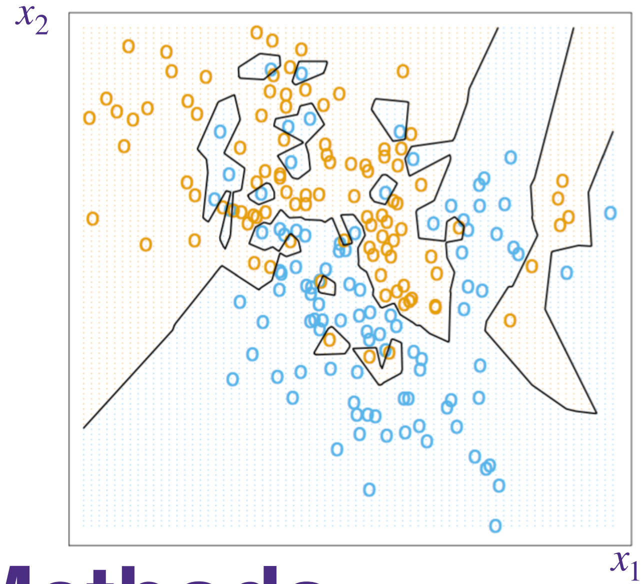
- Homework 3, due Saturday, February 26 midnight



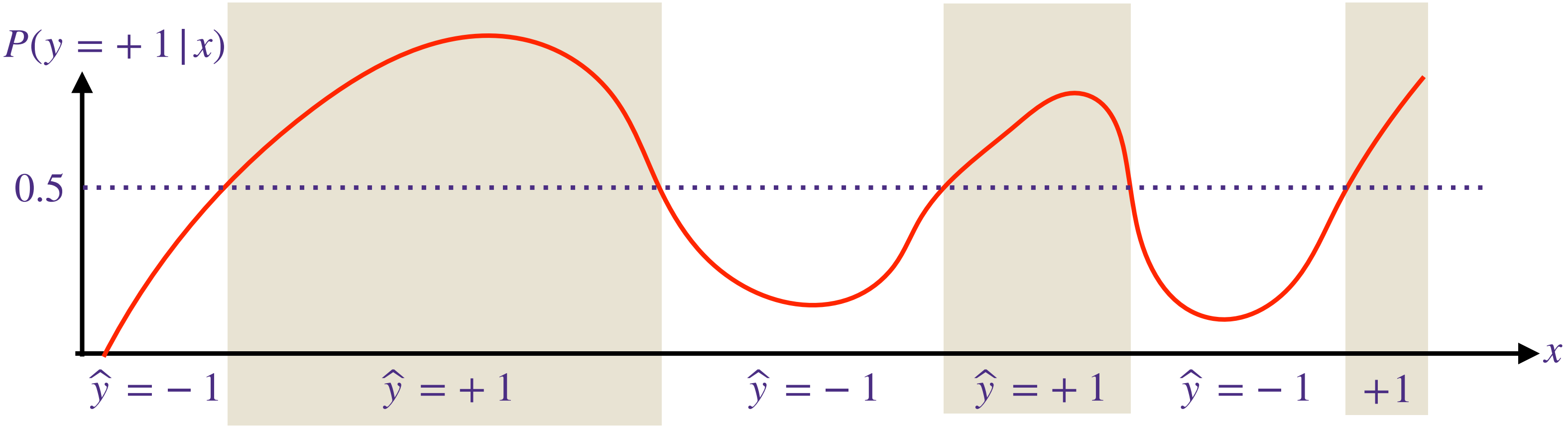
Lecture 21: Nearest Neighbor Methods

- Yet another non-linear model
    - Kernel method
    - Neural Network
    - Nearest Neighbor method
- A model is called “parametric” if the number of parameters do not depend on the number of samples
- A model is called “non-parametric” if the number of parameters increase with the number of samples

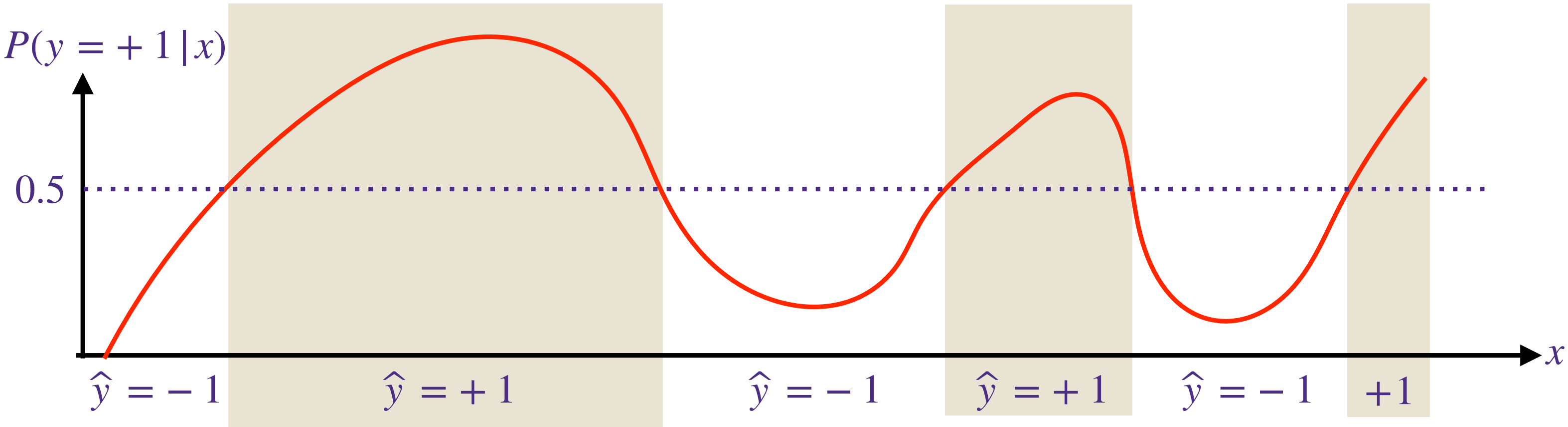
Recall Bayes optimal classifier

- Consider an example of binary classification on 1-dimensional $x \in \mathbb{R}$
- The problem is fully specified by the ground truths $P_{X,Y}(x, y)$
- Suppose for simplicity that $P_Y(y = +1) = P_Y(y = -1) = 1/2$
- Bayes optimal classifier minimizes the conditional error $P(\hat{y} \neq y \mid x)$ for every x, which can be written explicitly as

$$\hat{y} = \begin{cases} +1 & \text{if } P(+1 \mid x) > P(-1 \mid x) \\ -1 & \text{if } P(+1 \mid x) < P(-1 \mid x) \end{cases}$$



In practice we do not have $P(x, y)$

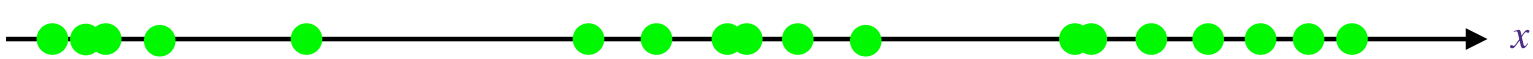


- Bayes optimal classifier $\hat{y} = \begin{cases} +1 \text{ if } P(+1 \mid x) > P(-1 \mid x) \\ -1 \text{ if } P(+1 \mid x) < P(-1 \mid x) \end{cases}$

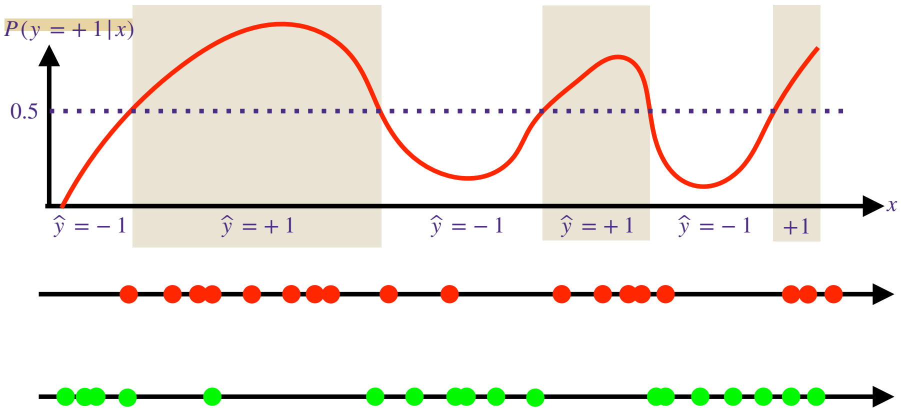
- How do we compare $P(y = +1 \mid x)$ and $P(y = -1 \mid x)$ from samples?

samples with $y = +1$

samples with $y = -1$



One way to approximate Bayes Classifier = local statistics



- Bayes optimal classifier

$$\hat{y} = \begin{cases} +1 & \text{if } P(+1\,|\,x) > P(-1\,|\,x) \\ -1 & \text{if } P(+1\,|\,x) < P(-1\,|\,x) \end{cases}$$

decision is based on $\dfrac{P(x, y=+1)}{P(x, y=-1)}$

- k-nearest neighbors classifier considers the k-nearest neighbors and takes a majority vote

$$\hat{y} = \begin{cases} +1, & \text{if (\# of +1 samples)} > \text{(\# of -1 samples)} \\ -1, & \text{if (\# of +1 samples)} < \text{(\# of -1 samples)} \end{cases}$$

- Decision is based on $\dfrac{\text{\# of +1 samples}}{\text{\# of -1 samples}}$

- Denote the n_r^+ as the number of samples within distance r from x with label $+1$, then

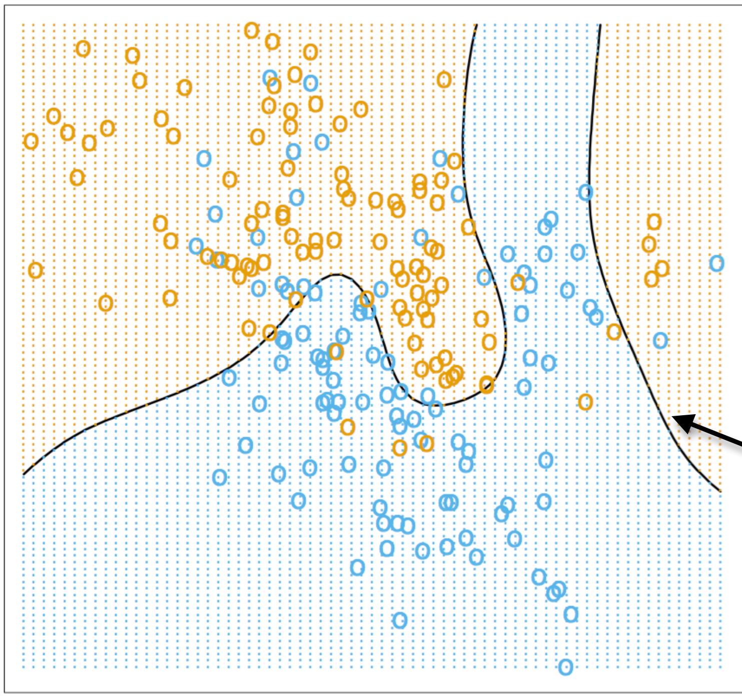
$$\frac{n_r^+}{n} \longrightarrow 2r \times P(x, y=+1)$$

  as we increase n and decrease r.

- If we take r to be the distance to the k-th neighbor from x, then

$$\frac{\text{\# of +1 samples}}{\text{\# of -1 samples}} \longrightarrow \frac{P(x, y=+1)}{P(x, y=-1)}$$

Some data, Bayes Classifier



Training data:

- True label: +1
- True label: -1

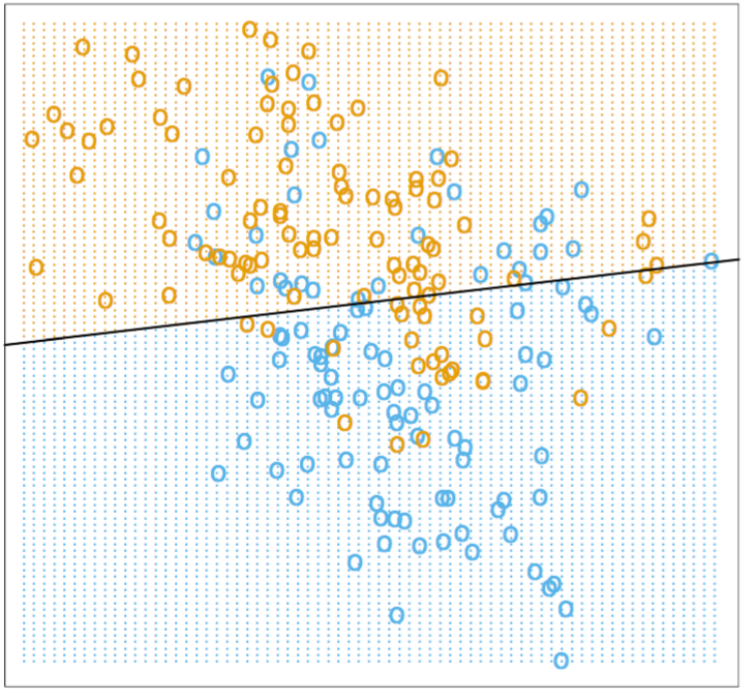
Optimal "Bayes" classifier:

$$\mathbb{P}(Y = 1 | X = x) = \frac{1}{2}$$

- Predicted label: +1
- Predicted label: -1

Figures from Hastie et al.

Linear Decision Boundary



Training data:

True label: +1

True label: -1

Learned:

Linear Decision boundary

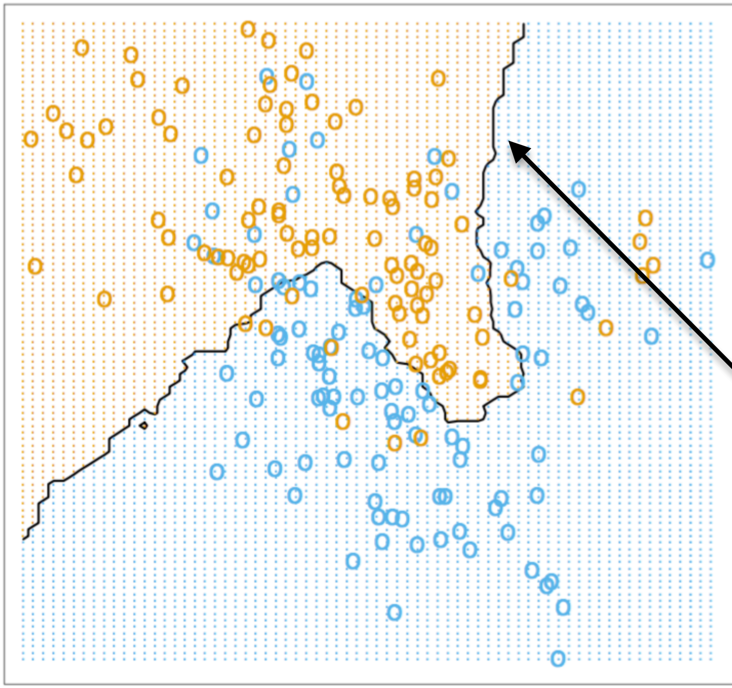
$$x^T w + b = 0$$

Predicted label: +1

Predicted label: -1

Figures from Hastie et al

k=15 Nearest Neighbor Boundary



Training data:

True label: +1

True label: -1

Learned:

15 nearest neighbor decision boundary (majority vote)

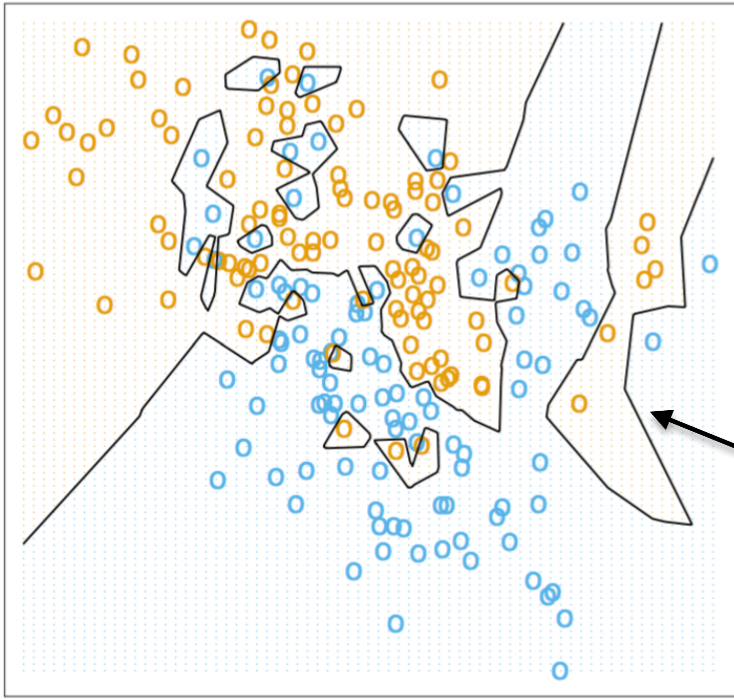
Predicted label: +1

Predicted label: -1

- Nearest neighbor gives non-linear decision boundaries
- What happens if we use a small k or a large k?

Figures from Hastie et al

k=1 Nearest Neighbor Boundary



Training data:

True label: +1

True label: -1

Learned:

1 nearest neighbor decision boundary (majority vote)

Predicted label: +1

Predicted label: -1

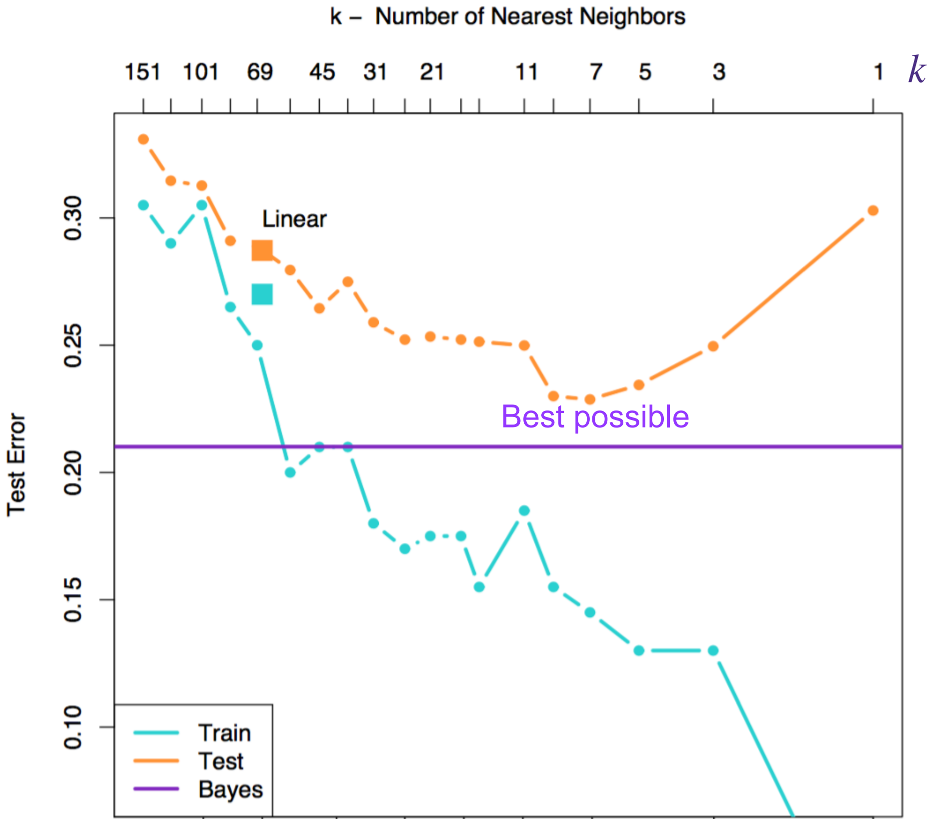
- With a small k, we tend to overfit.

Figures from Hastie et al

k-Nearest Neighbor Error

Model complexity low

Model complexity high



Bias-Variance tradeoff

As k->infinity?

Bias:

Variance:

As k->1?

Bias:

Variance:

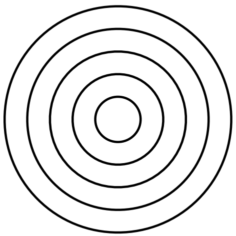
Figures from Hastie et al

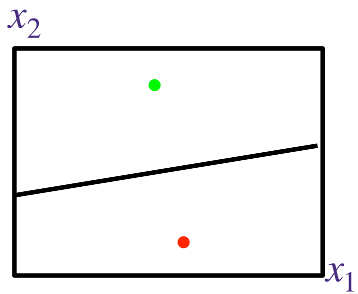
- The error achieved by Bayes optimal classifier provides a lower bound on what any estimator can achieve

Notable distance metrics (and their level sets)

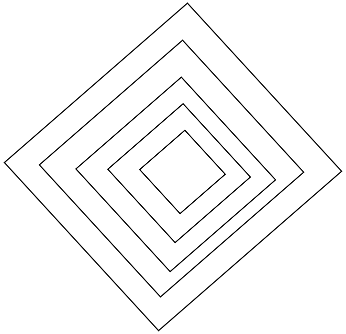
Consider 2 dimensional example with 2 data points with labels green, red,
and we show $k = 1$ nearest neighbor decision boundaries for various choices of distances

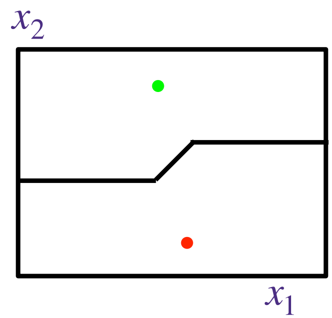
L$_2$ norm : $d(x, y) = \|x - y\|_2$

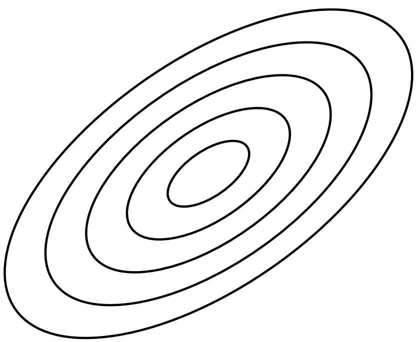


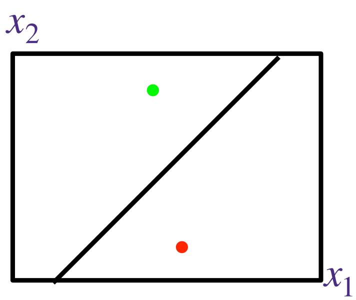


L$_1$ norm (taxi-cab)

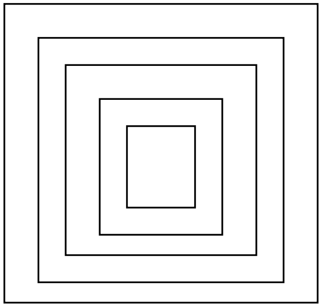


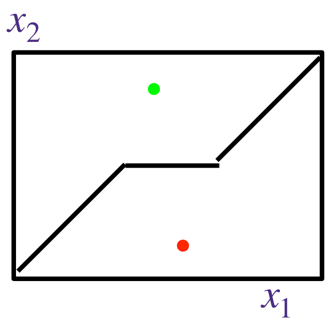






Mahalanobis norm: $d(x, y) = (x - y)^T M (x - y)$

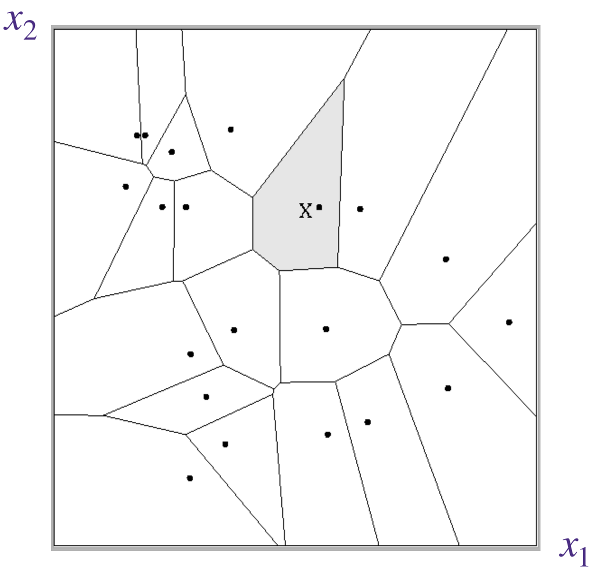


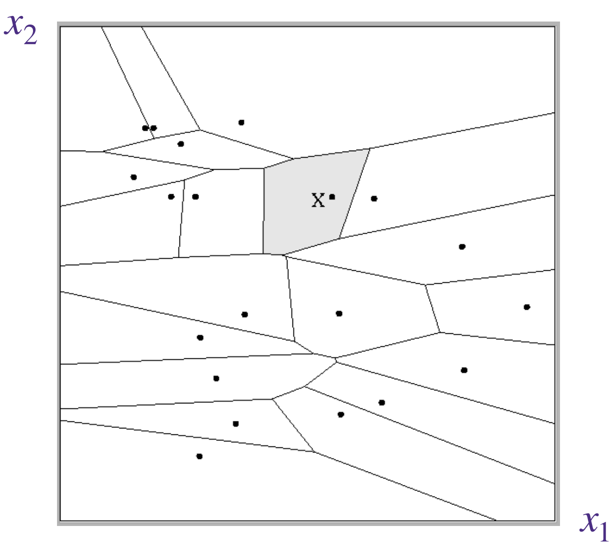


L-infinity *(max) norm*

$k = 1$ nearest neighbor

One can draw the nearest-neighbor regions in input space.





$Dist(\mathbf{x}^i,\mathbf{x}^j) = (x^i_1 - x^j_1)^2 + (x^i_2 - x^j_2)^2$ $\quad$ $Dist(\mathbf{x}^i,\mathbf{x}^j) = (x^i_1 - x^j_1)^2 + (3x^i_2 - 3x^j_2)^2$

The relative scalings in the distance metric affect region shapes

1 nearest neighbor guarantee - classification

$$\{(x_i, y_i)\}_{i=1}^n \qquad x_i \in \mathbb{R}^d, \quad y_i \in \{0,1\} \qquad (x_i, y_i) \overset{iid}{\sim} P_{XY}$$

Theorem[Cover, Hart, 1967] If P_X is supported everywhere in $\mathbb{R}^d$ and $P(Y = 1|X = x)$ is smooth everywhere, then as $n \to \infty$ the 1-NN classification rule has error at most twice the Bayes error rate.

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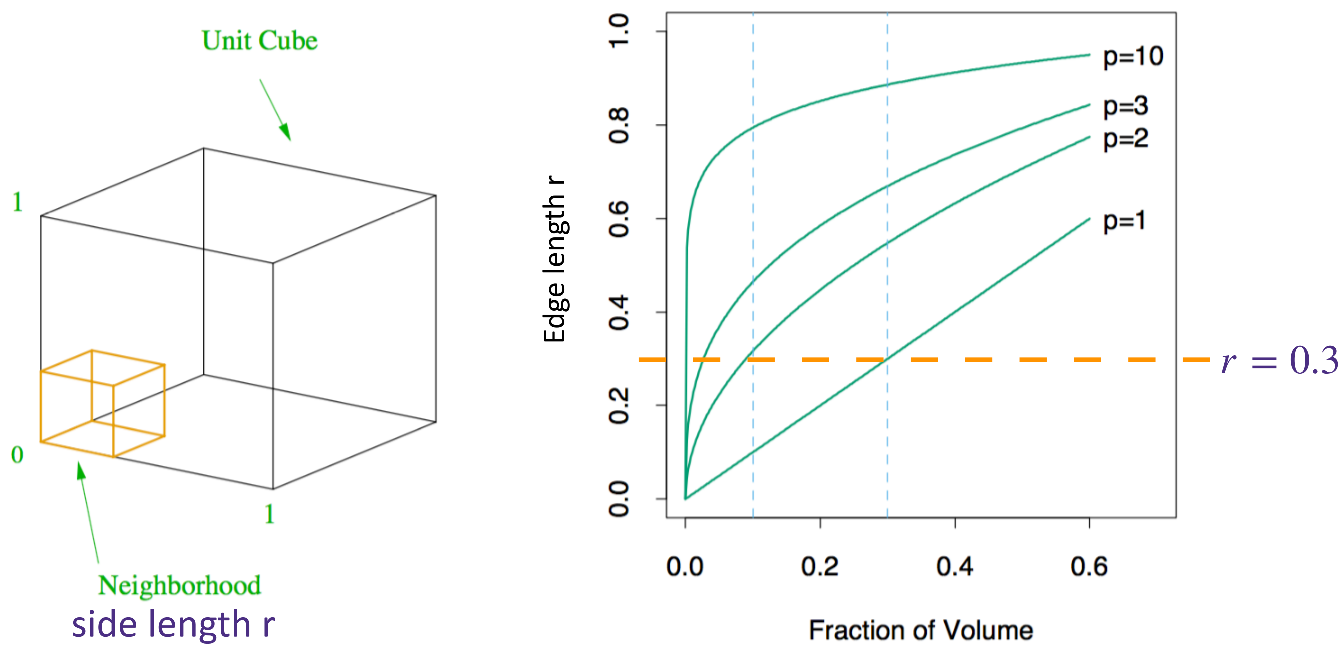
- Let x_{NN} denote the nearest neighbor at a point x
- First note that as $n \to \infty$, $P(y = +1 \,|\, x_{NN}) \to P(y = +1 \,|\, x)$
- Let $p^* = \min\{P(y = +1 \,|\, x), P(y = -1 \,|\, x)\}$denote the Bayes error rate
- At a point x,
  - Case 1: nearest neighbor is $+1$, which happens with $P(y = +1 \,|\, x)$ and the error rate is $P(y = -1 \,|\, x)$
  - Case 2: nearest neighbor is $+1$, which happens with $P(y = -1 \,|\, x)$ and the error rate is $P(y = +1 \,|\, x)$
- The average error of a 1-NN is

$$P(y = +1 \,|\, x)\, P(y = -1 \,|\, x) + P(y = -1 \,|\, x)\, P(y = +1 \,|\, x) \;= 2p^*(1 - p^*)$$

Curse of dimensionality Ex. 1

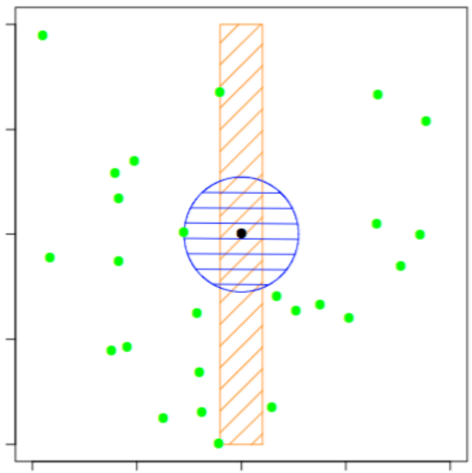


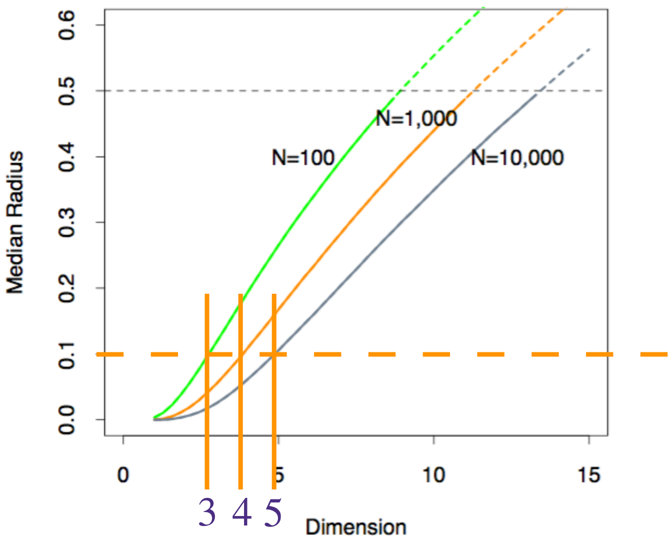
X is uniformly distributed over $[0,1]^p$. What is $\mathbb{P}(X \in [0,r]^p)$?

How many samples do we need so that a nearest neighbor is within a cube of side length r?

Curse of dimensionality Ex. 2

$$\{X_i\}_{i=1}^n \text{ are uniformly distributed over } [-.5, .5]^p.$$

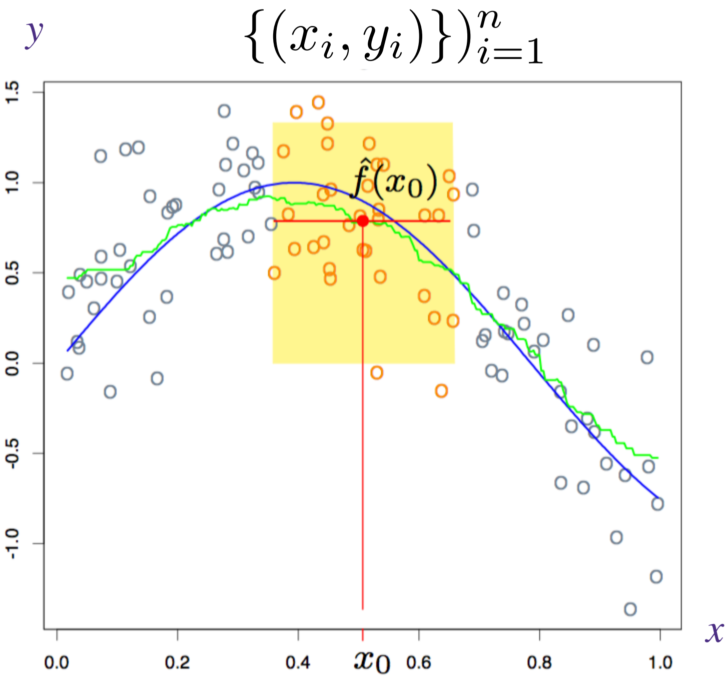




What is the median distance from a point at origin to its 1NN?

How many samples do we need so that a median Euclidean distance is within r?

Nearest neighbor regression



- What is the optimal classifier that minimizes MSE $\mathbb{E}[(\hat{y} - y)^2]$?

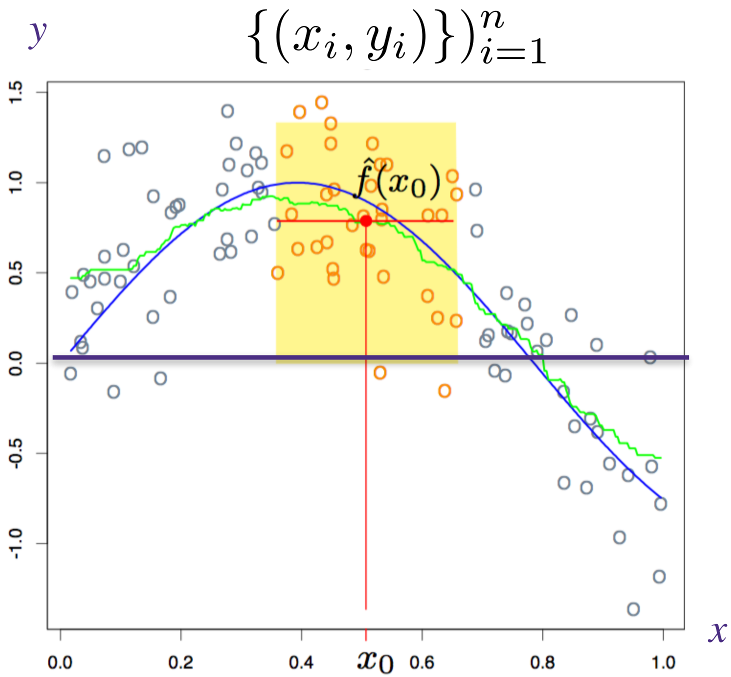
$$\hat{y} = \mathbb{E}[y \,|\, x]$$

- k-nearest neighbor regressor is

$$\hat{f}(x) = \frac{1}{k} \sum_{j \in \text{nearest neighbor}} y_j$$

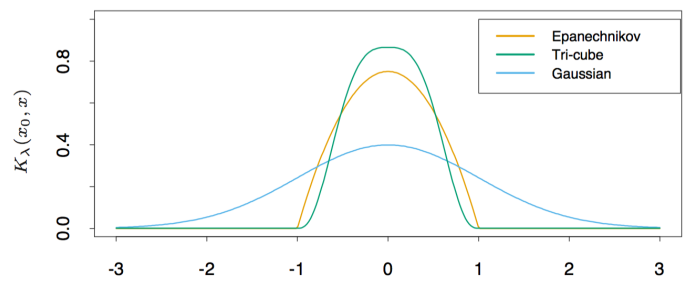
$$= \frac{\sum_{i=1}^n y_i \times \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}{\sum_{i=1}^n \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}$$

Nearest neighbor regression



In nearest neighbor methods, the "weight" changes abruptly

smoothing: $K(x,y)$

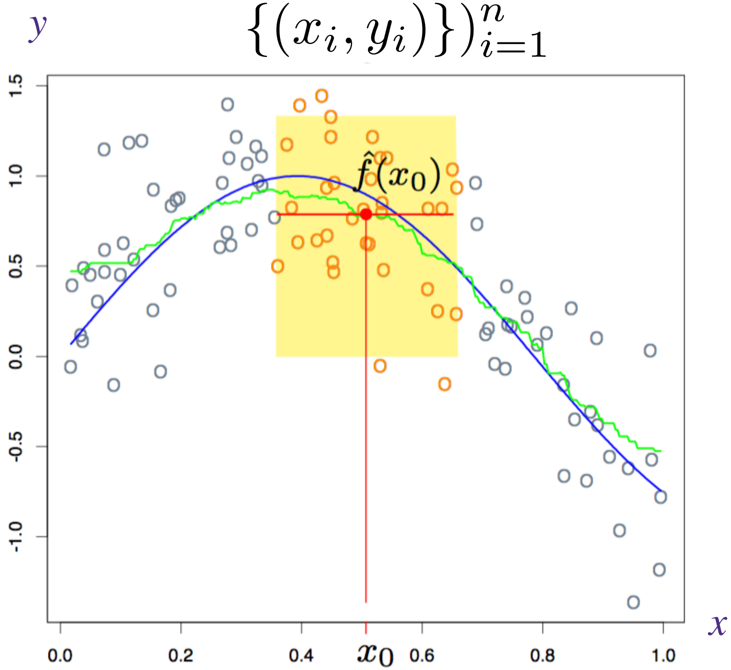


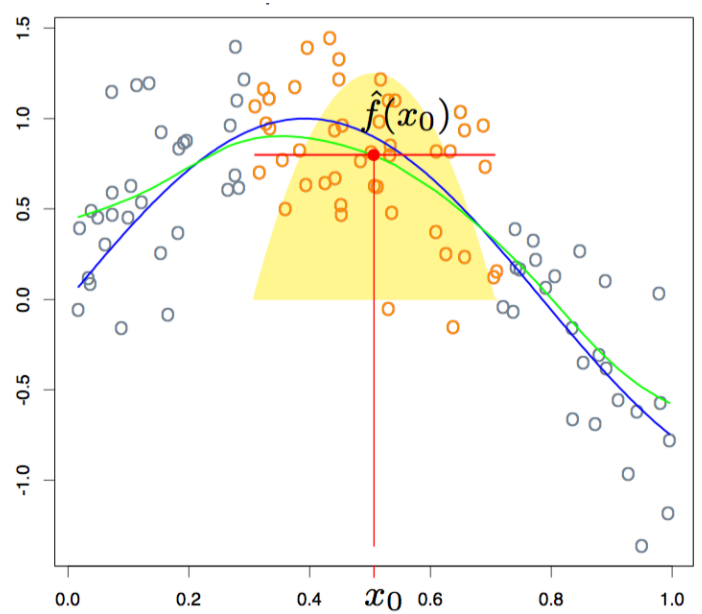
- k-nearest neighbor regressor is

$$\hat{f}(x_0) = \frac{\sum_{i=1}^n y_i \times \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}{\sum_{i=1}^n \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}$$

$$\widehat{f}(x_0) = \frac{\sum_{i=1}^n K(x_0, x_i) y_i}{\sum_{i=1}^n K(x_0, x_i)}$$

Nearest neighbor regression





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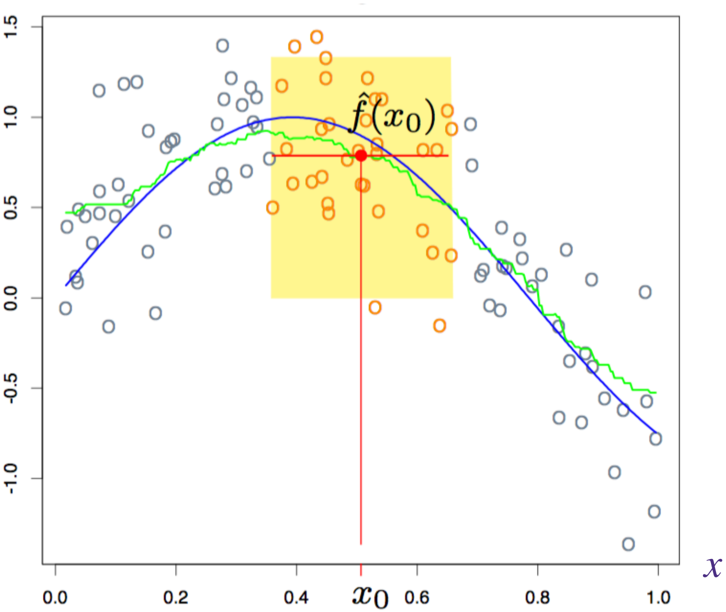
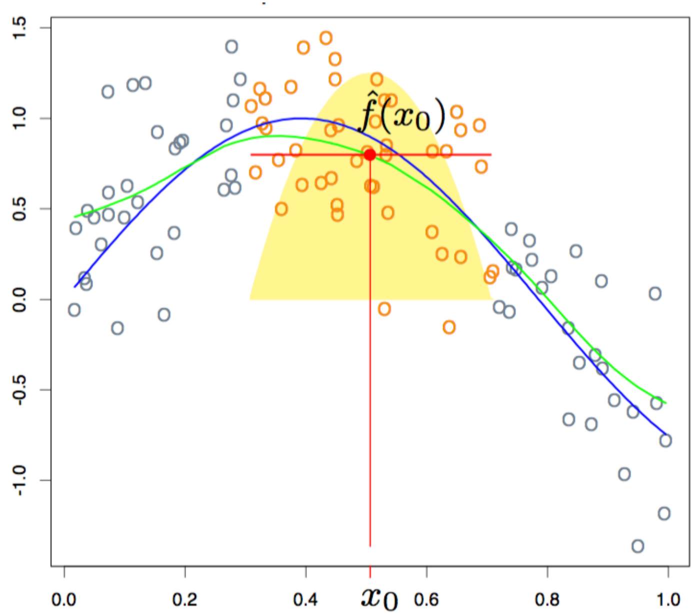
Nearest neighbor regression





Why just average them?

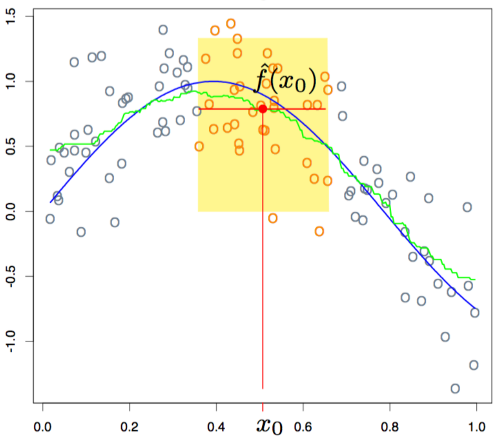
- k-nearest neighbor regressor is

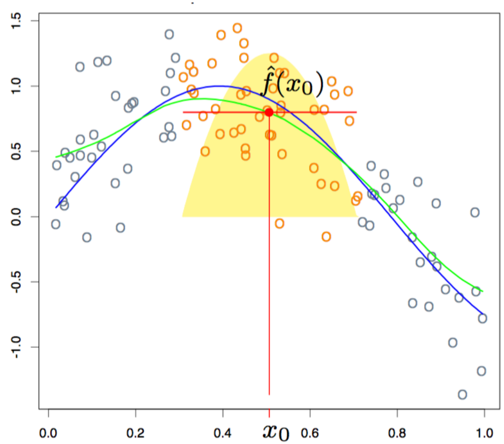
$$\hat{f}(x_0) = \frac{\sum_{i=1}^n y_i \times \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}{\sum_{i=1}^n \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}$$

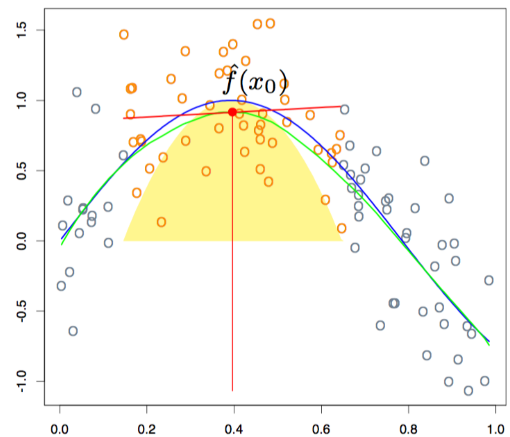
$$\widehat{f}(x_0) = \frac{\sum_{i=1}^n K(x_0, x_i) y_i}{\sum_{i=1}^n K(x_0, x_i)}$$

Nearest neighbor regression

$$\{(x_i, y_i)\}_{i=1}^n$$







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$$\hat{f}(x_0) = \frac{\sum_{i=1}^n y_i \times \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}{\sum_{i=1}^n \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}$$

$$\widehat{f}(x_0) = \frac{\sum_{i=1}^n K(x_0, x_i) y_i}{\sum_{i=1}^n K(x_0, x_i)}$$

$$\widehat{f}(x_0) = b(x_0) + w(x_0)^T x_0$$

$$w(x_0), b(x_0) = \arg\min_{w,b} \sum_{i=1}^n K(x_0, x_i)(y_i - (b + w^T x_i))^2$$

Local Linear Regression

Nearest Neighbor Overview

- Very simple to explain and implement
- No training! But finding nearest neighbors in large dataset at test can be computationally demanding (KD-trees help)
- You can use other forms of distance (not just Euclidean)
- Smoothing and local linear regression can improve performance (at the cost of higher variance)
- With a lot of data, “local methods” have strong, simple theoretical guarantees.
- Without a lot of data, neighborhoods aren’t “local” and methods suffer (curse of dimensionality).

Questions?