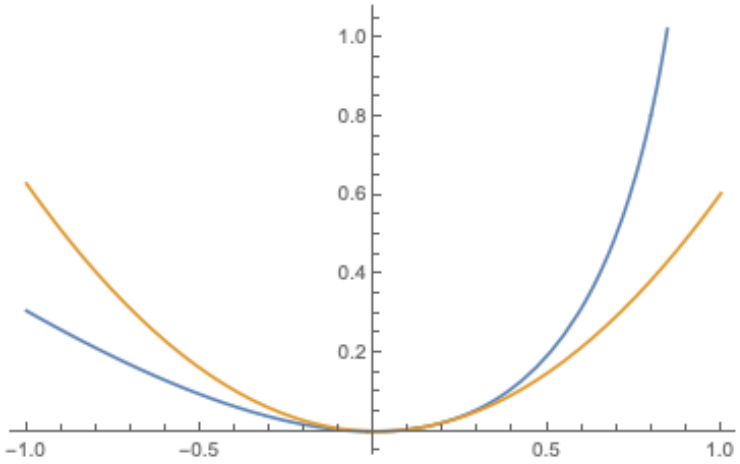
1. $1/2 \le \tilde{D}''(\boldsymbol{x}) \le 2$.
2. *For $x \ge 0$, we have $x/2 \le \tilde{D}'(\boldsymbol{x}) \le 2x$ and $-2x \le \tilde{D}'(-\boldsymbol{x}) \le -x/2$.*
3. $x^2/4 \le \tilde{D}(\boldsymbol{x}) \le x^2$.

What's happening here? We glue together $D(x)$ for small x with its quadratic approximation for $|x| > \epsilon$. For $x > \epsilon$, we "glue in" a Taylor series expansion based at $x = \epsilon$.

```
NumberForm[Series[Log[1 / (1 - x)] - x, {x, 0.1, 2}], 3]
```

```
nberForm=
0.00536 + 0.111 (x - 0.1) + 0.617 (x - 0.1)^2 + O[x - 0.1]^3
```

```
Plot[{Log[1 / (1 - x)] - x, 0.00536 + 0.111 (x - 0.1) + 0.617 (x - 0.1)^2}, {x, -1, 1}]
```




```
Plot[{Log[1 / (1 - x)] - x, 0.00536 + 0.111 (x - 0.1) + 0.617 (x - 0.1)^2}, {x, 0, 0.2}]
```

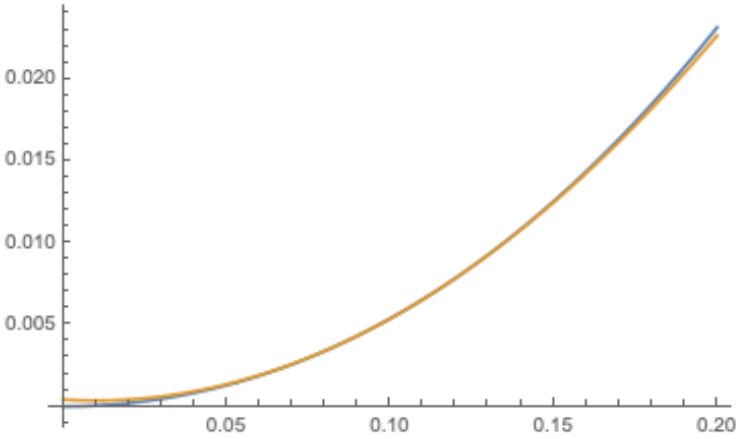


Figure 17.3: Plot showing $D(x) = -\log(1-x)$ and the quadratic approximation based at $x = 0.1$.

We also define

$$\tilde{D}_V(\boldsymbol{\delta}) = \sum_e \tilde{D}\left(\frac{\boldsymbol{\delta}(e)}{\boldsymbol{c}_+(e)}\right) + \tilde{D}\left(-\frac{\boldsymbol{\delta}(e)}{\boldsymbol{c}_-(e)}\right)$$

We can now introduce the smoothed optimization problem

$$\min_{\boldsymbol{\delta}\in\mathbb{R}^E} \quad \tilde{D}_V(\boldsymbol{\delta}) \tag{17.9}$$

$$\text{s.t. } \boldsymbol{B}\boldsymbol{\delta} = \alpha' F^* \boldsymbol{b}_{st} \qquad \text{“The Smoothed Update Problem”}$$

Note that $\tilde{D}_V(\boldsymbol{\delta})$ is strictly convex of over the feasible set, so the argmin is unique.

Pseudoclaim 17.1.7. *We can compute the argmin $\boldsymbol{\delta}^*$ of Problem* (17.9)*, the Smoothed Update Problem, using the Newton-Steps for K-stable Hessian convex functions that we saw in the previous chapter, in $\widetilde{O}(m)$ time.*

Sketch of proof. Problem (17.9) fits the class of problems for which we showed in the previous chapter that (appropriately scaled) Newton steps converge. This is true because the Hessian is always a 2-spectral approximation of the Hessian at $\tilde{D}_V(\boldsymbol{\delta}^*)$, as can be shown from Lemma 17.1.6. Because the Hessian of $\tilde{D}_V(\boldsymbol{\delta})$ is diagonal, and the constraints are flow constraints, each Newton step boils down to solving a Laplacian linear system, which can be done to high accuracy $\widetilde{O}(m)$ time. □

Remark 17.1.8. There are three things we need to modify to turn the pseudoclaim into a true claim, addressing the errors arising from both Laplacian solvers and Newton steps:

1. We need to rephrase the claim to so that we only claim $\boldsymbol{\delta}^*$ has been computed to high accuracy, rather than exactly.

2. We need to show that we can construct an initial guess to start off Newton's method $\boldsymbol{\delta}_0$ for which the value $\tilde{D}_V(\boldsymbol{\delta}_0)$ is not too large. (This is easy).

3. We need show that Newton steps converge despite using a Laplacian solver that doesn't give exact solutions, only high accuracy solutions. (Takes a bit of work, but is ultimately not too difficult).

Importantly, to ensure our overall interior point method still works, we also need to show that it converges, even if we're using approximate solutions everywhere. This also takes some work to show, again is not too difficult.

Local Agreement Implies Same Optimum.

Lemma 17.1.9. *Suppose $S \subseteq \mathbb{R}^n$ is a convex set, and let $f, g : S \to \mathbb{R}$ be convex functions. Let $\boldsymbol{x}^* = \arg\min_{\boldsymbol{x} \in S} f(\boldsymbol{x})$. Suppose f, g agree on a neighborhood of $\boldsymbol{x}^*$ in S (i.e. an open set containing $\boldsymbol{x}^*$). Then $\boldsymbol{x}^* = \arg\min_{\boldsymbol{x} \in S} g(\boldsymbol{x})$.*

Proof Sketch. We sketch the proof in the case when both f, g are differentiable: Observe that $\mathbf{0} = \boldsymbol{\nabla} f(\boldsymbol{x}^*) = \boldsymbol{\nabla} g(\boldsymbol{x}^*)$, and hence $g(\boldsymbol{x})$ is also minimized at $\boldsymbol{x}^*$. □

We define

$$\widehat{\boldsymbol{c}}(e) = \min(\boldsymbol{c}_+(e), \boldsymbol{c}_-(e)) \tag{17.10}$$

Lemma 17.1.10. *Suppose $\boldsymbol{\delta}^*$ is the argmin of Problem* (17.9)*, the Smoothed Update Problem, and $\left\| \overrightarrow{(\boldsymbol{\delta}^*(e)/\widehat{\boldsymbol{c}}(e))} \right\|_\infty < 0.1$. Then $\boldsymbol{\delta}^*$ is the argmin of Problem* (17.8)*.*

Proof. We observe that if $\left\|\overrightarrow{(\boldsymbol{\delta}^*(e)/\widehat{\boldsymbol{c}}(e))}\right\|_\infty < 0.1$, then $\tilde{D}_V(\boldsymbol{\delta}^*) = D_V(\boldsymbol{\delta}^*)$, and, for all $\boldsymbol{\tau} \in \mathbb{R}^m$ with norm

$$\left\|\overrightarrow{(\boldsymbol{\tau}(e)/\widehat{\boldsymbol{c}}(e))}\right\|_\infty < 0.1 - \left\|\overrightarrow{(\boldsymbol{\delta}^*(e)/\widehat{\boldsymbol{c}}(e))}\right\|_\infty$$

we have that $\tilde{D}_V(\boldsymbol{\delta}^* + \boldsymbol{\tau}) = D_V(\boldsymbol{\delta}^* + \boldsymbol{\tau})$. Thus $\tilde{D}_V$ and D_V agree on a neighborhood around $\boldsymbol{\delta}^*$ and hence by Lemma 17.1.9, we have that $\boldsymbol{\delta}^*$ is the argmin of Problem (17.8). □

17.1.5 Step size for divergence update

Definition 17.1.11 (*s-t well-conditioned* graph)**.** An undirected, capacitated multi-graph $G = (V, E, \boldsymbol{c})$ with source s and sink t is *s-t well-conditioned* if, letting U denote the maximum edge capacity $U = \|\boldsymbol{c}\|_\infty$, we have at least $\frac{2}{3}m$ multi-edges of capacity U going directly from s to t.

Remark 17.1.12. It is straightforward to make a graph s-t well-conditioned. We just add $2m$ new edges of capacity U directly between s and t. Given an exact maximum flow in the new graph, it is trivial to get one in the original graph: Just remove the flow on the new edges.

Definition 17.1.13. Given a *directed* graph $G = (V, E, \boldsymbol{c})$, the *symmetrization* of G is the undirected $\widehat{G} = (V, \widehat{E}, \widehat{\boldsymbol{c}})$ is the undirected graph given by

$$\{a, b\} \in \widehat{E} \text{ if } (a, b) \in E \text{ AND } (b, a) \in E$$

and

$$\widehat{\boldsymbol{c}}(\{a, b\}) = \min(\boldsymbol{c}(a, b), \boldsymbol{c}(b, a)).$$

Note that when $\widehat{G}_{\boldsymbol{f}}$ is the symmetrization of the residual graph $G_{\boldsymbol{f}}$ (which we defined in Chapter 11), then $\widehat{\boldsymbol{c}}$ matches exactly the definition of $\widehat{\boldsymbol{c}}$ in Equation (17.10).

Lemma 17.1.14. *Let G be an undirected, capacitated multi-graph $G = (V, E, \boldsymbol{c})$ which is s-t well-conditioned. Let $\boldsymbol{f}$ be the minimizer of Program* (17.2)*. Let $\widehat{G}_{\boldsymbol{f}}$ be the* symmetrization *of the residual graph $G_{\boldsymbol{f}}$ (in the sense of Lecture 10). Then there exists a flow $\hat{\boldsymbol{\delta}}$ which satisfies $\boldsymbol{B}\hat{\boldsymbol{\delta}} = \frac{1-\alpha}{5}F^*\boldsymbol{b}_{st}$ and is feasible in $\widehat{G}_{\boldsymbol{f}}$. Note that we can also state the feasibility in $\widehat{G}_{\boldsymbol{f}}$ as*

$$\left\|\overrightarrow{\left(\hat{\boldsymbol{\delta}}(e)/\widehat{\boldsymbol{c}}(e)\right)}\right\|_\infty \leq 1$$

Proof. We recall since $\boldsymbol{f}$ is the minimizer of Program (17.2), there exists dual-optimal voltages $\boldsymbol{x}$ such that

$$\boldsymbol{B}^\top \boldsymbol{x} = \boldsymbol{\nabla} V(\boldsymbol{f}) = \overrightarrow{\left(\frac{1}{\boldsymbol{c}(e) - \boldsymbol{f}(e)} - \frac{1}{\boldsymbol{c}(e) + \boldsymbol{f}(e)}\right)}$$

From Lecture 10, we know that there is flow $\bar{\boldsymbol{\delta}}$ that is feasible with respect to the residual graph capacities of the graph $G_{\boldsymbol{f}}$ such that $\boldsymbol{B}\bar{\boldsymbol{\delta}} = (1 - \alpha)F^*\boldsymbol{b}_{st}$. Note when treating $\bar{\boldsymbol{\delta}}$

as an undirected flow, feasibility in the residual graph means that $\overline{\boldsymbol{\delta}}(e) < \boldsymbol{c}(e) - \boldsymbol{f}(e)$ and $-\overline{\boldsymbol{\delta}}(e) < \boldsymbol{c}(e) + \boldsymbol{f}(e)$. Thus,

$$(1-\alpha)F^*\boldsymbol{b}_{st}^\top \boldsymbol{x} = \overline{\boldsymbol{\delta}}\boldsymbol{B}^\top \boldsymbol{x} = \sum_e \frac{\overline{\boldsymbol{\delta}}}{\boldsymbol{c}(e) - \boldsymbol{f}(e)} - \frac{\overline{\boldsymbol{\delta}}}{\boldsymbol{c}(e) + \boldsymbol{f}(e)} \leq m$$

Now, because the graph is s-t well-conditioned, there are at $\frac{2}{3}m$ edges directly from s to t with capacity U and each of these e satisfy by the Lagrangian gradient optimality condition (17.4)

$$\boldsymbol{b}_{st}^\top \boldsymbol{x} = \frac{1}{U - \boldsymbol{f}(e)} - \frac{1}{U + \boldsymbol{f}(e)}$$

Note that $\frac{2}{3}mU \leq F^* \leq mU$ because the graph is s-t well-conditioned. To complete the analysis, we consider three cases.

Case 1: $|\boldsymbol{f}(e)| \leq \frac{2}{3}U$. Then the capacity on each of these edges in the symmetrized residual graph $\widehat{G}_{\boldsymbol{f}}$ is at least $U/3$. As there are $\frac{2}{3}m$ of them, we get that there is a feasible flow in $\widehat{G}_{\boldsymbol{f}}$ of value at least $\frac{2}{9}mU \geq \frac{1}{10}F^*$.

Case 2: $\boldsymbol{f}(e) < -\frac{2}{3}U$. By the gradient condition, we have the same flow on all of the $\frac{2}{3}m$ s-t edges, adding up to at least $\frac{2}{3}mU$ going from t to s. This means that we must have at least $\frac{2}{3}mU$ flow going from s to t via the remaining edges. But, their combined capacity is at most $\frac{1}{3}mU$, so that cannot happen. Thus we can rule out this case entirely.

Case 3: $\boldsymbol{f}(e) > \frac{2}{3}U$. Then

$$\frac{m}{(1-\alpha)F^*} \geq \boldsymbol{b}_{st}^\top \boldsymbol{x} \geq \frac{1}{U - \boldsymbol{f}(e)} - \frac{1}{U + \boldsymbol{f}(e)} \geq \frac{4/5}{U - \boldsymbol{f}(e)}$$

So

$$U - \boldsymbol{f}(e) \geq \frac{4}{5}\frac{(1-\alpha)F^*}{m} \geq \frac{1}{2}(1-\alpha)U$$

In this case, the capacity on each of the $\frac{2}{3}m$ s-t edges with capacity U in G will have capacity $(1-\alpha)U/2$ in $\widehat{G}_{\boldsymbol{f}}$. This guarantees that there is feasible flow in $\widehat{G}_{\boldsymbol{f}}$ of value at least $\frac{1}{3}(1-\alpha)mU \geq \frac{1}{3}(1-\alpha)F^*$. □

Lemma 17.1.15. *Let* $0 < \alpha' \leq \frac{1-\alpha}{150\sqrt{m}}$. *Then the minimizer* $\boldsymbol{\delta}^*$ *of Problem* (17.9) *satisfies* $\left\|\overrightarrow{(\boldsymbol{\delta}^*(e)/\widehat{\boldsymbol{c}}(e))}\right\|_\infty < 0.1$.

Proof. By Lemma 17.1.14, there exists a flow $\hat{\boldsymbol{\delta}}$ which satisfies $\boldsymbol{B}\hat{\boldsymbol{\delta}} = \frac{1-\alpha}{5}F^*\boldsymbol{b}_{st}$ and $\left\|\overrightarrow{\left(\hat{\boldsymbol{\delta}}(e)/\widehat{\boldsymbol{c}}(e)\right)}\right\|_\infty \leq 1$. Hence for any $0 < \alpha' \leq \frac{1-\alpha}{150\sqrt{m}}$, the flow $\tilde{\boldsymbol{\delta}} = \alpha'\frac{5}{1-\alpha}\hat{\boldsymbol{\delta}}$ satisfies

$\boldsymbol{B}\tilde{\boldsymbol{\delta}} = \alpha' F^* \boldsymbol{b}_{st}$ and $\left\| \overrightarrow{\left(\tilde{\boldsymbol{\delta}}(e)/\widehat{\boldsymbol{c}}(e) \right)} \right\|_\infty \leq \frac{1}{30\sqrt{m}}$. This means that

$$\begin{aligned}
\tilde{D}_V(\tilde{\boldsymbol{\delta}}) &= \sum_e \tilde{D}\left(\frac{\tilde{\boldsymbol{\delta}}(e)}{\boldsymbol{c}_+(e)} \right) + \tilde{D}\left(-\frac{\tilde{\boldsymbol{\delta}}(e)}{\boldsymbol{c}_-(e)} \right) \\
&\leq \sum_e 4\left(\frac{\tilde{\boldsymbol{\delta}}(e)}{\boldsymbol{c}_+(e)} \right)^2 + 4\left(-\frac{\tilde{\boldsymbol{\delta}}(e)}{\boldsymbol{c}_-(e)} \right)^2 \\
&\leq \sum_e 8\left(\frac{\tilde{\boldsymbol{\delta}}(e)}{\widehat{\boldsymbol{c}}(e)} \right)^2 \\
&\leq 8/900 < 1/100.
\end{aligned}$$

This then means that the minimizer $\boldsymbol{\delta}^*$ of Problem (17.9) also satisfies $\tilde{D}_V(\tilde{\boldsymbol{\delta}}) < 1/100$.

$$\begin{aligned}
\left\| \overrightarrow{(\boldsymbol{\delta}^*/\widehat{\boldsymbol{c}}(e))} \right\|_\infty^2 &\leq \sum_e \left(\frac{\boldsymbol{\delta}^*(e)}{\boldsymbol{c}_+(e)} \right)^2 + \left(-\frac{\boldsymbol{\delta}^*(e)}{\boldsymbol{c}_-(e)} \right)^2 \\
&\leq \sum_e \tilde{D}\left(\frac{\boldsymbol{\delta}^*(e)}{\boldsymbol{c}_+(e)} \right) + \tilde{D}\left(-\frac{\boldsymbol{\delta}^*(e)}{\boldsymbol{c}_-(e)} \right) && \text{By Lemma 17.1.6.} \\
&= \tilde{D}_V(\tilde{\boldsymbol{\delta}}) < 1/100.
\end{aligned}$$

Hence $\left\| \overrightarrow{(\boldsymbol{\delta}^*/\widehat{\boldsymbol{c}}(e))} \right\|_\infty < 0.1$. □

Chapter 18

Distance Oracles

In this chapter, we learn about distance oracles as presented in the seminal paper [TZ05]. Distance Oracles are data structures that allow for any undirected graph $G = (V, E)$ to be stored compactly in a format that allows to query for the (approximate) distance between any two vertices u, v in the graph. The main result of this chapter is the following data structure.

Theorem 18.0.1. *There is an algorithm that, for any integer $k \geq 1$ and undirected graph $G = (V, E)$, computes a data structure that can be stored using $\tilde{O}(kn^{1+1/k})$ bits such that on querying any two vertices $u, v \in V$ returns in $O(k)$ time a distance estimate $\widetilde{\mathbf{dist}}(u, v)$ such that*

$$\mathbf{dist}(u, v) \leq \widetilde{\mathbf{dist}}(u, v) \leq (2k - 1) \cdot \mathbf{dist}(u, v).$$

The algorithm computes the data structure in expected time $\tilde{O}(kmn^{1/k})$.

Remark 18.0.2. Note that for $k = 1$, the theorem above is trivial: it can be solved by computing APSP and storing the distance matrix of G.

Remark 18.0.3. We point out that given space $O(n^{1+1/k})$, approximation $(2k-1)$ is the best that we can hope for according to a popular and widely believed conjecture that essentially says that there are unweighted graphs that have no cycle of length $(2k+1)$ but have $\tilde{\Omega}(n^{1+1/k})$ edges. A more careful analysis than we will carry out allows to shave all logarithmic factors from Theorem 18.0.1 and therefore the data structure is only a factor k off in space from optimal while also answering queries *extremely* efficiently. It turns out that the factor k can also be removed in space and query time (although currently preprocessing is quite expensive), see therefore the following (really involved) articles [Che14, Che15].

Remark 18.0.4. Also note that in directed graphs no such distance oracle is possible. Even maintaining the transitive closure (the information of who reaches who) can only be preserved if one stores $\tilde{\Omega}(n^2)$ bits.

18.1 Warm-up: A Distance Oracle for $k = 2$

Let us first describe the data structure for the case where $k = 2$. See therefore the pseudo-code below. Here we use the convention that $\mathbf{dist}(x, X)$ for some vertex $x \in V$ and some subset $X \subseteq V$ is the minimum distance from x to any $y \in X$, formally $\mathbf{dist}(x, X) = \min_{y \in X} \mathbf{dist}(x, y)$.

Algorithm 19: PREPROCESS(G)

Obtain S by sampling every vertex $v \in V$ i.i.d. with probability $n^{-1/2}$;
foreach $s \in S$ **do**
    Compute all distances from s to any other vertex $v \in V$;
    In a hash table $\mathcal{H}_s$ store for each $v \in V$ an entry with key v and value $\mathbf{dist}_G(s, v)$.
end
foreach $u \in V \setminus S$ **do**
    Find the *pivot* $p(u)$ of u to be some vertex in S that minimizes the distance to u;
    Store $p(u)$ along with $\mathbf{dist}_G(u, p(u)) = \mathbf{dist}_G(u, S)$;
    Find the *bunch* $B(u) = \{v \in V \mid \mathbf{dist}_G(u, v) < \mathbf{dist}_G(u, S)\}$;
    In a hash table $\mathcal{H}_u$ store for each $v \in B(v)$ an entry with key v and value $\mathbf{dist}_G(u, v)$.
end

The key to the algorithm is the definition of *pivots* and *bunches*. Below is an example that illustrates their definitions.

Without further due, let us discuss the query procedure which is depicted below. It essentially consists of checking whether the vertex v is already in the bunch of u in which case we have stored the distance $\mathbf{dist}_G(u, v)$ explicitly. Otherwise, it uses a detour via its pivot.

Algorithm 20: QUERY(u,v)

if $v \in \mathcal{H}_u$ **then return** value $\mathbf{dist}_G(u, v)$;
return $\mathbf{dist}_G(u, p(u)) + \mathbf{dist}_G(p(u), v)$ (the latter from $\mathcal{H}_{p(u)}$)

The second case is illustrated below.

Approximation Analysis. It is straight-forward to see that if we return in line 1 of the query algorithm, then we return the exact distance.

If we return in the second line, then we know that $v \notin B(u)$. By definition of a bunch this implies that

$$\mathbf{dist}(u, v) \geq \mathbf{dist}(u, S) = \mathbf{dist}(u, p(u)).$$

We can further use the triangle inequality to conclude that

$$\mathbf{dist}_G(p(u), v) \leq \mathbf{dist}(u, p(u)) + \mathbf{dist}(u, v)$$

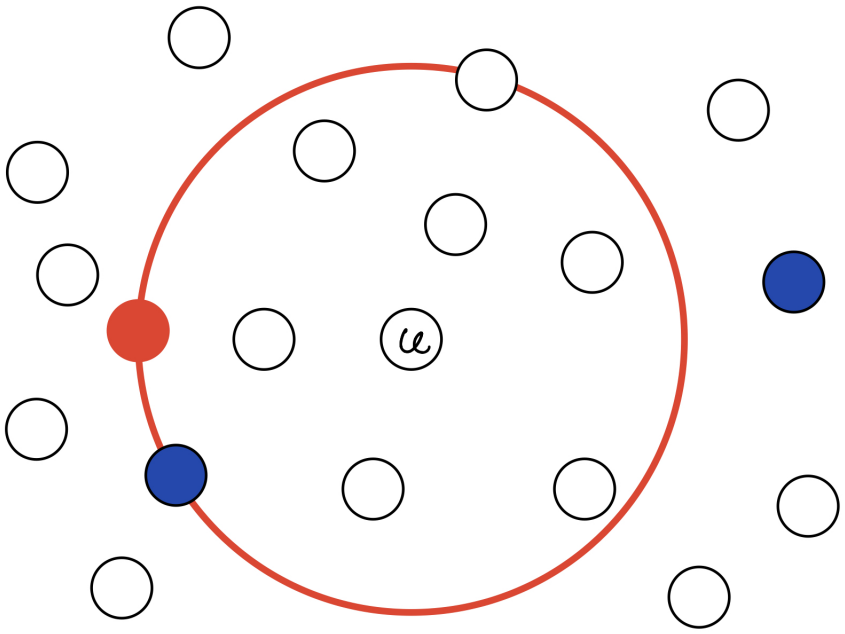


Figure 18.1: Graph G (without the edges) where vertices are drawn according to their distance from u. The blue and red vertices are in S. The red vertex is chosen to be the pivot $p(u)$. Note that another vertex in S could have been chosen to become the pivot. The bunch of u is the vertices that are strictly withing the red circle. In particular, both blue vertices, the red vertex and also the white vertex on the boundary of the red circle are *not* in the bunch $B(u)$.

Combining these two inequalities, we obtain

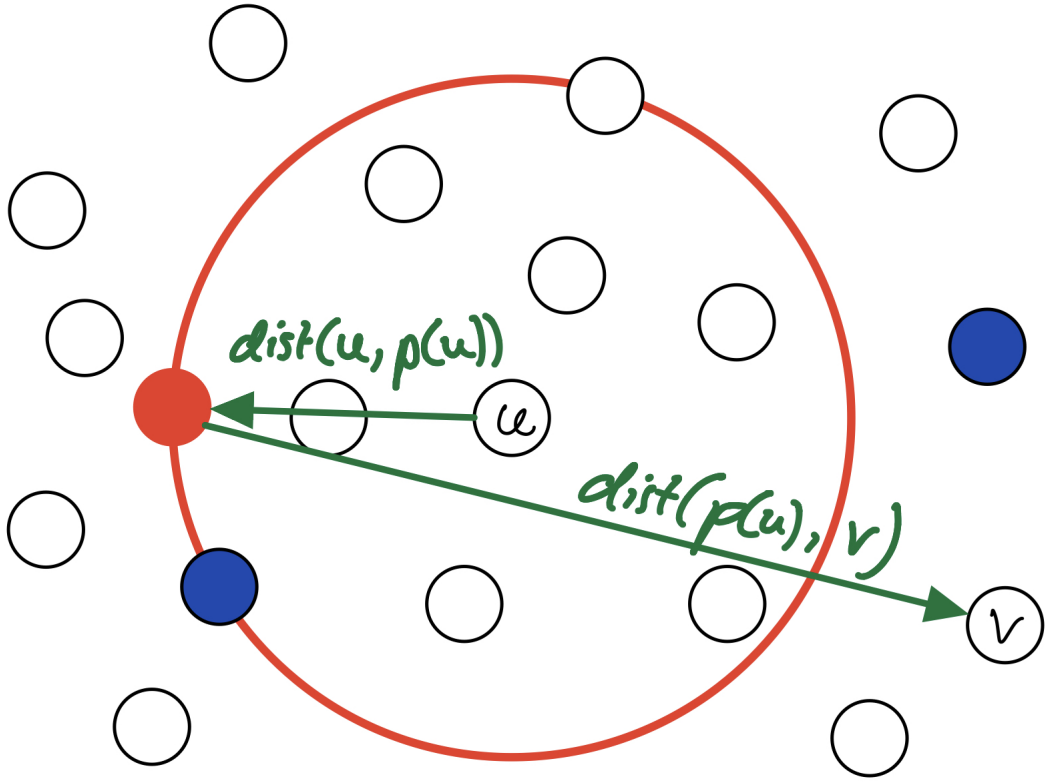
$$\mathbf{dist}_G(u, p(u)) + \mathbf{dist}_G(p(u), v) \leq 2 \cdot \mathbf{dist}(u, p(u)) + \mathbf{dist}(u, v) \leq 3 \cdot \mathbf{dist}(u, v).$$

We conclude that we obtain a 3-approximation.

Space Analysis. For each vertex $s \in S$, we store a hash-table with one entry for each vertex v. This can be stored with space $O(|S|n)$. We have by a standard Chernoff-bound that $|S| = \tilde{O}(\sqrt{n})$ w.h.p. so this becomes $\tilde{O}(n^{3/2})$.

Next, fix some $u \in V \setminus S$, and let us argue about the size of $B(u)$ (which asymptotically matches $|\mathcal{H}_u|$). We order the vertices $v_1, v_2, \ldots, v_n$ in V by their distance from u. Since we sample uniformly at random, by a simple Chernoff bound, we obtain that the first vertex v_i in $v_1, v_2, \ldots, v_n$ that is in S has $i = \tilde{O}(\sqrt{n})$ w.h.p.. But note that since only vertices that are *strictly* closer to u than v_i are in $B(u)$, this implies that $|B(u)| = \tilde{O}(\sqrt{n})$.

It remains to take a careful union bound over all bad events at every vertex $u \in V \setminus S$ to conclude that with high probability, the hash tables $\mathcal{H}_u$ for all $u \in V \setminus S$ combined take total space $\tilde{O}(|V \setminus S|\sqrt{n}) = \tilde{O}(n^{3/2})$. For the rest of the section, we condition on the event that each $|B(v)| = \tilde{O}(\sqrt{n})$ to use it as if it was a deterministic guarantee.



Preprocessing and Query Time. In order to find the distances stored in the hash tables $\mathcal{H}_s$ for $s \in S$, we can simply run Dijkstra from each $s \in S$ on the graph in total time $\tilde{O}(m|S|) = \tilde{O}(mn^{1/2})$.

To compute the *pivots* for each vertex u, we can insert a super-vertex s' and add an edge from s' to each $s \in S$ of weight 0. We can then run Dijkstra from s' on $G \cup \{s'\}$. Note that for each u, we have $\mathbf{dist}_{G\cup\{s'\}}(s', u) = \mathbf{dist}_G(p(u), u)$ and that $p(u)$ can be chosen to be the closest vertex on the path from s' to u that Dijkstra outputs along with the distances (recall that Dijkstra can output a shortest path tree). This takes $\tilde{O}(m)$ time.

It remains to compute the bunches $B(u)$. Here, we use duality: we define the cluster $C(w)$ for every vertex $w \in V \setminus S$ to be the set

$$C(w) = \{v \in V \mid \mathbf{dist}_G(v, w) < \mathbf{dist}_G(v, p(v))\}.$$

Note the subtle difference to the bunches in that membership of v now depends on $p(v)$ and *not* on $p(u)$! It is not hard to see that $u \in C(w) \iff w \in B(u)$. And it is straight-forward to compute the bunches from the clusters in time $O(\sum_v |B(v)|) = O(\sum_w |C(w)|) = \tilde{O}(n^{3/2})$.

Finally, it turns out that we can compute each $C(w)$ by running Dijkstra with a small modification.

Lemma 18.1.1 (Lemma 4.2 in [TZ05])**.** *Consider running Dijkstra from a vertex w but only relaxing edges incident to vertices v that satisfy $\mathbf{dist}_G(v, w) < \mathbf{dist}_G(v, p(v))$. Then,*

the algorithm computes $C(w)$ and all distances $\mathbf{dist}(v,w)$ *for* $v \in C(w)$ *in time* $\tilde{O}(|E(C(w))|)$ *where* $E(C(w))$ *are the edges that touch a vertex in* $C(w)$*.*

It remains to observe that the total time required to compute all clusters is

$$\tilde{O}(\sum_w |E(C(w))|) = \tilde{O}(\sum_{w, v \in C(w)} |E(v)|) = \tilde{O}(\sum_{v, w \in B(v)} |E(v)|) = \tilde{O}(\sum_v |E(v)||B(v)|).$$

But we have upper bounded $|B(v)| = \tilde{O}(\sqrt{n})$ for all v, thus each vertex just pays its degree $\tilde{O}(\sqrt{n})$ times and we get running time $\tilde{O}(m\sqrt{n})$.

Monte Carlo vs. Las Vegas. Note that the analysis above only guarantees that the algorithm works well with high probability. However, it is not hard to see that the algorithm can be transformed into a Las Vegas algorithm: whenever we find a bunch $B(v)$ whose size exceeds our $\tilde{O}(\sqrt{n})$ bound, we simply re-run the algorithm. This guarantees that the final data structure that we output indeed satisfies the guarantees stipulated in the theorem.

18.2 Distance Oracles for any $k \geq 2$

The generalization for all k's is rather straight-forward except for the query operation which works a bit magically. Let's first define the data structure by giving our new pre-processing algorithm.

Algorithm 21: PREPROCESS(G)

$S_1 = V$; $S_{k+1} = \emptyset$;
foreach $i \in [1,k]$ **do** Obtain S_{i+1} by sampling every $v \in S_i$ i.i.d. with prob. $n^{-1/k}$;
foreach $u \in V$ **do**
    foreach $i \in [1,k]$ **do**
        Let $p_i(u)$ be some vertex in S_i that minimizes the distance to u;
        Store $p_i(u)$ along with $\mathbf{dist}_G(u, p_i(u))$.
    end
    Let *bunch* $B(u) = \bigcup_i B_i(u)$ where $B_i(u) = \{v \in S_i \mid \mathbf{dist}_G(u,v) < \mathbf{dist}_G(u, S_{i+1})\}$;
    In a hash table $\mathcal{H}_u$ store for each $v \in B(u)$ an entry with key v and value $\mathbf{dist}_G(u,v)$.
end

Note that in a sense this algorithm is almost easier than the one for $k = 2$ since it treats each level in the same fashion. Here we ensure that the last set S_{k+1} is empty (which would happen with constant probability otherwise).

We make the implicit assumption throughout that $S_k \neq \emptyset$ so that $p_k(u)$ is well-defined for each u. We also define $\mathbf{dist}(x, X) = \infty$ if X is the empty set.

The drawing below illustrates the new definition of a bunch where we have chosen $k = 3$ to keep things simple.

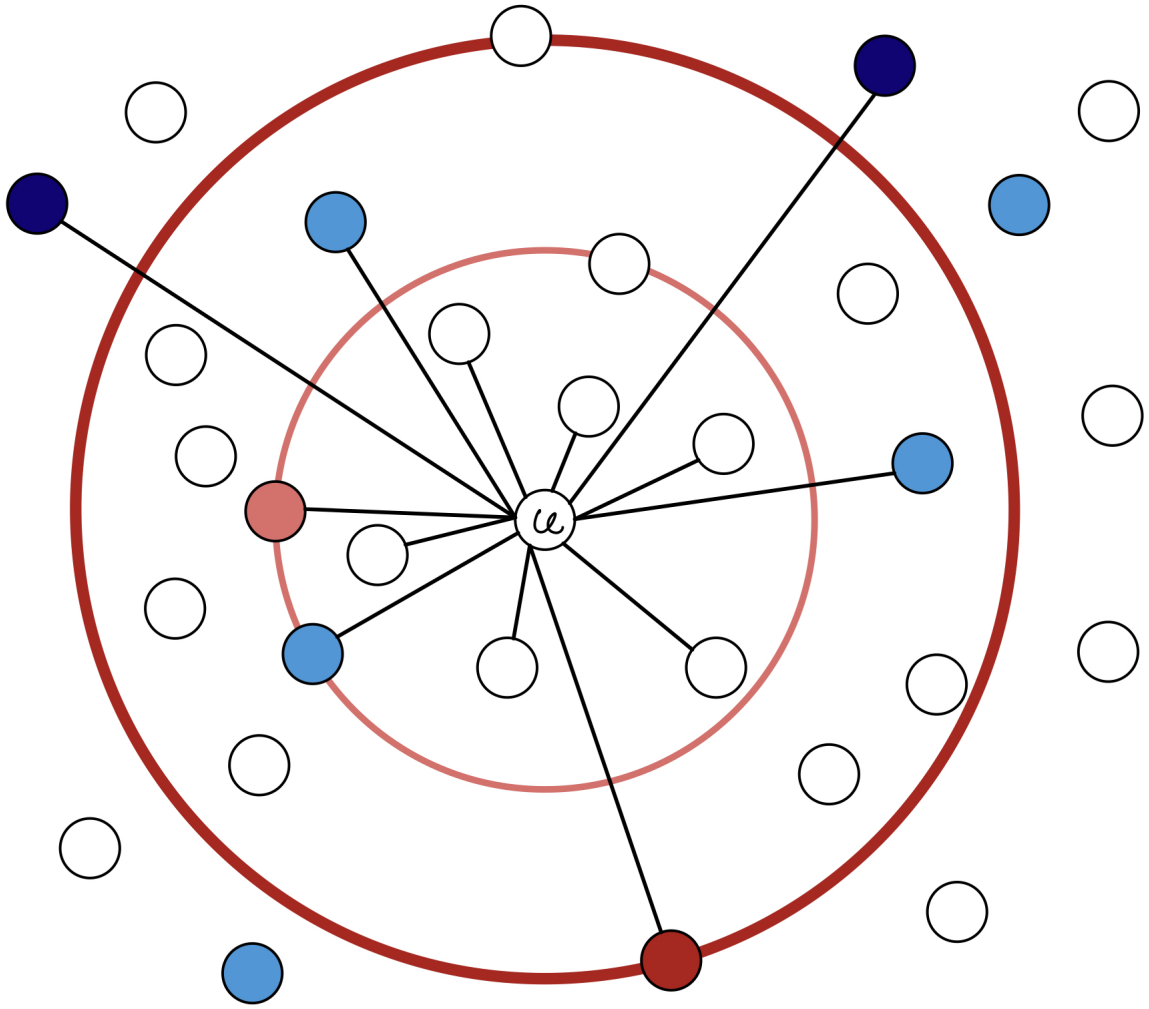


Figure 18.2: Graph G (without the edges) where vertices are drawn according to their distance from u. All vertices are in S_1. The blue and red vertices are in S_2. The dark blue and dark red vertices are also in S_3. Finally, we have $S_4 = \emptyset$. The light red vertex is chosen as pivot $p_2(u)$; the dark red vertex is chosen as pivot $p_3(u)$. The bunch $B(u)$ includes all vertices that have a black edge in this graph to u; in particular these are the white vertices within the circle drawn in light red ($B_1(u)$); the light blue vertices encircled by the dark red circle ($B_2(u)$); and all dark blue vertices ($B_3(u)$).

Before we explain the query procedure, let us give a (rather informal) analysis of the space required by our new data structure.

Space Analysis. We have for each vertex $u \in V$, and each $1 \leq i \leq k$ that the bunch $B_i(u)$ consists of all vertices in S_i that are closer to u than the closest vertex in S_{i+1}.

Now, order the vertices $x_1, x_2, \ldots$ in S_i by their distance from u. Since each vertex in S_i is sampled into S_{i+1} with probability $n^{-1/k}$, we have that with high probability some vertex x_i with $i = O(n^{1/k} \log n)$ is sampled into S_{i+1}. This ensures that $|B_i(u)| = \tilde{O}(n^{1/k})$ with high probability.

Applying this argument for all i, we have that $|B(u)| = \tilde{O}(k \cdot n^{1/k})$ for each u w.h.p. and therefore our space bound follows.

Preprocessing Time. Much like in the $k = 2$ construction, we can define for each $u \in S_i \setminus S_{i+1}$ the cluster $C(u) = \{v \in V \mid \mathbf{dist}_G(u, v) < \mathbf{dist}_G(u, S_{i+1})\}$. Extending our analysis from before using this new definition, we get construction time $\tilde{O}(kmn^{1/k})$.

Query Operation. A straight-forward way to query our new data structure for a tuple (u, v) would be to search for the smallest i such that $v \in B(p_i(u))$ and then return $\mathbf{dist}_G(u, p_i(u)) + \mathbf{dist}_G(p_i(u), v)$. This can be analyzed in the same way as we did for $k = 2$ to obtain stretch $4k - 3$[1].

However, we aim for stretch approximation $2k - 1$. We state below the pseudo-code to achieve this guarantee.

Algorithm 22: QUERY(u,v)

```
w ← u; i ← 1;
while w ∉ B(v) do
    i ← i + 1;
    (u, v) ← (v, u);
    w ← p_i(u)
end
return dist_G(u, w) + dist_G(w, v)
```

Our main tool in the analysis is the claim below where we define $\Delta = \mathbf{dist}_G(u, v)$.

Claim 18.2.1. *After the i^{th} iteration of the while-loop, we have* $\mathbf{dist}_G(u, w) \leq i\Delta$.

This implies our theorem, since we have at most $k - 1$ iterations, then w is a vertex in S_k and $S_k \subseteq B(x)$ for all vertices $x \in V$. Therefore we have that for the final w, we have $\mathbf{dist}_G(u, w) \leq (k - 1)\Delta$. It remains to conclude by the triangle inequality that

$$\mathbf{dist}_G(u, w) + \mathbf{dist}_G(w, v) \leq 2\mathbf{dist}_G(u, w) + \Delta \leq (2k - 1)\mathbf{dist}_G(u, v).$$

Proof of Claim 18.2.1. Let w_i, u_i, v_i denote the variables w, u, v after the i^{th} while-loop iteration (or right before for w_0, u_0, v_0).

For $i = 0$, we have that $w_0 = u_0$; thus, $\mathbf{dist}_G(u_0, w_0) = 0$.

[1] One can actually prove that this strategy gives an $4k - 5$ stretch with a little trick.

For $i \geq 1$, we want to prove that if the i^{th} while-loop iteration is executed then $\mathbf{dist}_G(u_i, w_i) \leq \mathbf{dist}_G(u_{i-1}, w_{i-1}) + \Delta$ (if it is not executed then the statement follows trivially).

In order to prove this, observe that by the while-loop condition, we must have had $w_{i-1} \notin B(v_{i-1})$, thus $\mathbf{dist}_G(v_{i-1}, w_{i-1}) \geq \mathbf{dist}_G(v_{i-1}, p_i(v_{i-1}))$.

But the while-iteration sets $u_i = v_{i-1}$ and $w_i = p_i(v_{i-1})$, and therefore we have

$$\begin{aligned}\mathbf{dist}_G(u_i, w_i) = \mathbf{dist}_G(v_{i-1}, p_i(v_{i-1})) &\leq \mathbf{dist}_G(v_{i-1}, w_{i-1}) = \mathbf{dist}_G(v_{i-1}, p_{i-1}(u_{i-1})) \\ &\leq \mathbf{dist}_G(u_{i-1}, p_{i-1}(u_{i-1})) + \mathbf{dist}_G(v_{i-1}, u_{i-1}) = \mathbf{dist}_G(u_{i-1}, w_{i-1}) + \Delta.\end{aligned}$$

□

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