MLCC 2015
Local Methods and Bias Variance Trade-Off

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About this class

1. Introduce a basic class of learning methods, namely **local methods**.
2. Discuss the fundamental concept of **bias-variance** trade-off to understand parameter tuning (a.k.a. model selection)

Outline

Learning with Local Methods

From Bias-Variance to Cross-Validation

The problem

What is the price of one house given its area?

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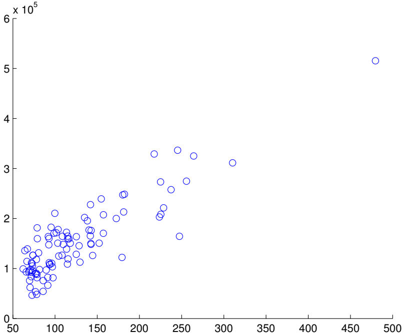
$x_1 = 62$	$y_1 = 99,200$
$x_2 = 64$	$y_2 = 135,700$
$x_3 = 65$	$y_3 = 93,300$
$x_4 = 66$	$y_4 = 114,000$
$\vdots$	$\vdots$



Let S the houses example dataset ($n = 100$)

$$S = \{(x_1, y_1), \ldots, (x_n, y_n)\}$$

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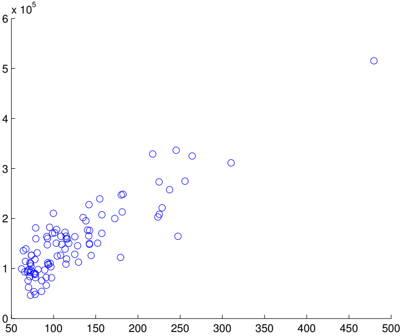

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Given a new point x^* we want to predict y^* by means of S.

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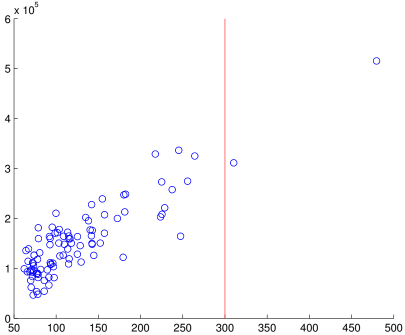

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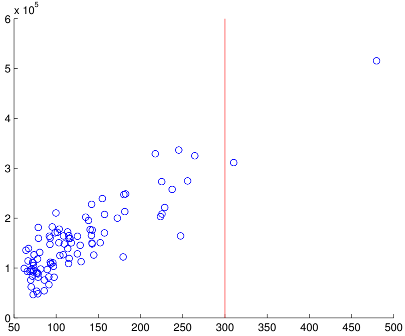

What is its price?

Nearest Neighbors

Nearest Neighbor: y^* is the same of the closest point to x^* in S.

$$y^* = 311,200$$

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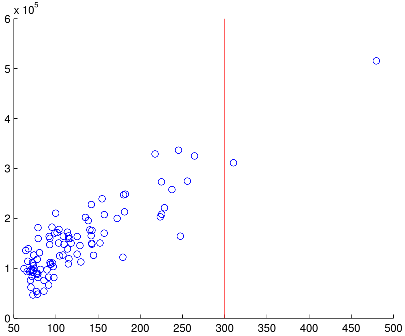

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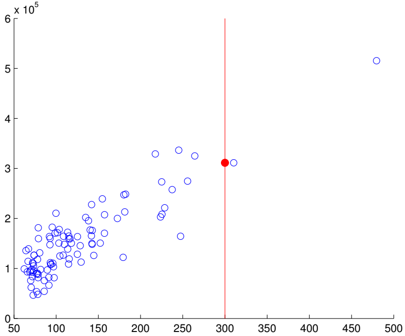

Nearest Neighbors

- $S = \{(x_i, y_i)\}_{i=1}^n$ with $x_i \in \mathbb{R}^D, y_i \in \mathbb{R}$
- x^* the new point $x^* \in \mathbb{R}^D$,
- y_{pred} the predicted output $y_{pred} = \hat{f}(x^*)$ where

$$f(x) = y_j \quad j = \arg \min_{i=1,\dots,n} \|x - x_i\|$$

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In general let $d : \mathbb{R}^D \times \mathbb{R}^D$ a distance on the input space, then

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Extensions

Nearest Neighbor takes y^* is the same of the closest point to x^* in S.

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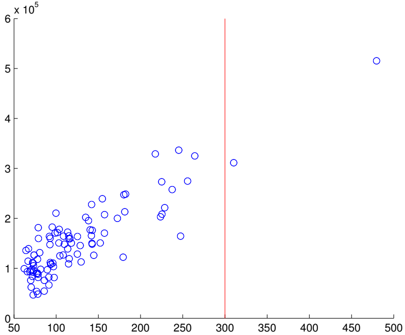

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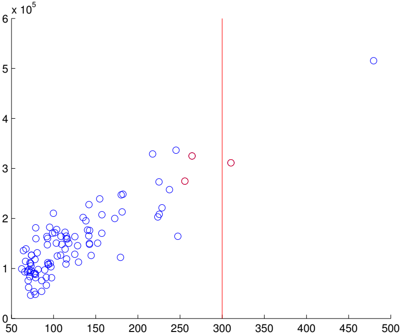

Can we do better? (for example using more points)

K-Nearest Neighbors

K-Nearest Neighbor: y^* is the mean of the values of the K closest point to x^* in S. If $K = 3$ we have

$$y^* = \frac{274,600 + 324,900 + 311,200}{3} = 303,600$$

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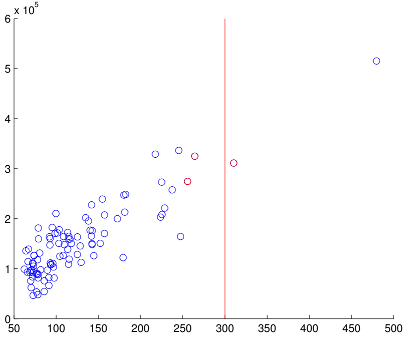

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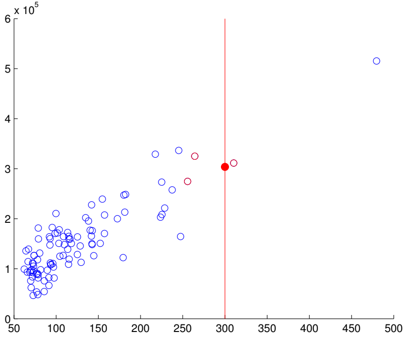

K-Nearest Neighbors

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- x^* the new point $x^* \in \mathbb{R}^D$,
- Let K be an integer $K << n$,
- $j_1, \ldots, j_K$ defined as $j_1 = \arg\min_{i \in \{1,\ldots,n\}} \|x - x_i\|$ and $j_t = \arg\min_{i \in \{1,\ldots,n\} \setminus \{j_1,\ldots,j_{t-1}\}} \|x - x_i\|$ for $t \in \{2, \ldots, K\}$,
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K-Nearest Neighbors (cont.)

$$f(x) = \frac{1}{K} \sum_{i=1}^{K} y_{j_i}$$

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K-Nearest Neighbors (cont.)

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- **General Metric** d f is the same, but $j_1, \ldots, j_K$ are defined as $j_1 = \arg\min_{i \in \{1,\ldots,n\}} d(x, x_i)$ and $j_t = \arg\min_{i \in \{1,\ldots,n\} \setminus \{j_1,\ldots,j_{t-1}\}} d(x, x_i)$ for $t \in \{2, \ldots, K\}$

Parzen Windows

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PARZEN WINDOWS:

$$\hat{f}(x) = \frac{\sum_{i=1}^{n} y_i k(x, x_i)}{\sum_{i=1}^{n} k(x, x_i)}$$

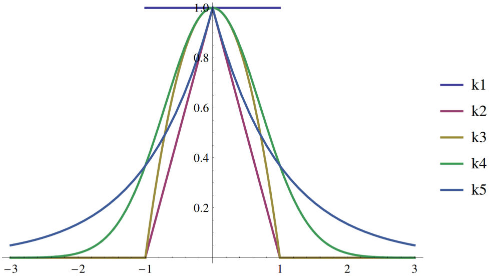
where k is a *similarity function*

- $k(x, x') \geq 0$ for all $x, x' \in \mathbb{R}^D$
- $k(x, x') \to 1$ when $\|x - x'\| \to 0$
- $k(x, x') \to 0$ when $\|x - x'\| \to \infty$

Parzen Windows

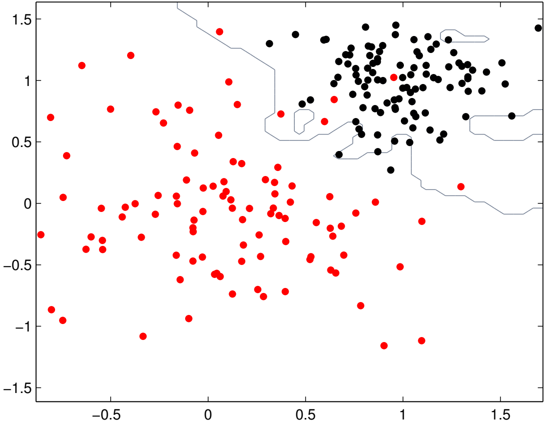
Examples of k

- $k_1(x,x') = \operatorname{sign}\left(1 - \frac{\|x-x'\|}{\sigma}\right)_+$ with a $\sigma > 0$
- $k_2(x,x') = \left(1 - \frac{\|x-x'\|}{\sigma}\right)_+$ with a $\sigma > 0$
- $k_3(x,x') = \left(1 - \frac{\|x-x'\|^2}{\sigma^2}\right)_+$ with a $\sigma > 0$
- $k_4(x,x') = e^{-\frac{\|x-x'\|^2}{2\sigma^2}}$ with a $\sigma > 0$
- $k_5(x,x') = e^{-\frac{\|x-x'\|}{\sigma}}$ with a $\sigma > 0$



K-NN example

K-Nearest neighbor depends on K.
When $K = 1$



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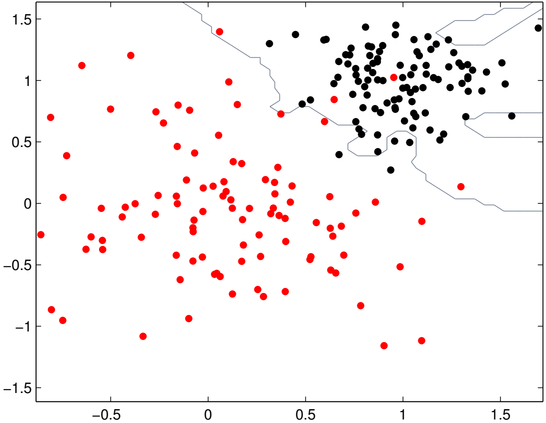
When $K = 2$



K-NN example

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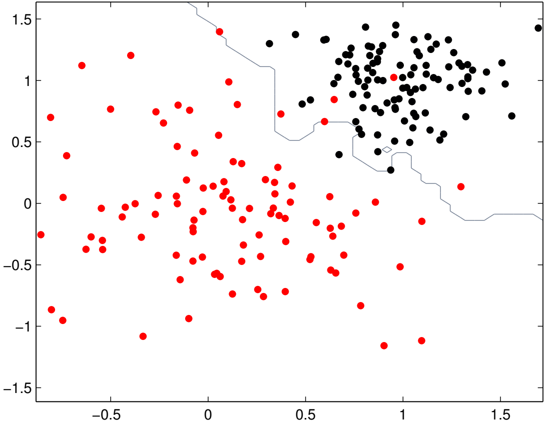
When $K = 3$



K-NN example

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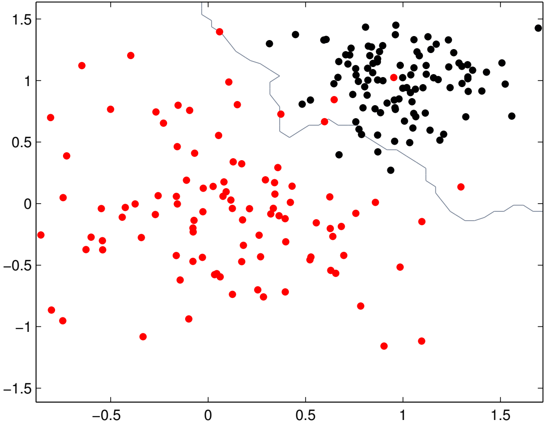
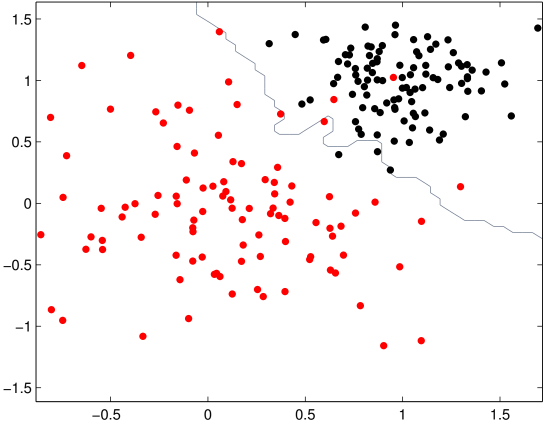
When $K = 4$



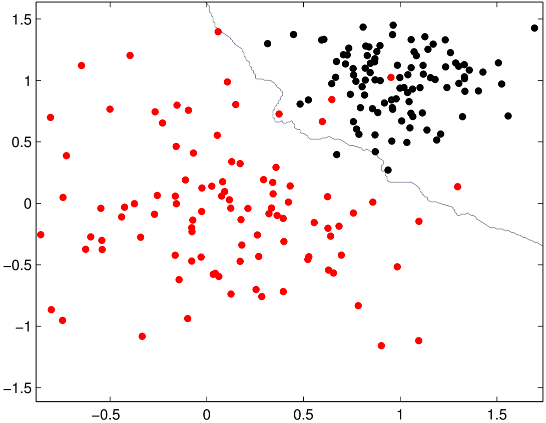
K-NN example

K-Nearest neighbor depends on K.
When $K = 5$



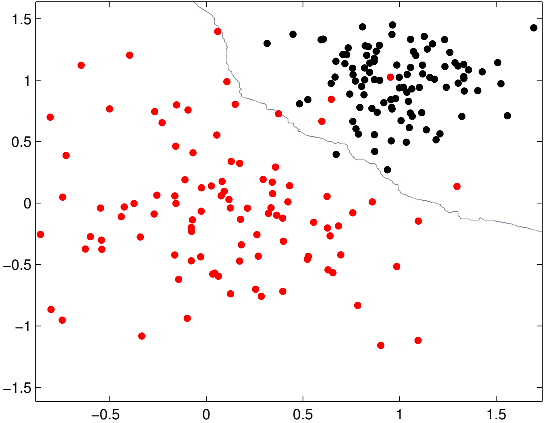
K-NN example

K-Nearest neighbor depends on K.
When $K = 9$



K-NN example

K-Nearest neighbor depends on K.
When $K = 15$



K-NN example

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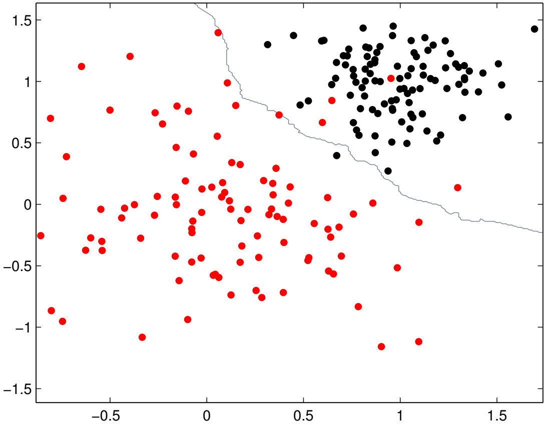

Changing K the result changes a lot! How to select K?

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Optimal choice for the Hyper-parameters

- $S = (x_i, y_i)_{i=1}^n$ training set. Name $Y = (y_1, \dots, y_n)$ and $X = (x_1^\top, \dots, x_n^\top)$.
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- $\hat{f}_{S,K}$ learned function (depends on S and K)

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Ideally! (In practice we don't have access to the distribution)

- We can still try to understand the above minimization problem: does a solution exists? What does it depend on?
- Yet, ultimately, we need something we can compute!

Example: regression problem

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that is

$$\mathcal{E}_K(x) = \mathbb{E}_S(f_*(x) - \hat{f}_{S,K}(x))^2 + \sigma^2$$

...

Bias Variance trade-off for K-NN

Define the *noisyless K-NN* (it is ideal!)

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Consider

$$\mathcal{E}_K(x) = \underbrace{(f_*(x) - \mathbb{E}_X \tilde{f}_{S,K}(x))^2}_{\text{bias}} + \underbrace{\mathbb{E}_S(\tilde{f}_{S,K}(x) - \hat{f}_{S,K}(x))^2 + \sigma^2}_{\text{variance}}$$

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Note that $\tilde{f}_{S,K}(x) = \mathbb{E}_{y|x} \hat{f}_{S,K}(x)$.
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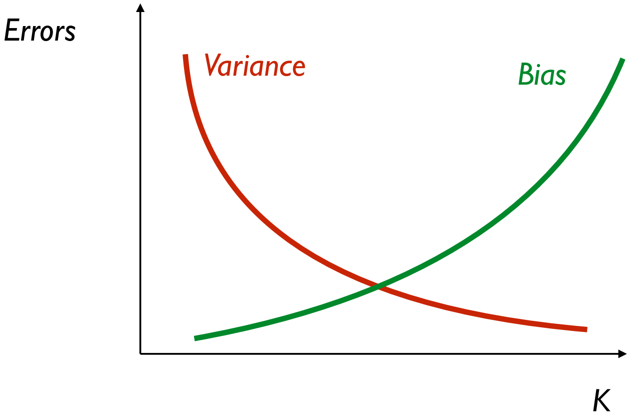
$$\mathcal{E}_K(x) = \underbrace{(f_*(x) - \mathbb{E}_X \tilde{f}_{S,K}(x))^2}_{\text{bias}} + \underbrace{\frac{\sigma^2}{K} + \sigma^2}_{\text{variance}}$$

...

Bias Variance trade-off



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How to choose K in practice?

- Idea: train on some data and validate the parameter on new unseen data as a proxy for the ideal case.

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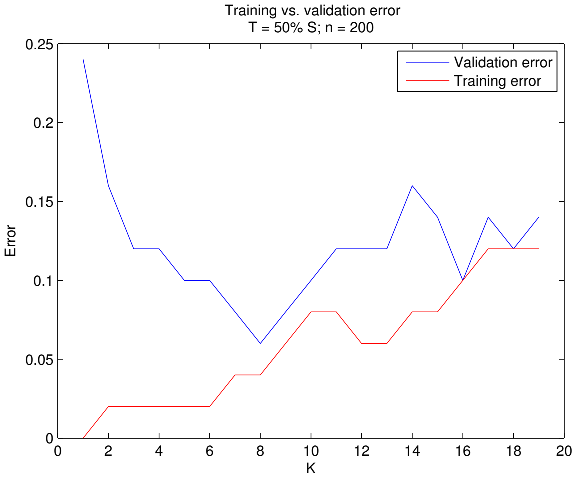
There are other related parameter selection methods (k-fold cross validation, leave-one out...).

Training and Validation Error behavior



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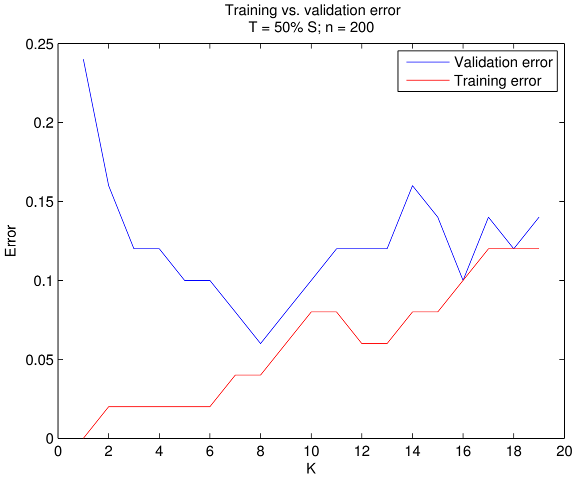

$\hat{K} = 8.$

Wrapping up

In this class we made our first encounter with learning algorithms (local methods) and the problem of tuning their parameters (via bias-variance trade-off and cross-validation) to avoid overfitting and achieve generalization.

Next Class

High Dimensions: Beyond local methods!