Non-Parametric Methods and Support Vector Machines

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Machine Learning

Outline

1. **Non-Parametric Methods**
   - K-NN
   - Parzen Windows
   - Local Models
2. **Support Vector Machines**
   - SVC
   - Slacks
   - Nonlinear SVC
   - Dual Problem
   - Kernel Trick

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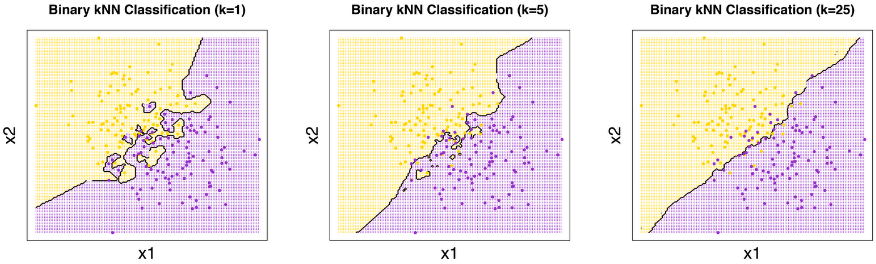
- Training algorithm? Simply "remember" $\mathbb{X}$ in storage

K-NN Methods II

- Could be very complex
- K is a hyperparameter controlling the model complexity



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- K-NN is also a ***lazy*** method since the prediction function f is obtained only before the prediction
  - Motivates the development of other ***local models***

Pros & Cons

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  - Almost no assumption on f other than ***smoothness***
    - High capacity/complexity
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  - Needs to deal with missing data (e.g., special distances)
  - Computationally expensive: $O(ND)$ time for making each prediction
    - Can speed up with index and/or approximation

Outline

Parzen Windows and Kernels

- Binary KNN classifier:

$$f(\boldsymbol{x}) = \operatorname{sign}\left(\sum_{i:\boldsymbol{x}^{(i)} \in \mathsf{KNN}(\boldsymbol{x})} y^{(i)}\right)$$

  - The "radius" of voter boundary depends on the input $\boldsymbol{x}$

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$$f(\boldsymbol{x}) = \mathrm{sign}\left(\sum_i y^{(i)} k(\boldsymbol{x}^{(i)}, \boldsymbol{x})\right)$$

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- How to act like soft K-NN?
- Gaussian RBF kernel:

$$k(\boldsymbol{x}^{(i)},\boldsymbol{x}) = \mathcal{N}(\boldsymbol{x}^{(i)} - \boldsymbol{x}; \boldsymbol{0}, \sigma^2 \boldsymbol{I})$$

- Or simply

$$k(\boldsymbol{x}^{(i)},\boldsymbol{x}) = \exp\left(-\gamma \|\boldsymbol{x}^{(i)} - \boldsymbol{x}\|^2\right)$$

- $\gamma \geq 0$ (or σ^2) is a hyperparameter controlling the smoothness of f

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Locally Weighted Linear Regression

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- In addition to the majority voting and average, we can define ***local models*** for lazy predictions
- E.g., in (eager) linear regression, we find $\boldsymbol{w} \in \mathbb{R}^{D+1}$ that minimizes SSE:

$$\arg\min_{\boldsymbol{w}} \sum_i (y^{(i)} - \boldsymbol{w}^\top \boldsymbol{x}^{(i)})^2$$

- Local model: to find $\boldsymbol{w}$ minimizing ***SSE local to the point $\boldsymbol{x}$ we want to predict***:

$$\arg\min_{\boldsymbol{w}} \sum_i k(\boldsymbol{x}^{(i)}, \boldsymbol{x})(y^{(i)} - \boldsymbol{w}^\top \boldsymbol{x}^{(i)})^2$$

  - $k(\cdot,\cdot) \in \mathbb{R}$ is an RBF kernel

Outline

Kernel Machines

- ***Kernel machines***:

$$f(\boldsymbol{x})=\sum_{i=1}^{N}c_i k(\boldsymbol{x}^{(i)},\boldsymbol{x})+c_0$$

- For example:
  - Parzen windows: $c_i = y^{(i)}$ and $c_0 = 0$
  - Locally weighted linear regression: $c_i = (y^{(i)} - \boldsymbol{w}^\top \boldsymbol{x}^{(i)})^2$ and $c_0 = 0$

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  - Locally weighted linear regression: $c_i = (y^{(i)} - \boldsymbol{w}^\top \boldsymbol{x}^{(i)})^2$ and $c_0 = 0$
- The variable $\boldsymbol{c} \in \mathbb{R}^N$ can be learned in either an eager or lazy manner
- Pros: complex, but highly accurate if regularized well

Sparse Kernel Machines

- To make a prediction, we need to store ***all*** examples
- May be infeasible due to
  - Large dataset (N)
  - Time limit
  - Space limit

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- May be infeasible due to
  - Large dataset (N)
  - Time limit
  - Space limit
- Can we make $\boldsymbol{c}$ ***sparse***?
  - I.e., to make $c_i \neq 0$ for only a small fraction of examples called ***support vectors***
- How?

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Separating Hyperplane I

- Model: $\mathbb{F} = \{f : f(\boldsymbol{x}; \boldsymbol{w}, b) = \boldsymbol{w}^\top \boldsymbol{x} + b\}$
  - A collection of hyperplanes
- Prediction: $\hat{y} = \text{sign}(f(\boldsymbol{x}))$

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$$\begin{aligned} \boldsymbol{w}^\top \boldsymbol{x}^{(i)} + b \geq 0, & \quad \text{if } y^{(i)} = 1 \\ \boldsymbol{w}^\top \boldsymbol{x}^{(i)} + b \leq 0, & \quad \text{if } y^{(i)} = -1 \end{aligned}$$

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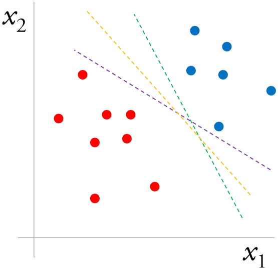
or simply

$$y^{(i)}(\boldsymbol{w}^\top \boldsymbol{x}^{(i)} + b) \geq 0$$

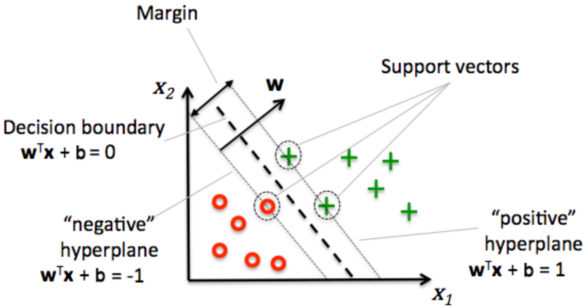
Separating Hyperplane II

- There are many feasible $\boldsymbol{w}$'s and b's when the classes are linearly separable
- Which hyperplane is the best?



Support Vector Classification

- ***Support vector classifier*** (SVC) picks one with ***largest margin***:
  - $y^{(i)}(\boldsymbol{w}^\top \boldsymbol{x}^{(i)} + b) \geq a$ for all i
  - Margin: $2a/\|\boldsymbol{w}\|$ [Homework]



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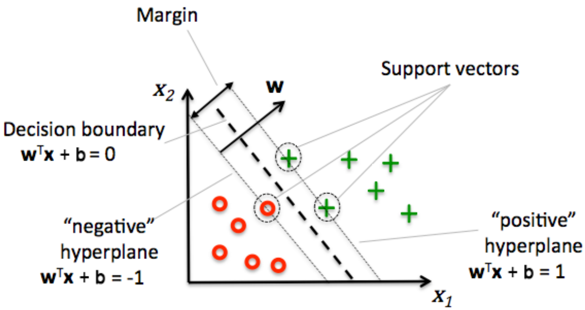

- With loss of generality, we let $a = 1$ and solve the problem:

$$\arg\min_{\boldsymbol{w},b} \frac{1}{2}\|\boldsymbol{w}\|^2$$
$$\text{sibject to } y^{(i)}(\boldsymbol{w}^\top \boldsymbol{x}^{(i)} + b) \geq 1, \forall i$$

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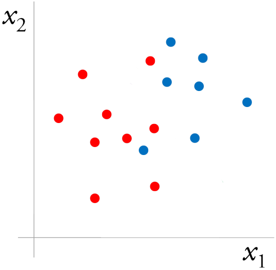
Overlapping Classes

- In practice, classes may be overlapping
  - Due to, e.g., noises or outliers



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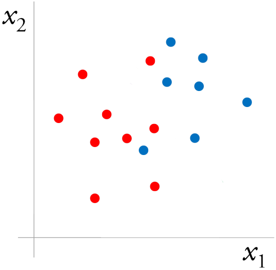


- The problem

$$\arg\min_{\boldsymbol{w},b} \frac{1}{2}\|\boldsymbol{w}\|^2$$
$$\text{sibject to } y^{(i)}(\boldsymbol{w}^\top \boldsymbol{x}^{(i)} + b) \geq 1, \forall i$$

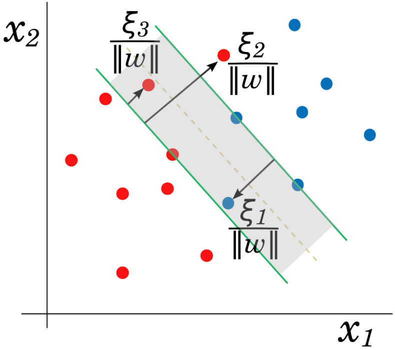
has no solution in this case. How to fix this?

Slacks

- SVC tolerates ***slacks*** that fall outside of the regions they ought to be
- Problem:

$$\arg\min_{\boldsymbol{w},b,\xi} \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{i=1}^{N}\xi_i$$
$$\text{sibject to } y^{(i)}(\boldsymbol{w}^\top \boldsymbol{x}^{(i)} + b) \geq 1 - \xi_i \text{ and } \xi_i \geq 0, \forall i$$

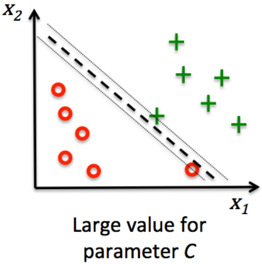
  - Favors large margin but also fewer slacks

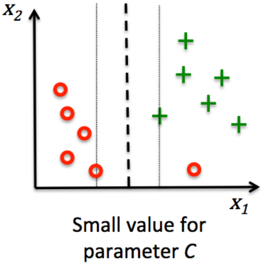


Hyperparameter C

$$\arg\min_{\boldsymbol{w},b,\xi} \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{i=1}^{N} \xi_i$$

- The hyperparameter C controls the tradeoff between
  - Maximizing margin
  - Minimizing number of slacks





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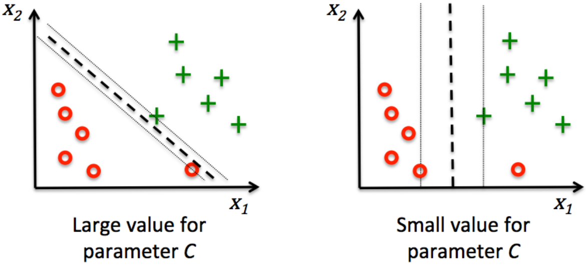

- Provides a geometric explanation to the weight decay

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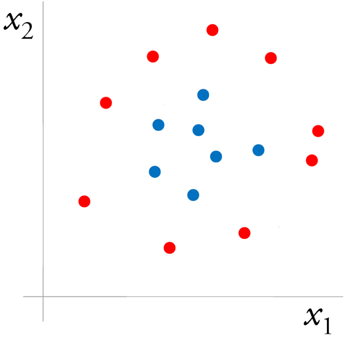
Nonlinearly Separable Classes

- In practice, classes may be nonlinearly separable



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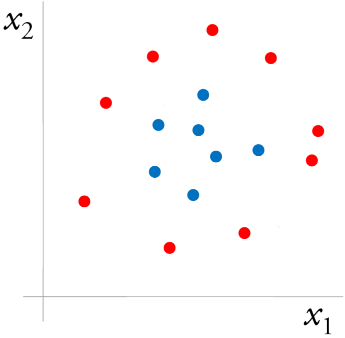

- SVC (with slacks) gives "bad" hyperplanes due to underfitting
- How to make it nonlinear?

Feature Augmentation

- Recall that in polynomial regression, we augment data features to make a linear regressor nonlinear

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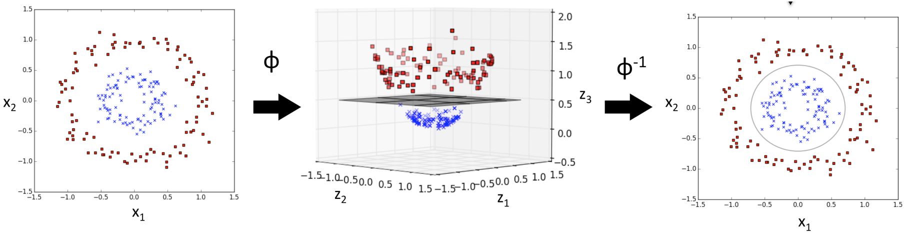
- We can can define a function $\Phi(\cdot)$ that maps each data point to a high dimensional space:

$$\arg\min_{\boldsymbol{w},b,\xi} \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_i \xi_i$$
$$\text{sibject to } y^{(i)}(\boldsymbol{w}^\top \Phi(\boldsymbol{x}^{(i)}) + b) \geq 1 - \xi_i \text{ and } \xi_i \geq 0, \forall i$$



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Time Complexity

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- The higher augmented feature dimension, the more variables in $\boldsymbol{w}$ to solve
- Can we solve $\boldsymbol{w}$ in time complexity that is independent with the mapped dimension?

Dual Problem

- Primal problem:

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- Dual problem:

$$\arg\max_{\alpha,\beta} \min_{\boldsymbol{w},b,\xi} L(\boldsymbol{w}, b, \xi, \alpha, \beta)$$
$$\text{subject to } \alpha \geq \mathbf{0}, \beta \geq \mathbf{0}$$

where $L(\boldsymbol{w}, b, \xi, \alpha, \beta) =$
$\frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_i \xi_t + \sum_i \alpha_i(1 - y^{(i)}(\boldsymbol{w}^\top \Phi(\boldsymbol{x}^{(i)}) + b) - \xi_i) + \sum_i \beta_i(-\xi_i)$

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- Primal problem is convex, so ***strong duality*** holds

Solving Dual Problem I

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- The inner problem

$$\min_{\boldsymbol{w},b,\xi} L(\boldsymbol{w}, b, \xi, \alpha, \beta)$$

  is convex in terms of $\boldsymbol{w}$, b, and ξ
- Let's solve it analytically:

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  is convex in terms of $\boldsymbol{w}$, b, and $\boldsymbol{\xi}$
- Let's solve it analytically:
- $\frac{\partial L}{\partial \boldsymbol{w}} = \boldsymbol{w} - \sum_i \alpha_i y^{(i)} \Phi(\boldsymbol{x}^{(i)}) = \boldsymbol{0} \Rightarrow \boldsymbol{w} = \sum_i \alpha_i y^{(i)} \Phi(\boldsymbol{x}^{(i)})$

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  $$\min_{\boldsymbol{w}, b, \xi} L(\boldsymbol{w}, b, \xi, \alpha, \beta)$$
  is convex in terms of $\boldsymbol{w}$, b, and ξ
- Let's solve it analytically:
- $\frac{\partial L}{\partial \boldsymbol{w}} = \boldsymbol{w} - \sum_i \alpha_i y^{(i)} \Phi(\boldsymbol{x}^{(i)}) = \boldsymbol{0} \Rightarrow \boldsymbol{w} = \sum_i \alpha_i y^{(i)} \Phi(\boldsymbol{x}^{(i)})$
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Solving Dual Problem I

- $L(\boldsymbol{w}, b, \xi, \alpha, \beta) =$
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- $\frac{\partial L}{\partial b} = \sum_i \alpha_i y^{(i)} = 0$
- $\frac{\partial L}{\partial \xi_i} = C - \alpha_i - \beta_i = 0 \Rightarrow \beta_i = C - \alpha_i$

Solving Dual Problem II

- $L(\boldsymbol{w},b,\xi,\alpha,\beta) =$
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- Outer maximization problem:

$$\arg\max_\alpha \mathbf{1}^\top\alpha - \tfrac{1}{2}\alpha^\top\boldsymbol{K}\alpha$$
$$\text{subject to } \mathbf{0} \leq \alpha \leq C\mathbf{1} \text{ and } \boldsymbol{y}^\top\alpha = 0$$

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Solving Dual Problem II

- Dual minimization problem of SVC:

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- Number of variables to solve? N instead of augmented feature dimension
- In practice, this problem is solved by specialized solvers such as the sequential minimal optimization (SMO) [3]
  - As $\boldsymbol{K}$ is usually ill-conditioned

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- For any $\boldsymbol{x}^{(i)}$ having $0 < \alpha_i < C$, we have

$$\beta_i = C - \alpha_i > 0 \Rightarrow \xi_i = 0,$$

$$(1 - y^{(i)}(\boldsymbol{w}^\top \Phi(\boldsymbol{x}^{(i)}) + b) - \xi_i) = 0 \Rightarrow b = y^{(i)} - \boldsymbol{w}^\top \Phi(\boldsymbol{x}^{(i)})$$

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- In practice, we usually take the average over ***all*** $\boldsymbol{x}^{(i)}$'s having $0 < \alpha_i < C$ to avoid numeric error

Outline

Kernel as Inner Product

- We need to evaluate $\Phi(\boldsymbol{x}^{(i)})^\top \Phi(\boldsymbol{x}^{(j)})$ when
  - Solving dual problem of SVC, where $K_{i,j} = y^{(i)} y^{(j)} \Phi(\boldsymbol{x}^{(i)})^\top \Phi(\boldsymbol{x}^{(j)})$
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  - E.g., let $\alpha = 1$, $\beta = 1$, $\gamma = 2$ and $\boldsymbol{a} \in \mathbb{R}^2$, then $\Phi(\boldsymbol{a}) = [1, \sqrt{2} a_1, \sqrt{2} a_2, a_1^2, a_2^2, \sqrt{2} a_1 a_2]^\top \in \mathbb{R}^6$

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Kernel Trick

- If we choose Φ induced by Polynomial or Gaussian RBF kernel, then

$$K_{i,j} = y^{(i)} y^{(j)} k(\boldsymbol{x}^{(i)}, \boldsymbol{x})$$

takes only $O(D)$ time to evaluate, and

$$f(\boldsymbol{x}) = \sum_i \alpha_i y^{(i)} k(\boldsymbol{x}^{(i)}, \boldsymbol{x}) + b$$

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- Independent with the augmented feature dimension
- α, β, and γ are new hyperparameters

Sparse Kernel Machines

- SVC is a kernel machine:

$$f(\boldsymbol{x}) = \sum_i \alpha_i y^{(i)} k(\boldsymbol{x}^{(i)}, \boldsymbol{x}) + b$$

- It is surprising that SVC works like K-NN in some sense

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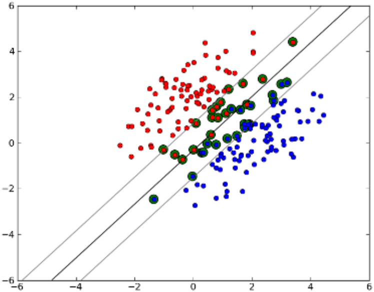
- However, SVC is a ***sparse*** kernel machine
- Only the ***slacks*** become the support vectors ($\alpha_i > 0$)



KKT Conditions and Types of SVs

- By KKT conditions, we have:
  - Primal feasibility: $y^{(i)}(\boldsymbol{w}^\top\Phi(\boldsymbol{x}^{(i)})+b)\geq 1-\xi_i$ and $\xi_i\geq 0$
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  - Since $\beta_i = C - \alpha_i \neq 0$, we have $\xi_i = 0$
- ***Bounded SVs*** ($\alpha_i = C$): $y^{(i)}(\boldsymbol{w}^\top \Phi(\boldsymbol{x}^{(i)}) + b) \leq 1$ (usually strict)
  - $1 - y^{(i)}(\boldsymbol{w}^\top \Phi(\boldsymbol{x}^{(i)}) + b) - \xi_i = 0$
  - Since $\beta_i = 0$, we have $\xi_i \geq 0$

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    - Usually wrapped by the 1-vs-1 technique for multi-class classification

Remarks II

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- Choose linear SVC (e.g., LIBLINEAR [2]) when
  - N is large (since nonlinear SVC does not scale), or
  - D is large (since classes may already be linearly separable)

Reference I

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