Going nonparametric:

Nearest neighbor and kernel regression

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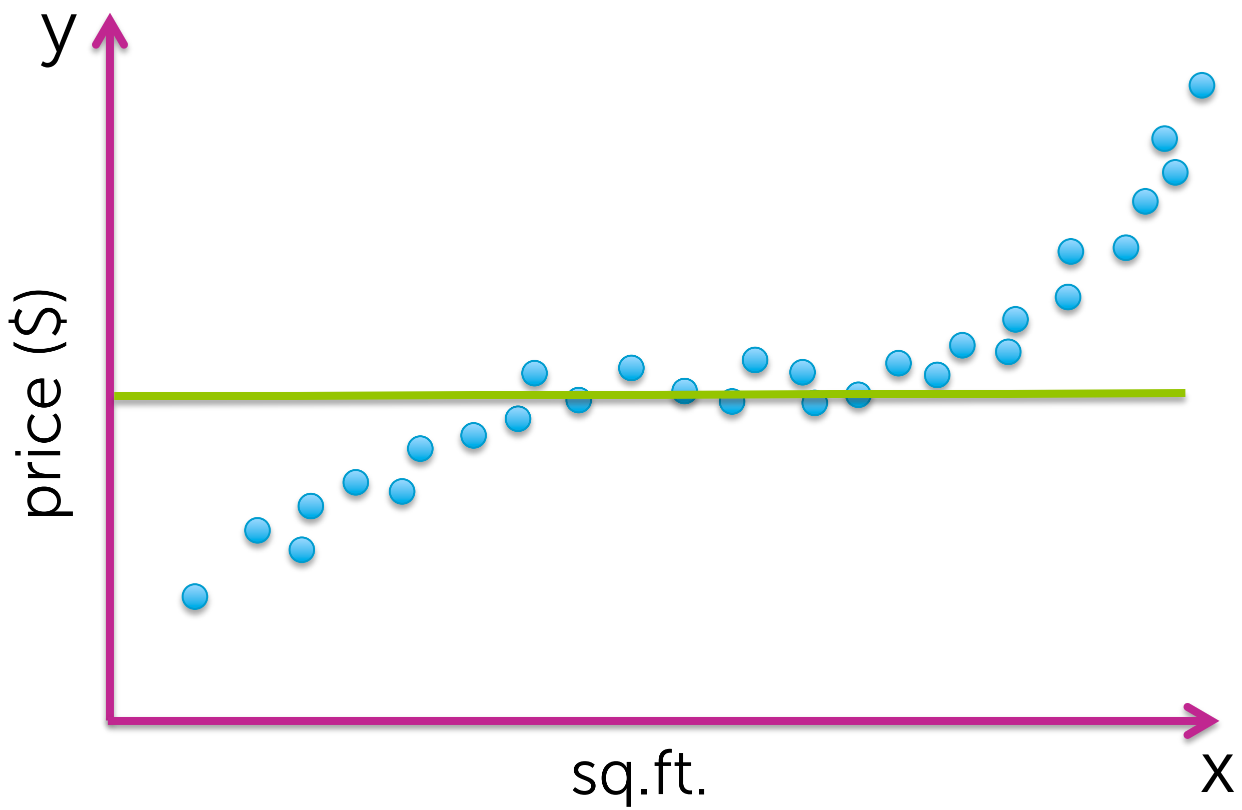
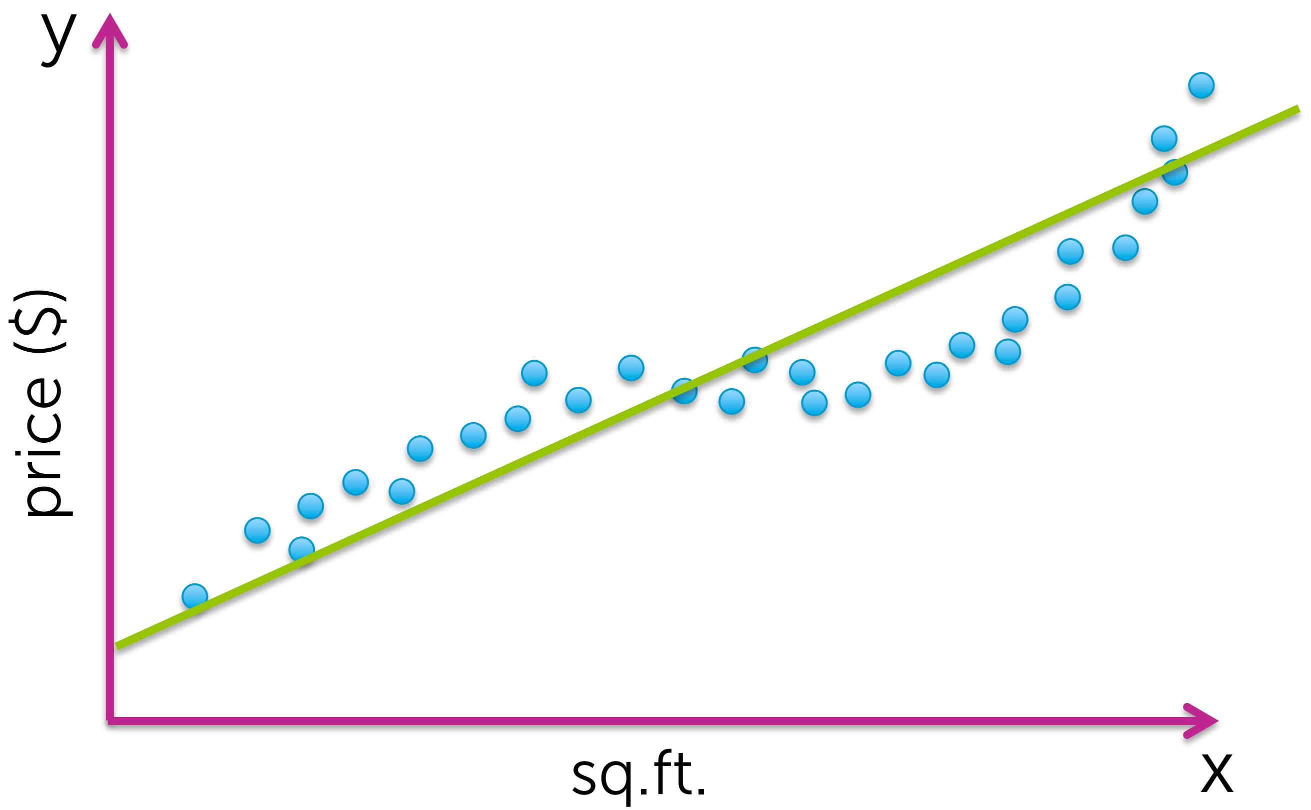
Fit globally vs. fit locally

Parametric models of f(x)



Parametric models of f(x)



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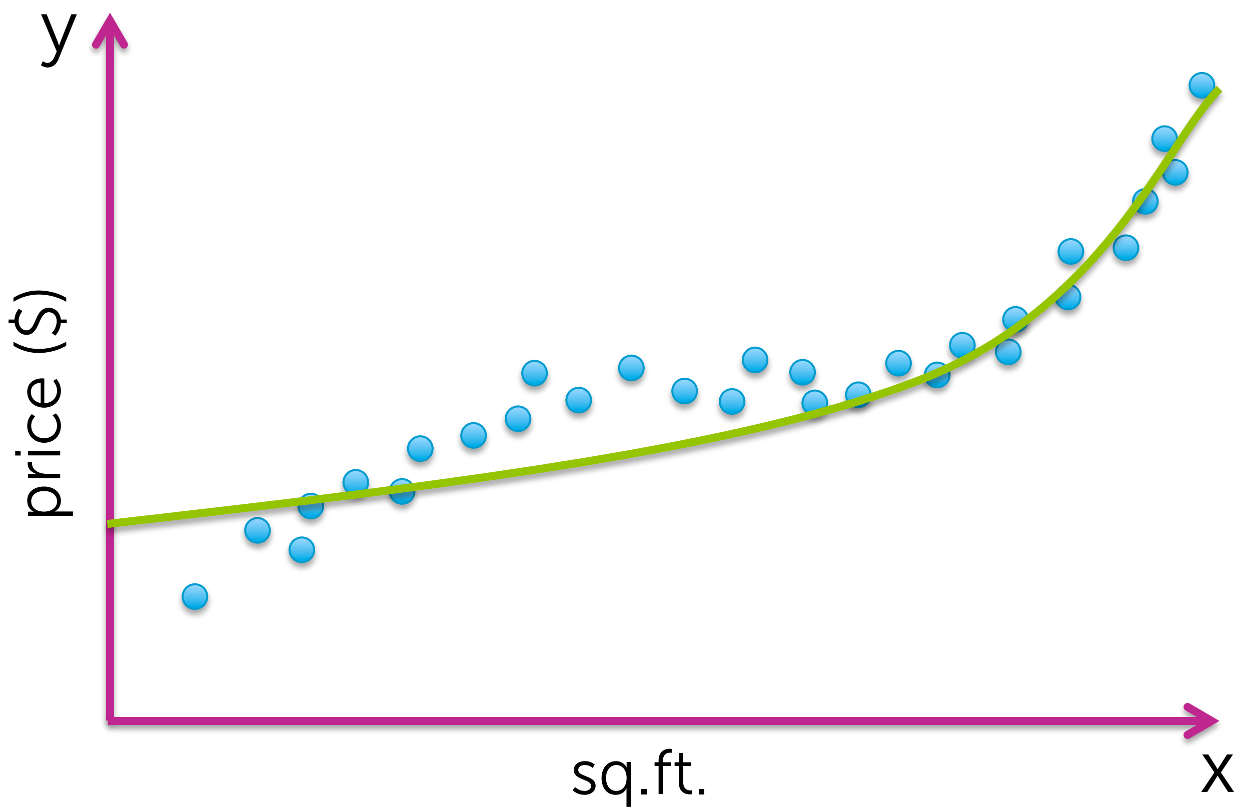
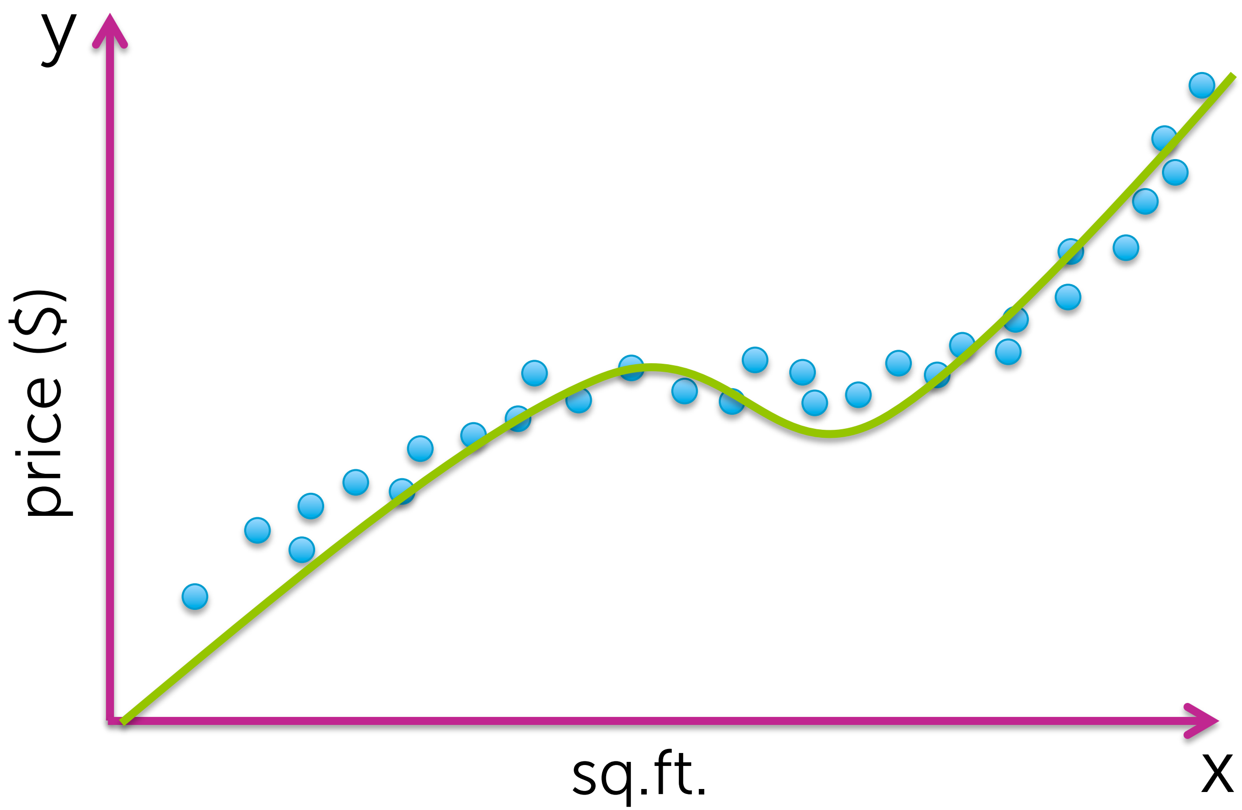
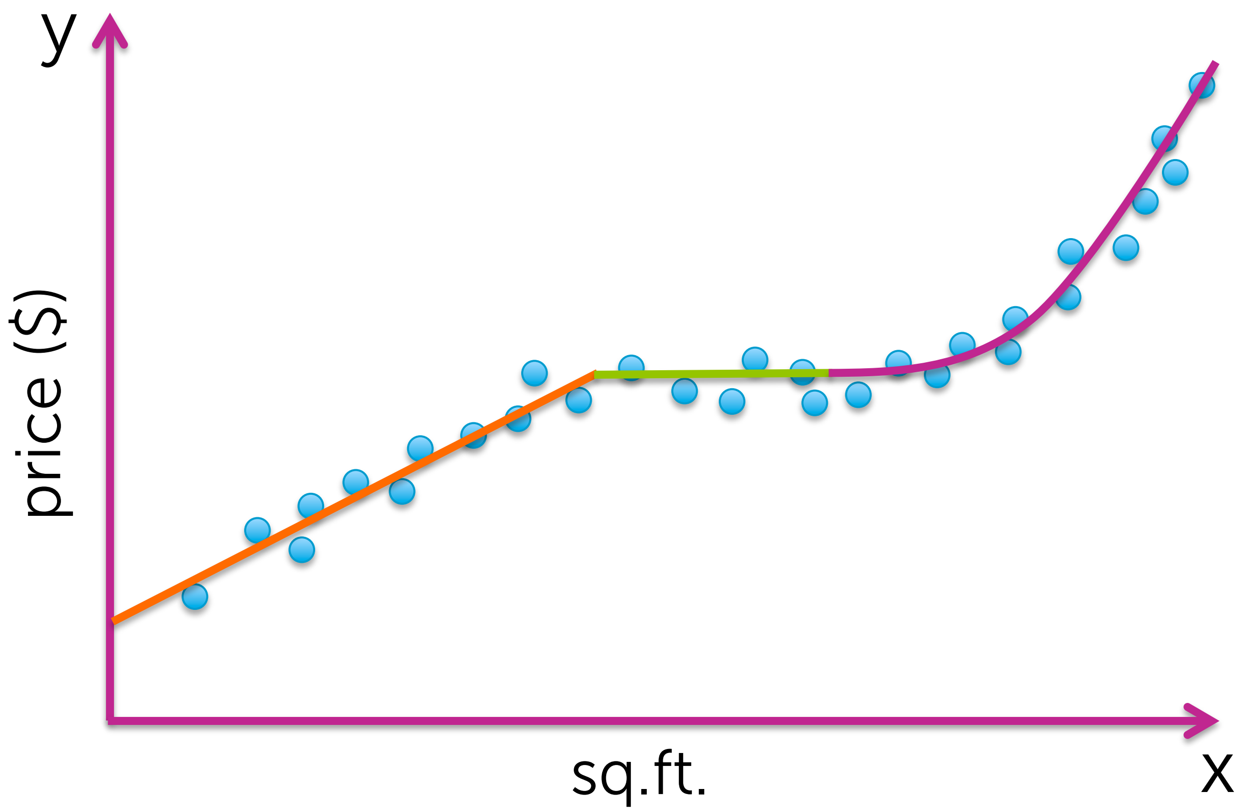


Parametric models of f(x)



f(x) is not really a polynomial



What alternative do we have?

If we:

- Want to allow flexibility in f(**x**) having local structure
- Don't want to infer "structural breaks"

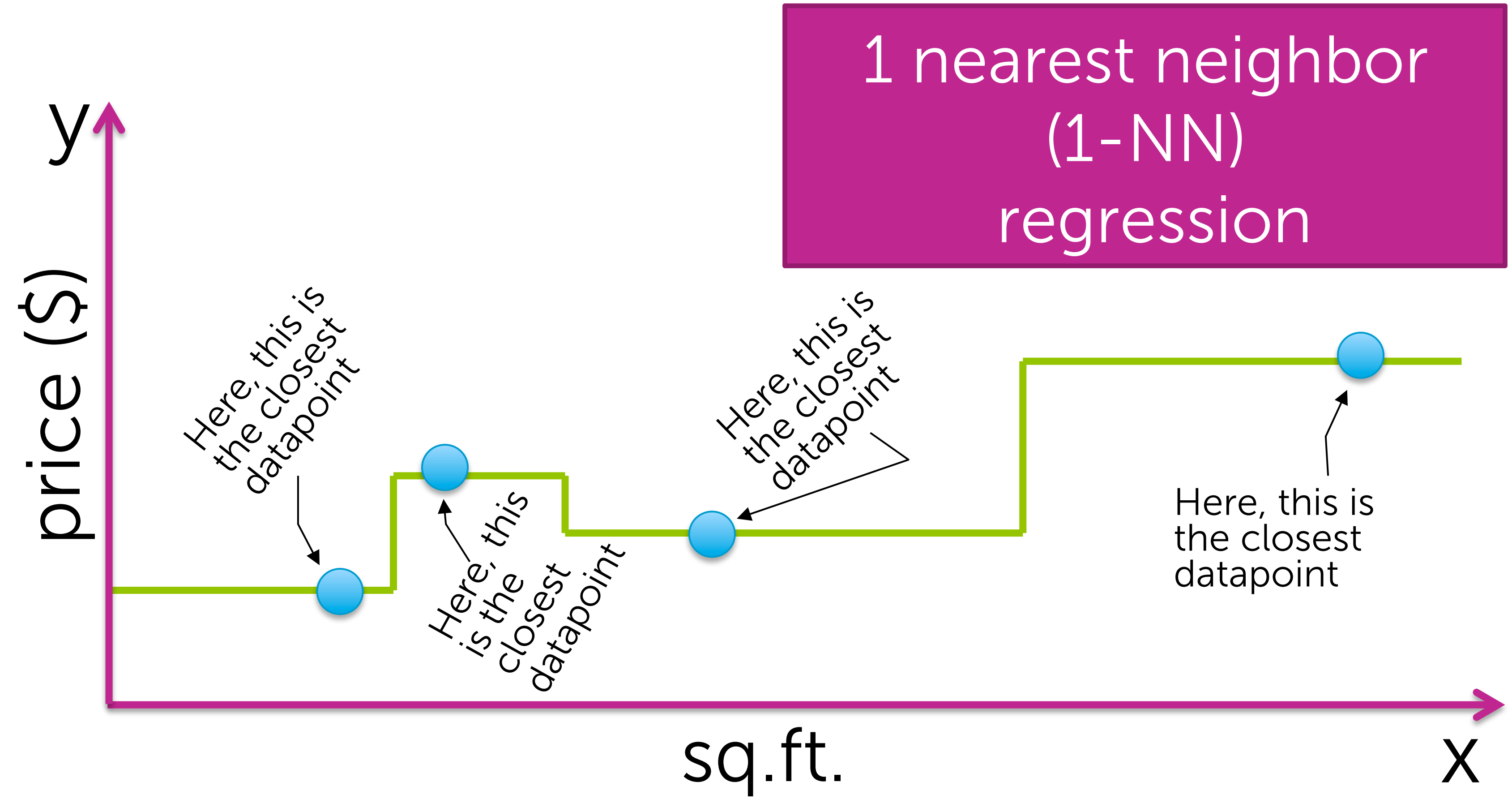
What's a simple option we have?

- Assuming we have plenty of data…

Simplest approach: Nearest neighbor regression

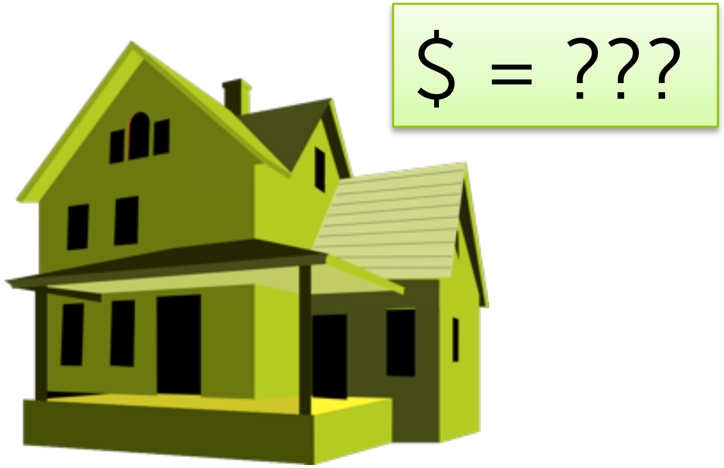
Fit locally to each data point

Predicted value = "closest" y_i



What people do naturally…

Real estate agent assesses value by finding sale of most similar house



1-NN regression more formally

Dataset of (🏠,\$) pairs: $(\mathbf{x}_1,y_1), (\mathbf{x}_2,y_2),\ldots,(\mathbf{x}_N,y_N)$

Query point: $\mathbf{x}_q$ ← \$?

big lime green house

1. Find "closest" $\mathbf{x}_i$ in dataset

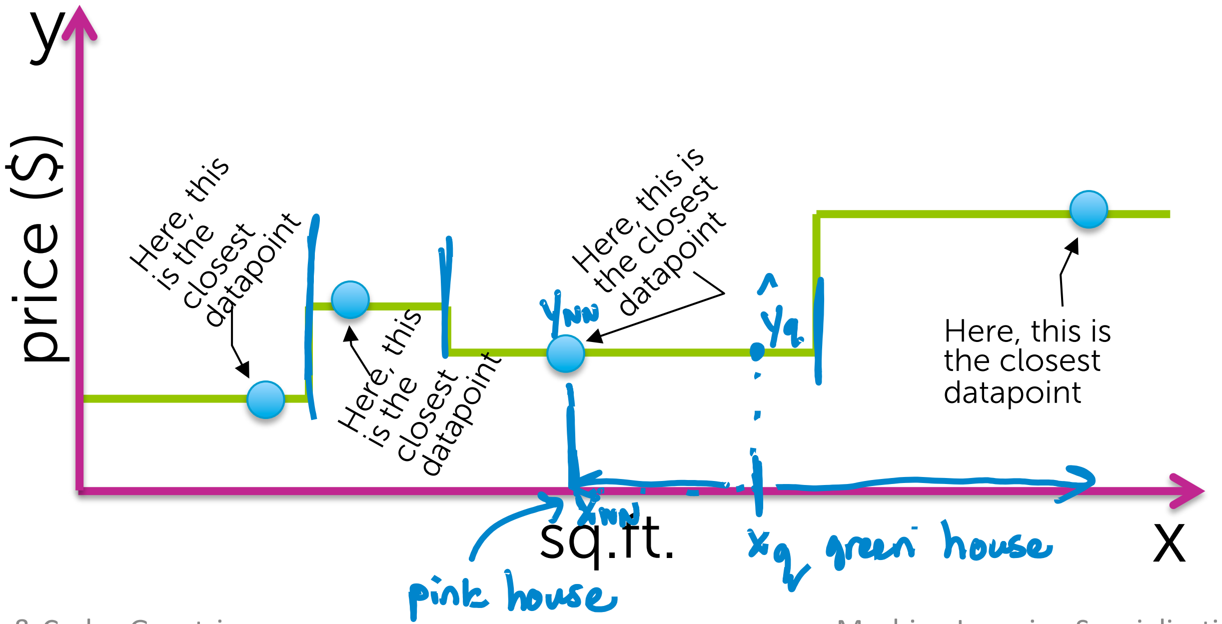
$$x_{NN} \leftarrow \min_i \text{distance}(x_i, x_q)$$

big pink house

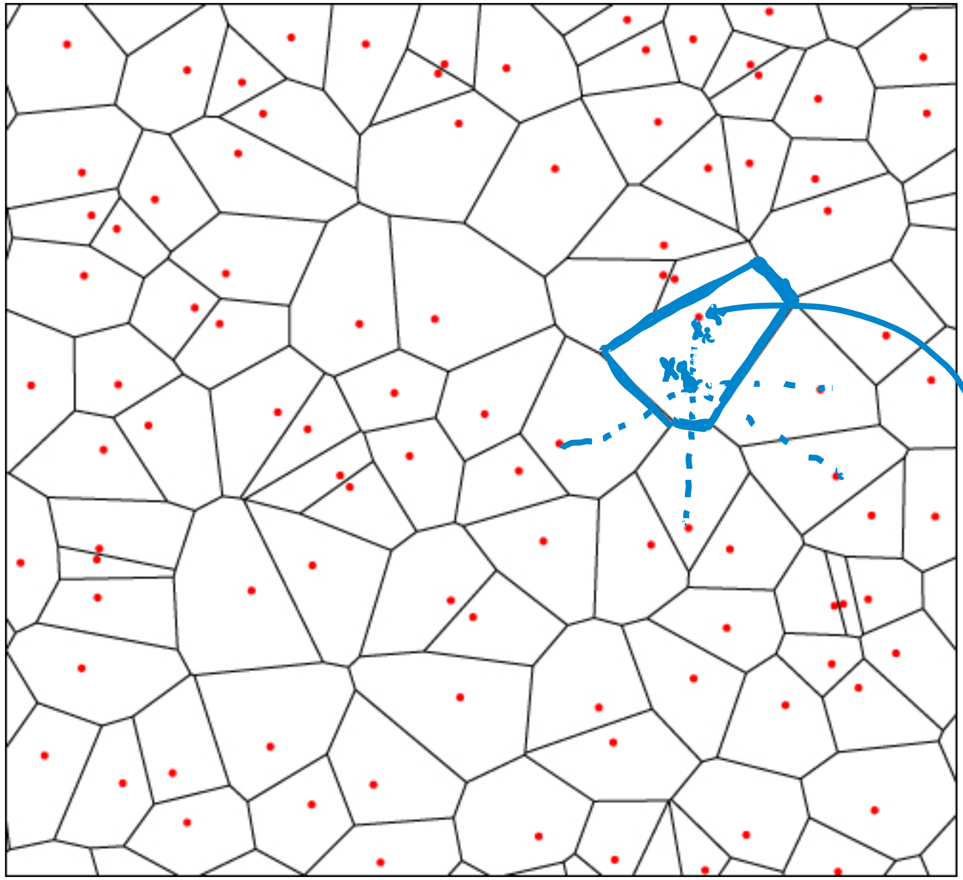
2. Predict

$$\hat{y}_q = y_{NN}$$

sales price of big pink house



Visualizing 1-NN in multiple dimensions



observation

Voronoi tesselation (or diagram):

- Divide space into N regions, each containing 1 datapoint
- Defined such that any **x** in region is "closest" to region's datapoint

x_q closer to x_i than any other x_j for $j \neq i$.

Don't explicitly form!

Distance metrics: Defining notion of "closest"

In 1D, just Euclidean distance:

$$\boxed{\text{distance}(x_j, x_q) = |x_j - x_q|}$$

In multiple dimensions:

- can define many interesting distance functions
- most straightforwardly, might want to weight different dimensions differently

Weighting housing inputs

Some inputs are more relevant than others

 # bedrooms
 # bathrooms
sq.ft. living
sq.ft. lot
floors
year built
year renovated
waterfront

Scaled Euclidean distance

Formally, this is achieved via

$$\text{distance}(\mathbf{x}_j, \mathbf{x}_q) = \sqrt{a_1(\mathbf{x}_j[1]-\mathbf{x}_q[1])^2 + \ldots + a_d(\mathbf{x}_j[d]-\mathbf{x}_q[d])^2}$$

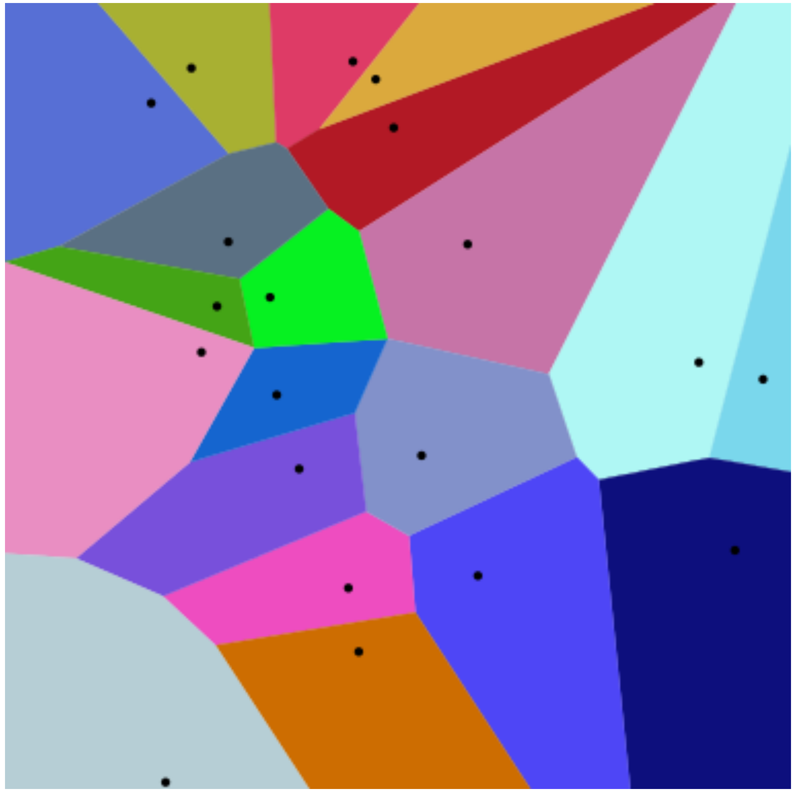
weight on each input
(defining relative importance)

Other example distance metrics:

- Mahalanobis, rank-based, correlation-based, cosine similarity, Manhattan, Hamming, …

Different distance metrics lead to different predictive surfaces

Euclidean distance



Manhattan distance

1-NN algorithm

Performing 1-NN search

- Query house: 

- Dataset: 

- **Specify:** Distance metric
- **Output:** Most similar house 

1-NN algorithm

closest house

Initialize **Dist2NN** = ∞,  = ∅

query house

For i=1,2,...,N

Compute: δ = **distance(** $_i$,  $_q$ **)**

If δ < **Dist2NN**

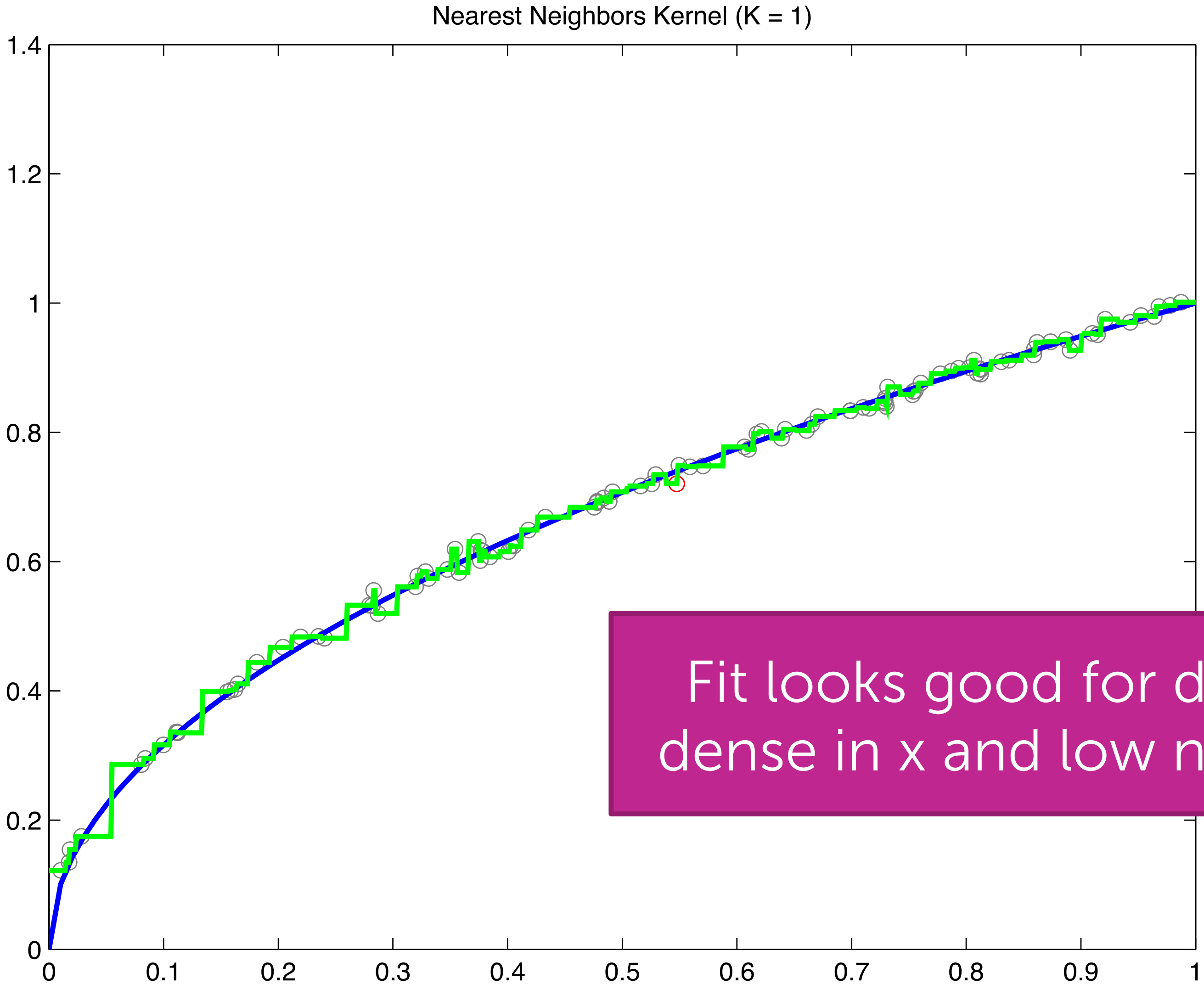
set   $_i$

set **Dist2NN** = δ

Return most similar house 

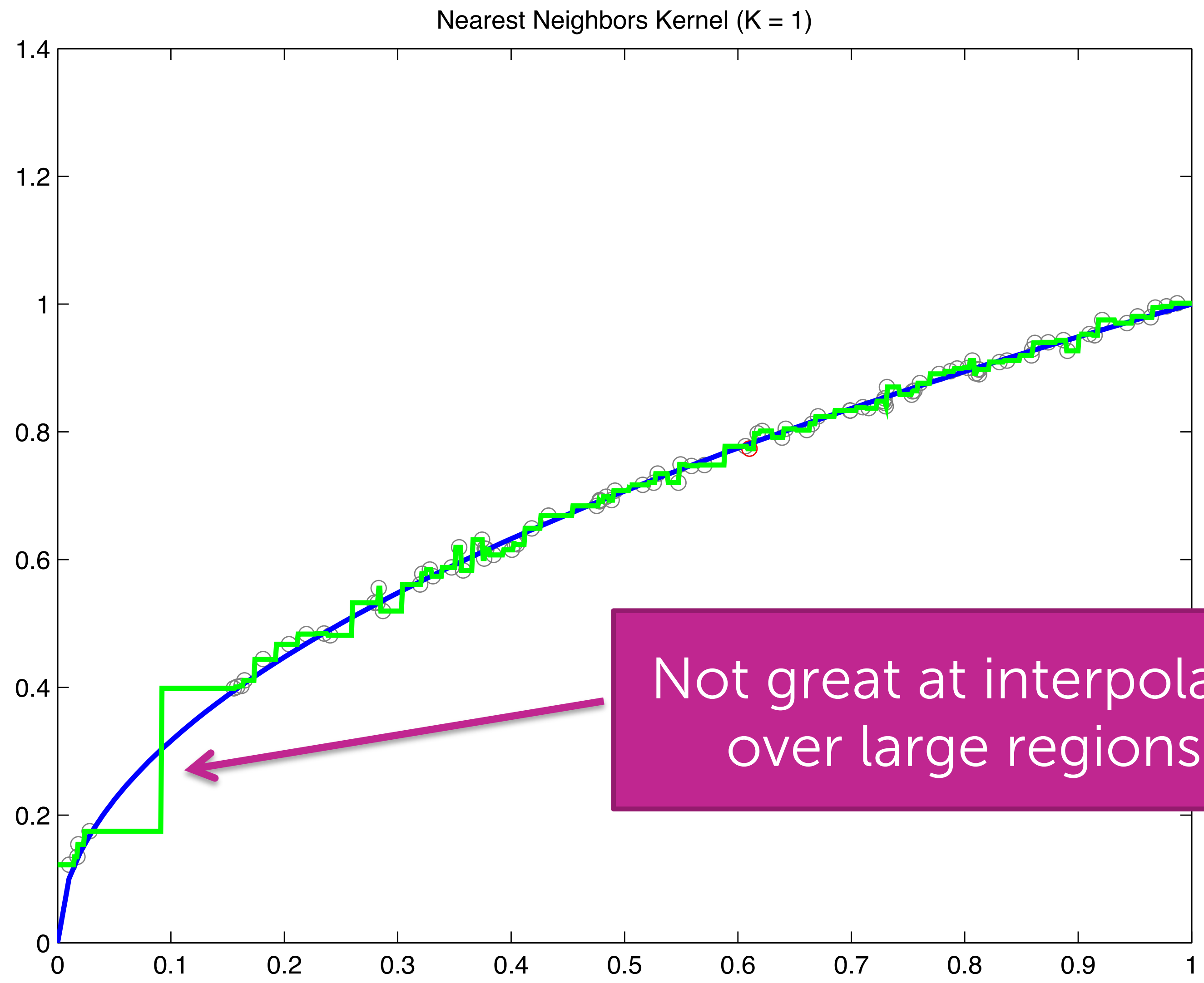
closest house
to query house

1-NN in practice



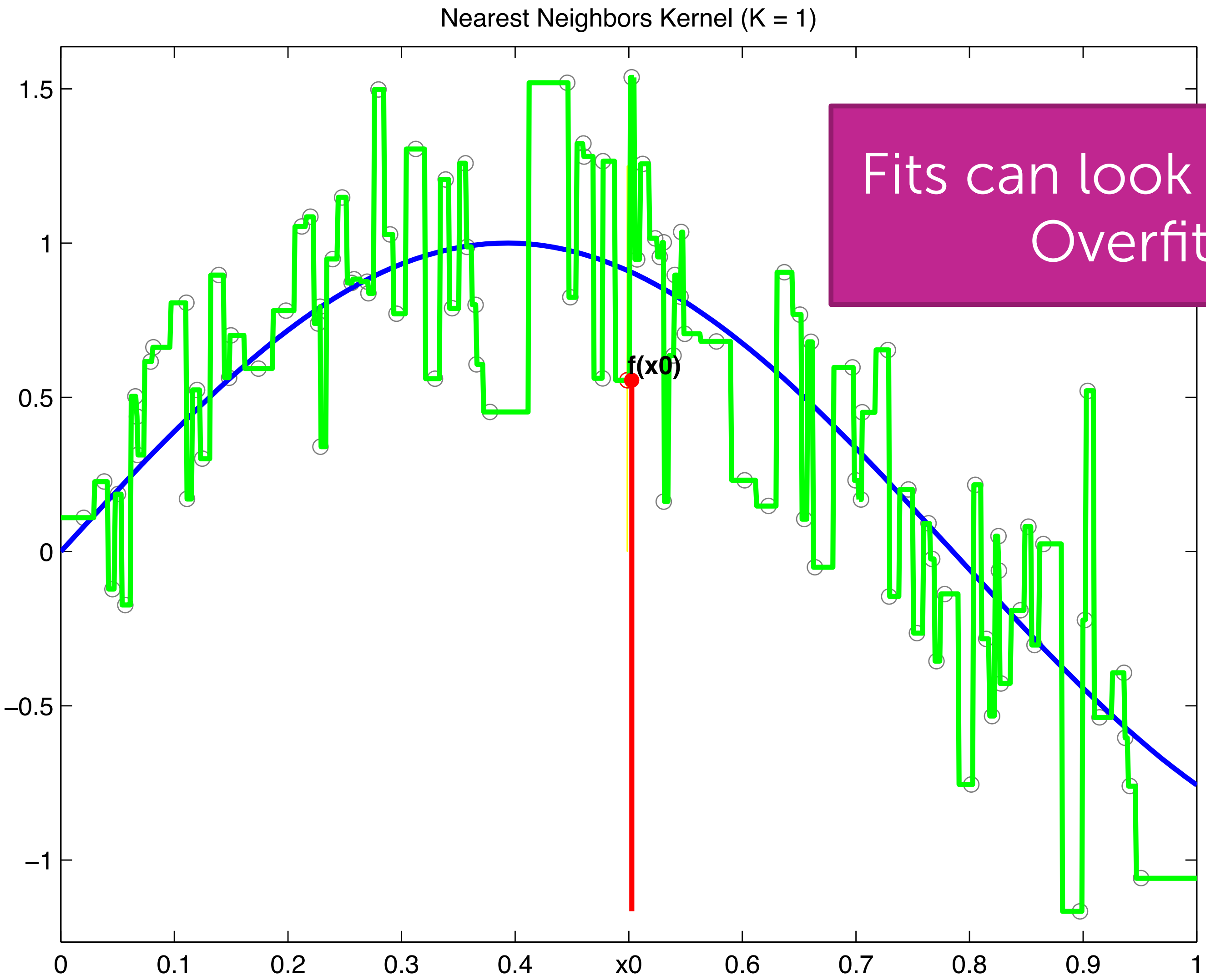
Fit looks good for data dense in x and low noise

Sensitive to regions with little data



Not great at interpolating over large regions…

Also sensitive to noise in data

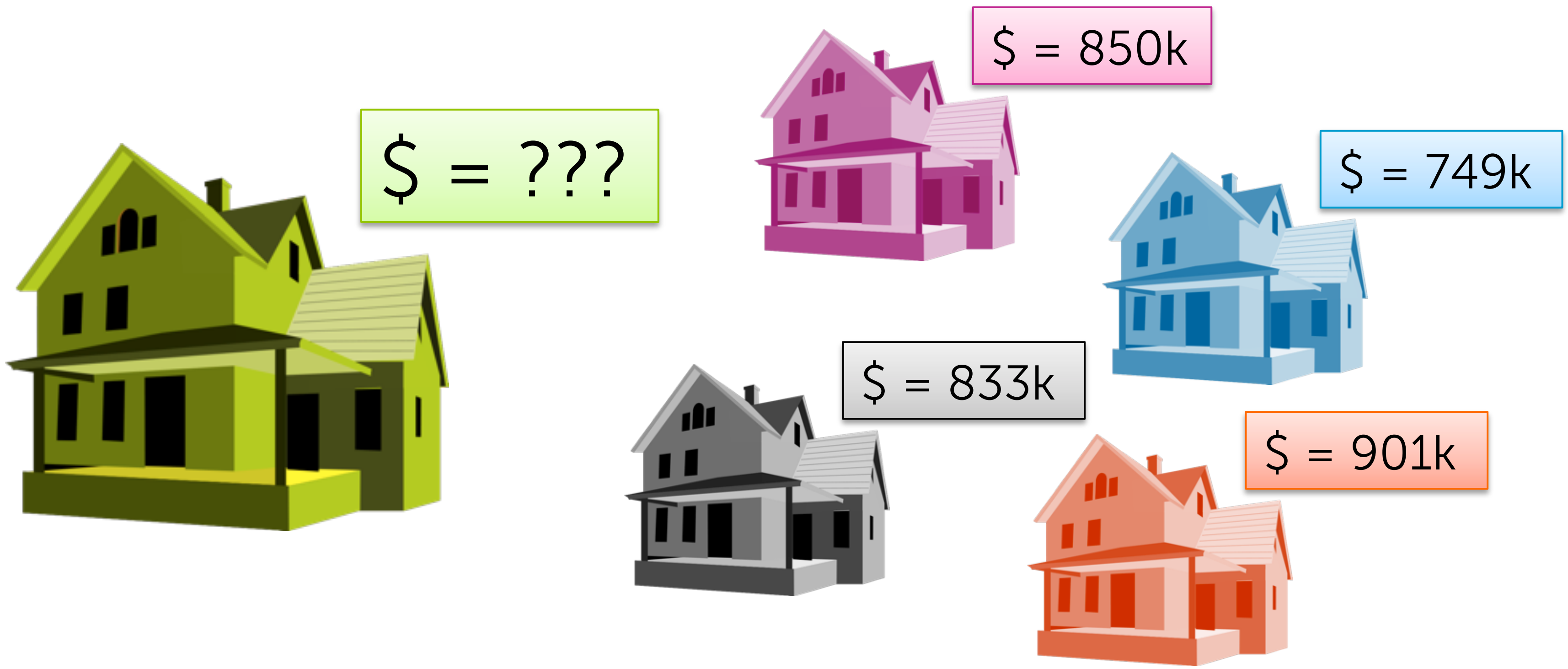


Fits can look quite wild…
Overfitting?

k-Nearest neighbors

Get more "comps"

More reliable estimate if you base estimate off of a larger set of comparable homes



k-NN regression more formally

Dataset of (,$) pairs: $(\mathbf{x}_1,y_1), (\mathbf{x}_2,y_2),\ldots,(\mathbf{x}_N,y_N)$

Query point: $\mathbf{x}_q$

1. Find k closest $\mathbf{x}_i$ in dataset

   $(x_{NN_1}, x_{NN_2}, \ldots, x_{NN_k})$ such that for any x_i not in nearest neighbor set,

   $$\text{distance}(x_i, x_q) \geq \text{distance}(x_{NN_k}, x_q)$$

2. Predict

   $$\hat{y}_q = \frac{1}{k}(y_{NN_1} + y_{NN_2} + \ldots + y_{NN_k})$$

   $$= \frac{1}{k}\sum_{j=1}^{k} y_{NN_j}$$

Performing k-NN search

- Query house: 
- Dataset: 
- **Specify:** Distance metric
- **Output:** Most similar houses

k-NN algorithm

sort first **k houses**
by distance to query house

Initialize **Dist2kNN** = sort($\delta_1,\ldots,\delta_k$) ← list of sorted distances

= so ,…, $_1$ $_k$ ← list of sorted houses

For i=k+1,…,N

query house

Compute: δ = **distance(** $_i$ **,** $_q$ **)**

If δ **< Dist2kNN**[k]

find j such that δ **> Dist2kNN**[j-1] but δ **< Dist2kNN**[j]

remove furthest house and shift queue:

[j+1] = [j:k

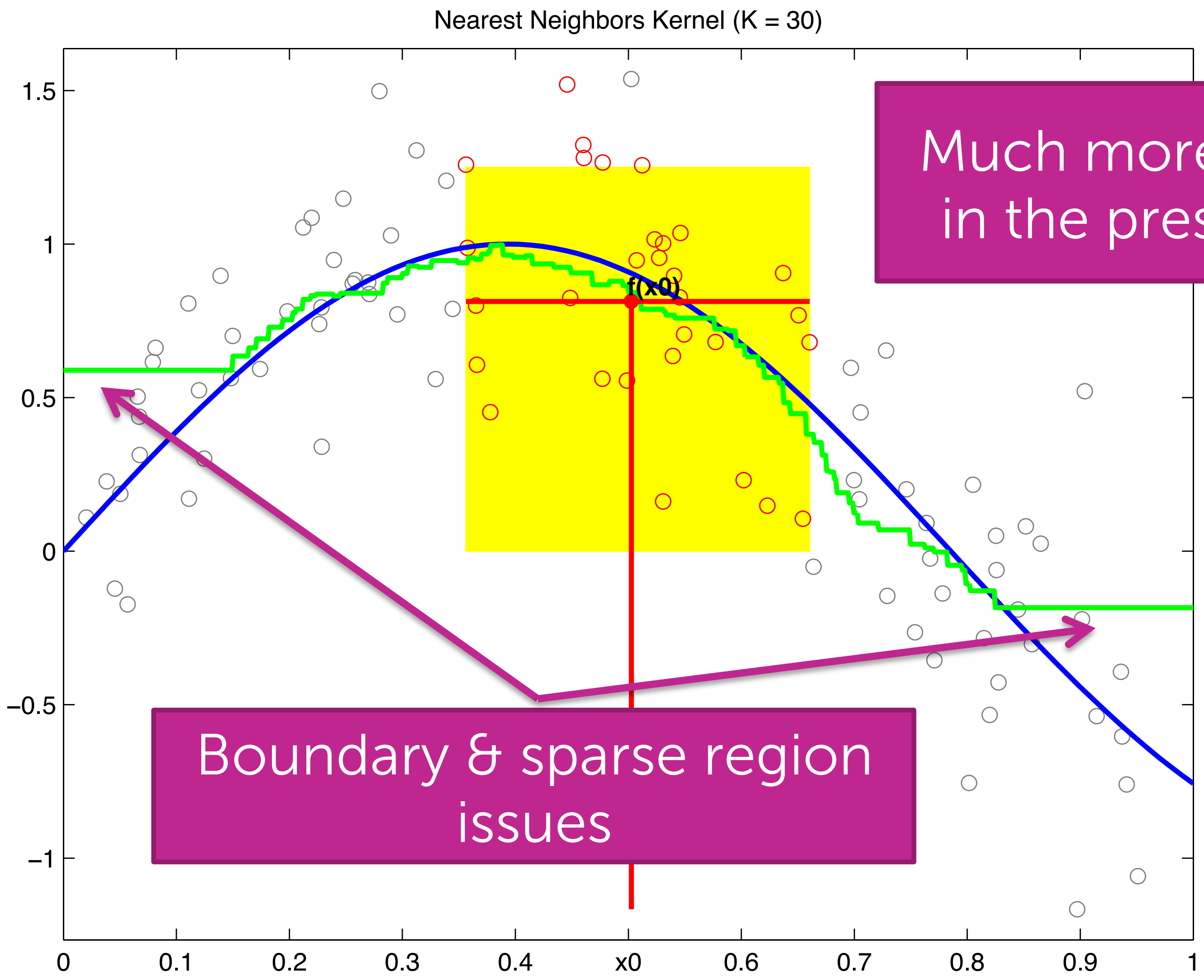
insert new NN

Dist2kNN[j+1:k] = **Dist2kNN**[j:k-1]

set **Dist2kNN**[j] = δ and = $_i$

Return k most similar houses ← closest houses to query house

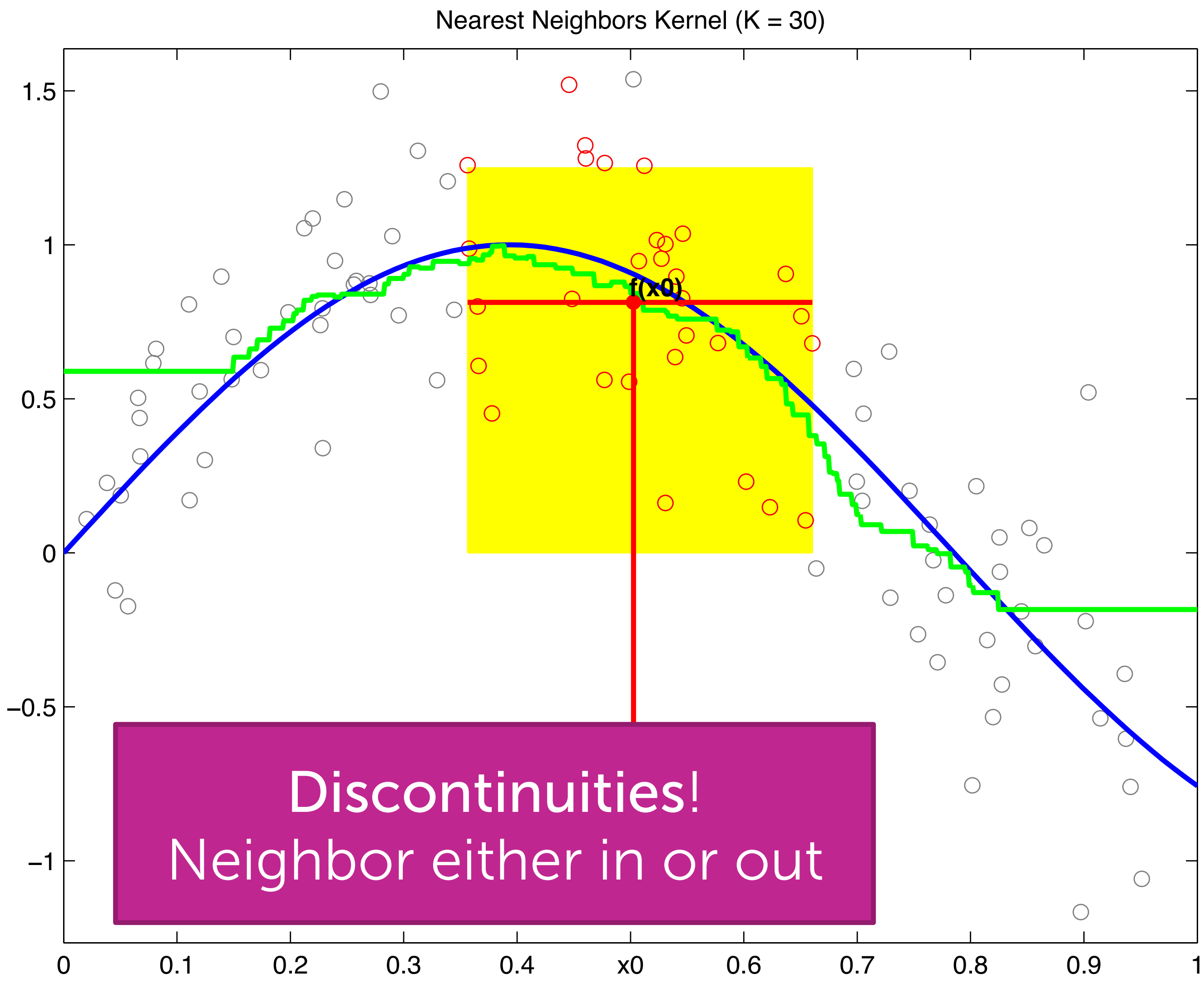
k-NN in practice



Much more reasonable fit in the presence of noise

Boundary & sparse region issues

k-NN in practice



Discontinuities!
Neighbor either in or out

Issues with discontinuities

Overall predictive accuracy might be okay, but…

For example, in housing application:

- If you are a buyer or seller, this matters
- Can be a jump in estimated value of house going just from 2640 sq.ft. to 2641 sq.ft.
- Don't really believe this type of fit

Weighted k-nearest neighbors

Weighted k-NN

Weigh more similar houses more than those less similar in list of k-NN

Predict:

weights on NN

$$\hat{y}_q = \frac{c_{qNN1} y_{NN1} + c_{qNN2} y_{NN2} + c_{qNN3} y_{NN3} + \ldots + c_{qNNk} y_{NNk}}{\sum_{j=1}^{k} c_{qNNj}}$$

How to define weights?

Want weight c_{qNNj} to be small when
  $\text{distance}(\mathbf{x}_{NNj},\mathbf{x}_q)$ large

and c_{qNNj} to be large when
  $\text{distance}(\mathbf{x}_{NNj},\mathbf{x}_q)$ small

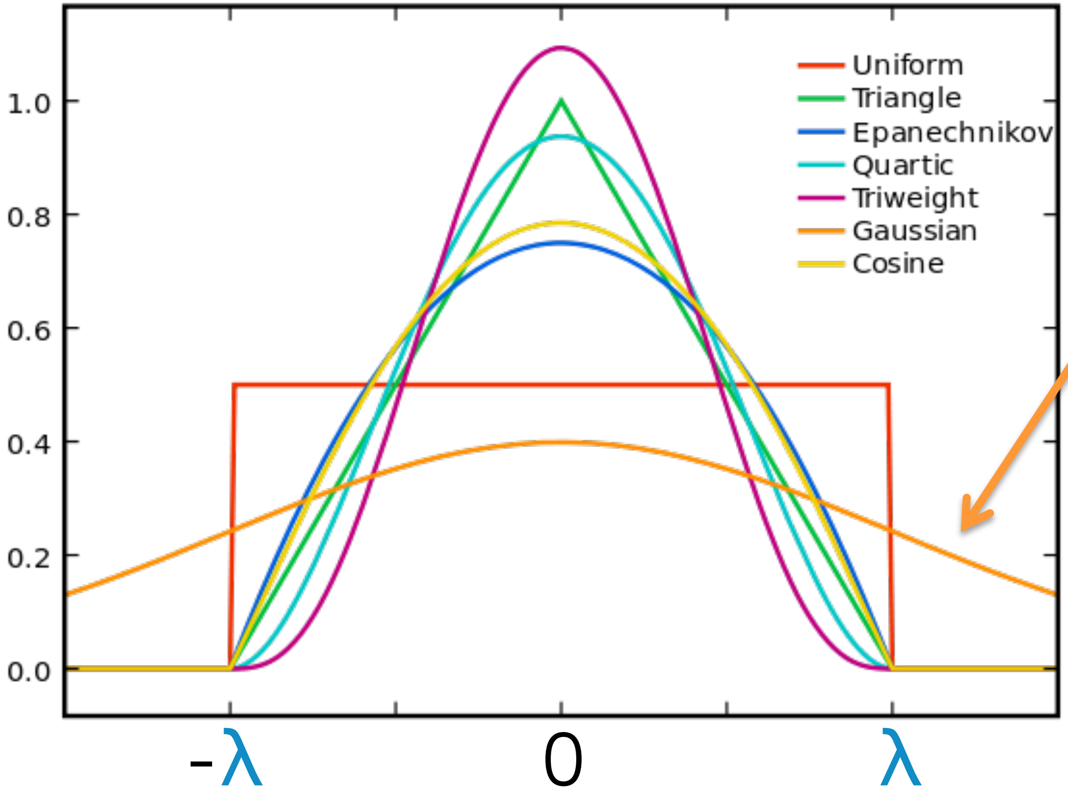
Simple method:

$$c_{qNN_j} = \frac{1}{\text{distance}(x_j, x_q)}$$

Kernel weights for d=1

Define: $c_{qNNj} = \text{Kernel}_\lambda(|x_{NNj} - x_q|)$

simple isotropic case



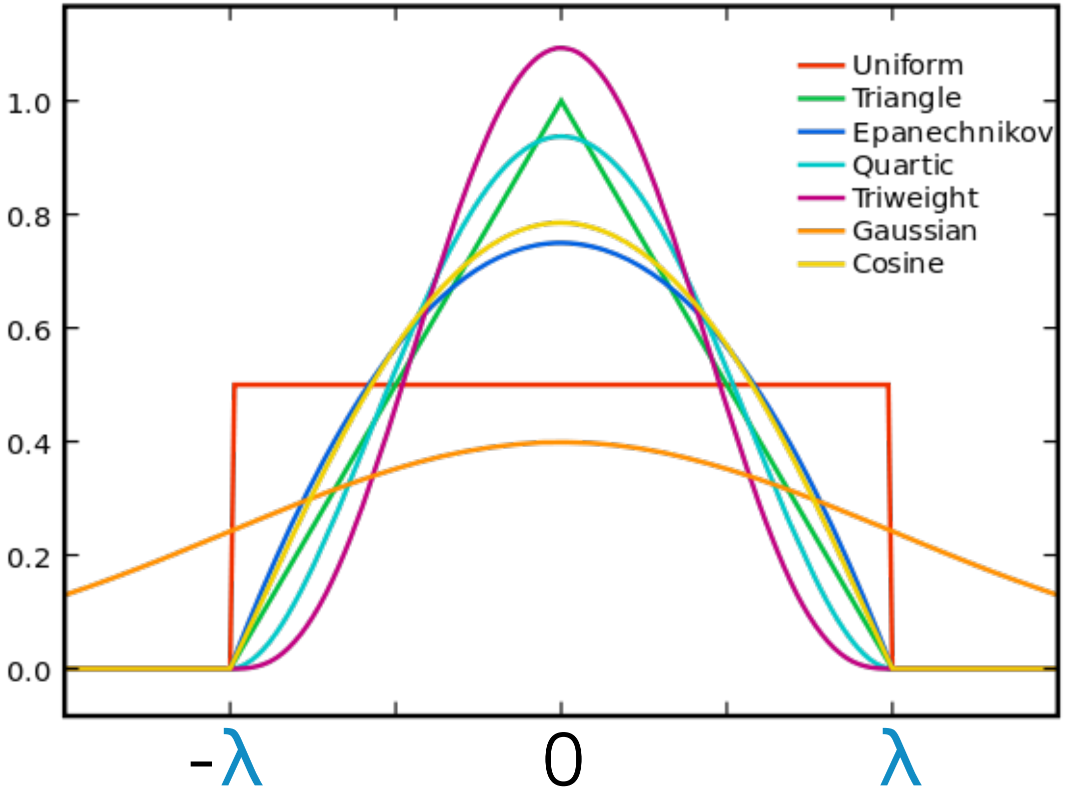
Gaussian kernel:

$$\text{Kernel}_\lambda(|x_i - x_q|) = \exp(-(x_i - x_q)^2/\lambda)$$

Note: never exactly 0!

Kernel weights for d≥1

Define: $c_{qNNj} = \text{Kernel}_{\lambda}(\text{distance}(\mathbf{x}_{NNj},\mathbf{x}_q))$



Kernel regression

Weighted k-NN

Weigh more similar houses more than those less similar in list of k-NN

Predict:

weights on NN

$$\hat{y}_q = \frac{c_{qNN1} y_{NN1} + c_{qNN2} y_{NN2} + c_{qNN3} y_{NN3} + \ldots + c_{qNNk} y_{NNk}}{\sum_{j=1}^{k} c_{qNNj}}$$

Kernel regression

Nadaraya-Watson kernel weighted average

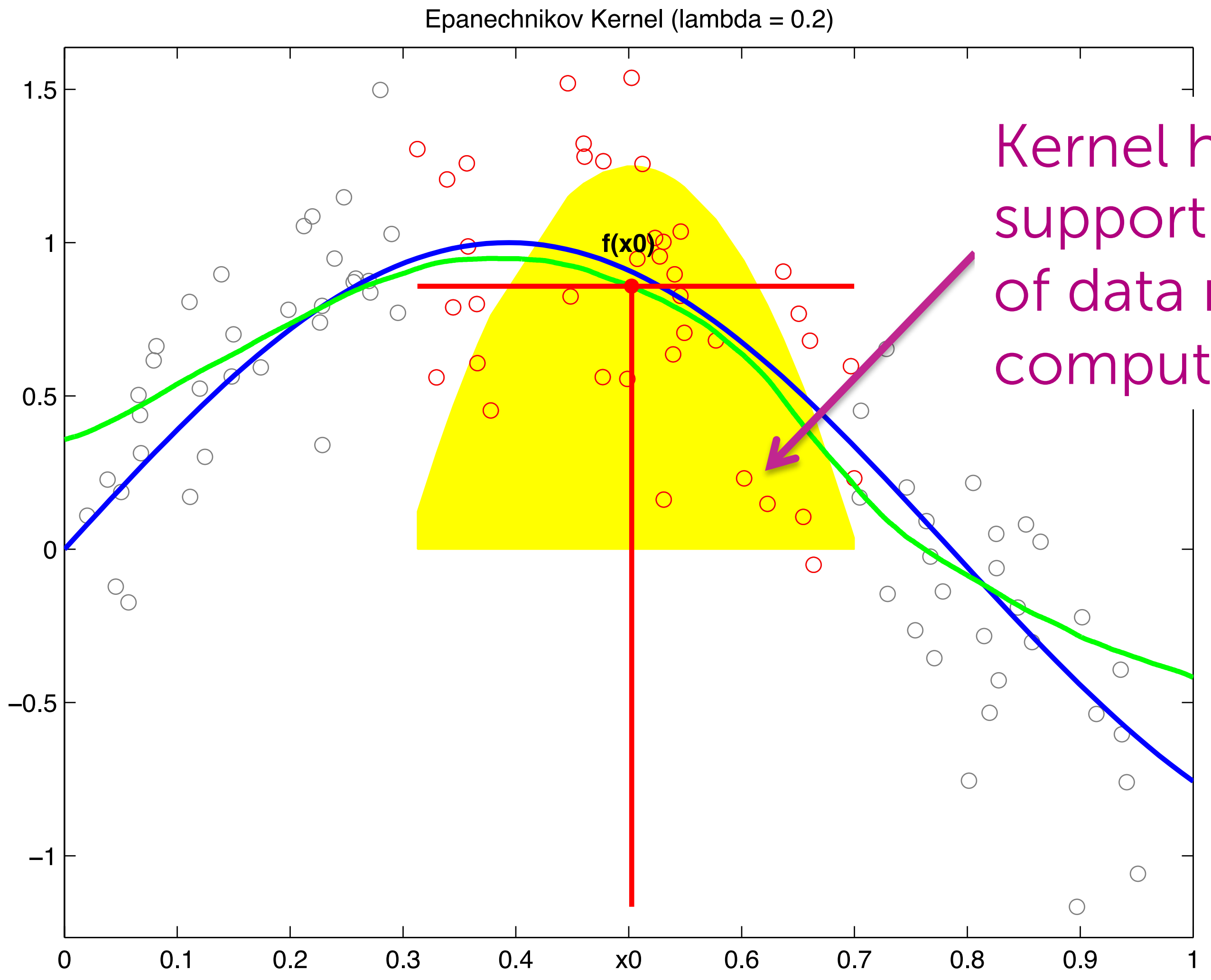
Instead of just weighting NN, weight *all* points

Predict:

weight on each datapoint

$$\hat{y}_q = \frac{\sum_{i=1}^{N} c_{qi} y_i}{\sum_{i=1}^{N} c_{qi}} = \frac{\sum_{i=1}^{N} \text{Kernel}_\lambda(\text{distance}(\mathbf{x}_i,\mathbf{x}_q)) * y_i}{\sum_{i=1}^{N} \text{Kernel}_\lambda(\text{distance}(\mathbf{x}_i,\mathbf{x}_q))}$$

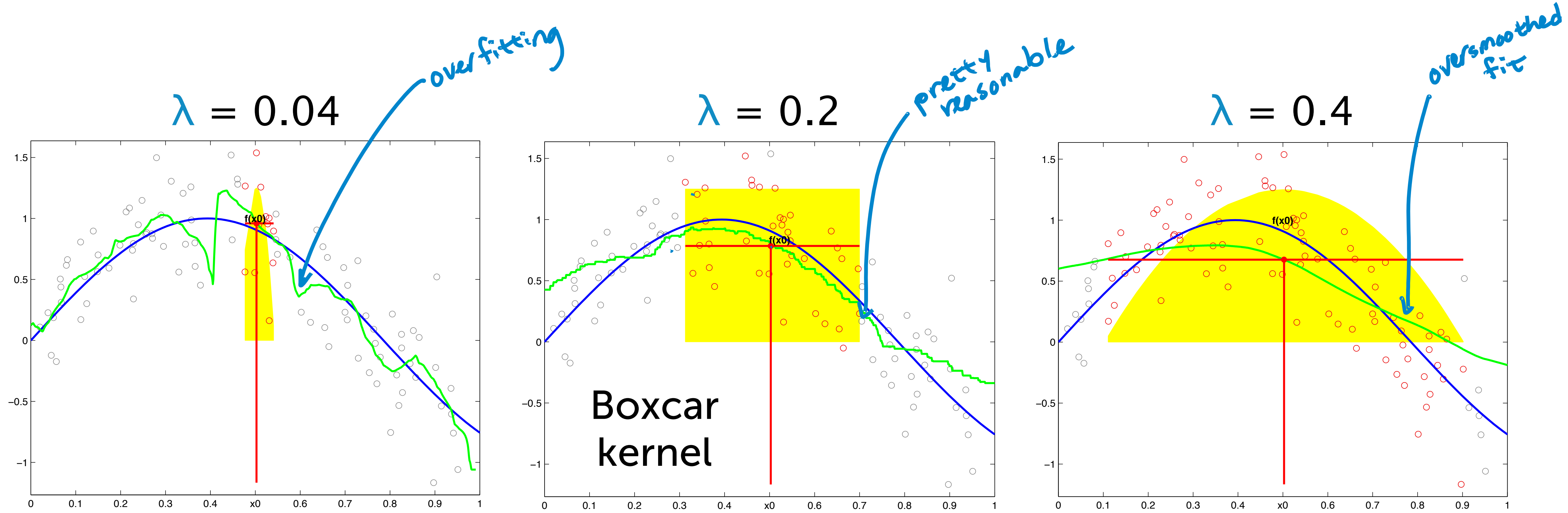
Kernel regression in practice



Kernel has bounded support…Only subset of data needed to compute local fit

Choice of bandwidth λ

Often, choice of kernel matters much less than choice of λ



Choosing λ (or k in k-NN)

How to choose? Same story as always…

Cross Validation

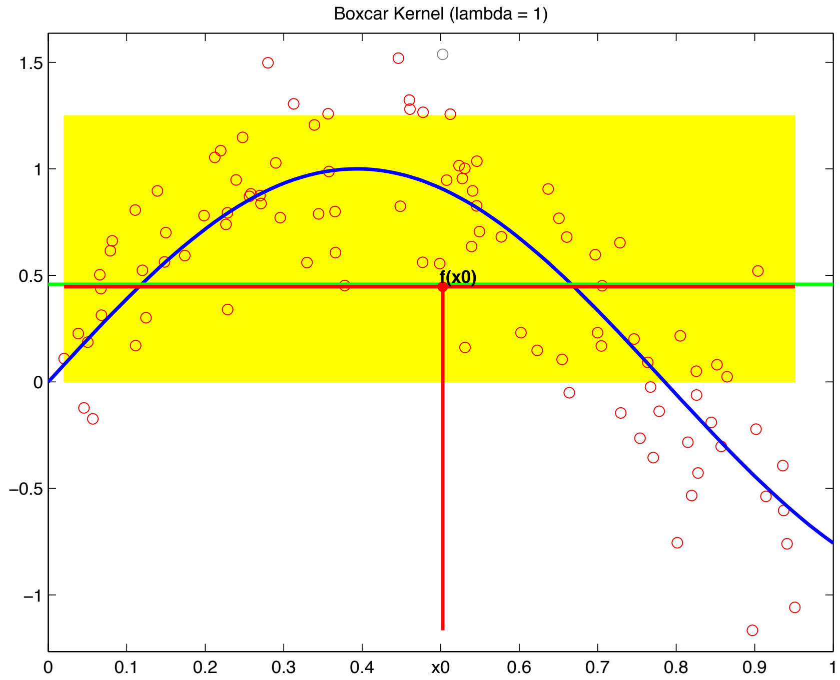
Formalizing the idea of local fits

Contrasting with global average

A globally constant fit weights all points equally

equal weight on each datapoint

$$\hat{y}_q = \frac{1}{N}\sum_{i=1}^{N} y_i = \frac{\sum_{i=1}^{N} c\, y_i}{\sum_{i=1}^{N} c}$$

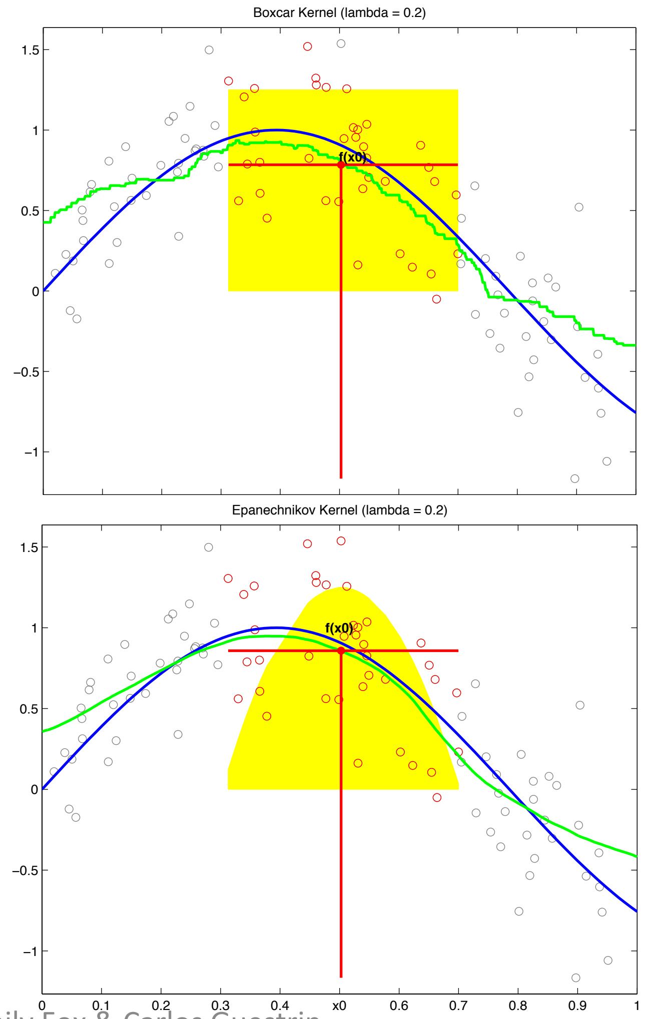


Contrasting with global average

Kernel regression leads to locally constant fit

– slowly add in some points and and let others gradually die off

$$\hat{y}_q = \frac{\sum_{i=1}^{N} \text{Kernel}_{\lambda}(\text{distance}(\mathbf{x}_i,\mathbf{x}_q)) * y_i}{\sum_{i=1}^{N} \text{Kernel}_{\lambda}(\text{distance}(\mathbf{x}_i,\mathbf{x}_q))}$$



Local linear regression

So far, discussed fitting constant function locally at each point

→ "locally weighted averages"

Can instead fit a line or polynomial locally at each point

→ "locally weighted linear regression"

Local regression rules of thumb

- Local linear fit reduces bias at boundaries with minimum increase in variance
- Local quadratic fit doesn't help at boundaries and increases variance, but does help capture curvature in the interior
- With sufficient data, local polynomials of odd degree dominate those of even degree

Recommended default choice:

local linear regression

Discussion on k-NN and kernel regression

Nonparametric approaches

k-NN and kernel regression are examples of nonparametric regression

General goals of nonparametrics:

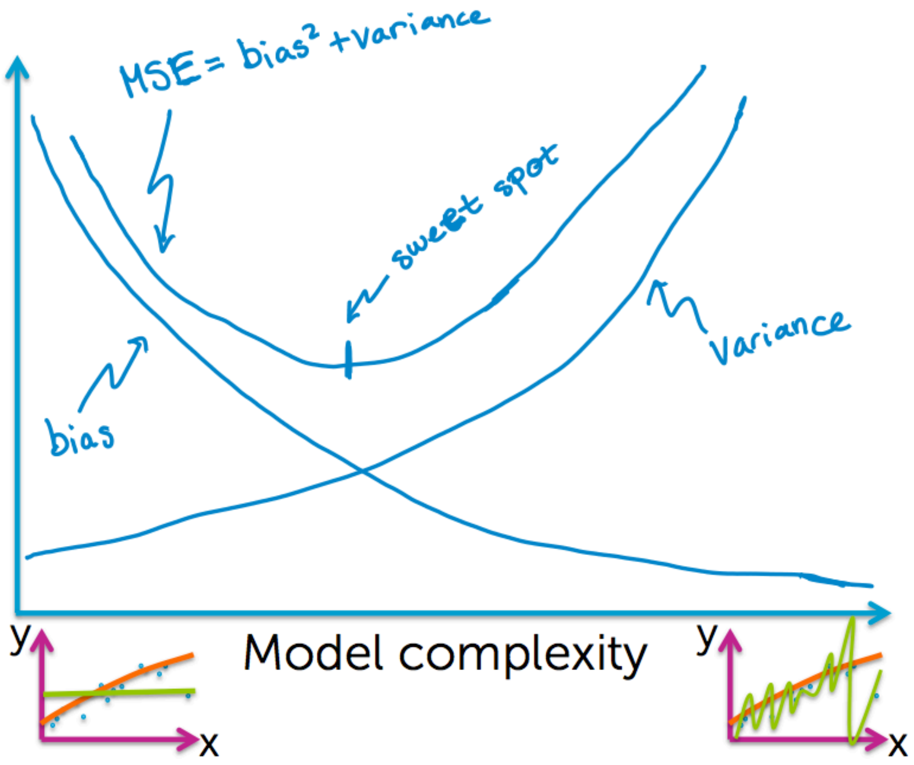
- Flexibility
- Make few assumptions about f(**x**)
- Complexity can grow with the number of observations N

Lots of other choices:

- Splines, trees, locally weighted structured regression models…

Limiting behavior of NN: Noiseless setting (ε_i=0)

In the limit of getting an infinite amount of noiseless data, the MSE of 1-NN fit goes to 0



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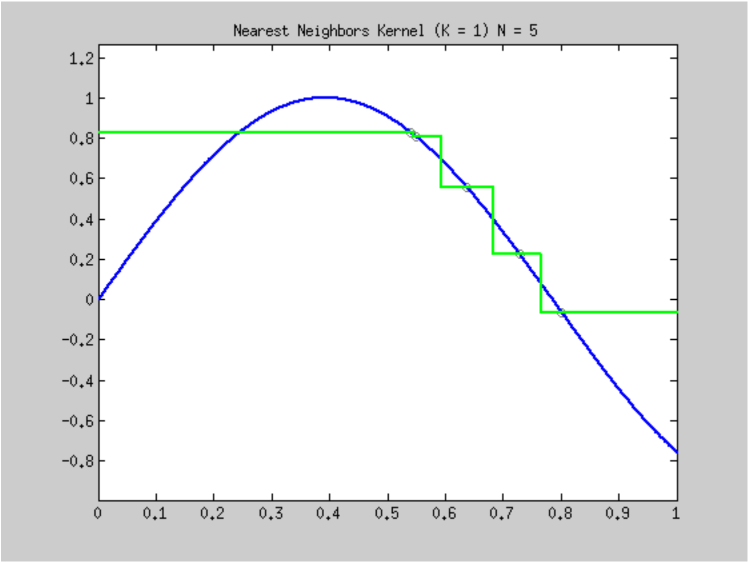
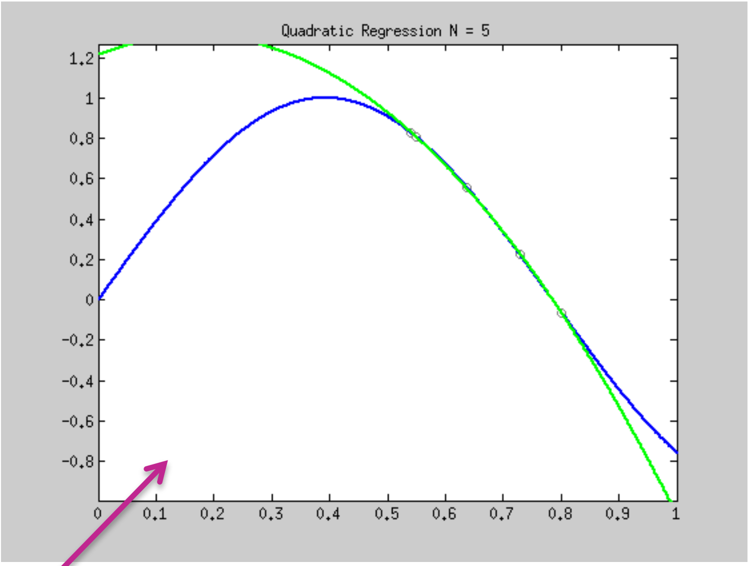


1-NN fit

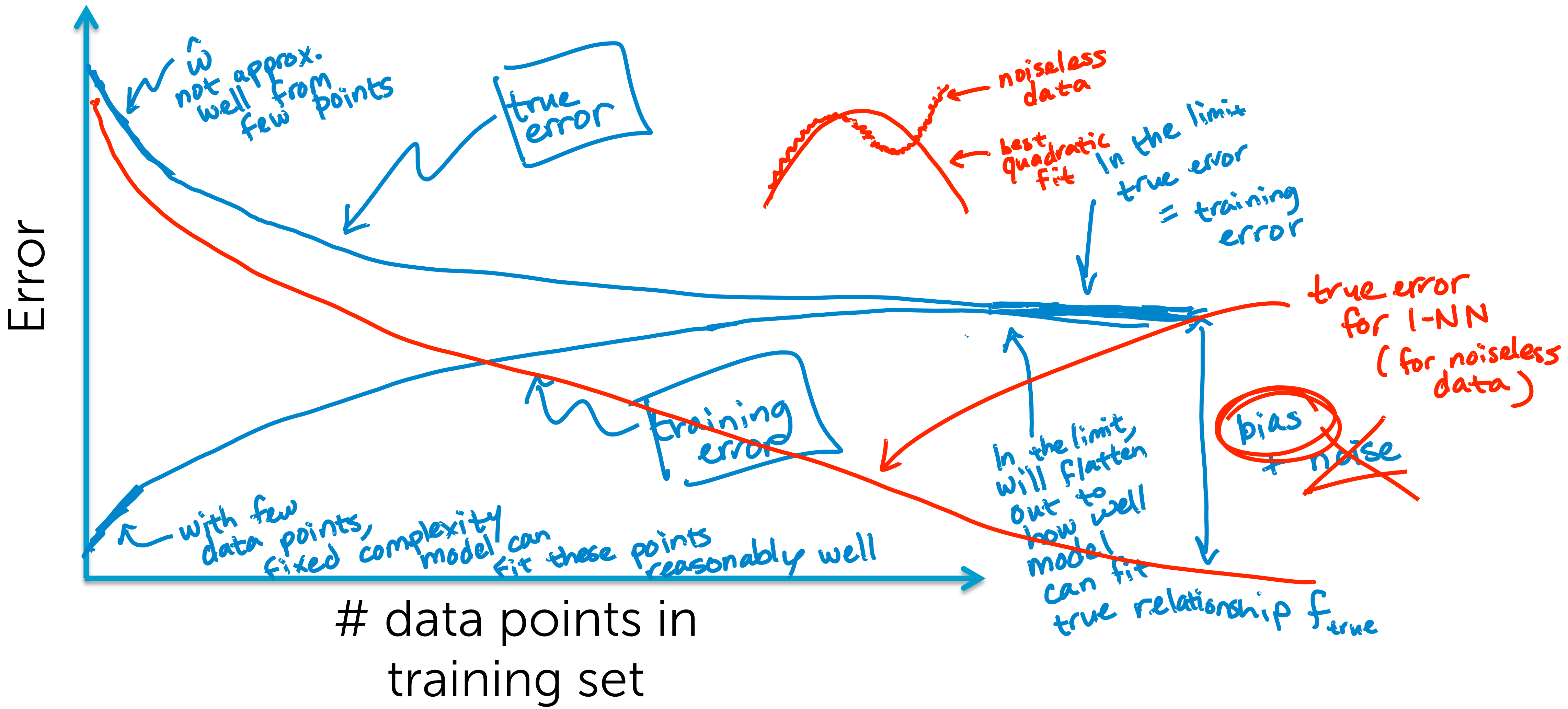


Quadratic fit

Not true for parametric models!

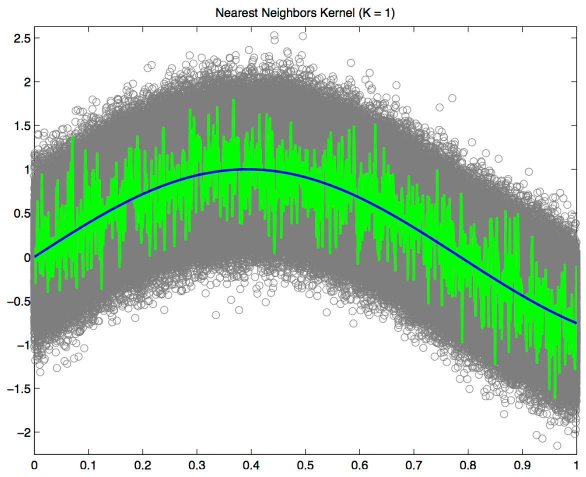
Error vs. amount of data

for a fixed model complexity

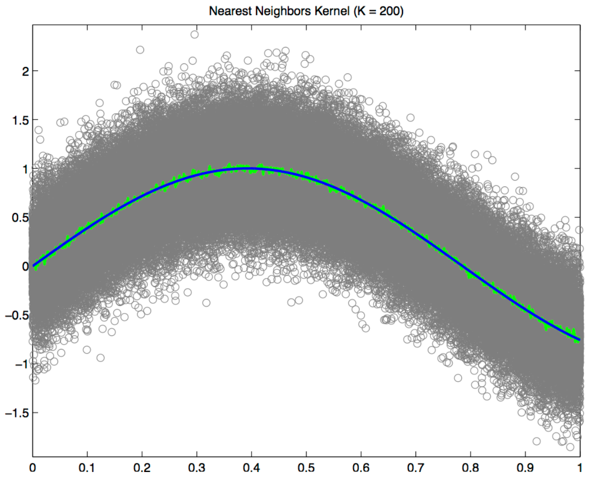


Limiting behavior of NN: Noisy data setting

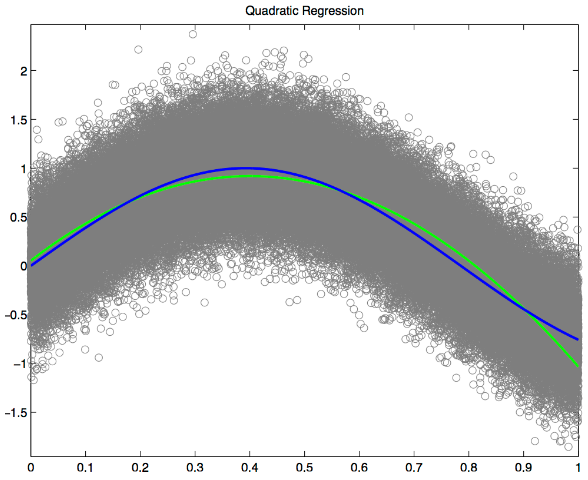
In the limit of getting an infinite amount of data, the MSE of NN fit goes to 0 if k grows, too



1-NN fit



200-NN fit



Quadratic fit

NN and kernel methods for large d or small N

NN and kernel methods work well when the data cover the space, but…

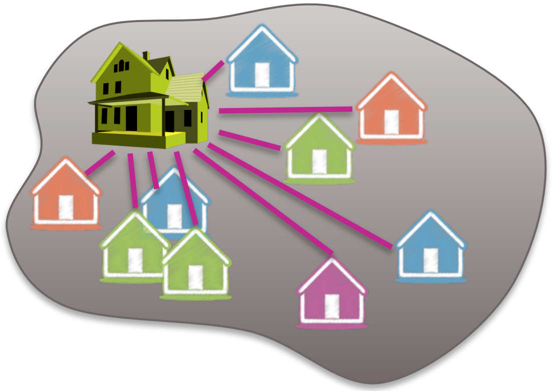
- the more dimensions d you have, the more points N you need to cover the space
- need $N = O(\exp(d))$ data points for good performance

This is where parametric models become useful…

Complexity of NN search

Naïve approach: **Brute force search**

- Given a query point $\mathbf{x}_q$
- Scan through each point $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$
- O(N) distance computations per 1-NN query!
- O(Nlogk) per k-NN query!

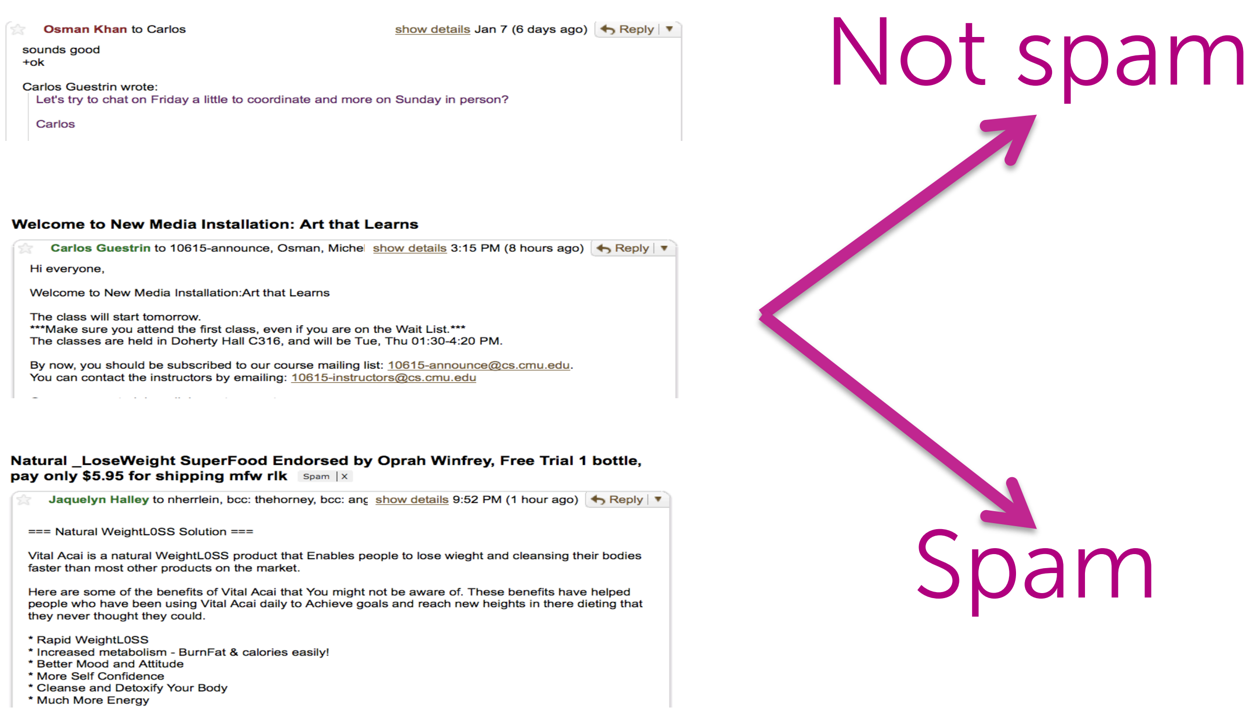


What if N is huge???
(and many queries)

Will talk more about efficient methods in
Clustering & Retrieval course

k-NN for classification

Recall classification task: Spam filtering example



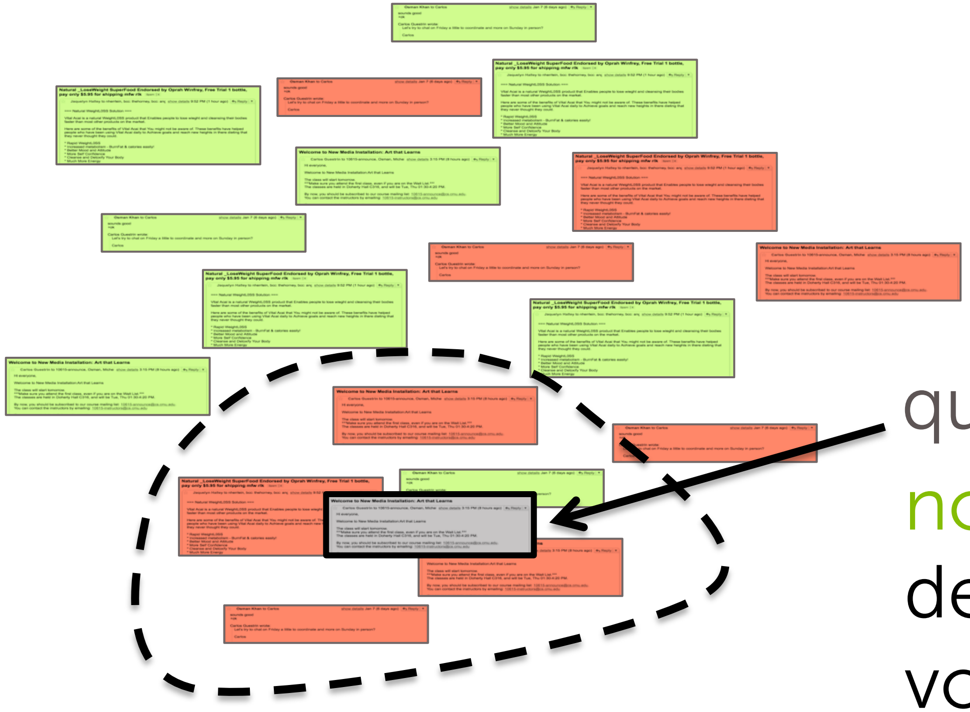
Input: **x**

Output: y

Text of email, sender, IP,...

Using k-NN for classification

Space of labeled emails (not spam vs. spam), organized by similarity of text



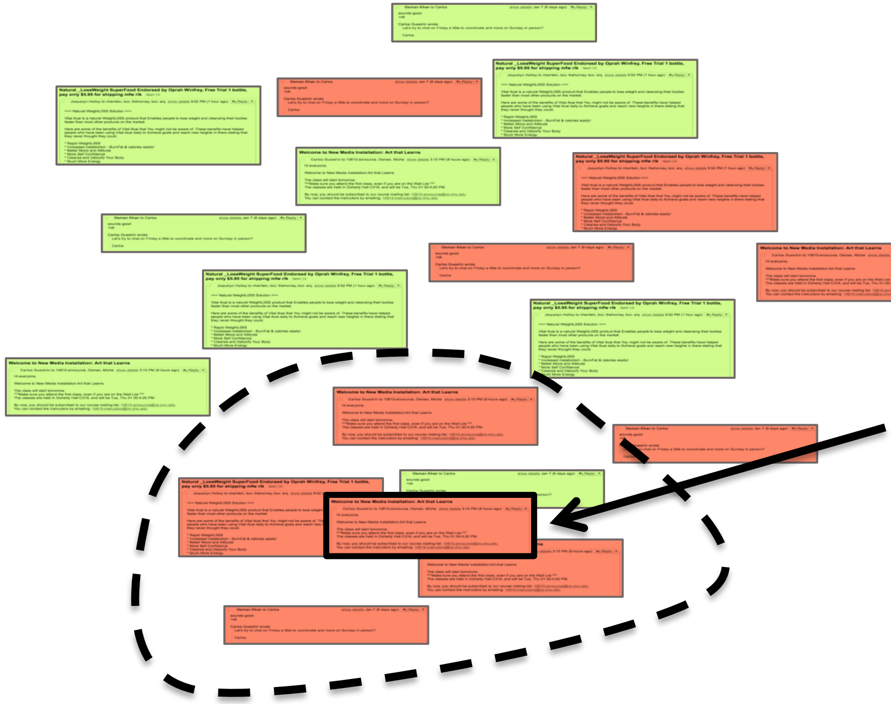
query email

not spam vs. spam

decide via majority vote of k-NN

Using k-NN for classification

Space of labeled emails (not spam vs. spam), organized by similarity of text



query email

not spam vs. $\boxed{\text{spam}}$

decide via majority vote of k-NN

Summary for nearest neighbor and kernel regression

What you can do now…

- Motivate the use of nearest neighbor (NN) regression
- Define distance metrics in 1D and multiple dimensions
- Perform NN and k-NN regression
- Analyze computational costs of these algorithms
- Discuss sensitivity of NN to lack of data, dimensionality, and noise
- Perform weighted k-NN and define weights using a kernel
- Define and implement kernel regression
- Describe the effect of varying the kernel bandwidth λ or # of nearest neighbors k
- Select λ or k using cross validation
- Compare and contrast kernel regression with a global average fit
- Define what makes an approach nonparametric and why NN and kernel regression are considered nonparametric methods
- Analyze the limiting behavior of NN regression
- Use NN for classification