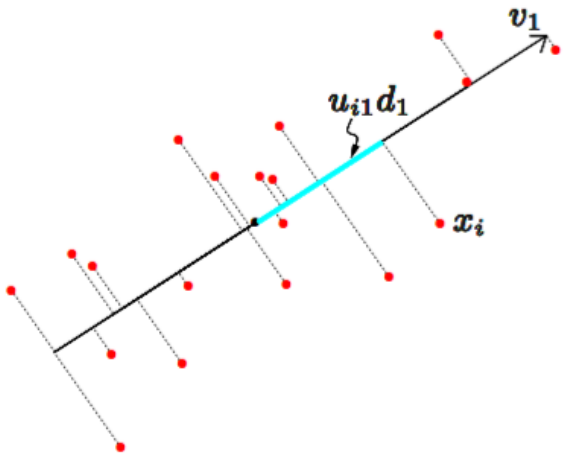
PCA: Efficient computation and some cool applications

PCA: a high-fidelity linear projection

Given $x_i \in \mathbb{R}^d$ and some $q < d$ consider

$$\min_{\mathbf{V}_q} \sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||^2.$$



where $\mathbf{V}_q = [v_1, v_2, \ldots, v_q]$ is orthonormal:

$$\mathbf{V}_q^T \mathbf{V}_q = I_q$$

$\mathbf{V}_q$ are the first q eigenvectors of Σ

$\mathbf{V}_q$ are the first q *principal components*

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$$

Principal Component Analysis (PCA) projects $(\mathbf{X} - \mathbf{1}\bar{x}^T)$ down onto $\mathbf{V}_q$

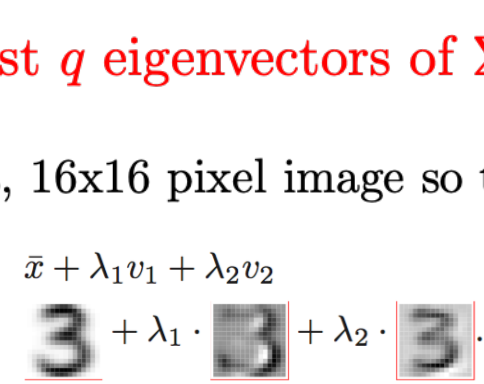
$$(\mathbf{X} - \mathbf{1}\bar{x}^T)\mathbf{V}_q = \mathbf{U}_q \mathrm{diag}(d_1, \ldots, d_q) \qquad \mathbf{U}_q^T \mathbf{U}_q = I_q$$

PCA on MNIST

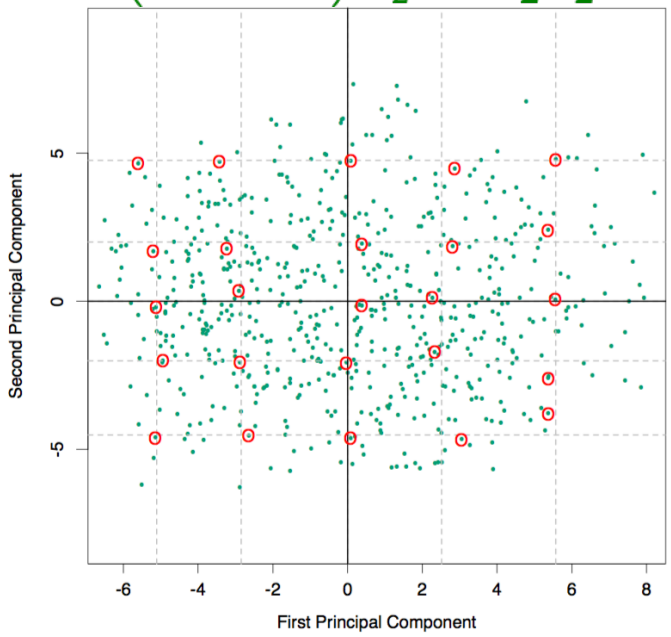
$\mathbf{V}_q$ are the first q eigenvectors of Σ and SVD $\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T$

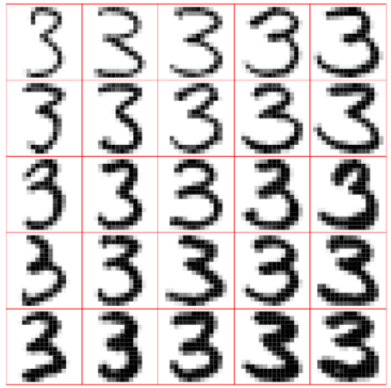
Handwritten 3's, 16x16 pixel image so that $x_i \in \mathbb{R}^{256}$

$$\begin{aligned} \hat{f}(\lambda) &= \bar{x} + \lambda_1 v_1 + \lambda_2 v_2 \\ &= \bar{x} + \lambda_1 \cdot \quad + \lambda_2 \cdot \quad . \end{aligned}$$



$$(\mathbf{X} - \mathbf{1}\bar{x}^T)\mathbf{V}_2 = \mathbf{U}_2\mathbf{S}_2 \in \mathbb{R}^{n \times 2}$$





$\mathbf{diag(S)}$

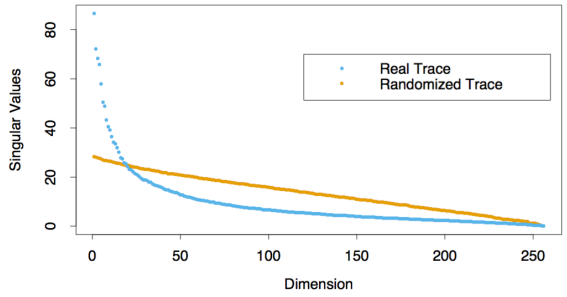
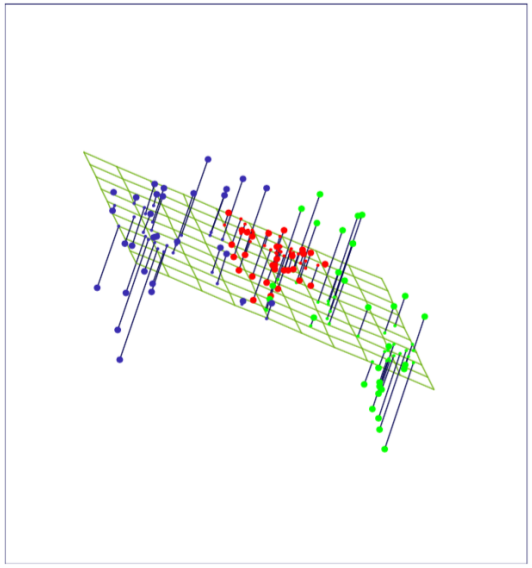


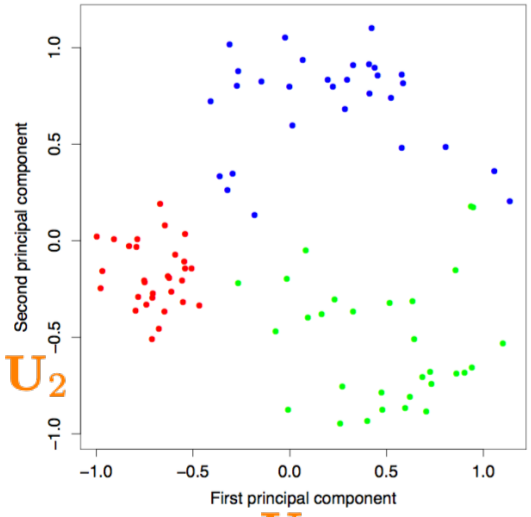
FIGURE 14.24. *The 256 singular values for the digitized threes, compared to those for a randomized version of the data (each column of* $\mathbf{X}$ *was scrambled).*

SVD and PCA

$\mathbf{V}_q$ are the first q eigenvectors of Σ and SVD $\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{USV}^T$



$\mathbf{X} - \mathbf{1}\bar{x}^T$



$\mathbf{U}_2$

$\mathbf{U}_1$

How do we compute the principal components?

1. Power iteration
2. **Solving for a singular value decomposition (SVD)**

Singular Value Decomposition (SVD)

Theorem (SVD): Let $\mathbf{A} \in \mathbb{R}^{m \times n}$ with rank $r \leq \min\{m, n\}$. Then $\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^T$ where $\mathbf{S} \in \mathbb{R}^{r \times r}$ is diagonal with positive entries, $\mathbf{U}^T\mathbf{U} = I$, $\mathbf{V}^T\mathbf{V} = I$.

$$\mathbf{A}^T\mathbf{A}v_i =$$

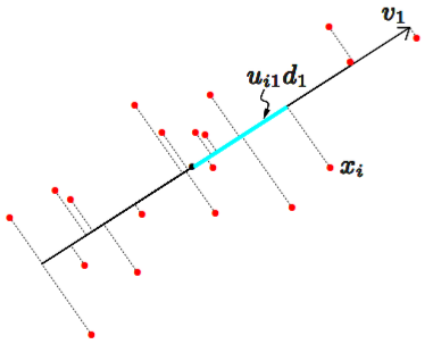
$$\mathbf{A}\mathbf{A}^T u_i =$$

How do we compute the principal components?

1. **Power iteration**
2. Solving for a singular value decomposition (SVD)

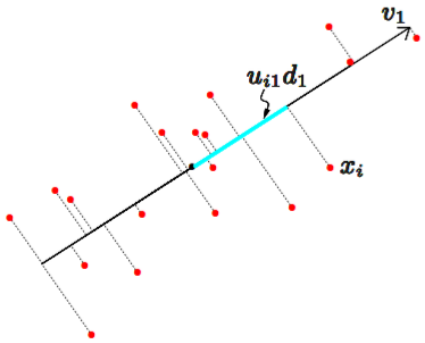
Power method - one vector at a time

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T \qquad v_* = \arg\max_{v} \; v^T \Sigma v$$



Power method - one vector found iteratively

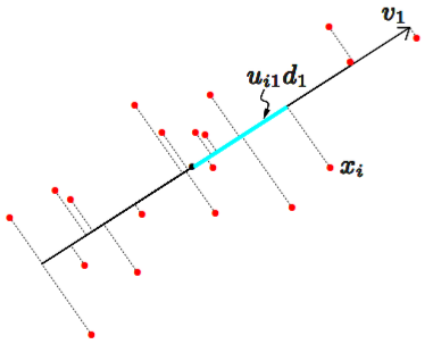
$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T \qquad v_* = \arg\max_{v} v^T \Sigma v$$



$$z_0 \sim \mathcal{N}(0, I) \qquad \text{Iterate:} \quad z_{t+1} = \frac{\Sigma z_t}{\|\Sigma z_t\|_2}$$

Power method - one vector found iteratively

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T \qquad v_* = \arg\max_{v} v^T \Sigma v$$

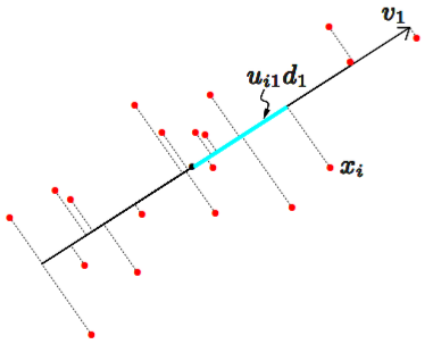


$$z_0 \sim \mathcal{N}(0, I) \qquad \text{Iterate:} \quad z_{t+1} = \frac{\Sigma z_t}{\|\Sigma z_t\|_2}$$

To analyze write: $\Sigma = \mathbf{V}\mathbf{D}\mathbf{V}^T \qquad z_t =: \mathbf{V}\alpha_t$

Power method - analysis

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T \qquad v_* = \arg\max_{v} v^T \Sigma v$$



$z_0 \sim \mathcal{N}(0, I)$ Iterate: $z_{t+1} = \dfrac{\Sigma z_t}{\|\Sigma z_t\|_2}$

To analyze write: $\Sigma = \mathbf{V}\mathbf{D}\mathbf{V}^T \qquad z_t =: \mathbf{V}\alpha_t$

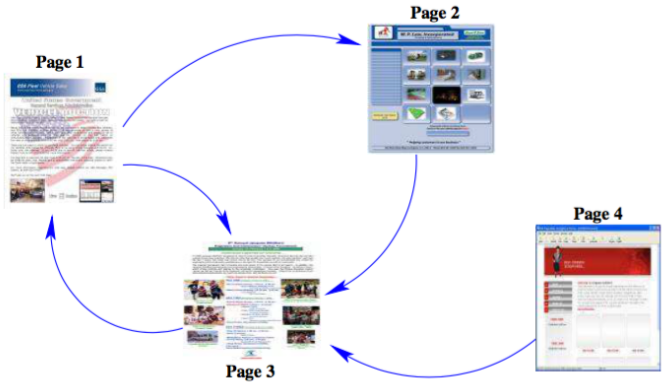
$$\alpha_{t+1} = \mathbf{V}^T z_{t+1} = \frac{\mathbf{V}^T \Sigma z_t}{\|\Sigma z_t\|} = \frac{\mathbf{D}\alpha_t}{\|\mathbf{D}\alpha_t\|} = \frac{\mathbf{D}^2\alpha_{t-1}}{\|\mathbf{D}^2\alpha_{t-1}\|} = \frac{\mathbf{D}^t\alpha_0}{\|\mathbf{D}^t\alpha_0\|}$$

$$\mathbf{D}^t = (\mathbf{D}_{1,1})^t(\mathbf{D}/\mathbf{D}_{1,1})^t \to (\mathbf{D}_{1,1})^t \mathbf{e}_1\mathbf{e}_1^T \text{ since } \mathbf{D}_{i,i}/\mathbf{D}_{1,1} < 1$$

Markov chains - PageRank

$$L_{i,j} = \mathbf{1}\{\text{page } j \text{ points to page } i\}$$

$$\mathbf{L} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$



Google PageRank of page i:

$$p_i = (1-\lambda) + \lambda \sum_{j=1}^{n} \frac{L_{i,j}}{c_j} p_j$$

$$c_j = \sum_{k=1}^{n} L_{j,k}$$

Markov chains - PageRank

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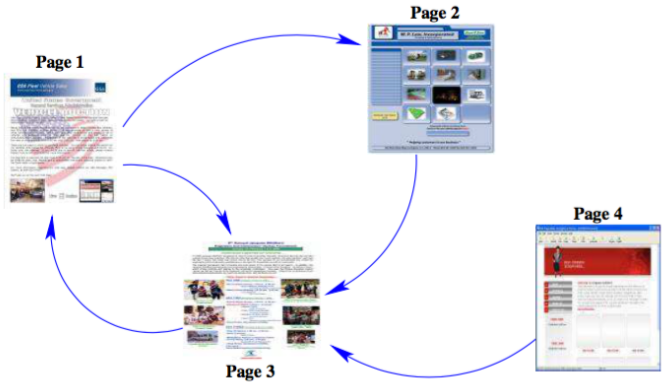

Google PageRank of pages given by:

$$\mathbf{p} = (1-\lambda)\mathbf{1} + \lambda \mathbf{L}\mathbf{D}_c^{-1}\mathbf{p}$$

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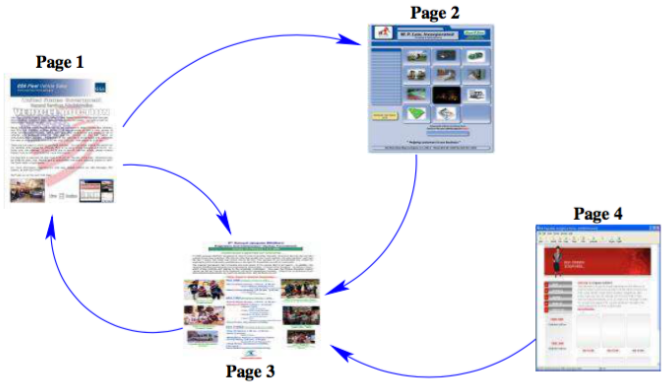


Google PageRank of pages given by:

$$\mathbf{p} = (1-\lambda)\mathbf{1} + \lambda \mathbf{L}\mathbf{D}_c^{-1}\mathbf{p}$$

Set arbitrary normalization: $\mathbf{1}^T\mathbf{p} = n$ so that

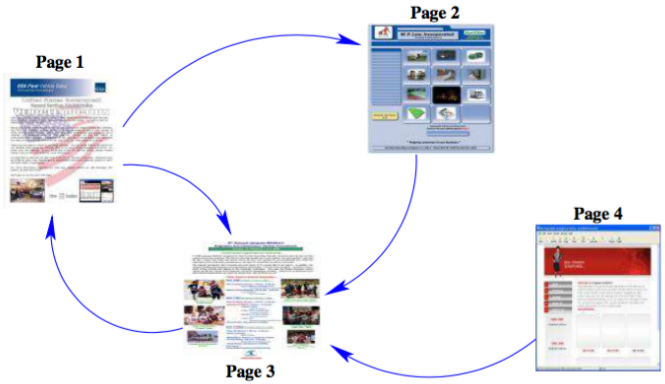
$$\mathbf{p} = \left((1-\lambda)\mathbf{1}\mathbf{1}^T/n + \lambda \mathbf{L}\mathbf{D}_c^{-1}\right)\mathbf{p}$$

$$=: \mathbf{A}\mathbf{p}$$

Markov chains - PageRank

$$L_{i,j} = \mathbf{1}\{\text{page } j \text{ points to page } i\}$$

$$\mathbf{L} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$



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Set arbitrary normalization: $\mathbf{1}^T\mathbf{p} = n$ so that

$$\begin{aligned} \mathbf{p} &= \left((1-\lambda)\mathbf{1}\mathbf{1}^T/n + \lambda \mathbf{L}\mathbf{D}_c^{-1}\right)\mathbf{p} \\ &=: \mathbf{A}\mathbf{p} \end{aligned}$$

$\mathbf{p}$ is an eigenvector of $\mathbf{A}$ with eigenvalue 1! And by the properties stochastic matrices, it corresponds to the *largest* eigenvalue

Markov chains - PageRank

$$L_{i,j} = \mathbf{1}\{\text{page } j \text{ points to page } i\}$$

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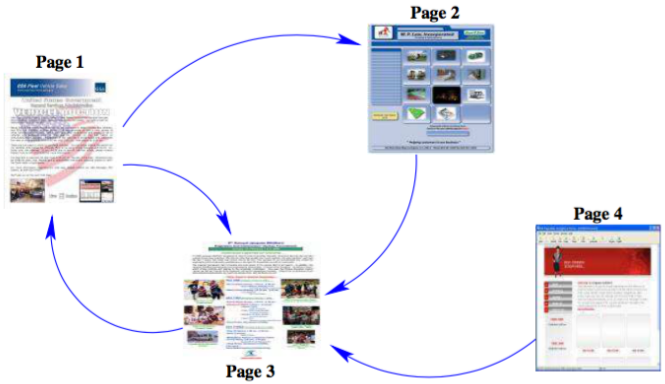

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$$=: \mathbf{A}\mathbf{p}$$

$\mathbf{p}$ is an eigenvector of $\mathbf{A}$ with eigenvalue 1! And by the properties stochastic matrices, it corresponds to the *largest* eigenvalue

Solve using power method: $\mathbf{p}_{k+1} = \dfrac{\mathbf{A}\mathbf{p}_k}{\mathbf{1}^T\mathbf{A}\mathbf{p}_k/n}$ $\mathbf{p}_0 \sim \text{uniform}([0,1]^n)$

PCA and SVD take-aways

PCA finds a d-dimensional representation with:

- Highest variance in any d-dimensional space
- Lowest reconstruction error
- spanned by the top d eigenvectors of covariance matrix

How to find the top d eigenvectors?

- SVD: $(X - I\,\mu) := A = U\,S\,V^T$
  - **V are the eigenvectors of A^TA**
  - U are the eigenvectors of AA^T
- Power method

This is one way to represent data in lower dimensions: there are others with other properties

- E.g., that approximately maintain pairwise distances

Miscellaneous fun stuff!

AKA choose your own adventure

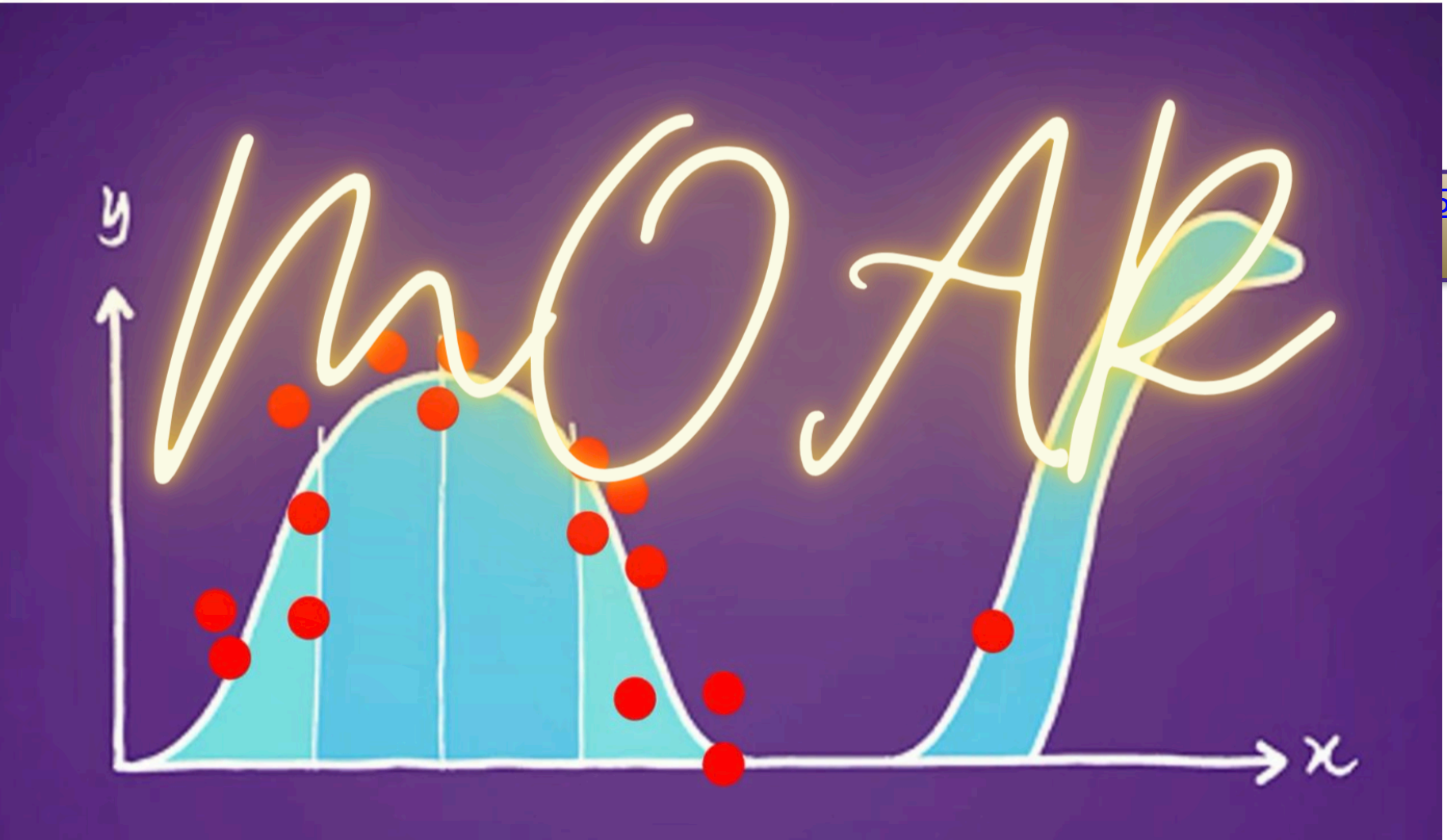
What's next?

Theory + Practice

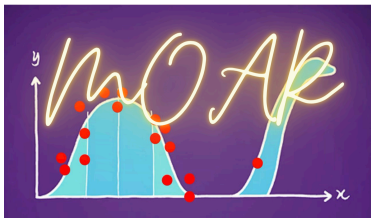
Theory

Practice

- What if our data is not IID?



What's next?



Theory + Practice

Theory

Practice

- What if our data is not IID?
  - If the shift is **in response to our learning**
    - Manipulating that change

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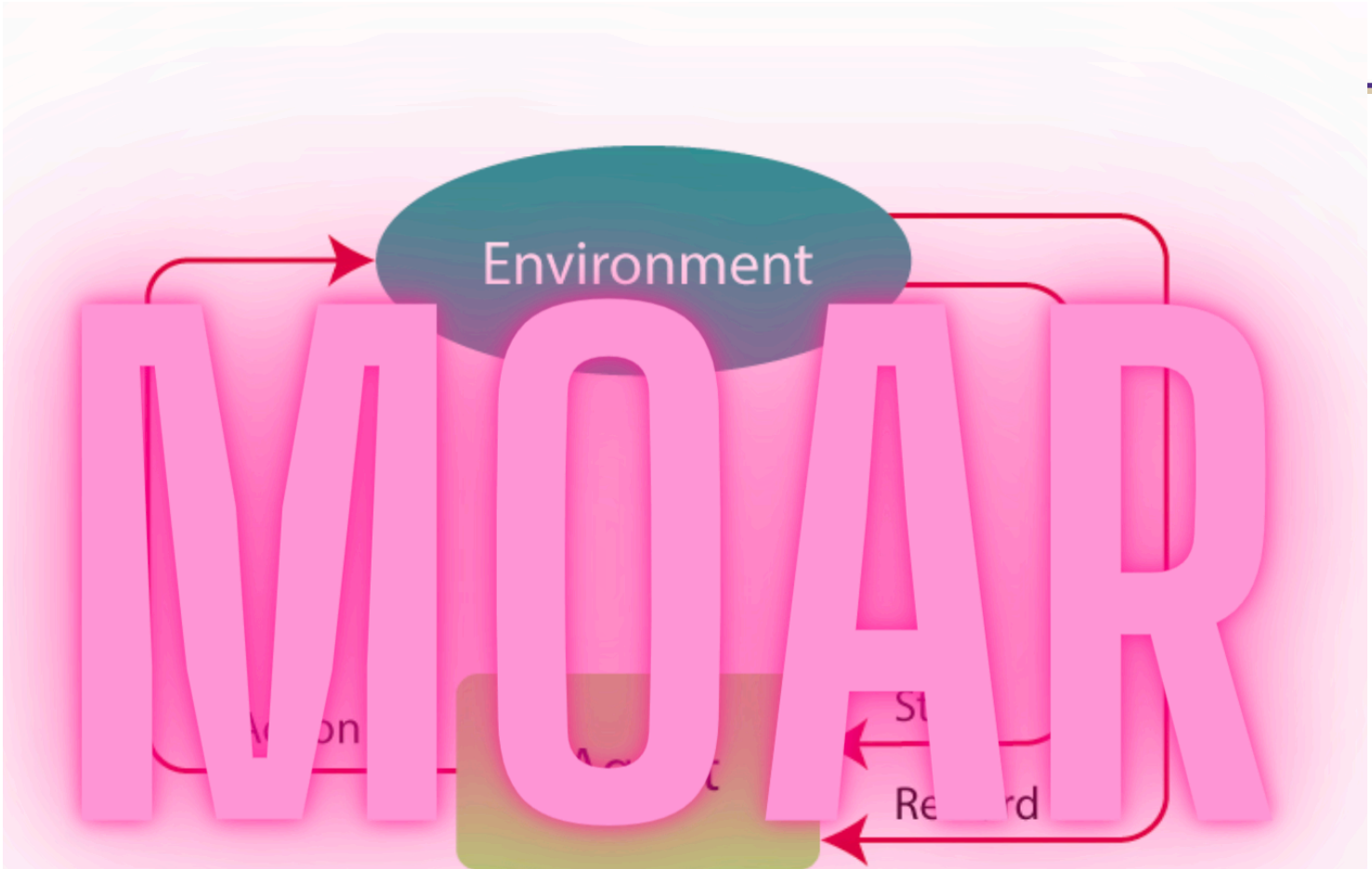
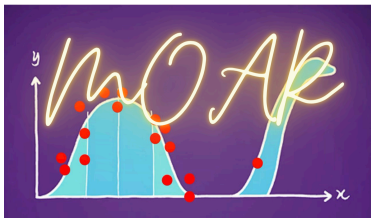


What's next?



Theory + Practice

Theory

Practice

- What if our data is not IID?
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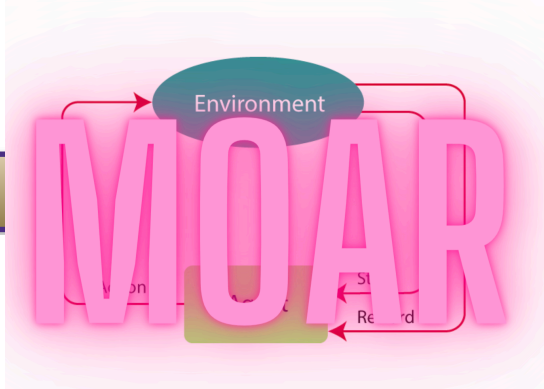
    - Manipulating that change

Reinforcement Learning (CSE542)



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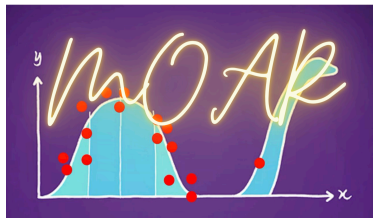
What's next?

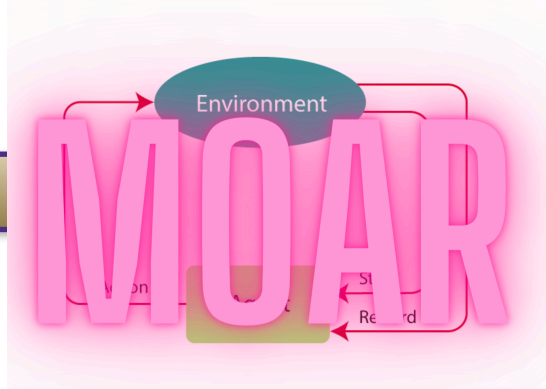


Theory + Practice

Theory

Practice

- What if our data is not IID?
  - If the shift is **in response to our learning**
    - Manipulating that change



Reinforcement Learning (CSE542)

Robotics (CSE478, CSE 571, …)

…5),

  - Be robust to those change

Interactive learning (CSE541), Online learnin

Adversarial robustness

  - If the shift is **independent of our learning**

Repeated retraining,

distributionally robust optimization, ….

What's next?

Theory + Practice

Theory

Practice

- What if I care about understanding text?

  Natural Language Processing (CSE447, 517)

  Linguistics

  Large language models

- What if I care about understanding images/video?

  Graphics (CSE457, CSE557)

  Computer Vision (CSE455, CSE576)

What's next?

Theory + Practice

Theory

Practice

- What if I loved neural networks and I need moooooooaaaaar?

Deep Learning (CSE 490, CSE543)

Natural Language Processing (CSE447, 517)

Computer Vision (CSE455, CSE576)

What's next?

Theory + Practice

Theory

Practice

- What if I loved proofs and talking about convergence and I need moooooooaaaaar?

EE 511, STAT 527, STAT 535, STAT 538,
STAT 539, CSE 541, CSE 515, Advanced Machine Learning, Optimization, …

Graphical models! (CSE 515), taught by me this fall!

What's next?

Theory + Practice

Theory

Practice

- What if I want to know about practical advice for data collection/ data cleaning + preprocessing?

  CSE 547

- What if I want to know about possible real-world impact of these design choices?

  Fairness in ML (taught intermittently)

- What if I want to know more about structured learning / origin stories of ML?

  CSE 415, 473, 573, 574

What's next?

Theory + Practice

Theory

Practice

- What if I want to know about generating data?

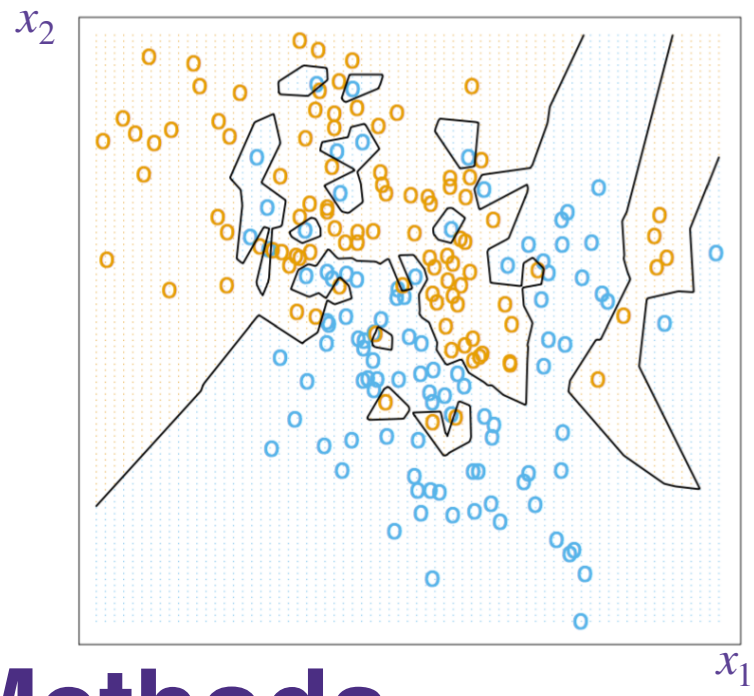
  GANS

  LLMS

- What if I care about biology/health?

  CSE427, 428, 487, 488, 527, 528, 529

Nonparametric models for classification



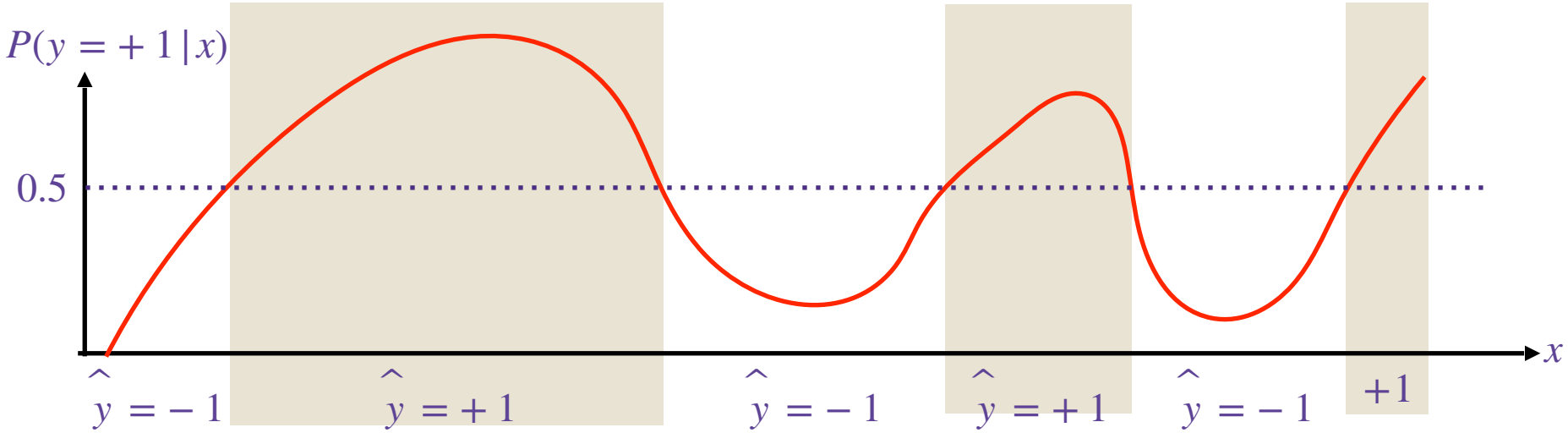
Nearest Neighbor Methods

- 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

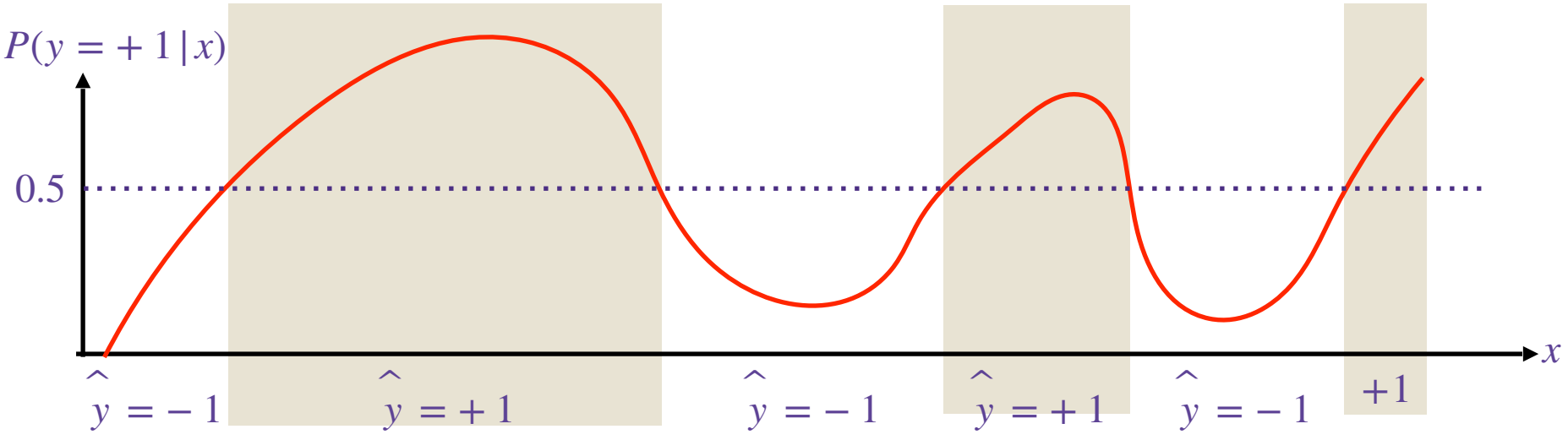
Recall Bayes optimal classifier

- 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 $P(\hat{y} \neq y \,|\, x)$ for every x, which can be written explicitly as

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



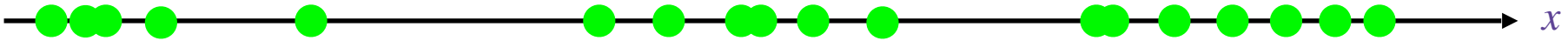
In practice we do not have $P(x, y)$



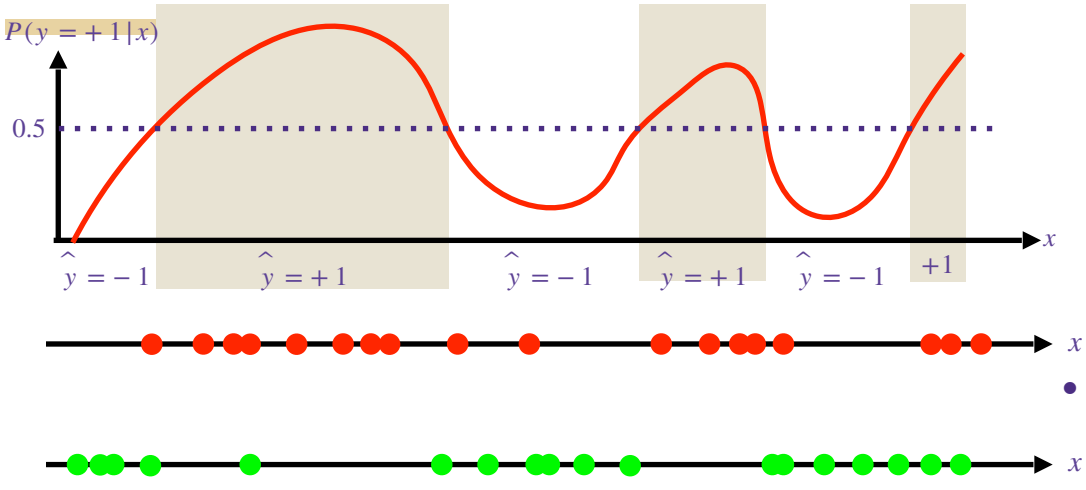
- Bayes optimal classifier $\hat{y} = \begin{matrix} +1 \text{ if } P(+1 \mid x) > P(-1 \mid x) \\ -1 \text{ if } P(+1 \mid x) < P(-1 \mid x) \end{matrix}$
- How do we compare $P(y = +1 \mid x)$ and $P(y = -1 \mid x)$ from samples?

samples with $y = +1$

samples with $y = -1$



One way to approximate Bayes Classifier = local statistics



- Bayes optimal classifier

$$\hat{y} = +1 \text{if} P(+1|x) > P(-1|x)$$
$$-1 \text{if} P(+1|x) < P(-1|x)$$

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

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

- 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

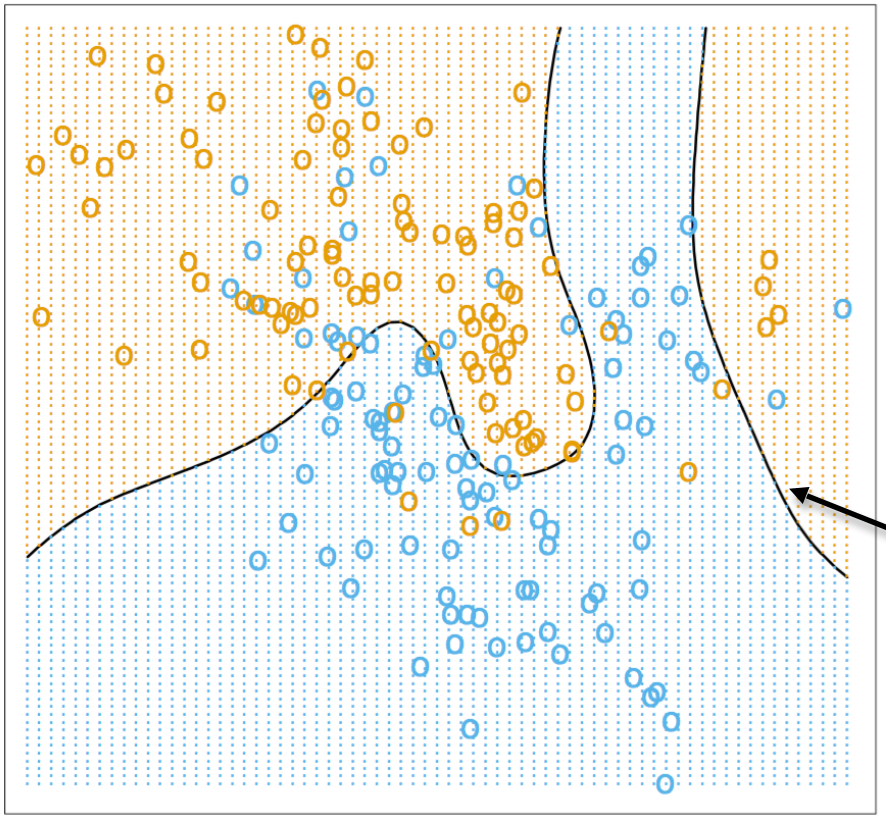
$$\frac{n_r^+}{n} \longrightarrow 2r \times P(x, y=+1)$$

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:

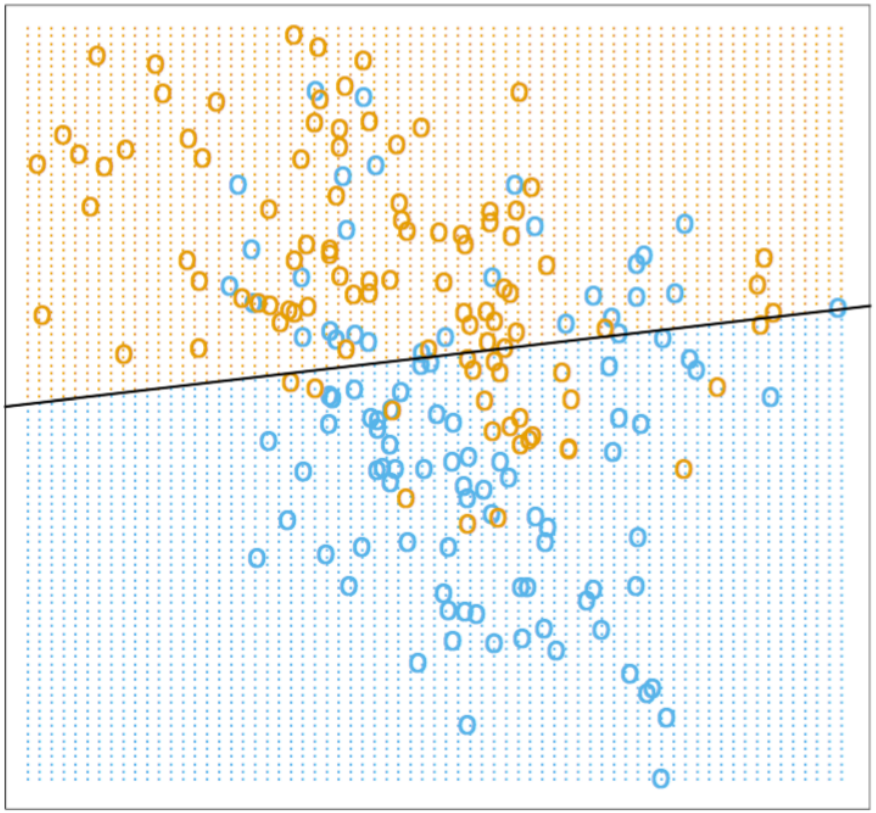
$$\mathbb{P}(Y = 1|X = x) = \frac{1}{2}$$

Predicted label: +1

Predicted label: -1

Figures from Hastie et al.

Linear Decision Boundary



Training data:

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

Learned:

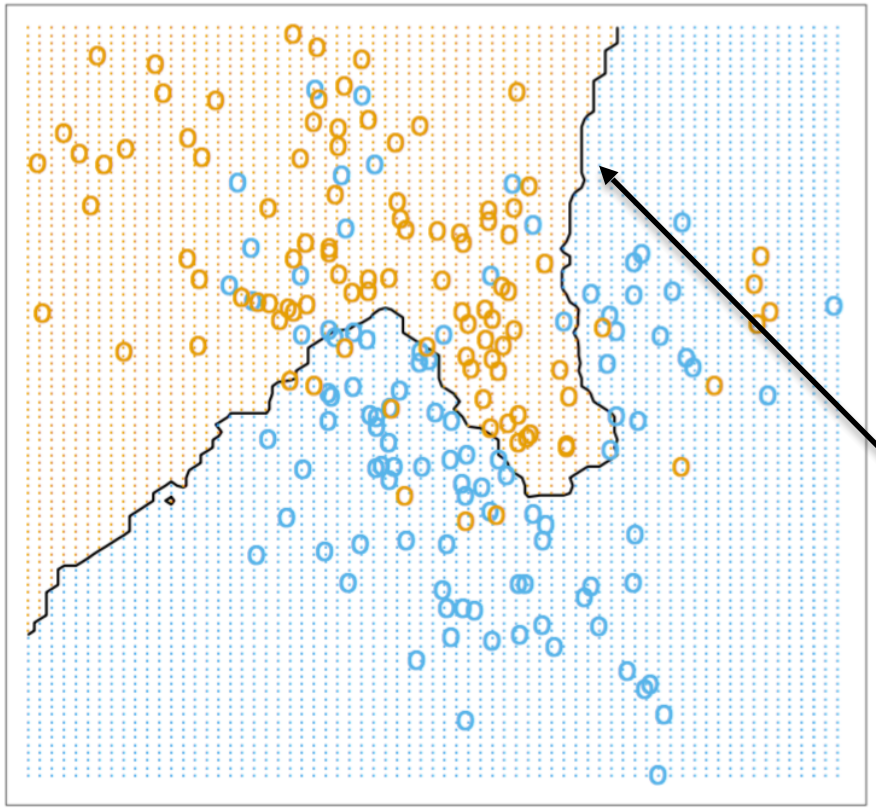
Linear Decision boundary

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

- 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)

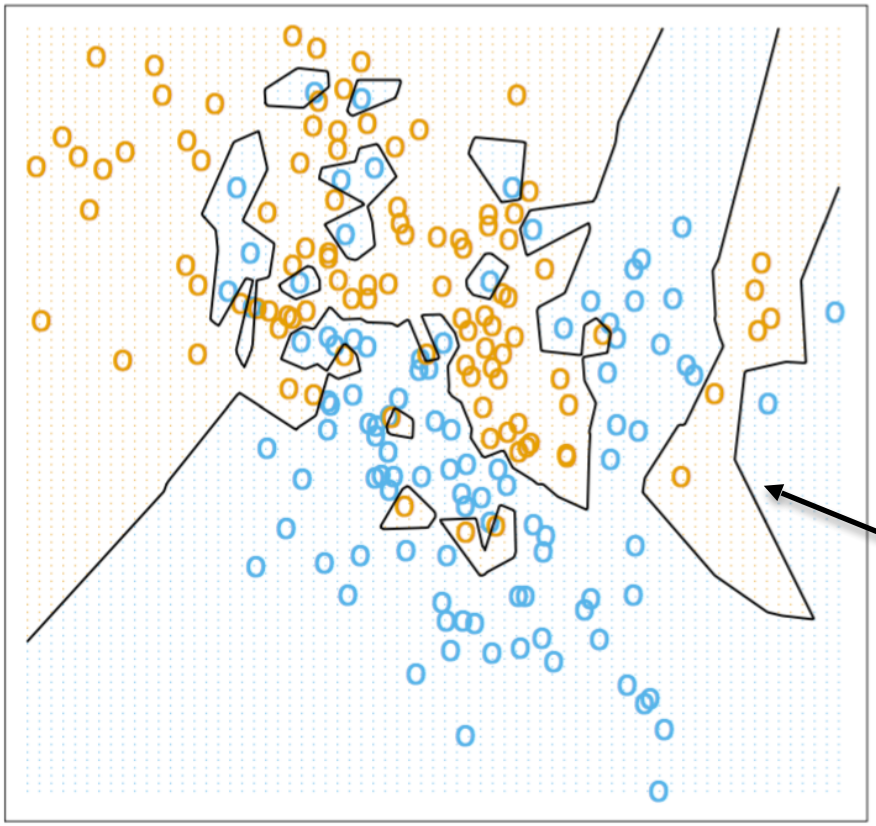
Predicted label: +1

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

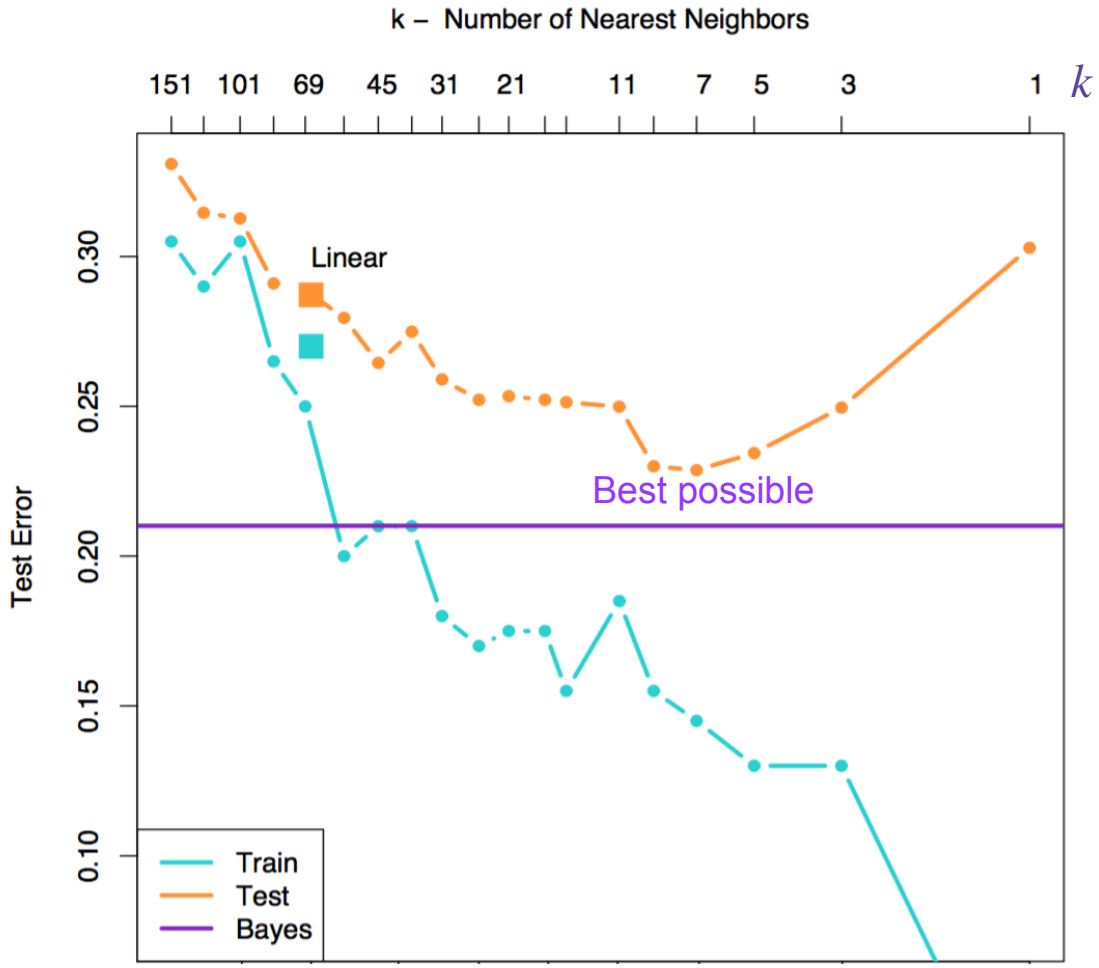
- With a small k, we tend to overfit.

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:

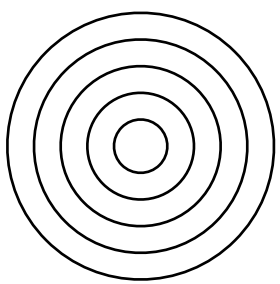
Figures from Hastie et al

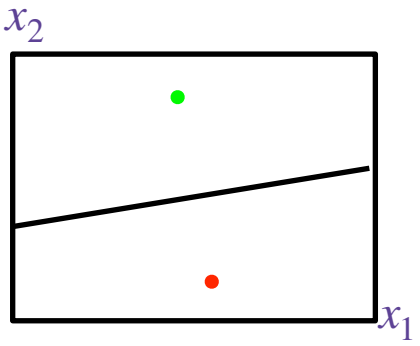
- The error achieved by Bayes optimal classifier provides a lower bound on what any estimator can achieve

Notable distance metrics (and their level sets)

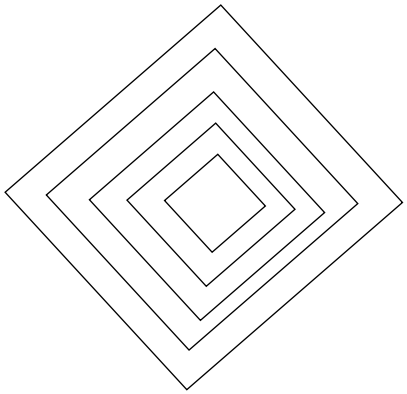
Consider 2 dimensional example with 2 data points with labels green, red,
and we show $k = 1$nearest neighbor decision boundaries for various choices of distances

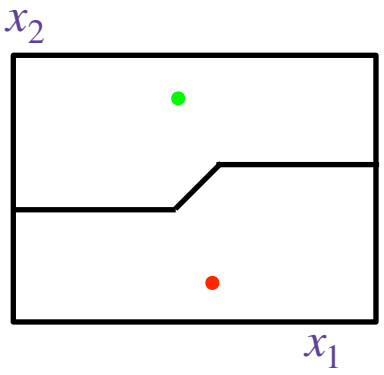
L_2 norm : $d(x, y) = \| x - y \|_2$

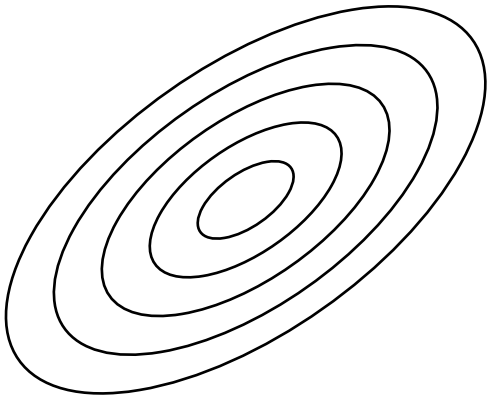


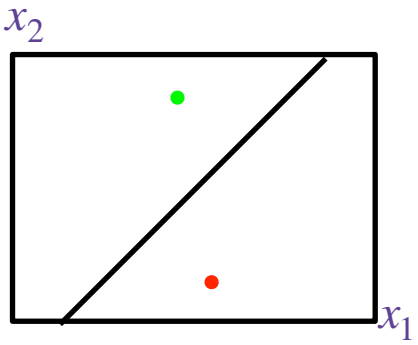


L_1 norm (taxi-cab)

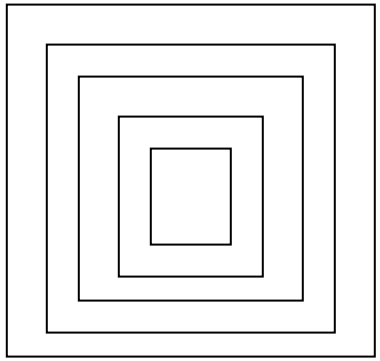




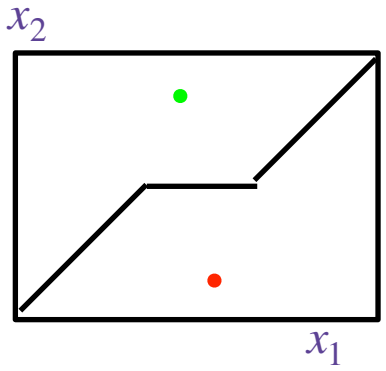




Mahalanobis norm: $d(x, y) = (x - y)^T M(x - y)$

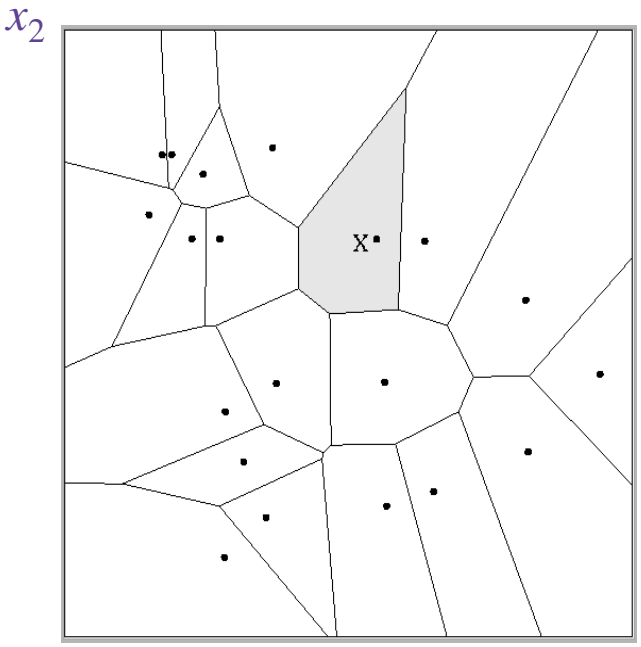


L-infinity *(max) norm*



$k = 1$ nearest neighbor

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



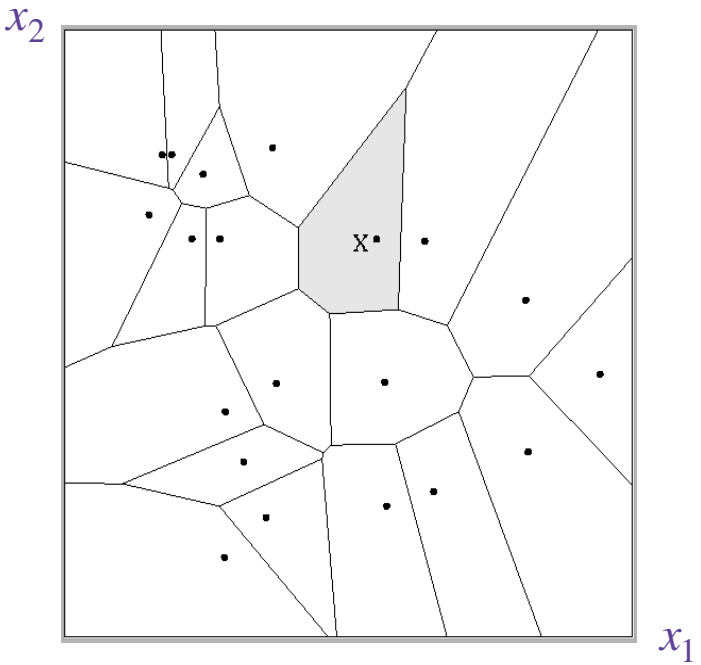
x_2

x_1

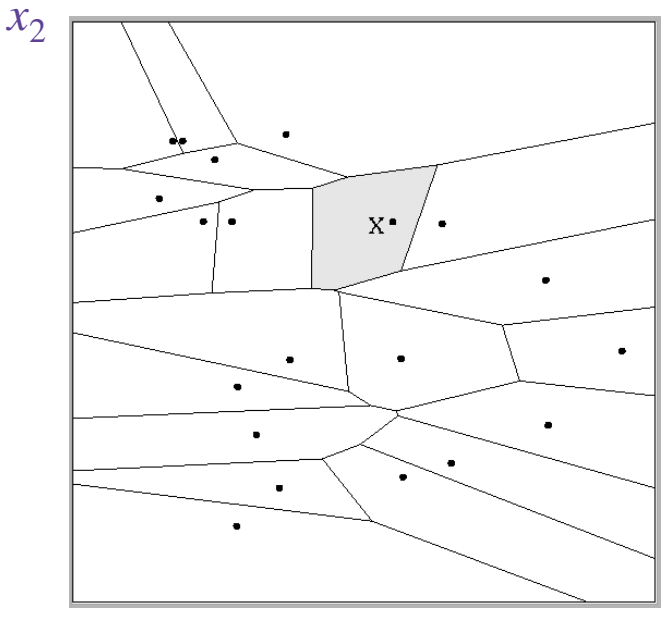
$$Dist(\mathbf{x}^i,\mathbf{x}^j) = (x^i_1 - x^j_1)^2 + (x^i_2 - x^j_2)^2$$

$k = 1$ nearest neighbor

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



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



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

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.

1 nearest neighbor guarantee - classification

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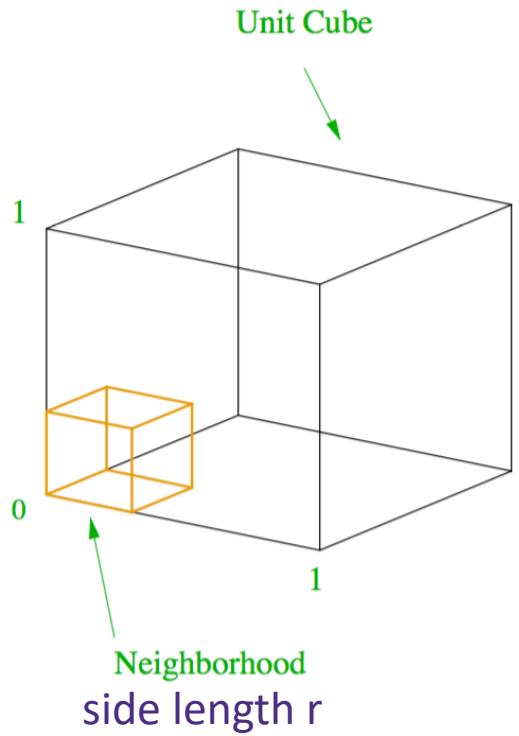
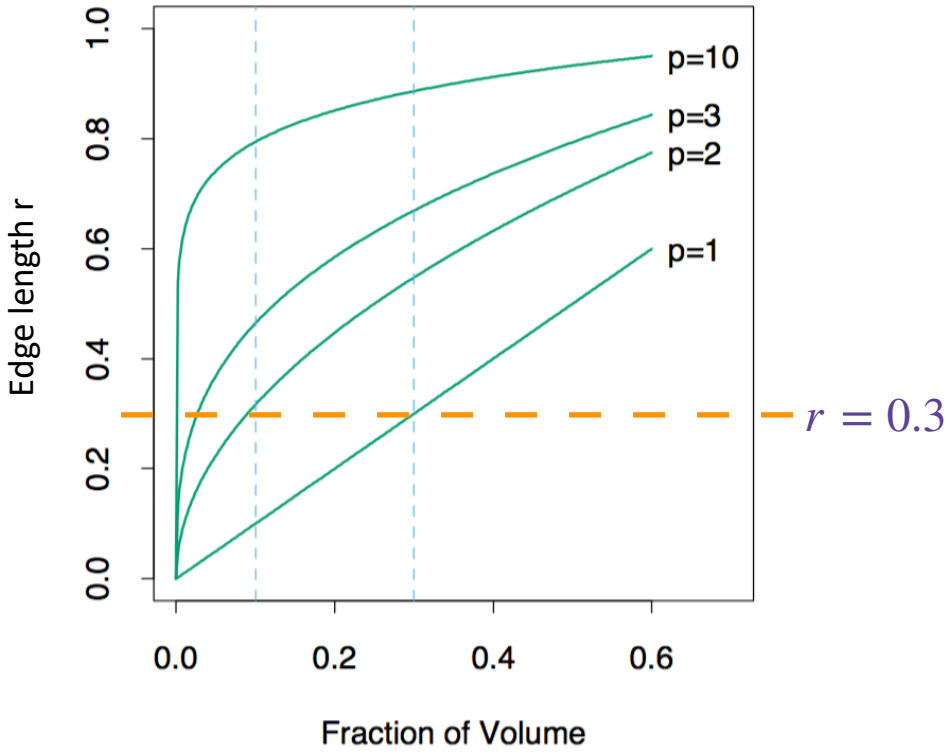
- Let x_{NN} denote the nearest neighbor at a point x
- First note that as $n \to \infty, P(y = +1 \,|\, x_{NN}) \to P(y = +1 \,|\, x)$
- Let $p^* = min\{P(y = +1 \,|\, x), P(y = -1 \,|\, x)\}$ denote the Bayes error rate
- At a point x,
  - Case 1: nearest neighbor is $+1$, which happens with $P(y =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



side length r

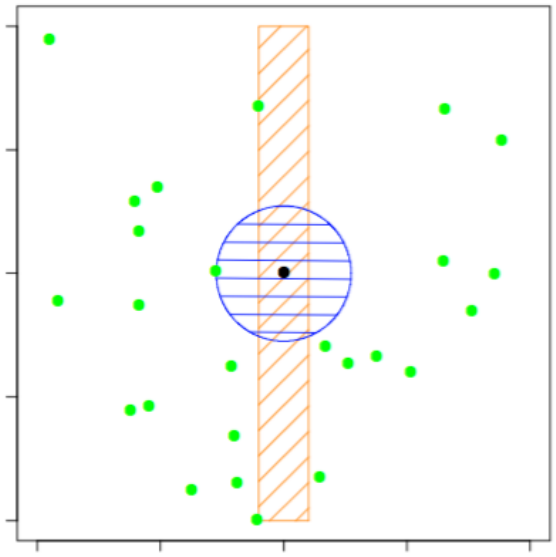


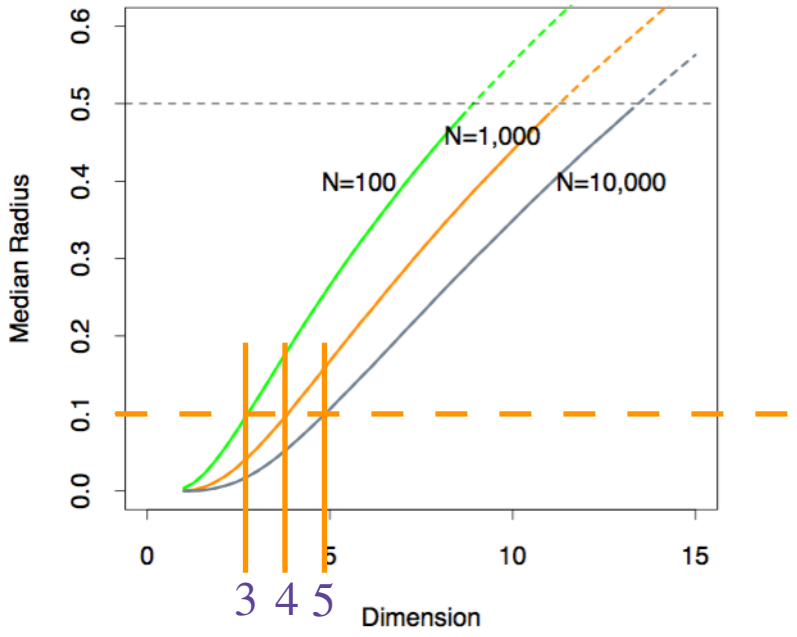
X is uniformly distributed over $[0,1]^p$. What is $\mathbb{P}(X \in [0,r]^p)$?

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

Curse of dimensionality Ex. 2

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

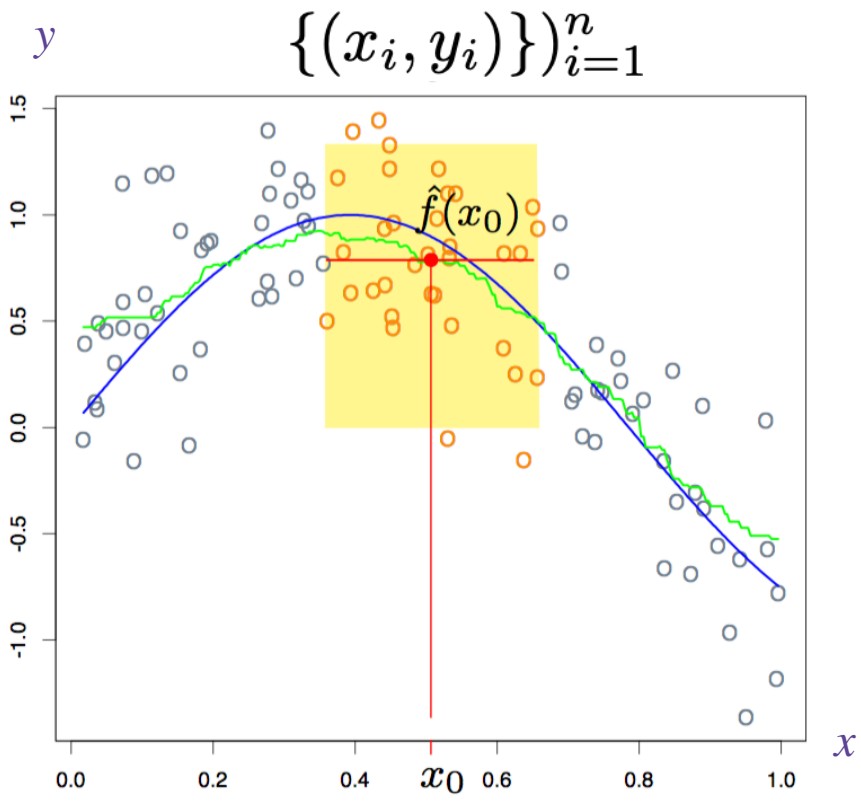




What is the median distance from a point at origin to its 1NN?

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 $\mathbb{E}[(\hat{y} - y)^2]$?

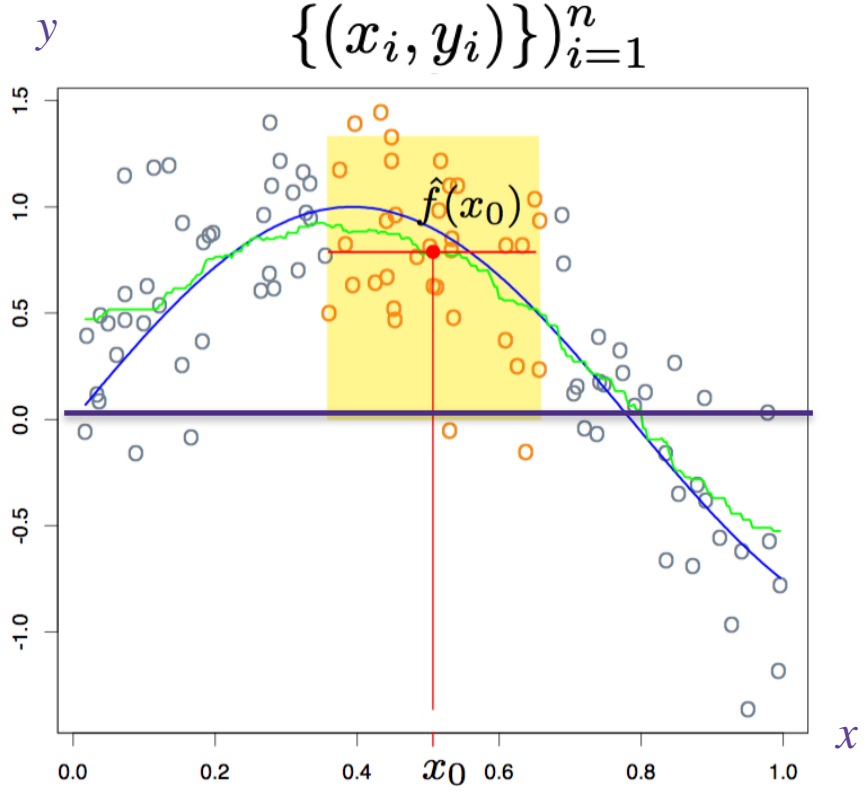
$$\hat{y} = \mathbb{E}[y \mid x]$$

- k-nearest neighbor regressor is

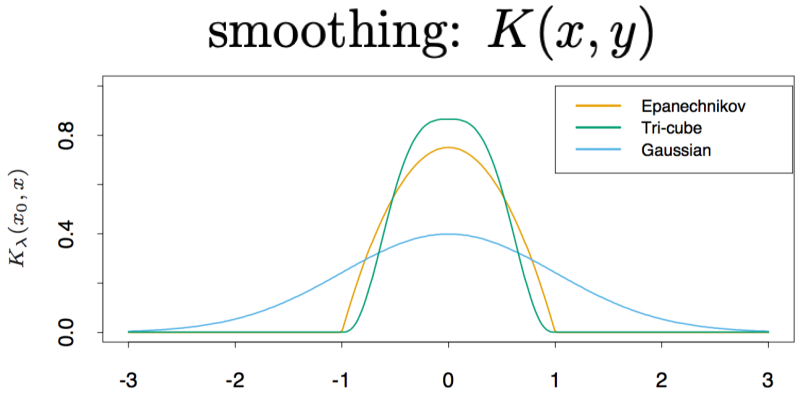
$$\hat{f}(x) = \frac{1}{k} \sum_{j \in \text{nearest neighbor}} y_j$$

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

Nearest neighbor regression



In nearest neighbor methods, the "weight" changes abruptly

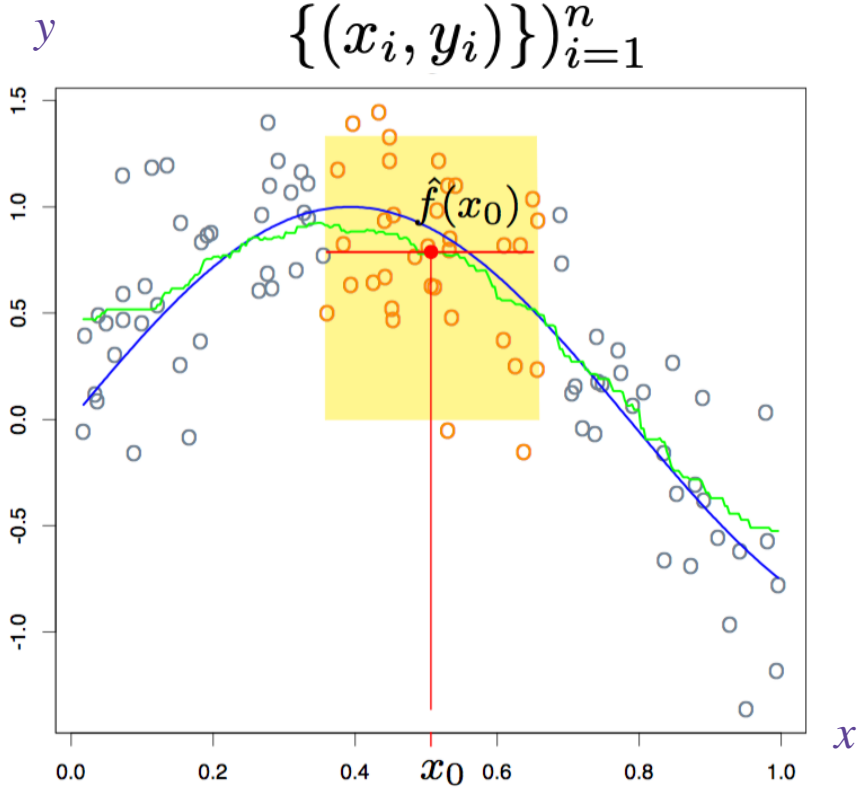


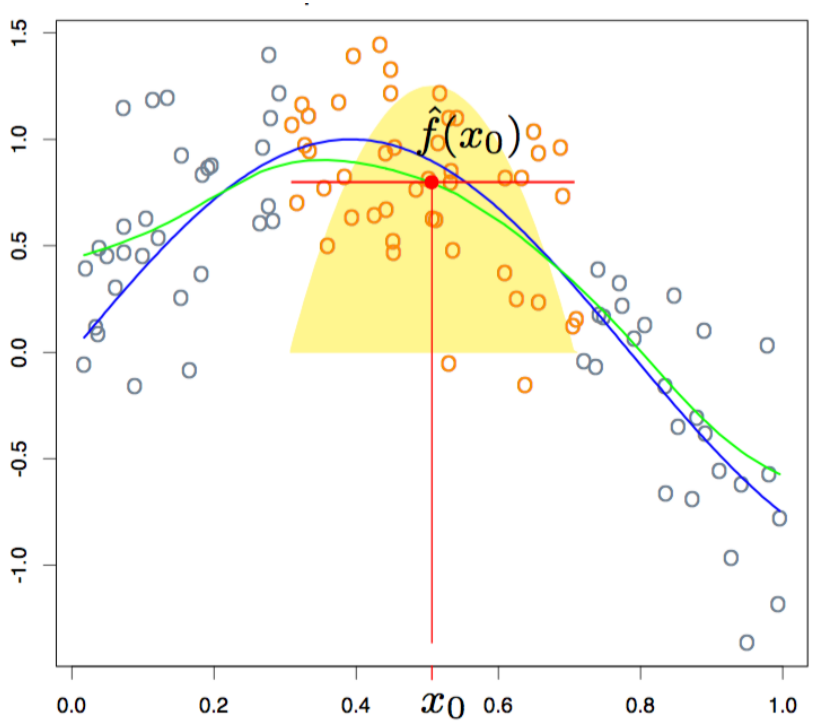
- k-nearest neighbor regressor is

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

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

Nearest neighbor regression



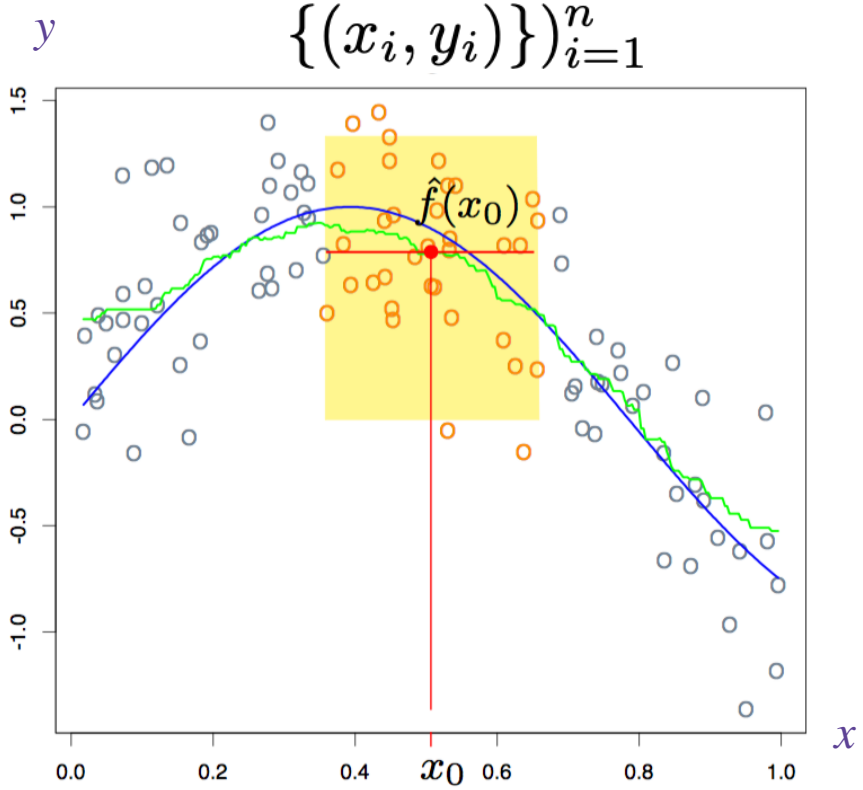


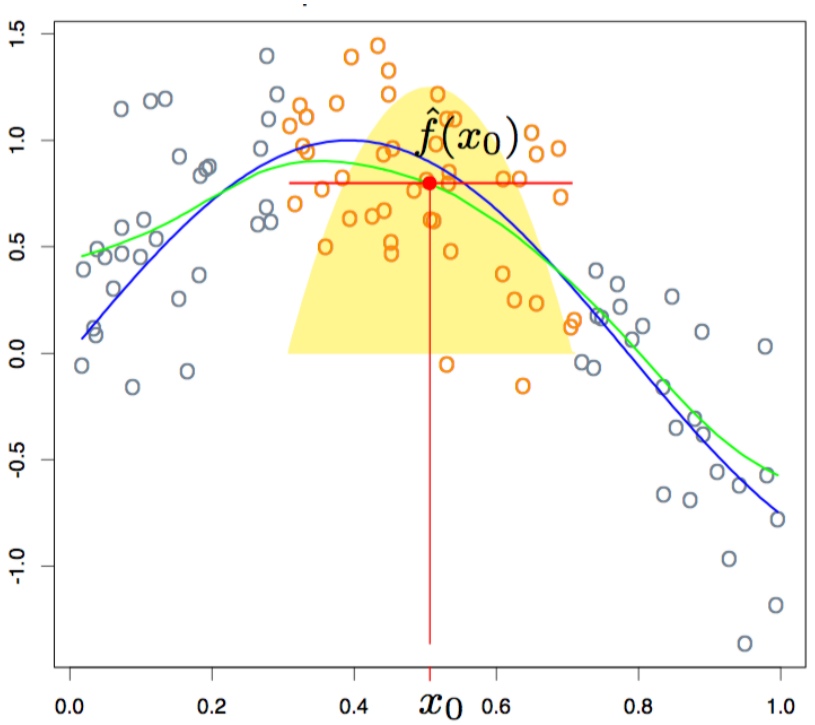
- k-nearest neighbor regressor is

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

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

Nearest neighbor regression





Why just average them?

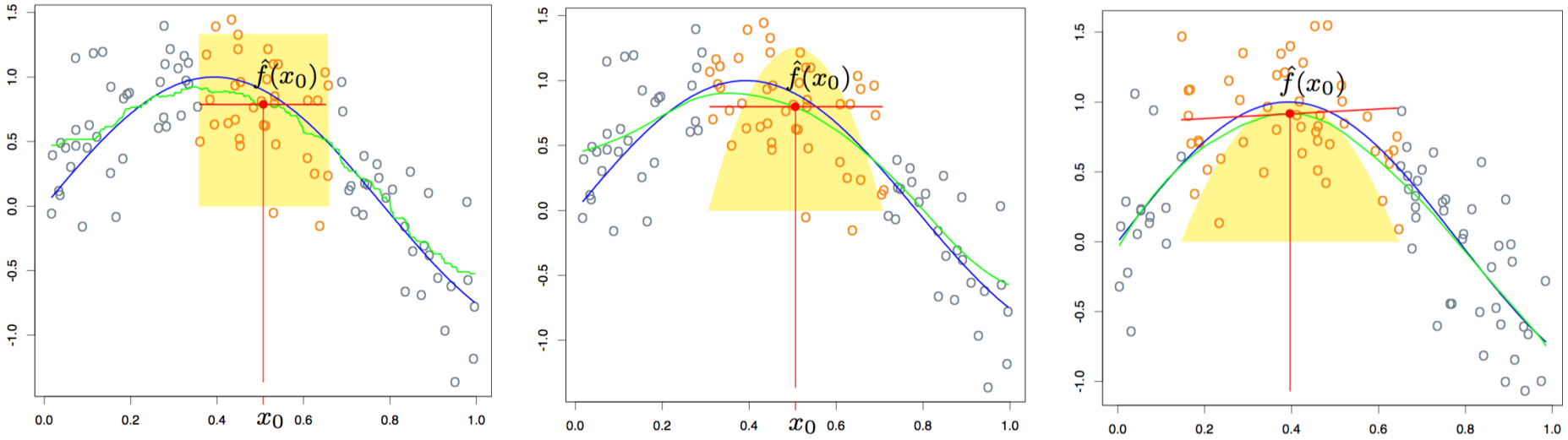
- k-nearest neighbor regressor is

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

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

Nearest neighbor regression

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



- k-nearest neighbor regressor is

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

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

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

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

Local Linear Regression

Nearest Neighbor Overview

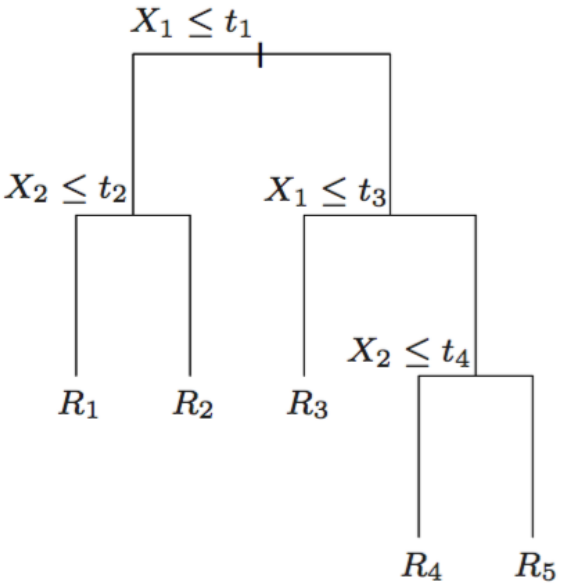
- Very simple to explain and implement
- No training! But finding nearest neighbors in large dataset at test can be computationally demanding (KD-trees help)
- You can use other forms of distance (not just Euclidean)
- Smoothing and local linear regression can improve performance (at the cost of higher 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).

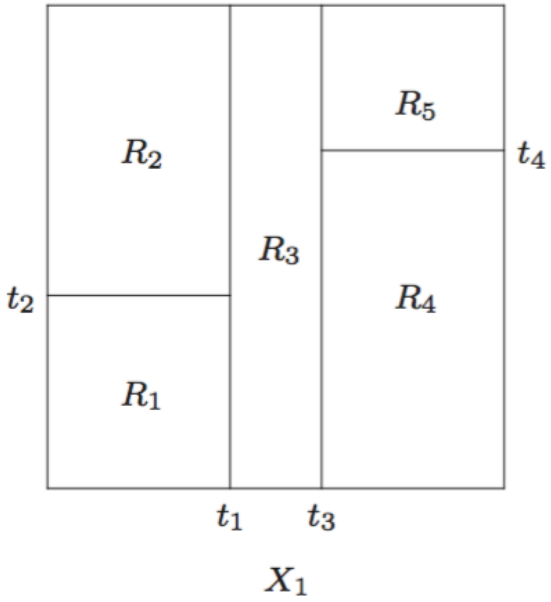
Questions?

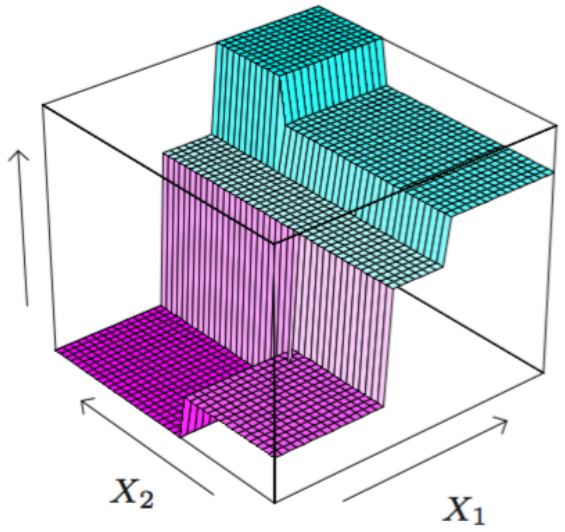
Trees

Trees

Example: binary tree with splits along axes







$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m).$$

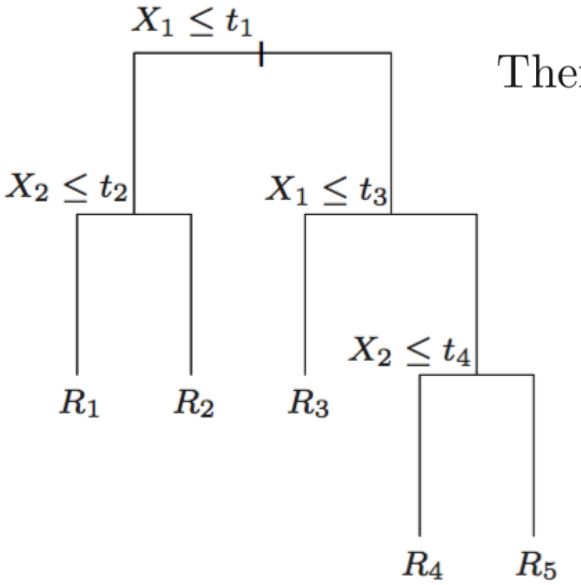
Regression Trees

$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m).$$

$$\hat{c}_m = \text{ave}(y_i | x_i \in R_m).$$

Binary tree with splits along axes.

How do you build the tree / find the splits?



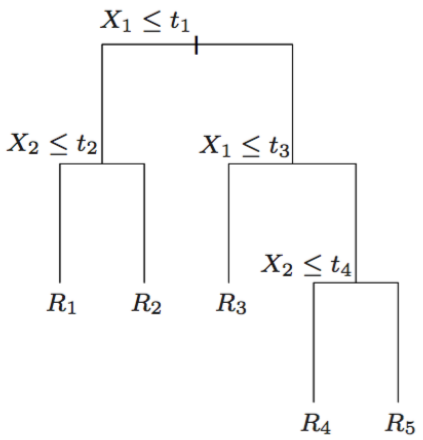
$$R_1(j,s) = \{X | X_j \le s\} \text{ and } R_2(j,s) = \{X | X_j > s\}.$$

Then we seek the splitting variable j and split point s that solve

$$\min_{j,\, s} \left[\min_{c_1} \sum_{x_i \in R_1(j,s)} (y_i - c_1)^2 + \min_{c_2} \sum_{x_i \in R_2(j,s)} (y_i - c_2)^2 \right].$$

Learning decision trees

- Start from empty decision tree
- Split on next best attribute (feature)
  - Use, for example, information gain to select attribute
  - Split on $\arg\max_i IG(X_i) = \arg\max_i H(Y) - H(Y \mid X_i)$
- Recurse
- Prune

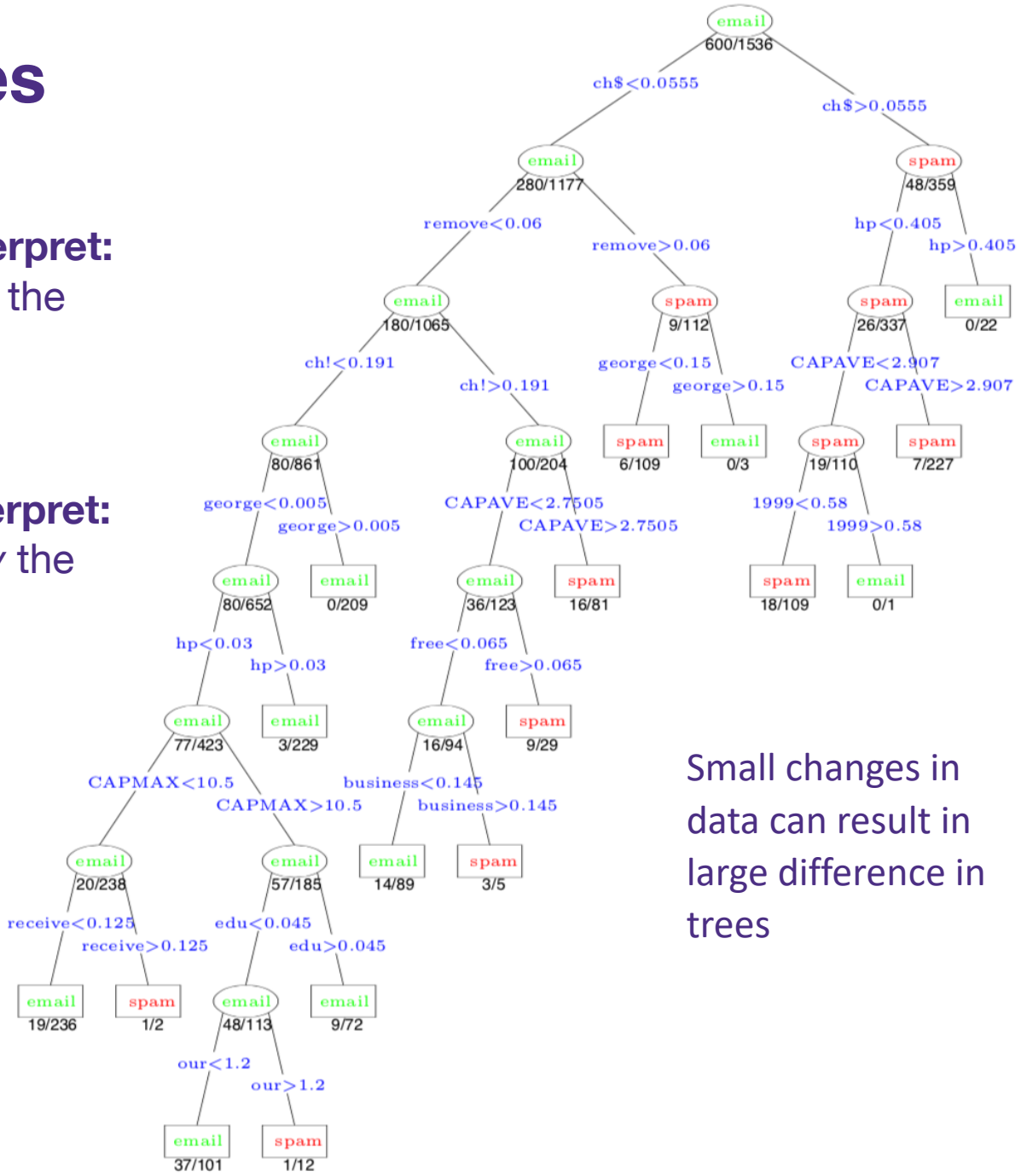


$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m).$$

Decision Trees

Trees are easy to interpret:
- You can explain *how* the classifier came to the conclusion it did

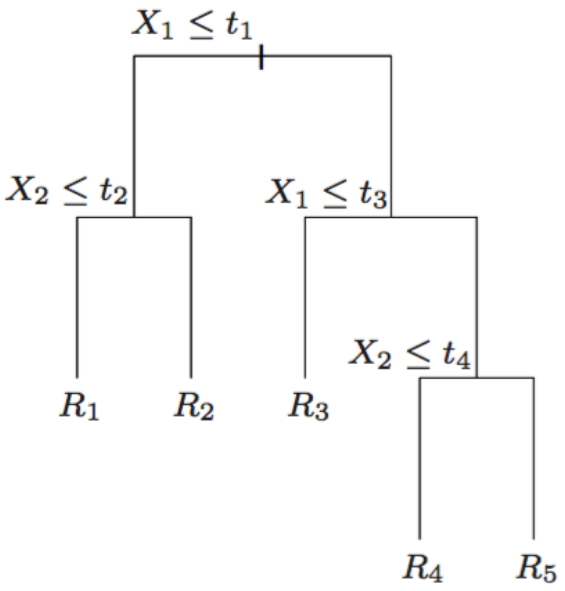
Trees are hard to interpret:
- Tough to explain *why* the classifier came to the conclusion it did



Small changes in data can result in large difference in trees

Trees

$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m).$$



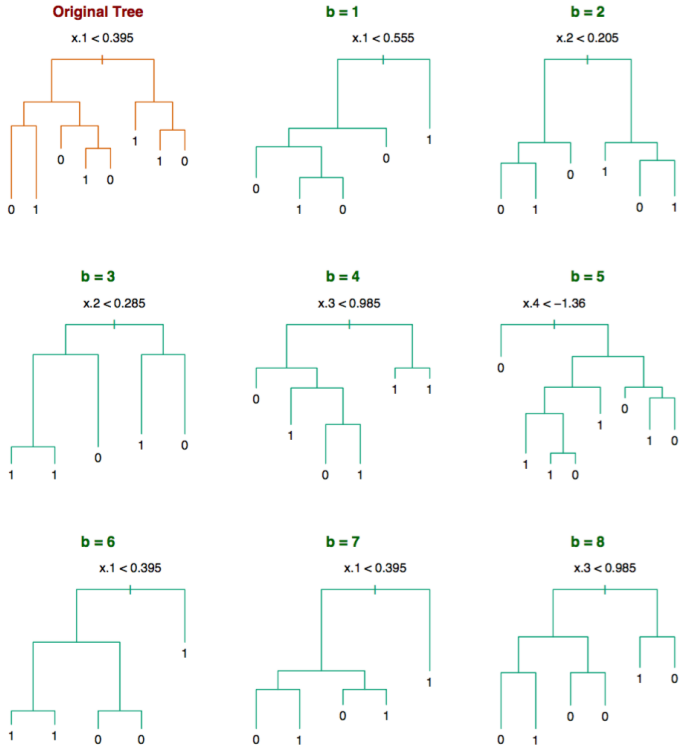
- Trees
  - **have low bias, high variance**
  - deal with categorial variables well
  - intuitive, interpretable
  - good software exists

Random Forests

Random Forests

Tree methods have **low bias** but **high variance**.

One way to reduce variance is to construct a lot of “lightly correlated” trees and average them:



“Bagging:” Bootstrap aggregating

Random Forests

Algorithm 15.1 *Random Forest for Regression or Classification.*

1. For $b = 1$ to B:

   (a) Draw a bootstrap sample $\mathbf{Z}^*$ of size N from the training data.

   (b) Grow a random-forest tree T_b to the bootstrapped data, by recursively repeating the following steps for each terminal node of the tree, until the minimum node size n_{min} is reached.

      i. Select m variables at random from the p variables.

      ii. Pick the best variable/split-point among the m.

      iii. Split the node into two daughter nodes.

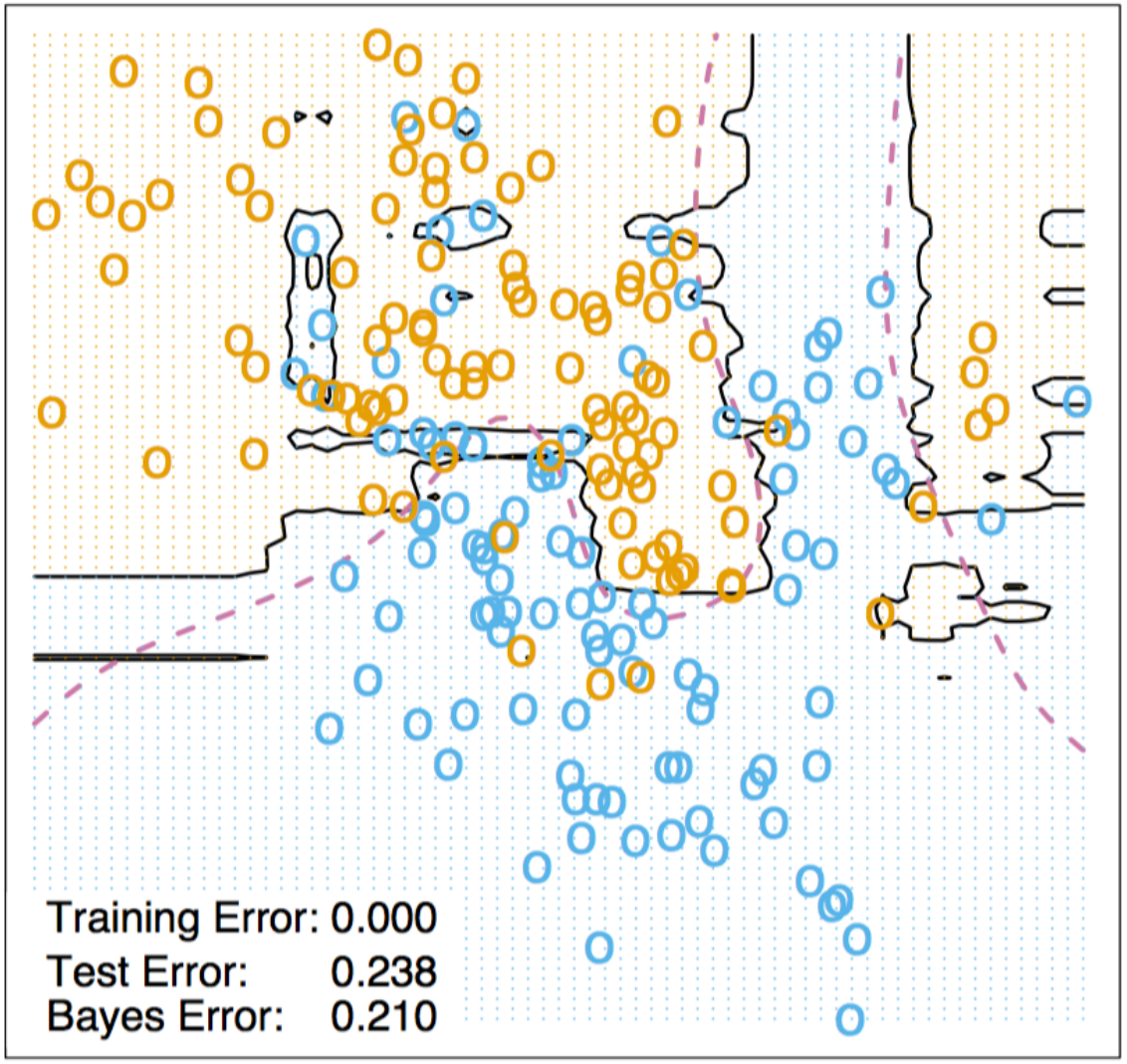
2. Output the ensemble of trees $\{T_b\}_1^B$.

To make a prediction at a new point x:

Regression: $\hat{f}_{\text{rf}}^B(x) = \frac{1}{B}\sum_{b=1}^B T_b(x)$.

Classification: Let $\hat{C}_b(x)$ be the class prediction of the bth random-forest tree. Then $\hat{C}_{\text{rf}}^B(x) = \textit{majority vote}\ \{\hat{C}_b(x)\}_1^B$.

Random Forest - Decision Boundary Example



Random Forest

Given random variables $Y_1, Y_2, \ldots, Y_B$ with
$\mathbb{E}[Y_i] = y$, $\mathbb{E}[(Y_i - y)^2] = \sigma^2$, $\mathbb{E}[(Y_i - y)(Y_j - y)] = \rho\sigma^2$

Assume bias = 0

σ^2 **Variance of individual predictor**

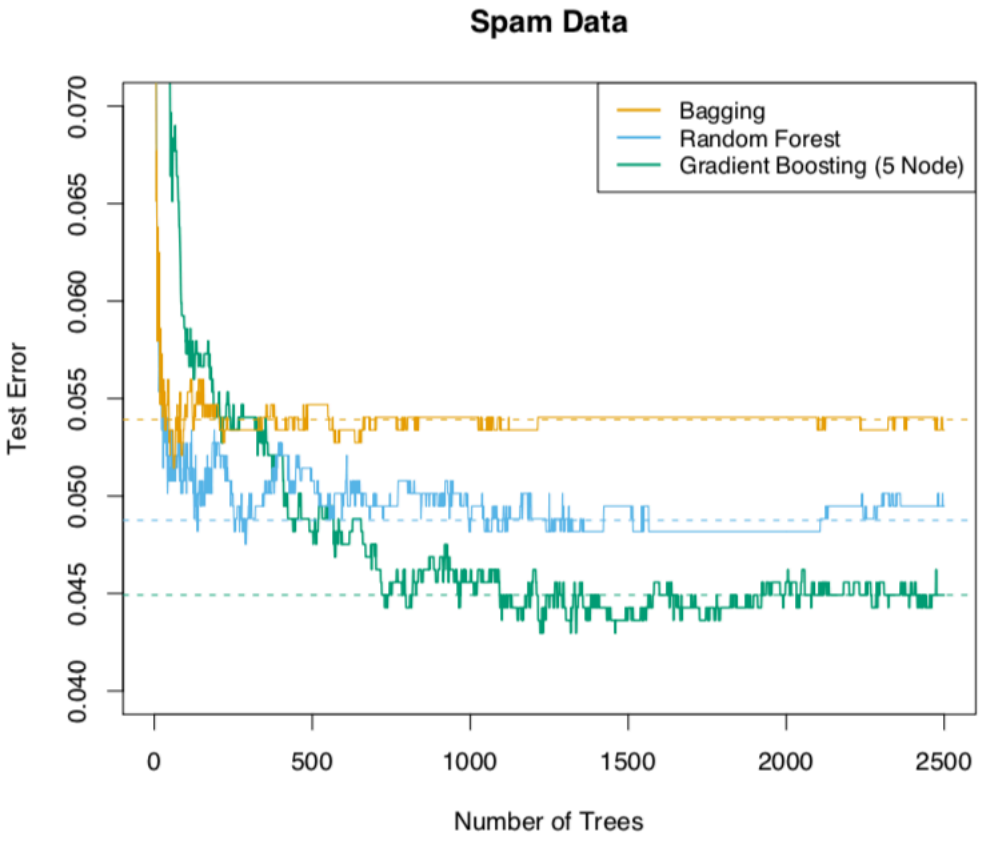
$\rho\sigma^2$ **Correlation between predictors**

The Yi's are identically distributed but **not** independent

$$\mathbb{E}[(\frac{1}{B}\sum_{i=1}^{B} Y_i - y)^2] =$$

Random Forest

The power of weakly correlated predictors:



Bagging: Averaged trees trained on bootstrapped datasets that used **all d variables**

Random forest: Averaged trees trained on bootstrapped datasets that used **m < d random variables**

Gradient boosting: ignore for now

Takeaway: reducing correlation improves performance!

Random Forests

- Random Forests
  - **have low bias, low variance**
  - deal with categorial variables well
  - not that intuitive or interpretable
  - Notion of confidence estimates
  - good software exists

Boosting and Additive Models

Boosting

- 1988 Kearns and Valiant: “Can **weak learners** be combined to create a **strong learner?**”

Weak learner definition (informal):

An algorithm $\mathcal{A}$ is a *weak learner* for a hypothesis class $\mathcal{H}$ that maps $\mathcal{X}$ to $\{-1, 1\}$ if for all input distributions over $\mathcal{X}$ and $h \in \mathcal{H}$, we have that $\mathcal{A}$ correctly classifies h with error at most $1/2 - \gamma$

- 1990 Robert Schapire: “Yup!”
- 1995 Schapire and Freund: “Practical for 0/1 loss” AdaBoost
- 2001 Friedman: “Practical for arbitrary losses”

Additive models

- Given: $\{(x_i, y_i)\}_{i=1}^n \quad x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$
- Generate **random** functions: $\phi_t : \mathbb{R}^d \to \mathbb{R} \quad t = 1, \ldots, p$
- Learn some weights: $\widehat{w} = \arg\min_w \sum_{i=1}^n \text{Loss}\left(y_i, \sum_{t=1}^p w_t \phi_t(x_i)\right)$
- Classify new data: $f(x) = \text{sign}\left(\sum_{t=1}^p \widehat{w}_t \phi_t(x)\right)$

Additive models

- Given: $\{(x_i, y_i)\}_{i=1}^n \quad x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$

$$\phi_t : \mathbb{R}^d \to \mathbb{R} \quad t = 1, \ldots, p$$

- Generate **random** functions:

$$\widehat{w} = \arg\min_w \sum_{i=1}^n \text{Loss}\left(y_i, \sum_{t=1}^p w_t \phi_t(x_i)\right)$$

- Learn some weights:

$$f(x) = \text{sign}\left(\sum_{t=1}^p \widehat{w}_t \phi_t(x)\right)$$

An interpretation:
Each $\phi_t(x)$ is a classification rule that we are assigning some weight $\widehat{w}_t$

- Classify new data:

$$\widehat{w}, \widehat{\phi}_1, \ldots, \widehat{\phi}_t = \arg\min_{w, \phi_1, \ldots, \phi_p} \sum_{i=1}^n \text{Loss}\left(y_i, \sum_{t=1}^p w_t \phi_t(x_i)\right)$$

is in general computationally hard

Forward Stagewise Additive models

$b(x, \gamma)$ is a function with parameters γ Examples: $b(x, \gamma) = \frac{1}{1 + e^{-\gamma^T x}}$

$b(x, \gamma) = \gamma_1 \mathbf{1}\{x_3 \leq \gamma_2\}$

Algorithm 10.2 *Forward Stagewise Additive Modeling.*

1. Initialize $f_0(x) = 0$.
2. For $m = 1$ to M:
   (a) Compute

$$(\beta_m, \gamma_m) = \arg\min_{\beta,\gamma} \sum_{i=1}^{N} L(y_i, f_{m-1}(x_i) + \beta b(x_i; \gamma)).$$

   (b) Set $f_m(x) = f_{m-1}(x) + \beta_m b(x; \gamma_m)$.

Idea: greedily add one function at a time

Forward Stagewise Additive models

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AdaBoost: $b(x, \gamma)$: classifiers to $\{-1, 1\}$

$$L(y, f(x)) = \exp(-yf(x))$$

Forward Stagewise Additive models

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Boosted Regression Trees:

$L(y, f(x)) = (y - f(x))^2$

$b(x, \gamma)$: regression trees

Forward Stagewise Additive models

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Boosted Regression Trees: $L(y, f(x)) = (y - f(x))^2$

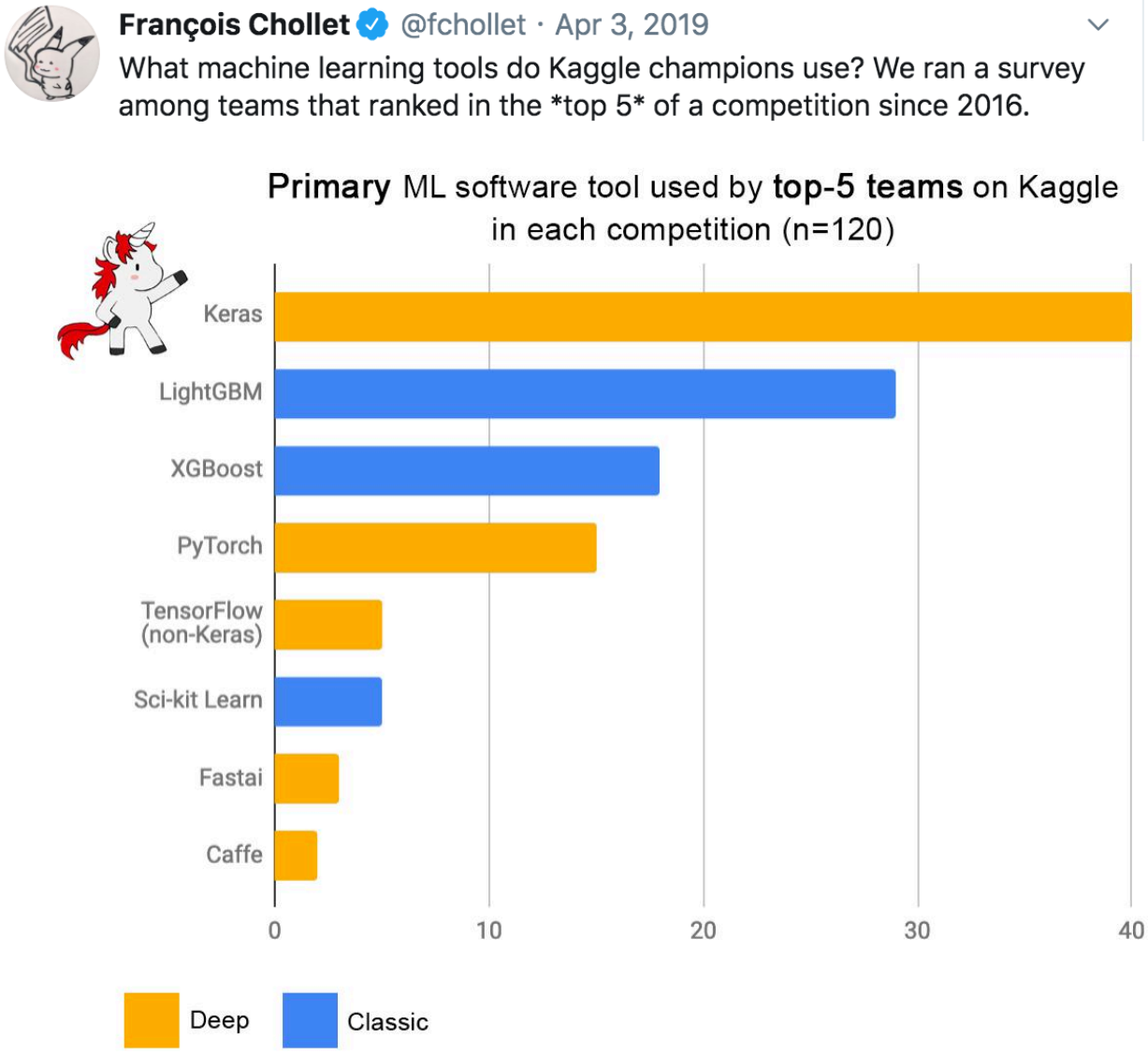
$$\begin{aligned} L(y_i, f_{m-1}(x_i) + \beta b(x_i; \gamma)) &= (y_i - f_{m-1}(x_i) - \beta b(x_i; \gamma))^2 \\ &= (r_{im} - \beta b(x_i; \gamma))^2, \qquad r_{im} = y_i - f_{m-1}(x_i) \end{aligned}$$

Efficient: No harder than learning regression trees!

Additive models

- Boosting is popular at parties: Invented by theorists, heavily adopted by practitioners.
- Computationally efficient with “weak” learners. But can also use trees! Boosting can scale.
- Gradient boosting generalization with good software packages (e.g., *XGBoost)*. Effective on Kaggle

Additive models



Bagging versus Boosting

- Bagging *averages* many **low-bias**, **lightly dependent** classifiers to reduce the variance
- Boosting *learns* linear combination of **high-bias**, **highly dependent** classifiers to reduce error

Last slide of the quarter!