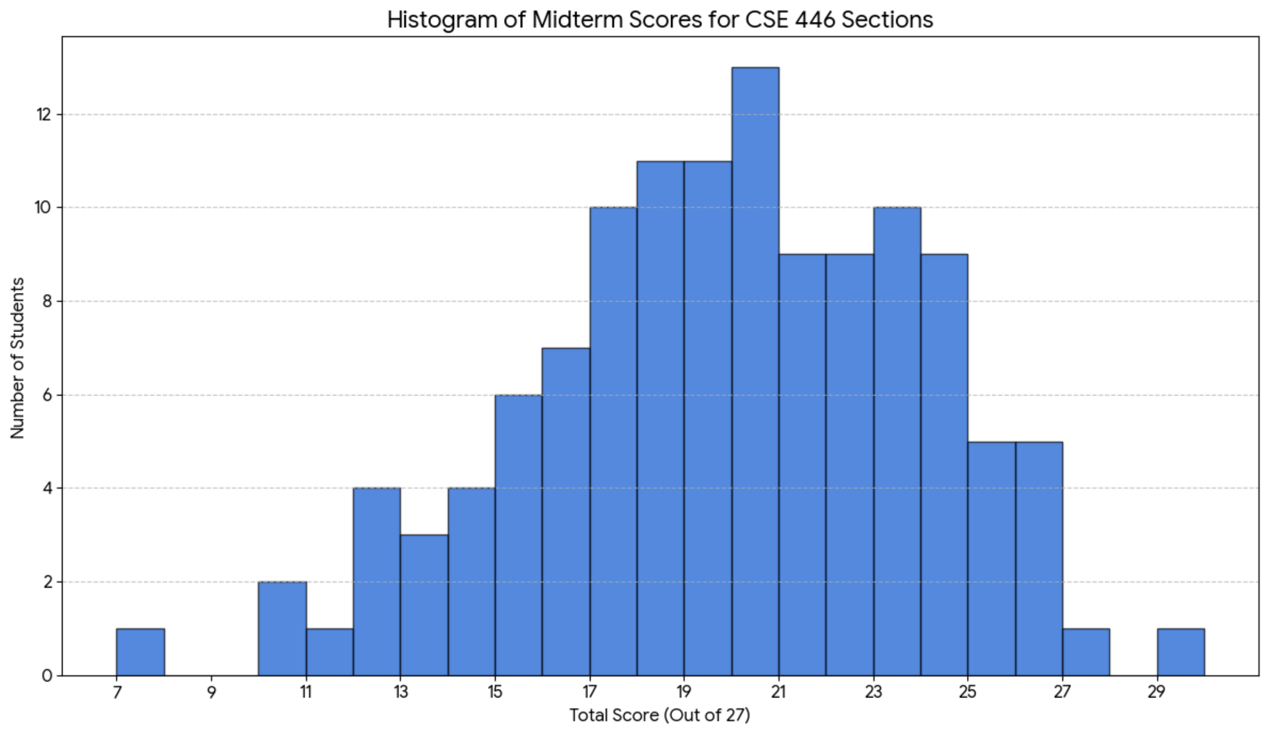
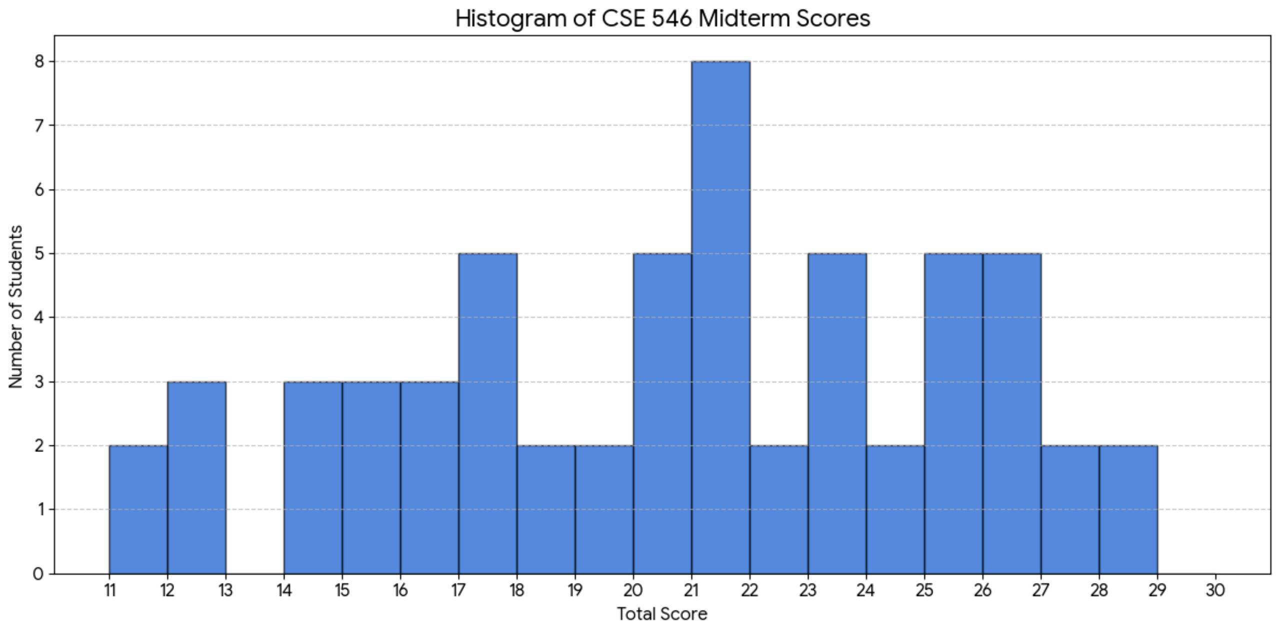
Midterm results: CSE 446

- Median: 20.0 / 27
- Standard deviation: 4.14



Midterm results: CSE 546

- Median: 21.4 / 27
- Standard deviation: 4.64



Midterm results

- Exam scores are imperfect metrics
- Midterm is 20% of course grade – you can still do well

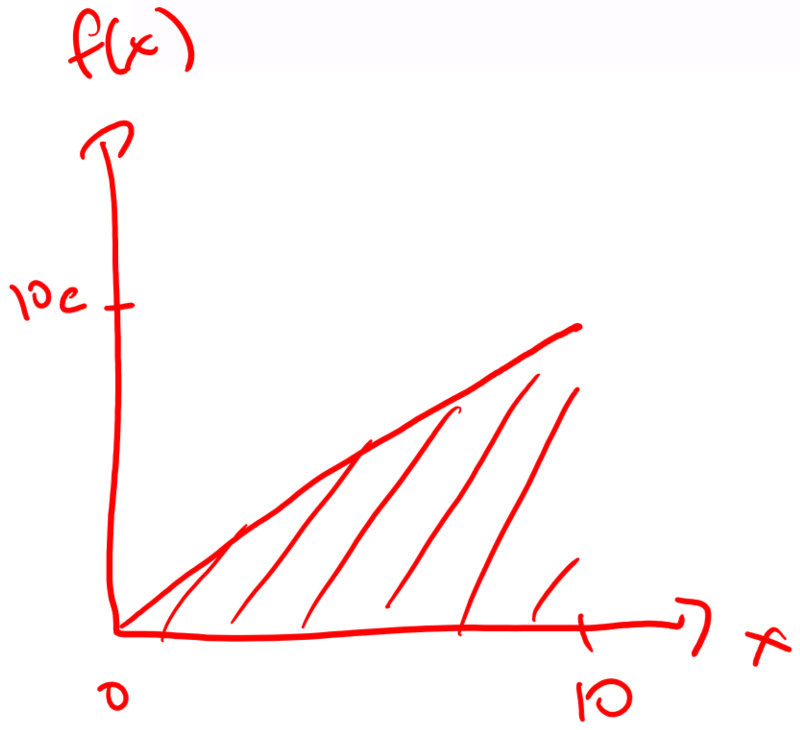
- You can submit regrade requests 11/12 @ 11:59PM
- Clarifications? Come to OH or post on Ed
- You may pick up your cheat sheets after class

Q7

7. 1 point

Give a value for the constant $c \in \mathbb{R}$ that makes f a valid PDF:

$$f(x) = \begin{cases} cx, & \text{if } 0 < x < 10 \\ 0, & \text{otherwise} \end{cases}$$



want:

① $\int_{-\infty}^{\infty} f(x)\,dx = 1$

② $f(x) \geq 0 \quad \forall x \in \mathbb{R}$

$50c = 1$

$c = \frac{1}{50}$

Q9

9. 1 point

Assume we have n training data points sampled from some population distribution, which we then use to train a model. Is leave-one-out cross validation (LOOCV) error (1) typically a slight underestimate, (2) an unbiased estimator, or (3) typically a slight overestimate of the true (population) error of the final model trained on all n data points? Briefly explain your answer.

Final model trained on n data points

LOOCV models trained on $n-1$ data points

↑ training data, ↓ error

$\Rightarrow$ overestimate

Q11

$(X^TX)^{-1}X^Ty$ ← $+\lambda I$

11. Consider the following linear regression setting. Let $X \in \mathbb{R}^{n\times d}$, $\lambda \geq 0$, and suppose $y \in \mathbb{R}^n$ is drawn from a Gaussian, $y \sim \mathcal{N}(Xw, \sigma^2 I)$ for some $w \in \mathbb{R}^d$, $\sigma^2 > 0$. Let

$$\widehat{w} = \arg\min_{w\in\mathbb{R}^d} \|Xw - y\|_2^2 + \lambda\|w\|_2^2.$$

(a) 1 point

If $n < d$ and $\lambda = 0$, how many solutions does the above optimization problem have?

Answer: ∞

(b) 1 point

If $n < d$ and $\lambda > 0$, how many solutions does the above optimization problem have?

Answer: 1

(c) 1 point

Fill in the blanks with **increases/decreases/does not change**. As σ^2 **increases**:

The bias of $\widehat{w}$ unchanged

The variance of $\widehat{w}$ ↑

The irreducible error ↑

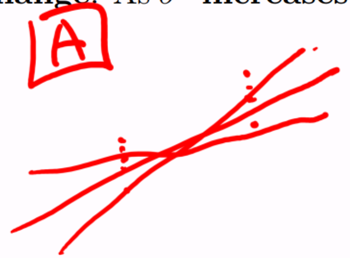
imagine $n=1$, $d=2$

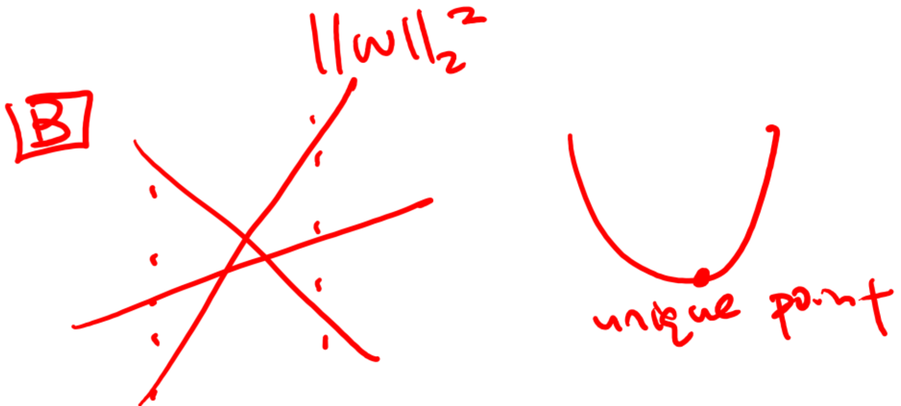
$y=5$

$x_1=1$, $x_2=2$

want:
$w_1x_1 + w_2x_2 = y$

$w_1=1$, $w_2=2$
$w_1=3$, $w_2=1$
⋮
} have 0 MSE





Q19

19. You train a logistic regression classifier with features $x = (x_1, x_2)$, using

$$P(y = 1|x) = \sigma(w_0 + w_1 x_1 + w_2 x_2), \quad \text{where } \sigma(z) = \frac{1}{1 + e^{-z}}.$$

a) 1 point

Describe the geometric shape of the decision boundary in this feature space.

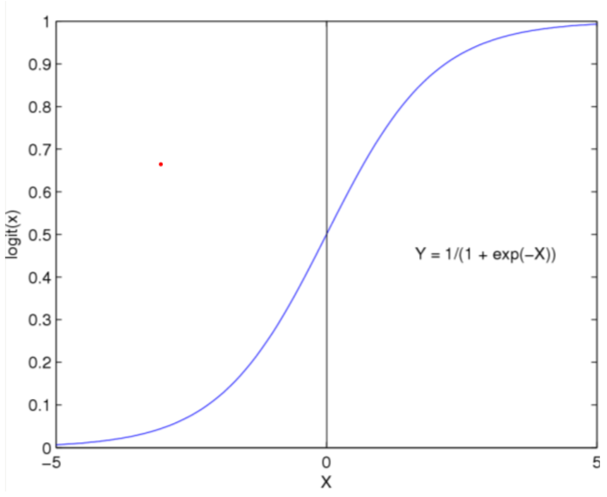
Modeling conditional probabilities

$$\widehat{w}_{\text{MLE}} = \text{argmax}_w \sum_{i=1}^{n} \log P_w(y_i|x_i)$$

- Logistic regression uses a model specialized for (binary) classification:

$$P(Y = 1|X = x) = \frac{1}{1 + e^{-w^\top x}}$$

$$P(Y = 0|X = x) = \frac{e^{-w^\top x}}{1 + e^{-w^\top x}}$$



Sigmoid for binary classification

- What's the shape of the decision rule $P(Y = 1|X) \geq P(Y = 0|X)$?

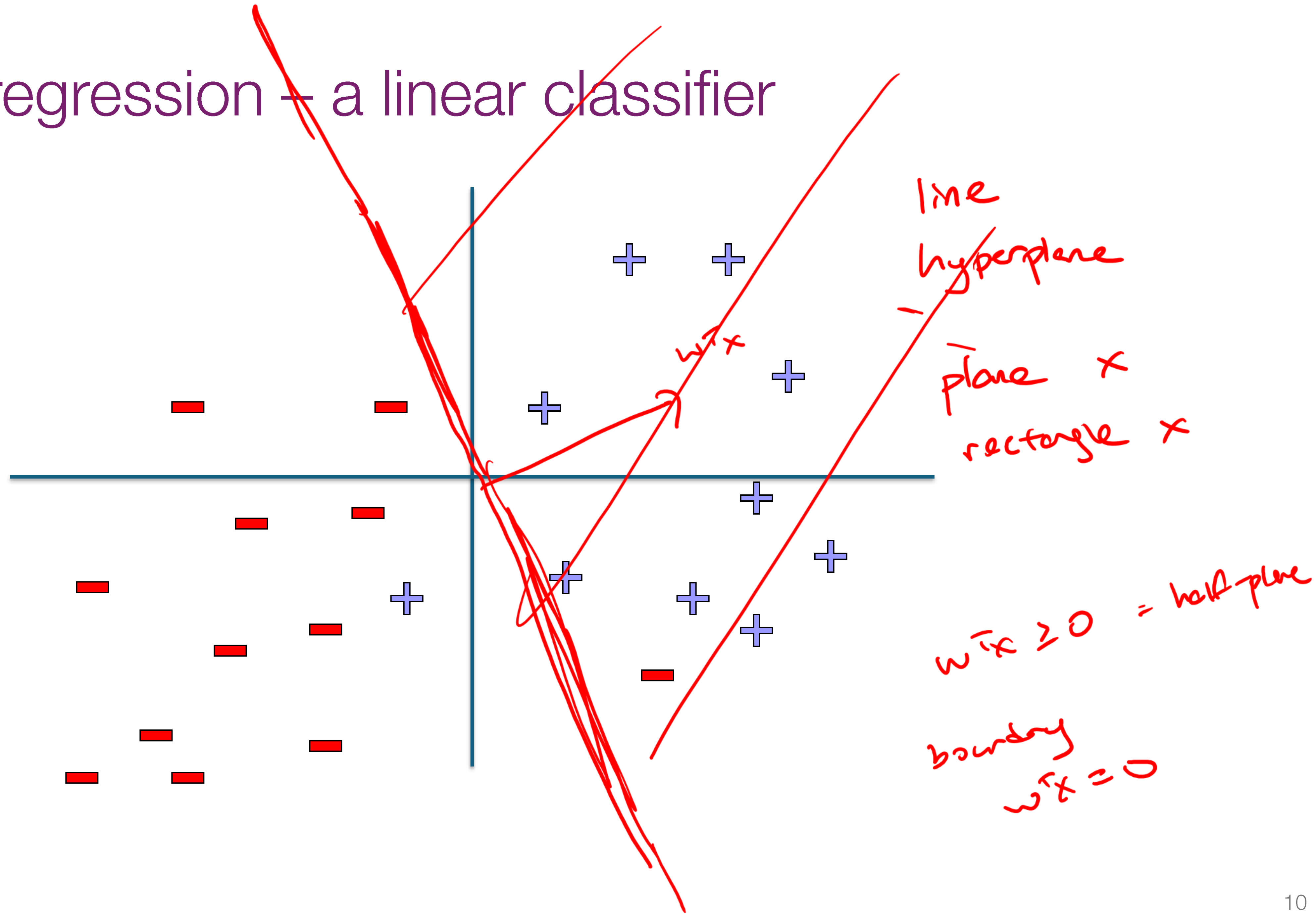
$p(y=1 \mid x) = \frac{1}{1+e^{-w^T x}}$, $p(y=0 \mid x) = \frac{e^{-w^T x}}{1+e^{-w^T x}}$

$\log \frac{p(y=1 \mid x)}{p(y=0 \mid x)} = w^T x$

$\Rightarrow \quad w^T x \geq 0$

decision rule

Logistic regression – a linear classifier



Q19

19. You train a logistic regression classifier with features $x = (x_1, x_2)$, using

$$P(y = 1|x) = \sigma(w_0 + w_1 x_1 + w_2 x_2), \quad \text{where } \sigma(z) = \frac{1}{1 + e^{-z}}.$$

a) 1 point

Describe the geometric shape of the decision boundary in this feature space.

21. **[Extra credit. Not attempting this question will not affect your grade.]** Consider linear regression on 2-dimensional data, where the features of the i-th data point are denoted $(x_1^{(i)}, x_2^{(i)}) \in \mathbb{R}^2$ and the target of the i-th data point is $y^{(i)} \in \mathbb{R}$. There are n training data points, $\{(x_1^{(i)}, x_2^{(i)}), y^{(i)}\}_{i=1}^n$. Assume that the following always holds in the training data, for all $i = 1, 2, \ldots, n$:

$$x_2^{(i)} = 2x_1^{(i)}$$
$$y^{(i)} = 5x_1^{(i)}.$$

x_1	x_2	y
1	2	5
2	4	10
	⋮	

1. 1 point Suppose we train a ridge regression model, i.e., we solve

$$\hat{w} = \arg\min_{(w_1,w_2)\in\mathbb{R}^2} \underbrace{\sum_{i=1}^{n}\left(w_1 x_1^{(i)} + w_2 x_2^{(i)} - y^{(i)}\right)^2}_{\text{MSE}} + \underbrace{\lambda\left(w_1^2 + w_2^2\right)}_{R}$$

with $\lambda > 0$. What is $\hat{w}$ in the limit as $\lambda \to 0$ from above? Hint: It is not necessary to formally take the limit; just assume λ is vanishingly small but positive.

Key observations:

(1) MSE will be 0 (if $\lambda \to 0$)
↑ infinite number of solutions

(2) Regularizer will choose among solutions with MSE 0

$w_1 x_1 + w_2 x_2 = y$

$\Rightarrow w_1 x_1 + 2w_2 x_1 = 5x_1$

$\Rightarrow w_1 + 2w_2 = 5$

solve $\min_w \; w_1^2 + w_2^2$

s.t. $w_1 + 2w_2 = 5$

$\Rightarrow \hat{w} = (1, 2)$

21. **[Extra credit. Not attempting this question will not affect your grade.]** Consider linear regression on 2-dimensional data, where the features of the i-th data point are denoted $(x_1^{(i)}, x_2^{(i)}) \in \mathbb{R}^2$ and the target of the i-th data point is $y^{(i)} \in \mathbb{R}$. There are n training data points, $\{(x_1^{(i)}, x_2^{(i)}), y^{(i)}\}_{i=1}^n$. Assume that the following always holds in the training data, for all $i = 1, 2, \ldots, n$:

$$x_2^{(i)} = 2x_1^{(i)}$$
$$y^{(i)} = 5x_1^{(i)}.$$

2. [1 point] Now suppose we train a Lasso regression model, i.e., we solve

$$\hat{w} = \arg \min_{(w_1, w_2) \in \mathbb{R}^2} \sum_{i=1}^{n} \left(w_1 x_1^{(i)} + w_2 x_2^{(i)} - y^{(i)}\right)^2 + \lambda\left(|w_1| + |w_2|\right)$$

with $\lambda > 0$. What is $\hat{w}$ in the limit as $\lambda \to 0$ from above? Hint: It is not necessary to formally take the limit; just assume λ is vanishingly small but positive.

solve $\min |w_1| + |w_2|$

s.t. $w_1 + 2w_2 = 5$

$\hat{w} = (0, 5/2)$

$\|(0, 5/2)\|_2^2 = 6.25$

$\|(1, 2)\|_2^2 = 5$

$2.5^2 = 6.25$

Non-parametric methods: Nearest neighbors

CSE 446/546

Sewoong Oh & Pang Wei Koh

Parametric vs non-parametric

linear reg
logistic reg
NNs ...

- A model is <u>parametric</u> if # parameters does not depend on # samples

- A model is <u>non-parametric</u> if # parameters increases with # samples
  - Does not mean absence of parameters!

$\{w^T x : w \in \mathbb{R}^d\}$

Why non-parametric models?

$x \in \mathbb{R}, \quad y \in \{0, 1\}$

Idea: Scale model complexity with data

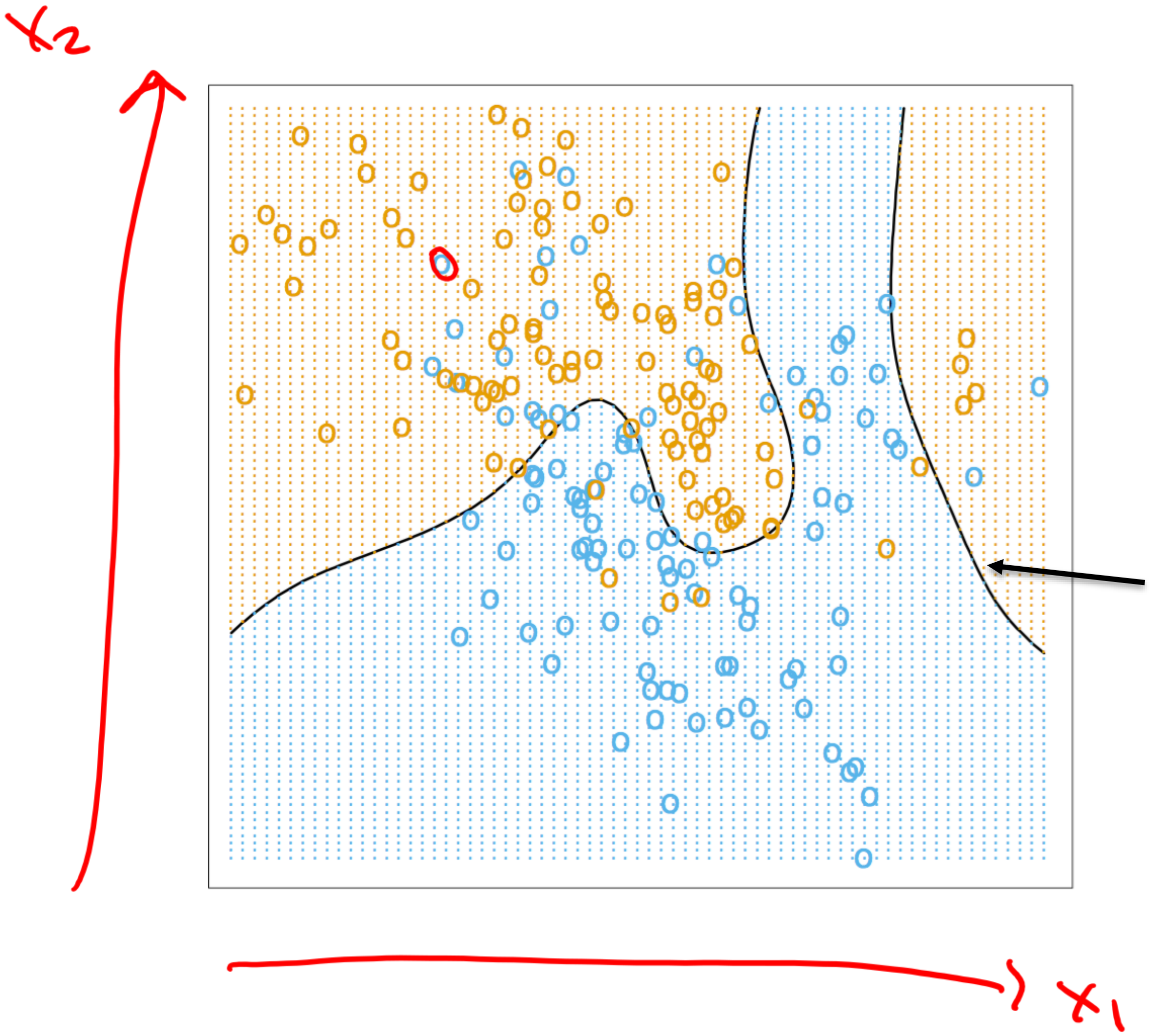
This lecture: k nearest neighbors

- Assume we have a classification task
- To classify a new point x:
  - Find its k nearest neighbors in the training data
  - Set y to be the majority vote of the labels of these nearest neighbors

- Design choices / hyperparameters:
  - Number of nearest neighbors k
  - Distance metric
  - Aggregation method

Example: Bayes classifier

$x \in \mathbb{R}^2$



Training data:

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

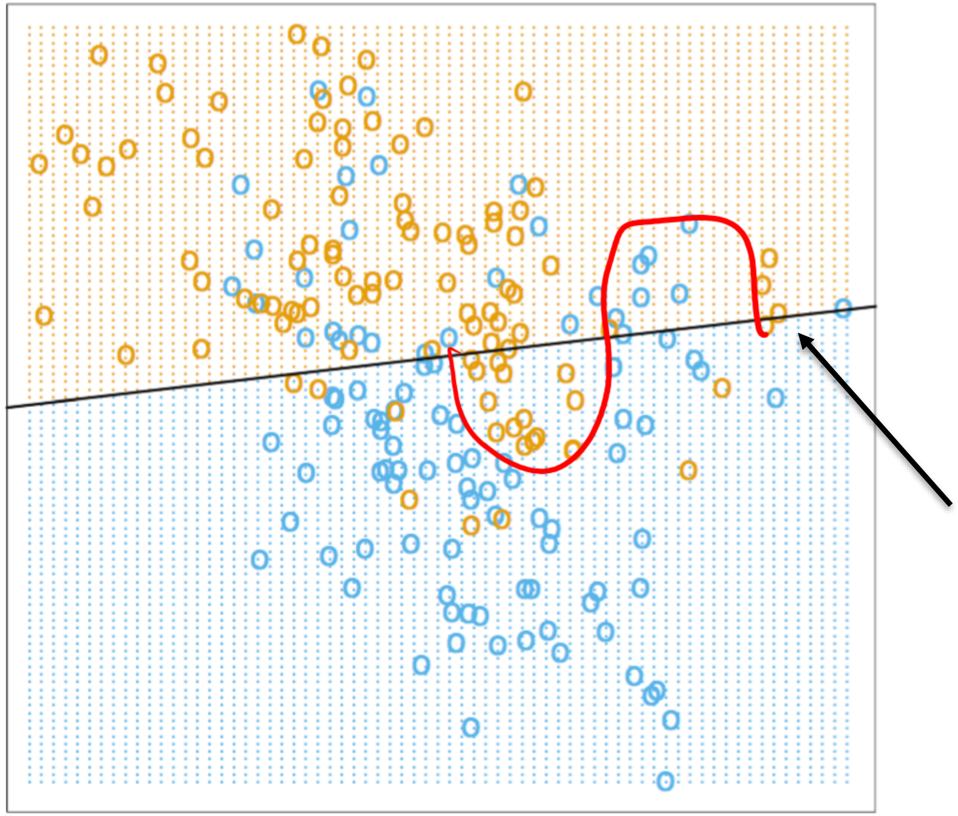
Optimal Bayes classifier:

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

- 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:

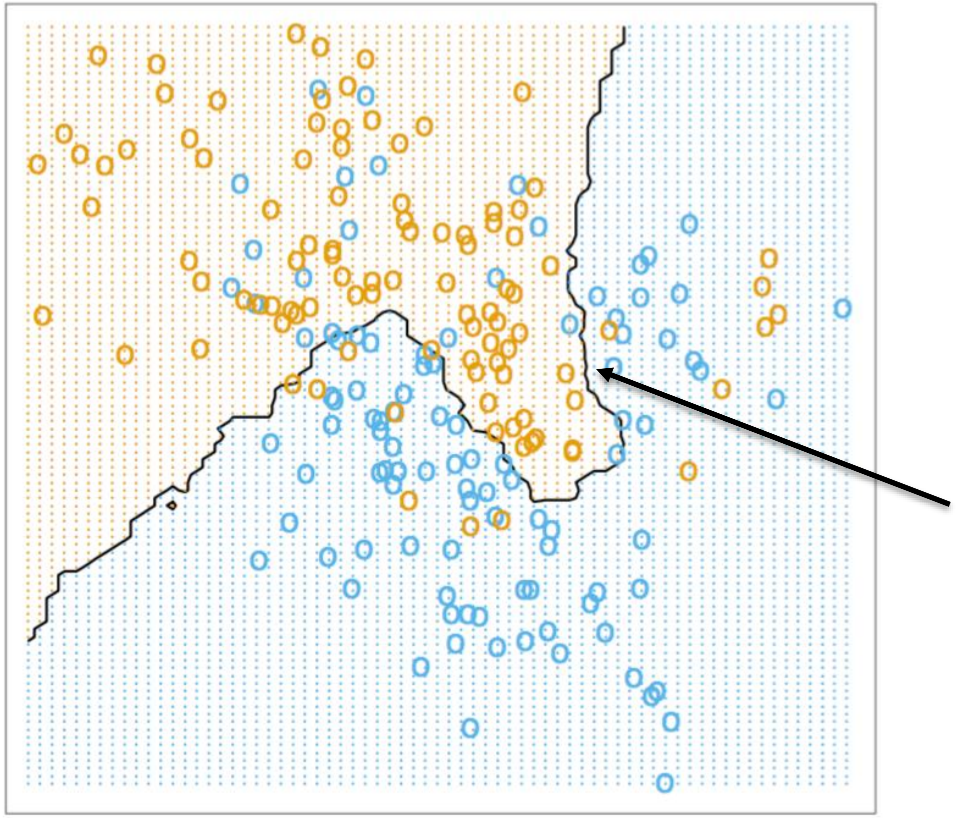
$$x^T w + b = 0$$

Predicted label: +1

Predicted label: -1

Figures from Hastie et al.

$k = 15$ nearest neighbors boundary



Training data:

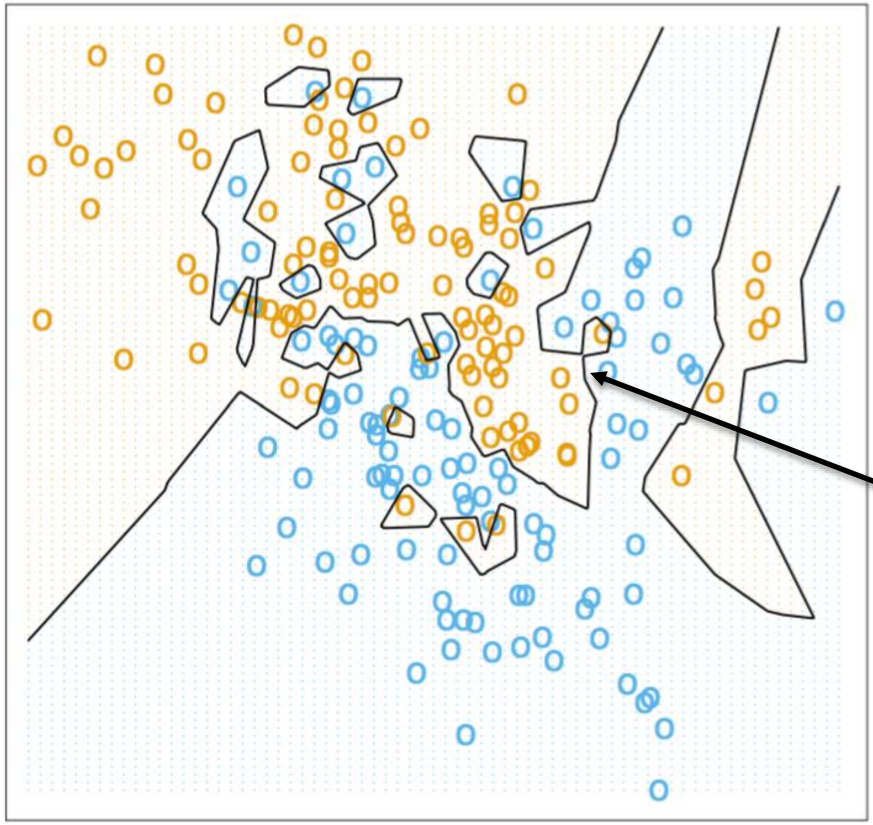
- True label: +1
- True label: -1

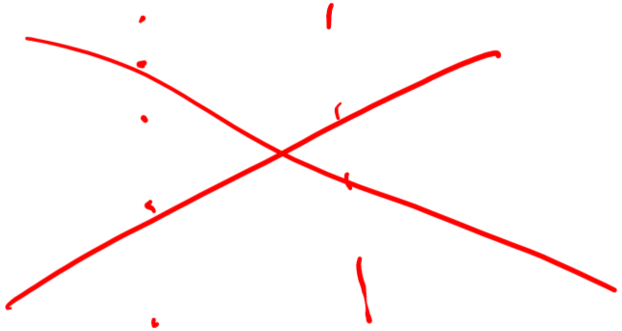
15 nearest neighbors decision boundary (majority vote)

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

Figures from Hastie et al.

$k = 1$ nearest neighbor boundary





Training data:

True label: +1

True label: -1

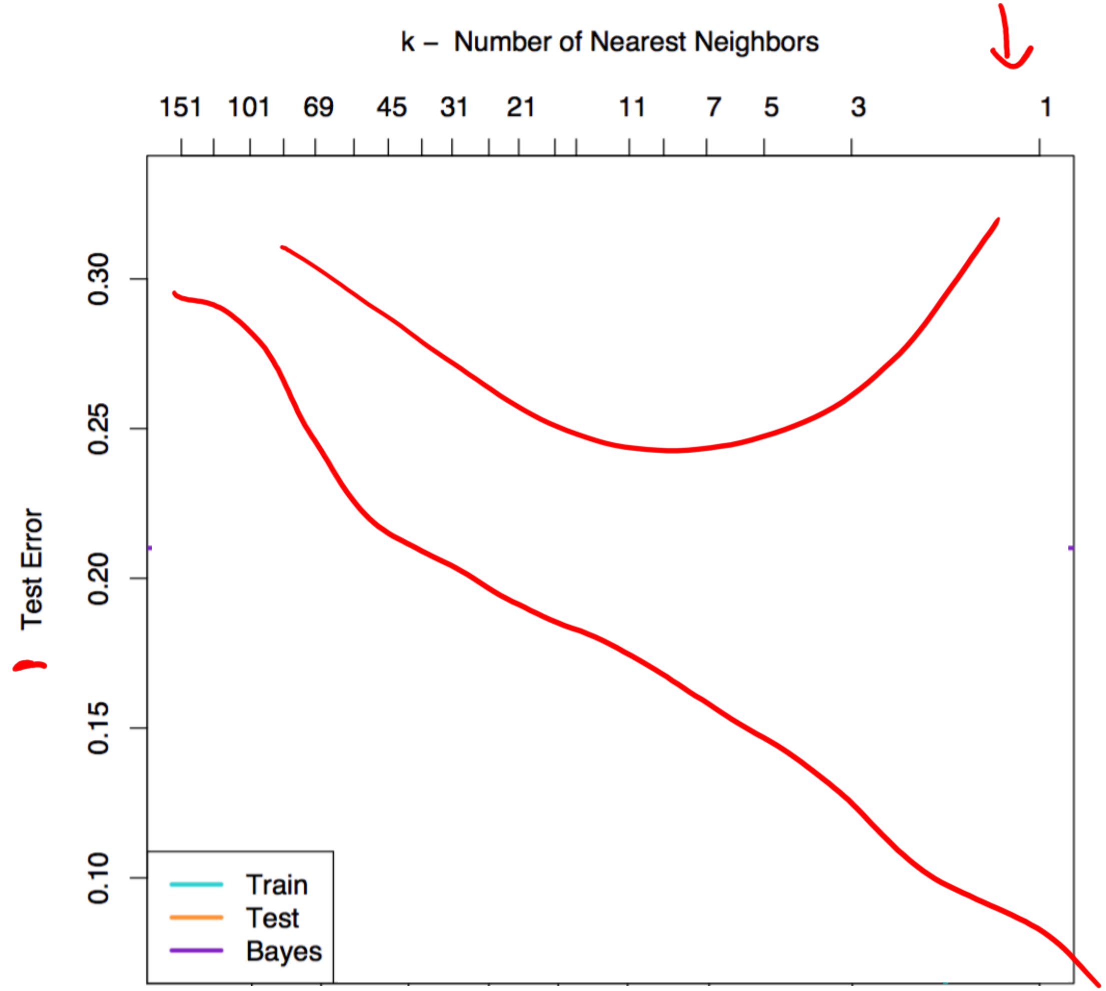
1 nearest neighbor decision boundary (majority vote)

Predicted label: +1

Predicted label: -1

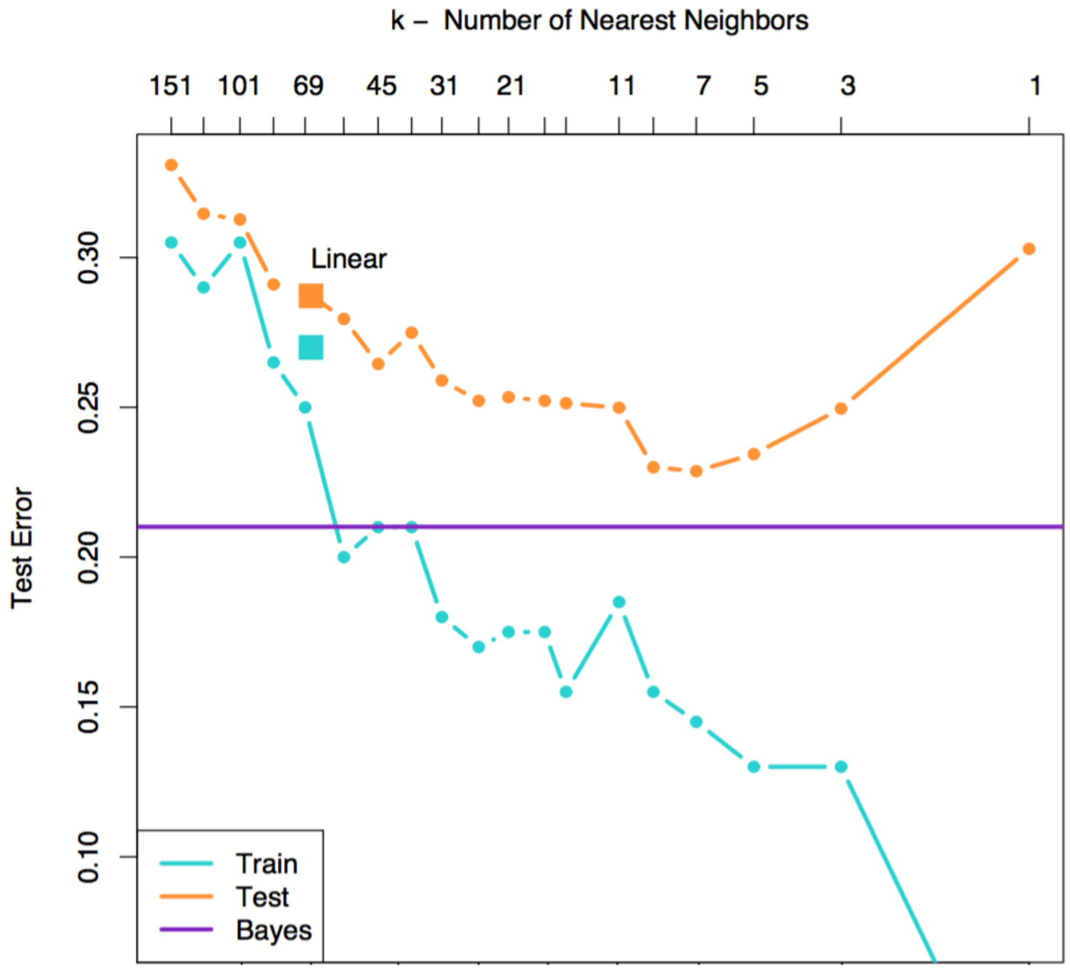
Figures from Hastie et al.

k nearest neighbors error



Figures from Hastie et al.

k nearest neighbors error



As k gets larger:

Bias: ↑

Variance: ↓

Figures from Hastie et al.

Parametric vs non-parametric

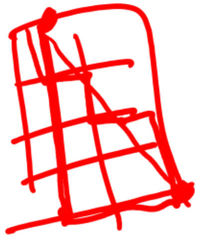
- A model is <u>parametric</u> if # parameters does not depend on # samples

After training, discard training data

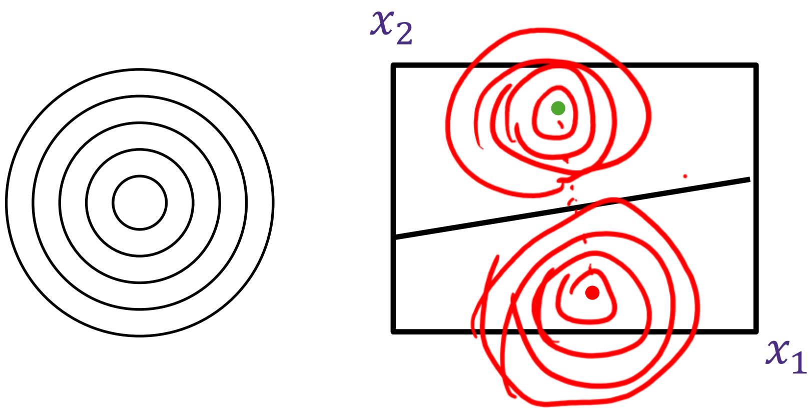
- A model is <u>non-parametric</u> if # parameters increases with # samples

Typically, keep training data

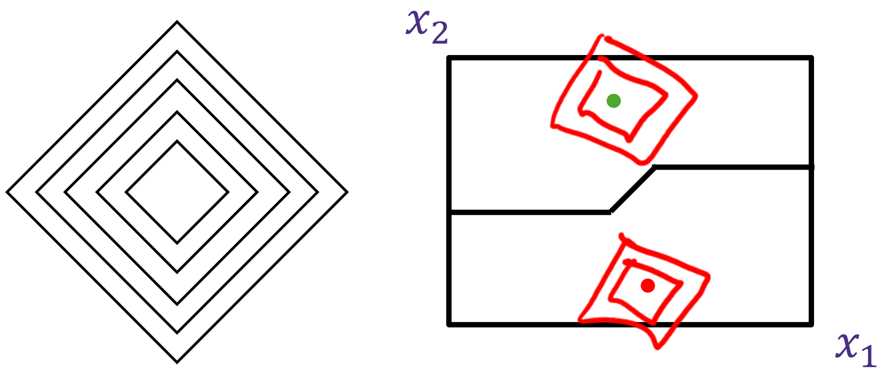
Notable distance metrics & level sets



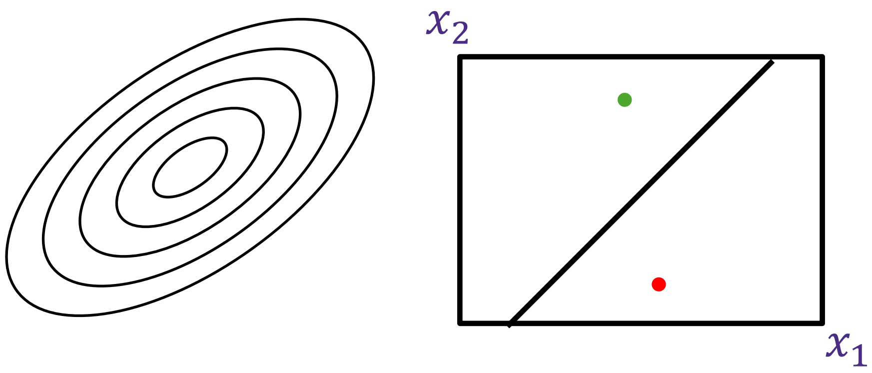
ℓ_2 norm (Euclidean) $d(u,v) = \|u-v\|_2^2$



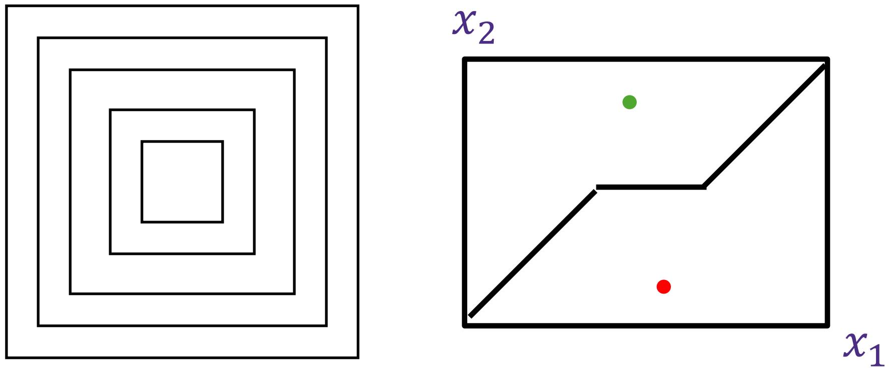
ℓ_1 norm (Manhattan, taxicab) $d(u,v) = \|u-v\|_1 = \sum_{i=1} |u_i - v_i|$



Mahalanobis norm $d(u,v) = (u-v)^T M (u-v)$

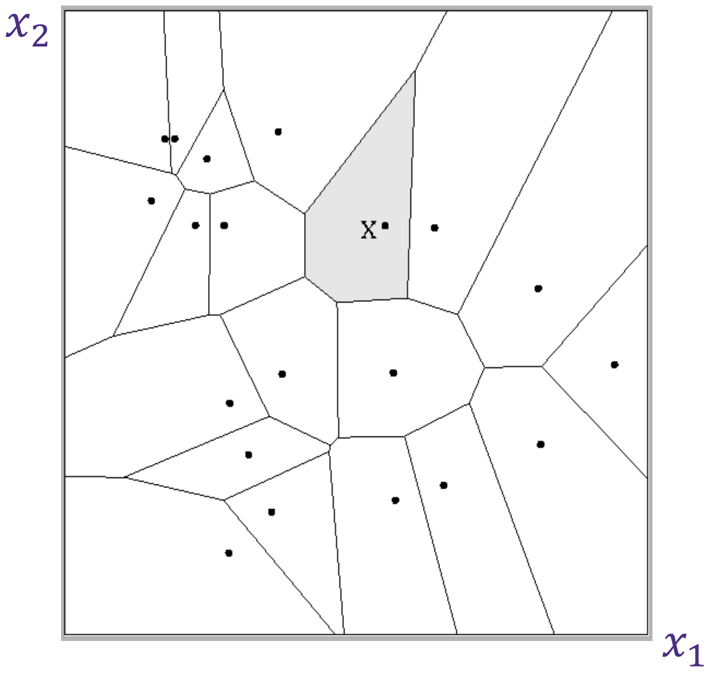


ℓ_∞ norm (max)

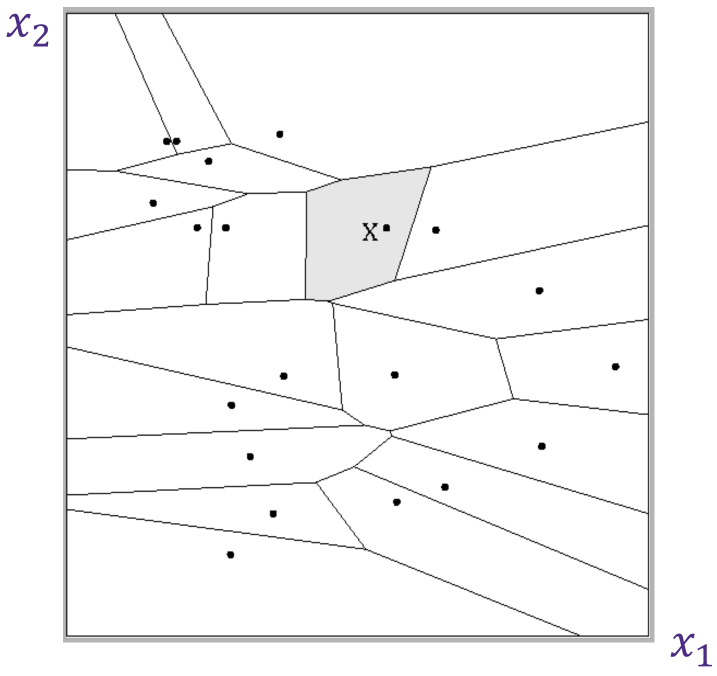


Example: distance metrics with $k = 1$ NN

$d(x, x') = (x_1 - x_1')^2 + (x_2 - x_2')^2$



$d(x, x') = (x_1 - x_1')^2 + 9(x_2 - x_2')^2$



Learned distance metrics

Training data

Test data

Dog

Cat

1-NN classification: Theoretical guarantees

Given test point x, let x_{NN} be nearest neighbor in D_{train}, y, y_{NN} binary

Error if $y \neq y_{NN}$

Case 1: $y_{NN} = 1$, $y = 0$ w.p. $p(y=1 \mid x_{NN})\, p(y=0 \mid x)$

Case 2: $y_{NN} = 0$, $y = 1$ w.p. $p(y=0 \mid x_{NN})\, p(y=1 \mid x)$

As $n \to \infty$, $p(y \mid x_{NN}) \to p(y \mid x)$ (under regularity conditions)

Error:

$$2\, p(y=1 \mid x)\, p(y=0 \mid x) \text{ as } n \to \infty$$

$$= 2p^*(1-p^*)$$

$$\leq 2p^*$$

Define Bayes error

$$p^* = \min\{p(y=1 \mid x), p(y=0 \mid x)\}$$

1-NN classification: Theoretical guarantees

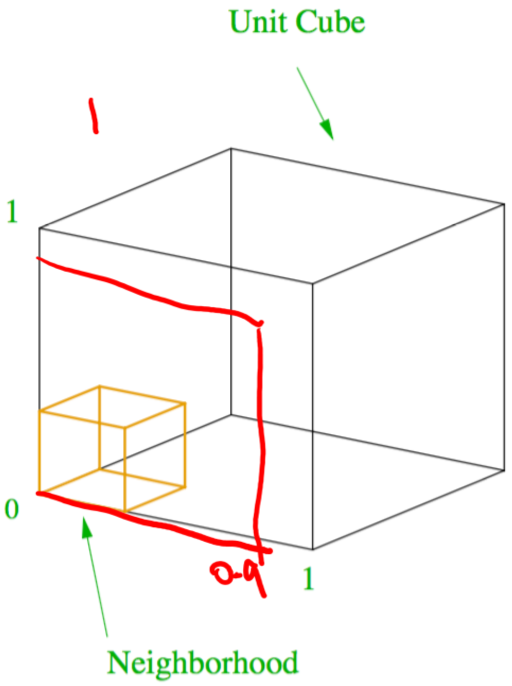
Theorem[Cover, Hart, 1967] If P_X is supported everywhere in $\mathbb{R}^d$ and $P(Y = 1|X = x)$ is smooth everywhere, then as $n \to \infty$ the 1-NN classification rule has error at most twice the Bayes error rate.

x

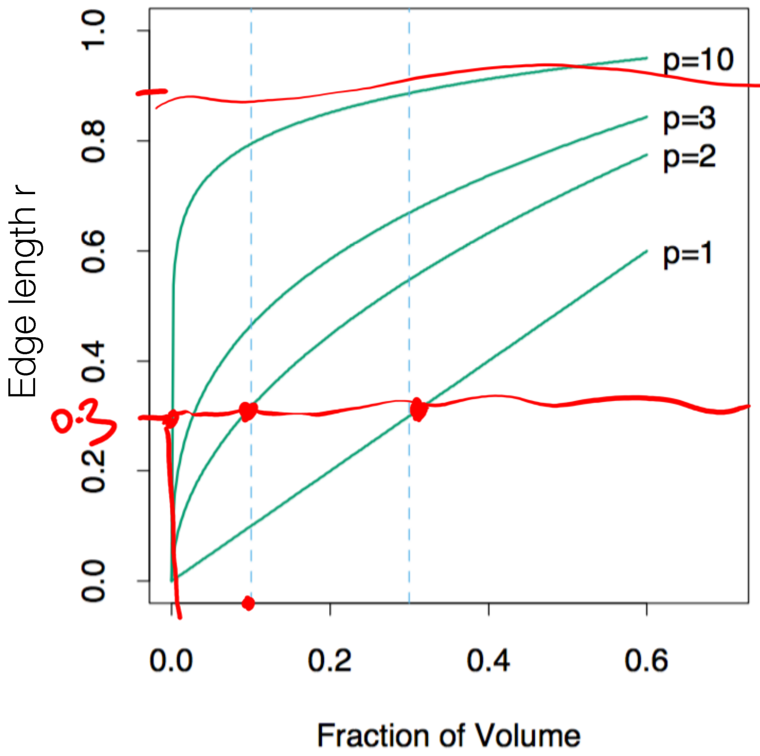
p(y=1|x) = 99%

p(y=0|x) = 1%

Curse of dimensionality, example 1



side length r

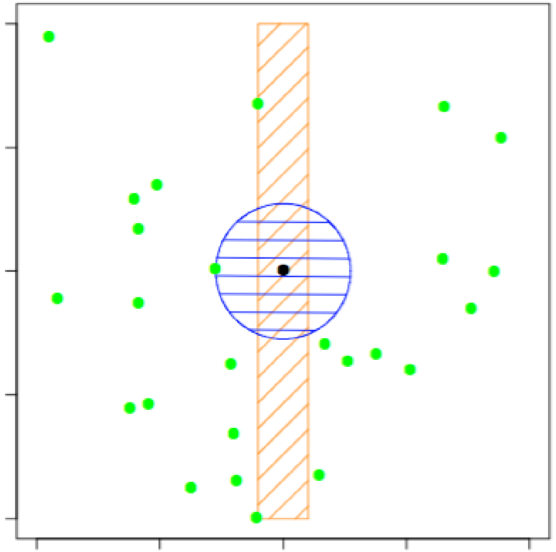


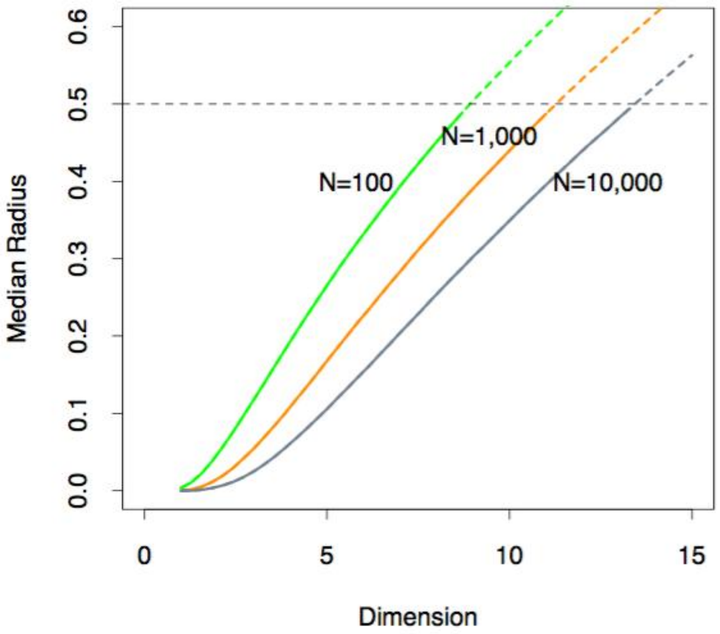
X is uniformly distributed over $[0,1]^p$. What is $\mathbb{P}(X \in [0,r]^p)$?

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

Curse of dimensionality, example 2

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

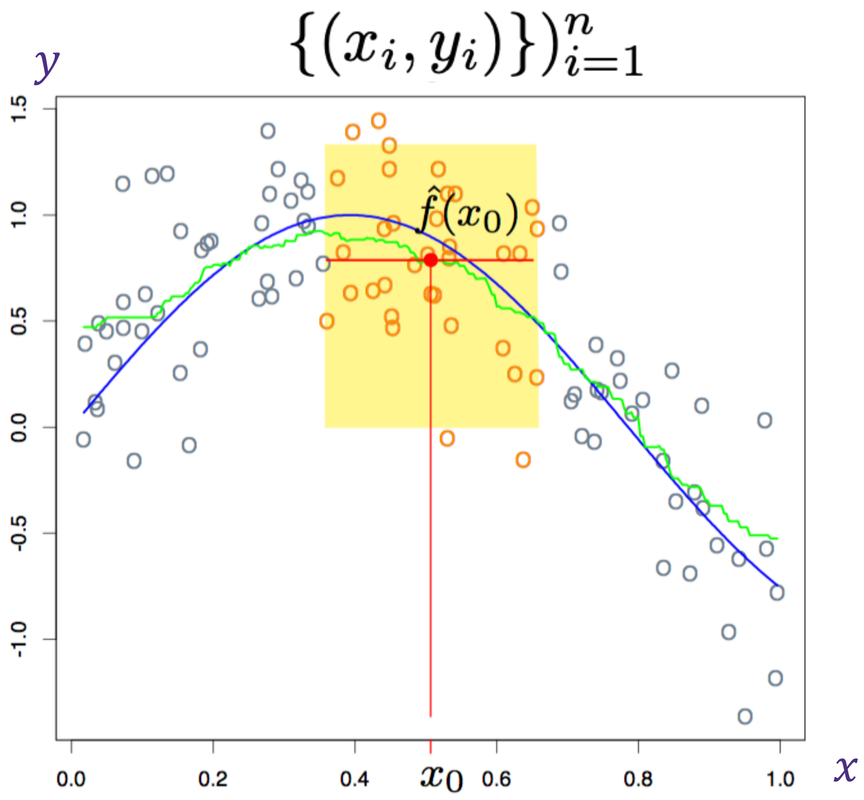




What is the median distance from a point at origin to its 1NN?

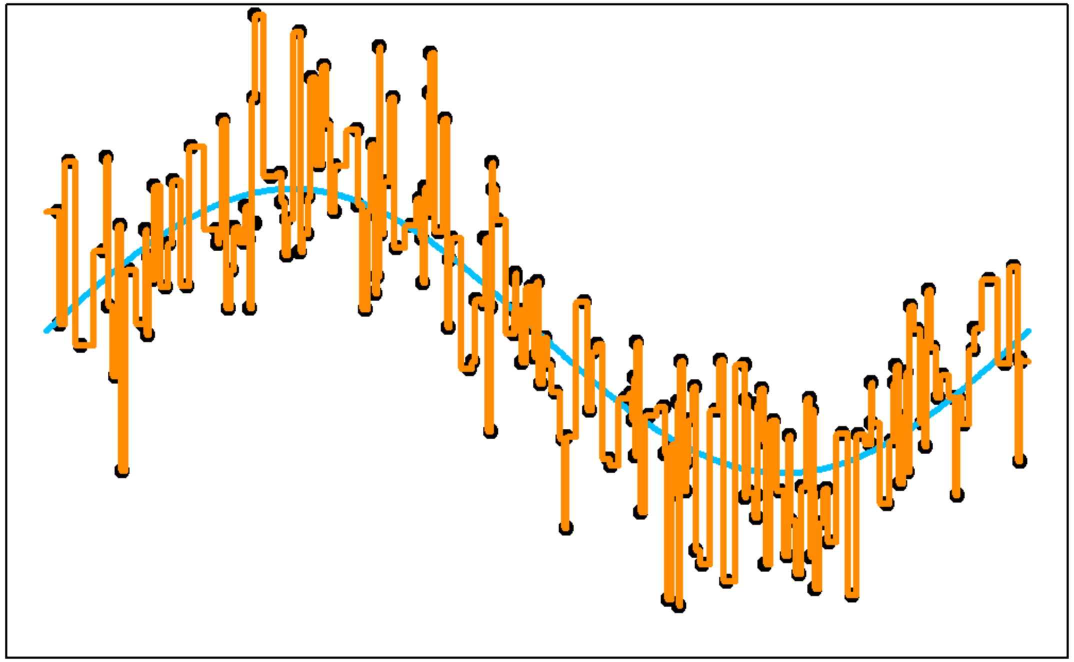
How many samples do we need so that a median Euclidean distance is within r?

Nearest neighbor regression



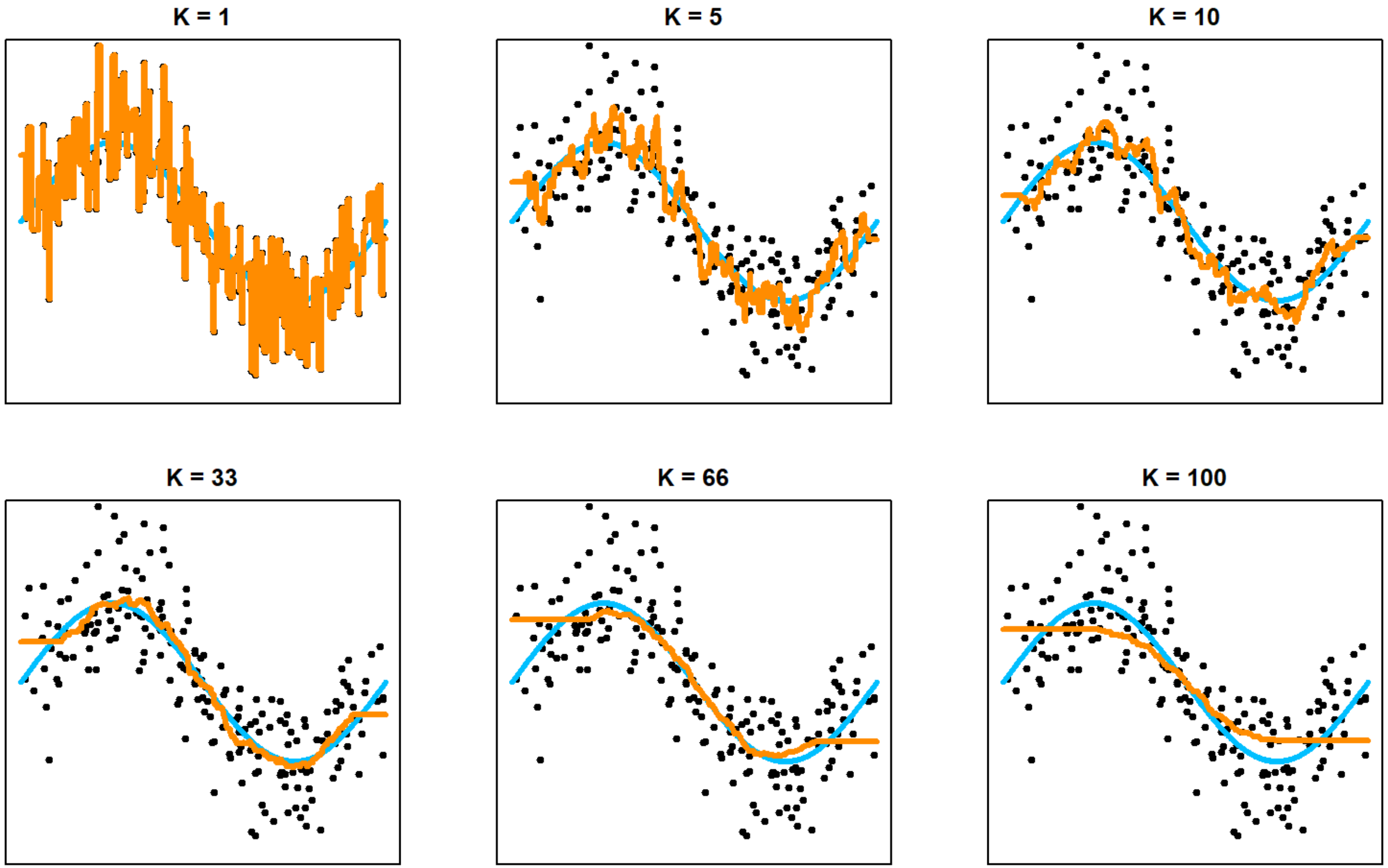
Overfitting

1-Nearest Neighbor Regression



Figures from Ruoqing Zhu, Stat 542

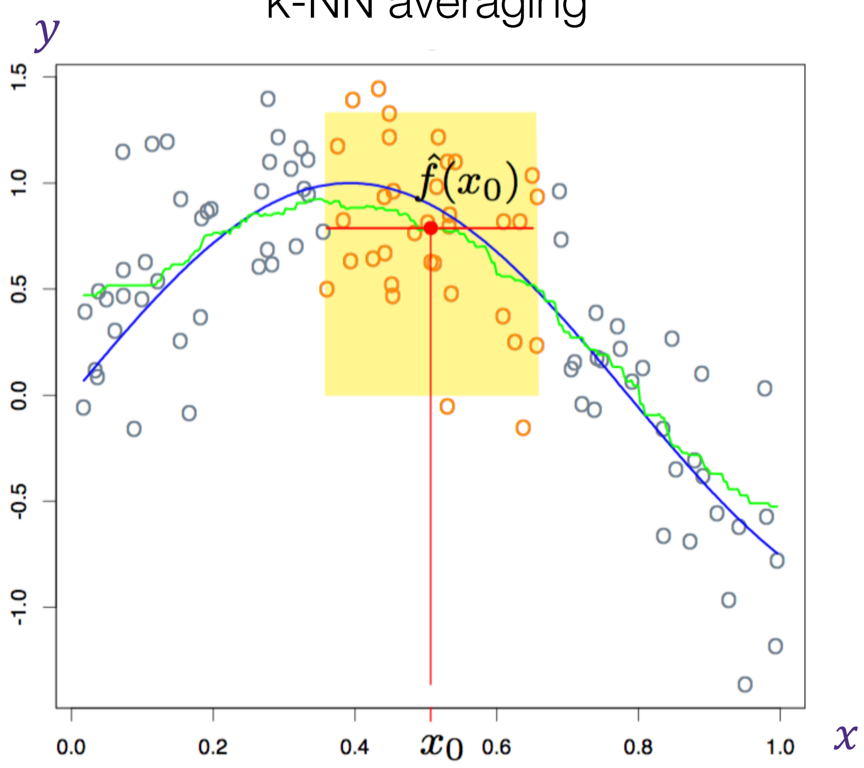
Bias vs variance



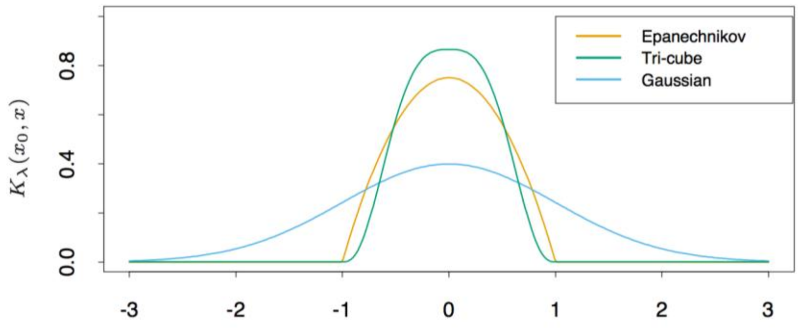
Figures from Ruoqing Zhu, Stat 542

Smoothed nearest neighbor regression

k-NN averaging



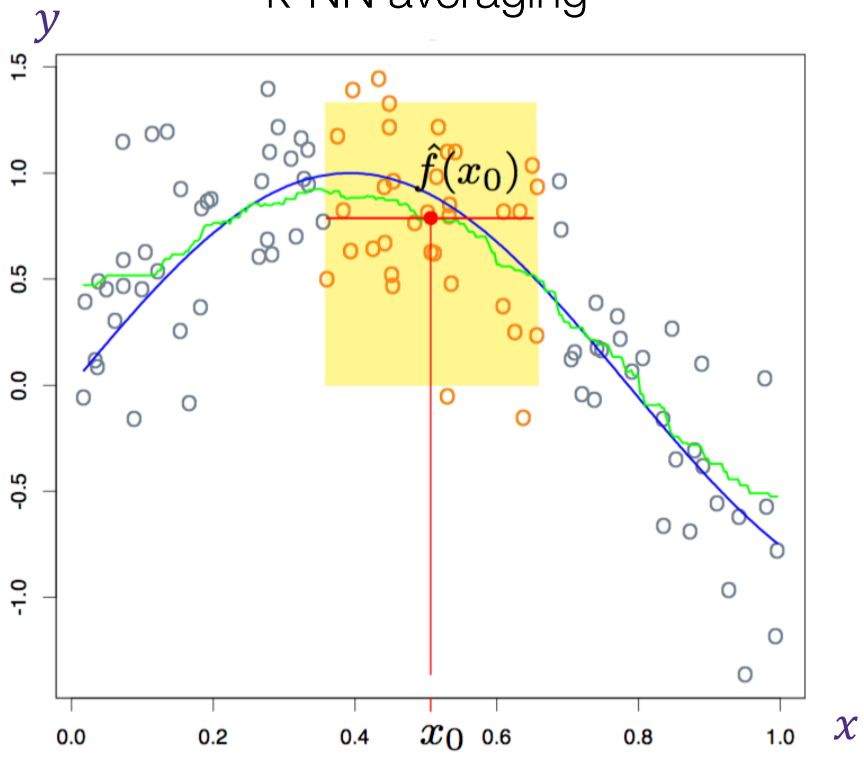
smoothing: $K(x, y)$



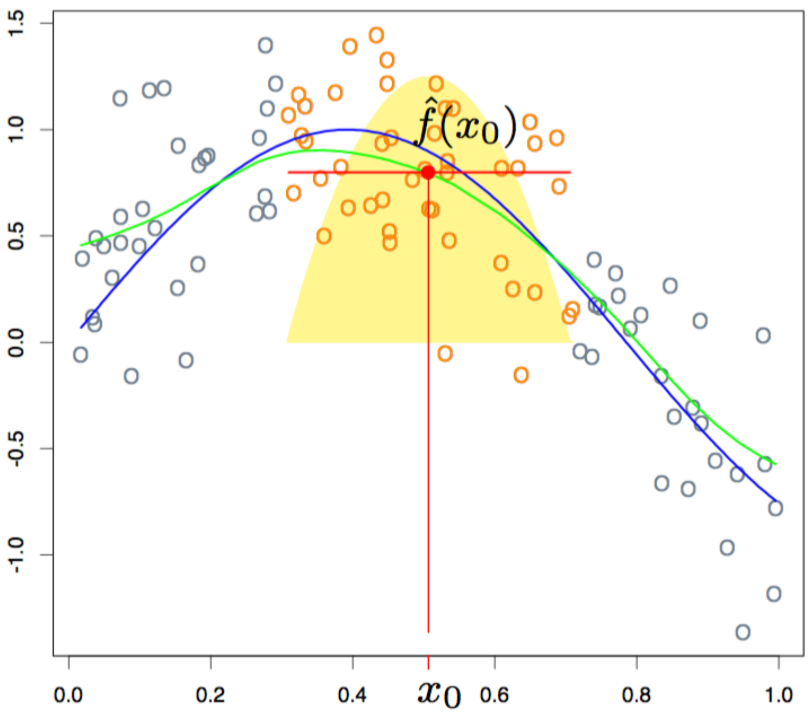
$$\hat{f}(x) = \frac{\sum_{i=1}^{n} K\left(x, x^{(i)}\right) y^{(i)}}{\sum_{i=1}^{n} K\left(x, x^{(i)}\right)}$$

Smoothed nearest neighbor regression

k-NN averaging



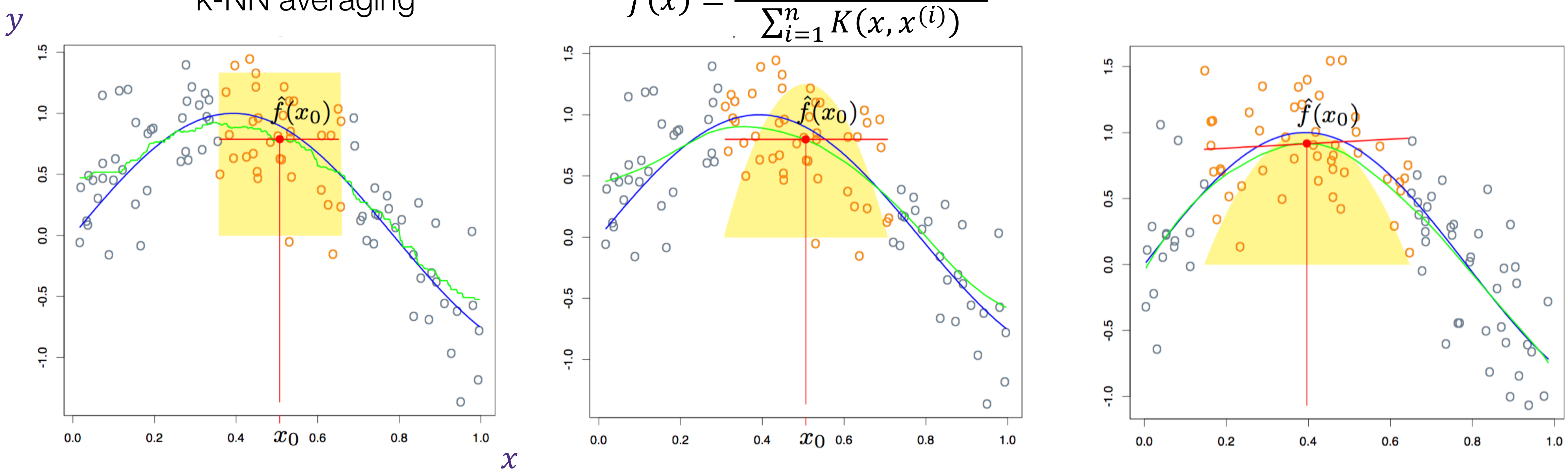
$$\hat{f}(x) = \frac{\sum_{i=1}^{n} K\left(x, x^{(i)}\right) y^{(i)}}{\sum_{i=1}^{n} K\left(x, x^{(i)}\right)}$$



Locally linear regression

k-NN averaging

$$\hat{f}(x) = \frac{\sum_{i=1}^{n} K\left(x, x^{(i)}\right) y^{(i)}}{\sum_{i=1}^{n} K\left(x, x^{(i)}\right)}$$



Have we seen non-parametric methods before?

- Kernel methods can be non-parametric:

$$f(x) = \sum_{i=1}^{n} \alpha_i \, K\left(x^{(i)}, x\right)$$

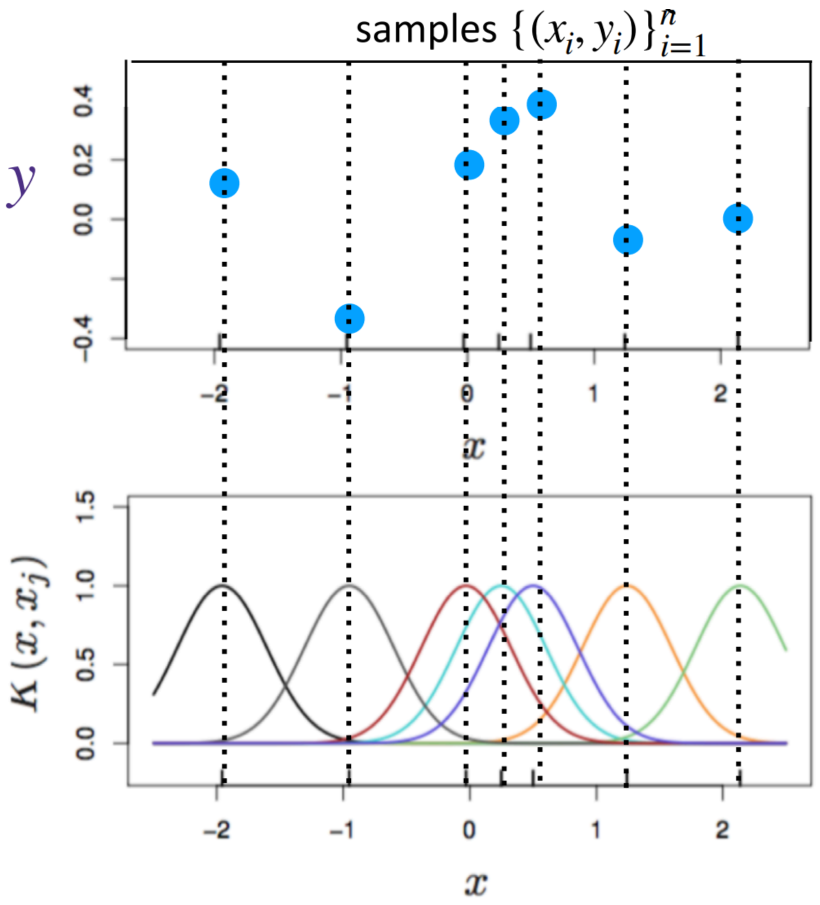
parameters goes up with # data

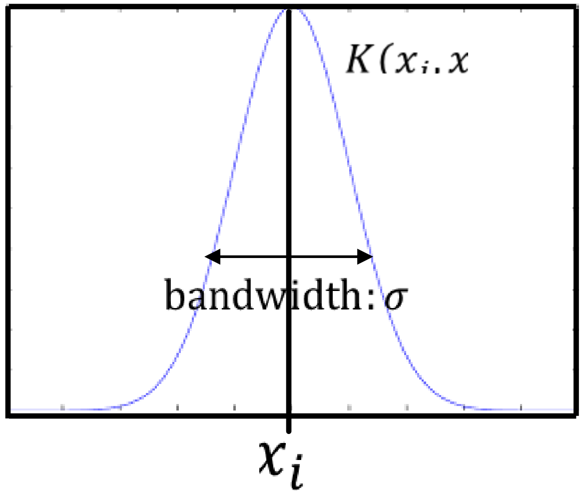
- Compare with (smoothed) nearest neighbors:

$$\hat{f}(x) = \frac{\sum_{i=1}^{n} K\left(x, x^{(i)}\right) y^{(i)}}{\sum_{i=1}^{n} K\left(x, x^{(i)}\right)}$$

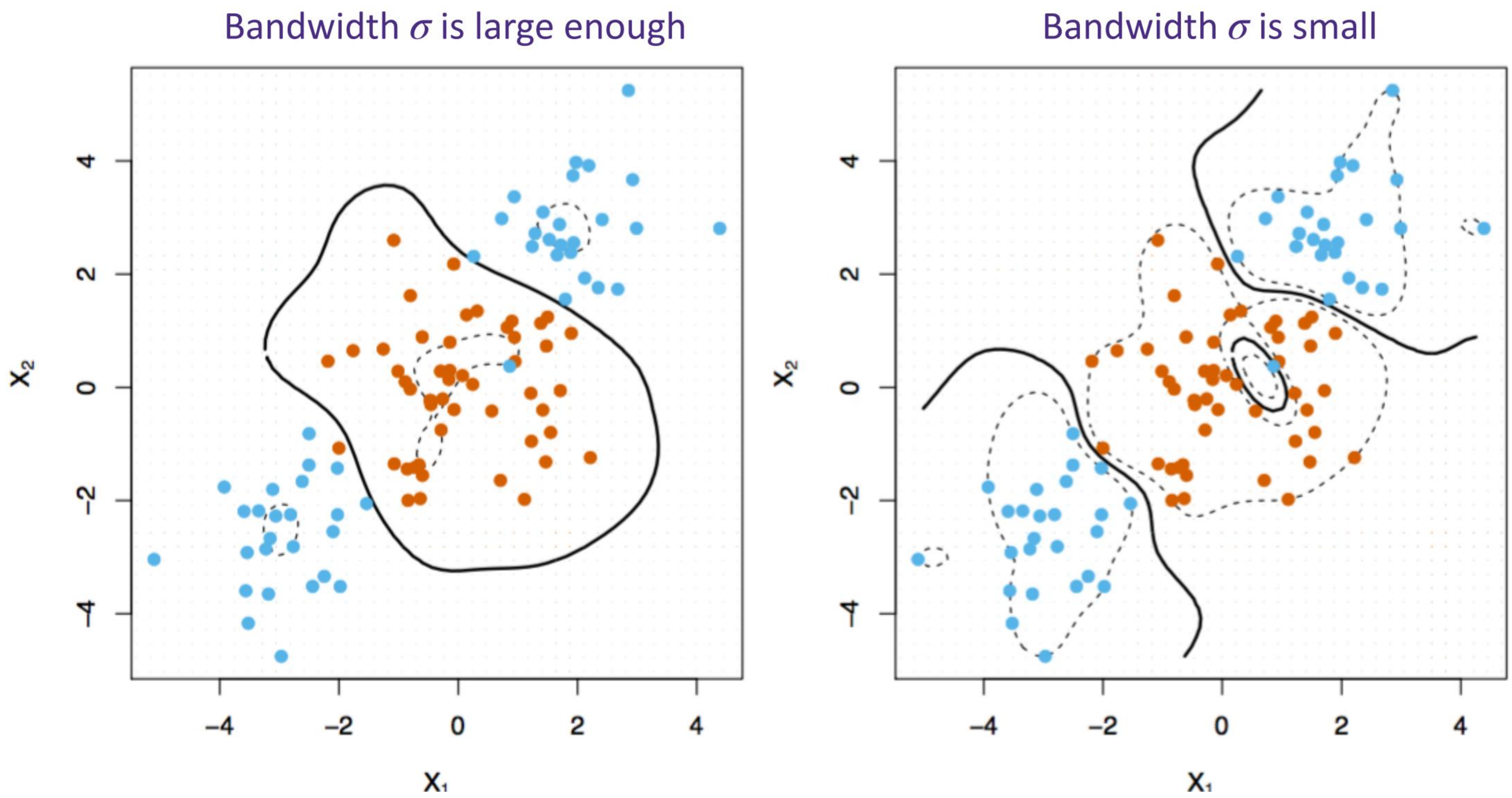
The Radial Basis Function (RBF) kernel $\exp\left(-\frac{\|x^{(i)}-x\|_2^2}{2\sigma^2}\right)$

$$f(x) = \sum_{i=1}^{n} \alpha_i K\left(x^{(i)}, x\right)$$





The Radial Basis Function (RBF) kernel $\exp\left(-\frac{\|x^{(i)}-x\|_2^2}{2\sigma^2}\right)$



Kernel methods

$$f(x) = \sum_{i=1}^{n} \alpha_i \, K\left(x^{(i)}, x\right)$$

- Learning with RBF kernels can be seen as a soft, learned version of “nearest” neighbors
- $K\left(x^{(i)}, x\right) = \phi\left(x^{(i)}\right)^{\top} \phi(x)$ defines “similarity” between $x^{(i)}$ and x
- How many parameters?

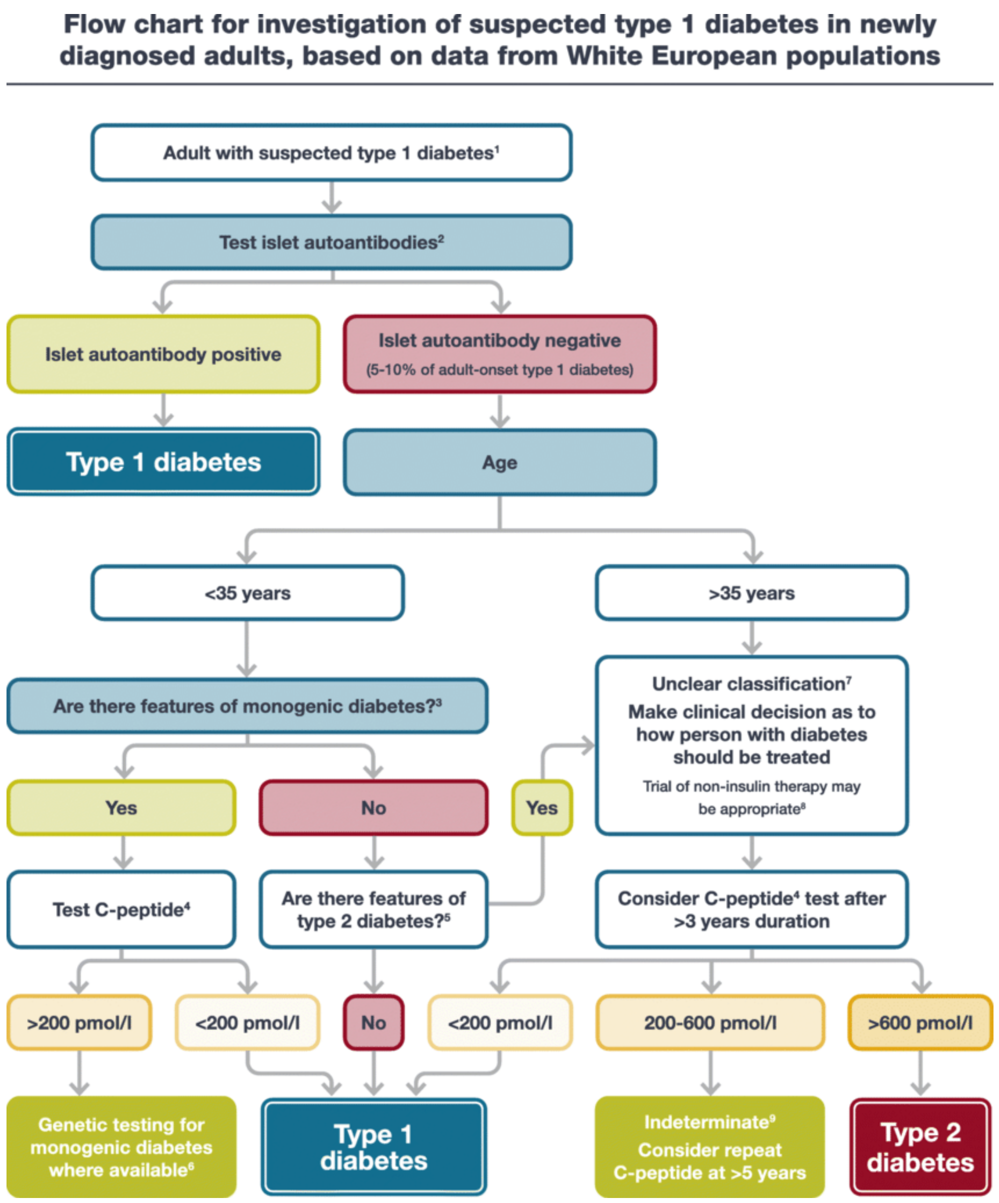
Takeaways

- k-NN is very simple to explain and implement
- No training! But inference can still be computationally demanding.
- 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)

Non-parametric methods: Trees

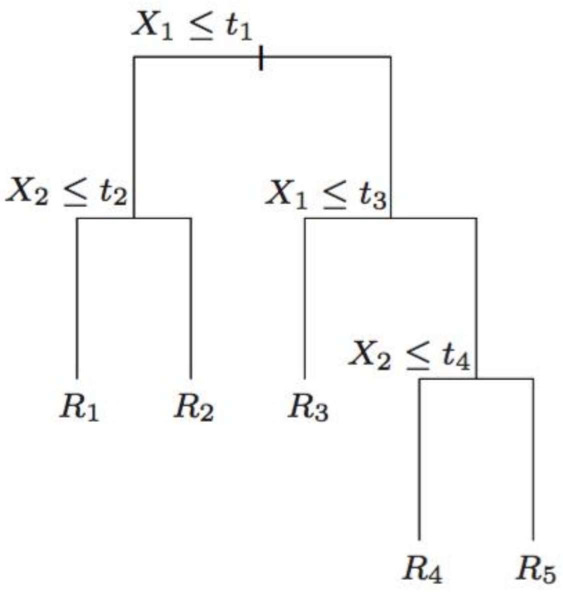
CSE 446/546

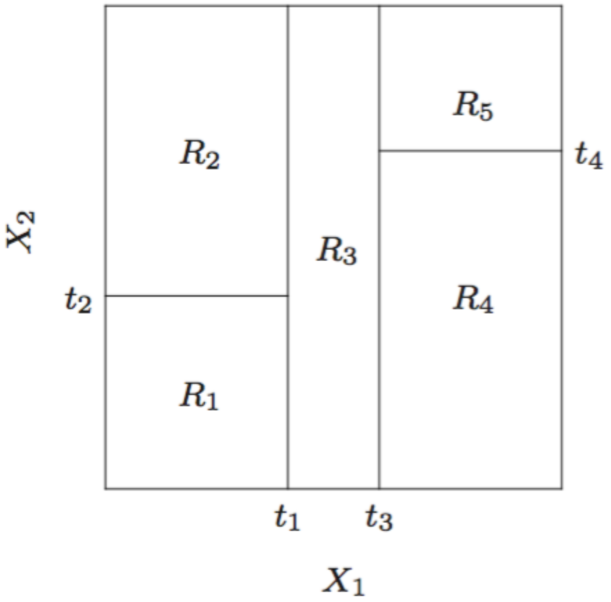
Sewoong Oh & Pang Wei Koh



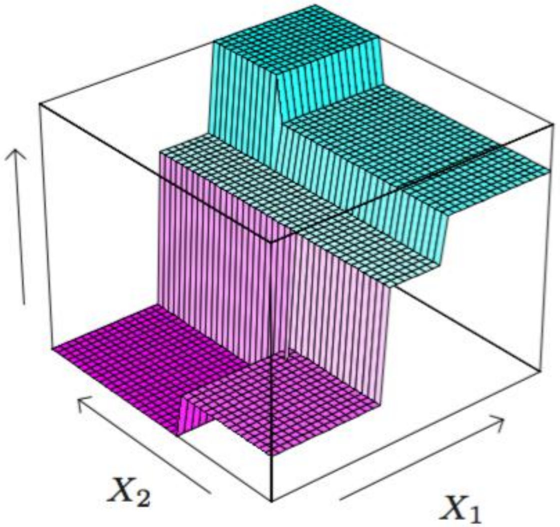
Holt et al., 2021

Decision / Regression trees





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



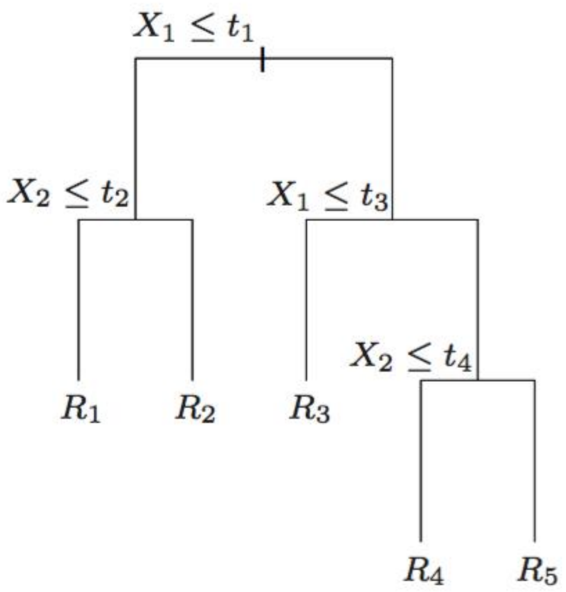
Generic algorithm for building trees

1. Start from empty decision tree
2. Recursively, for each node:
   - Iterate through all features and compute how good it'd be to split on each feature
   - Split on the "best" feature
3. Prune

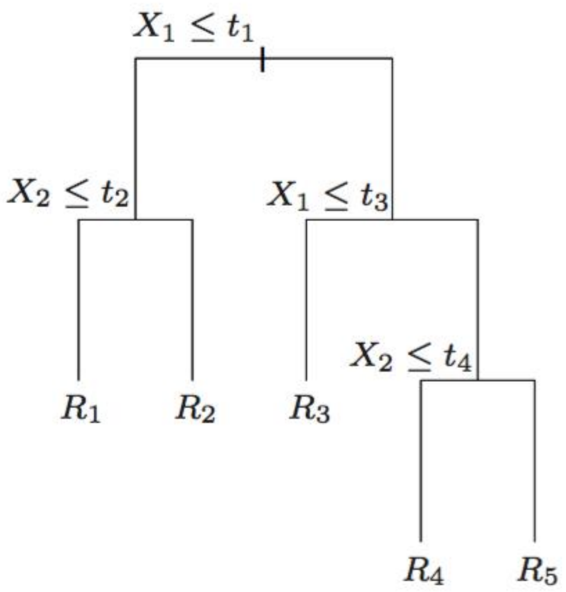
Design choices:

- Termination condition
- Tree complexity
- Splitting criterion
- Pruning

Splitting regression trees



Splitting decision trees



Interpreting trees

Trees are “easy” to interpret:

- You can explain how the classifier came to the conclusion it did

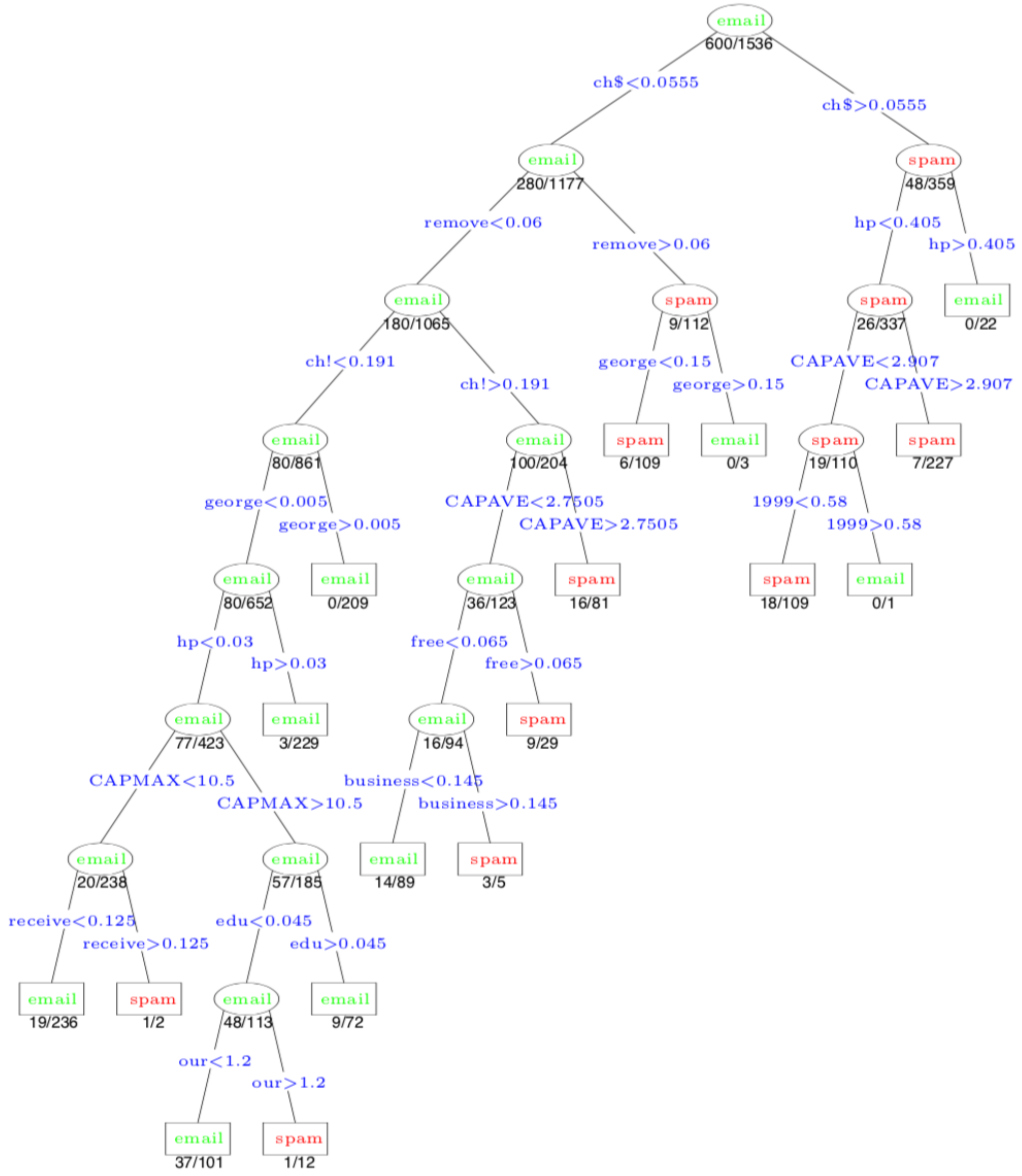
Interpreting trees

Trees are "easy" to interpret:

- You can explain <u>how</u> the classifier came to the conclusion it did

Trees are hard to interpret:

- Tough to explain <u>why</u> the classifier came to the conclusion it did
- Small changes in data can result in large difference in trees

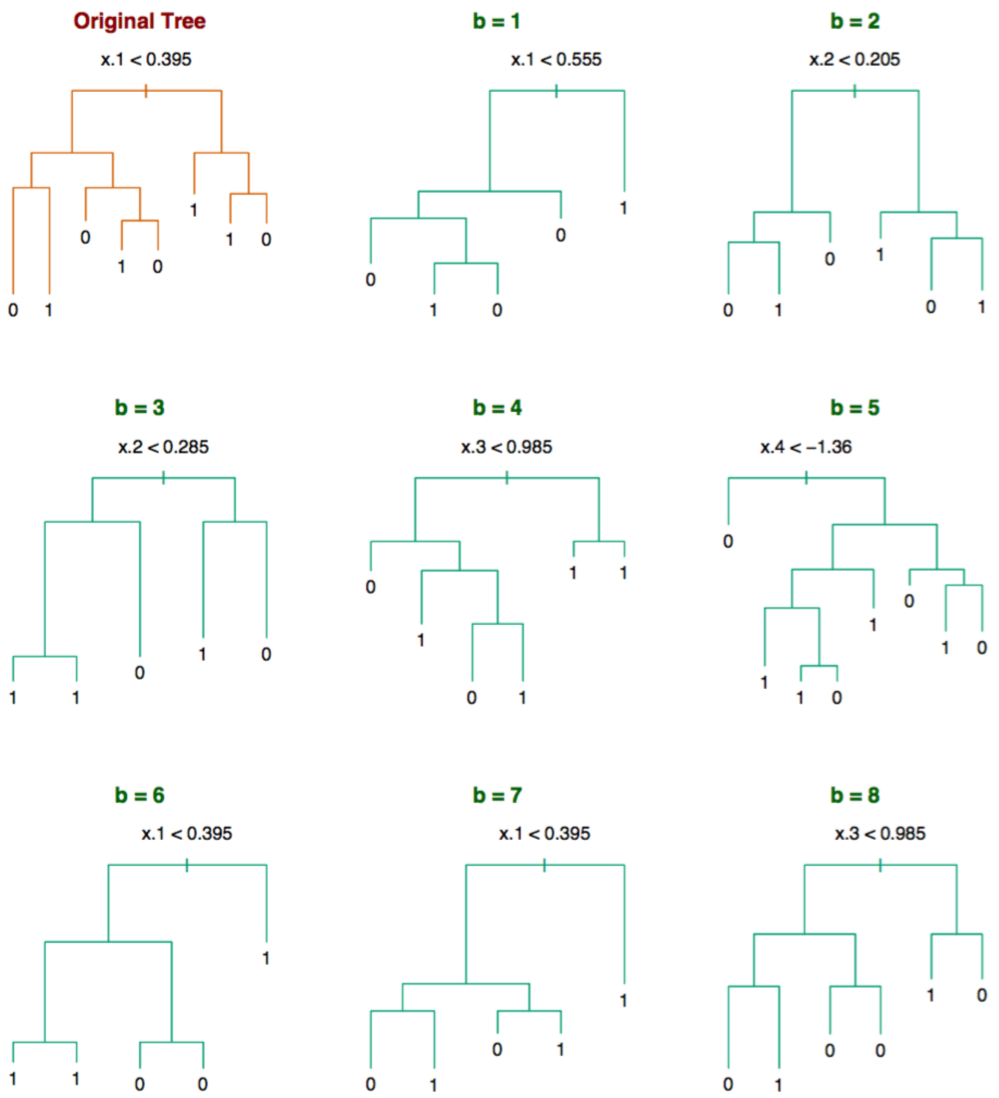


Summary so far

- Trees have bias, variance
- Deal with categorial variables well
- Intuitive, “interpretable”
- Good software exists
- Some theoretical guarantees

Random forests

- Forest = many trees
- Tree methods have low bias but high variance
- We can reduce variance by constructing many "lightly correlated" trees and averaging 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.

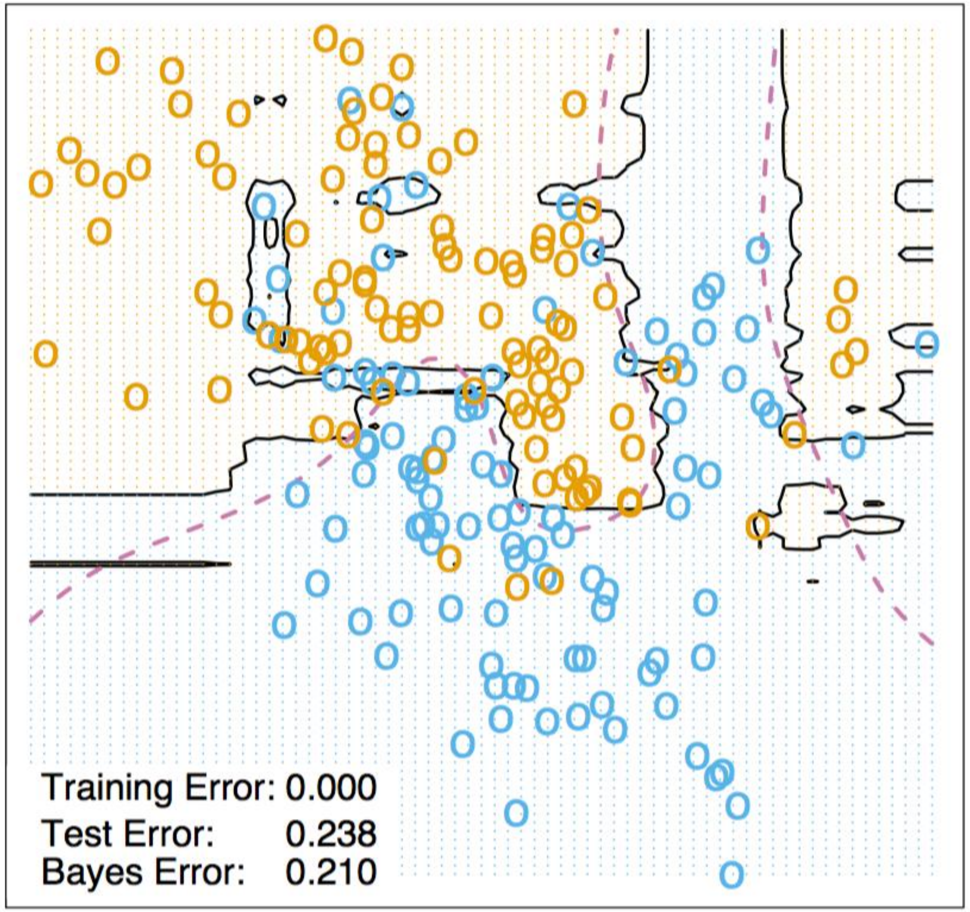
2. Output the ensemble of trees $\{T_b\}_1^B$.

To make a prediction at a new point x:

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

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

Random forests: Decision boundary example

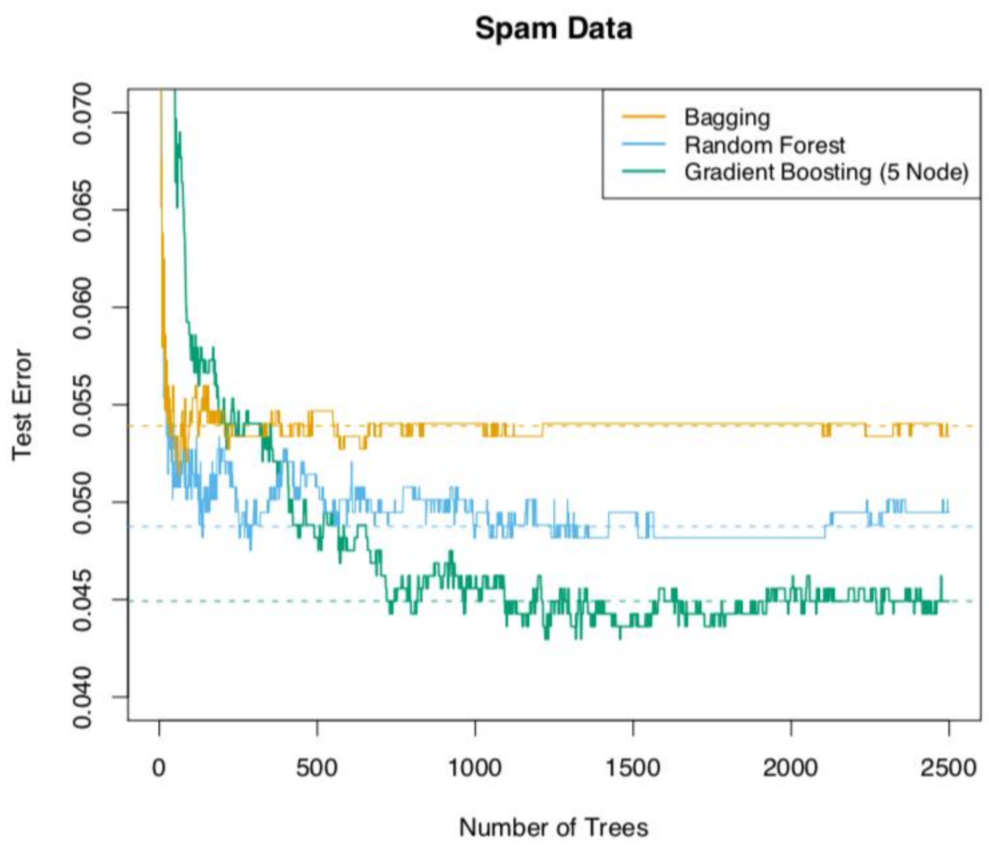


Random forests

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

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

The power of weakly correlated predictors



Bagging: Averaged trees on bootstrapped datasets using all d features

Random forest: Averaged trees on bootstrapped datasets using m randomly selected features

Takeaway: reducing correlation improves performance!

Summary so far

- Random forests have bias, variance
- Deal with categorical variables well
- Not that intuitive nor "interpretable"
- Gives some notion of confidence estimates
- Good software exists
- Some theoretical guarantees

Boosting and additive models

Instead of ensembling bootstrapped models, can we:

- Keep the idea of ensembling / combining simpler models, but
- Not necessarily have the models be identically distributed?

Key idea: Given a current collection of models, add a new model that focuses on what the previous models got wrong

Additive models

Forward stagewise additive models

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

Forward stagewise additive models

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

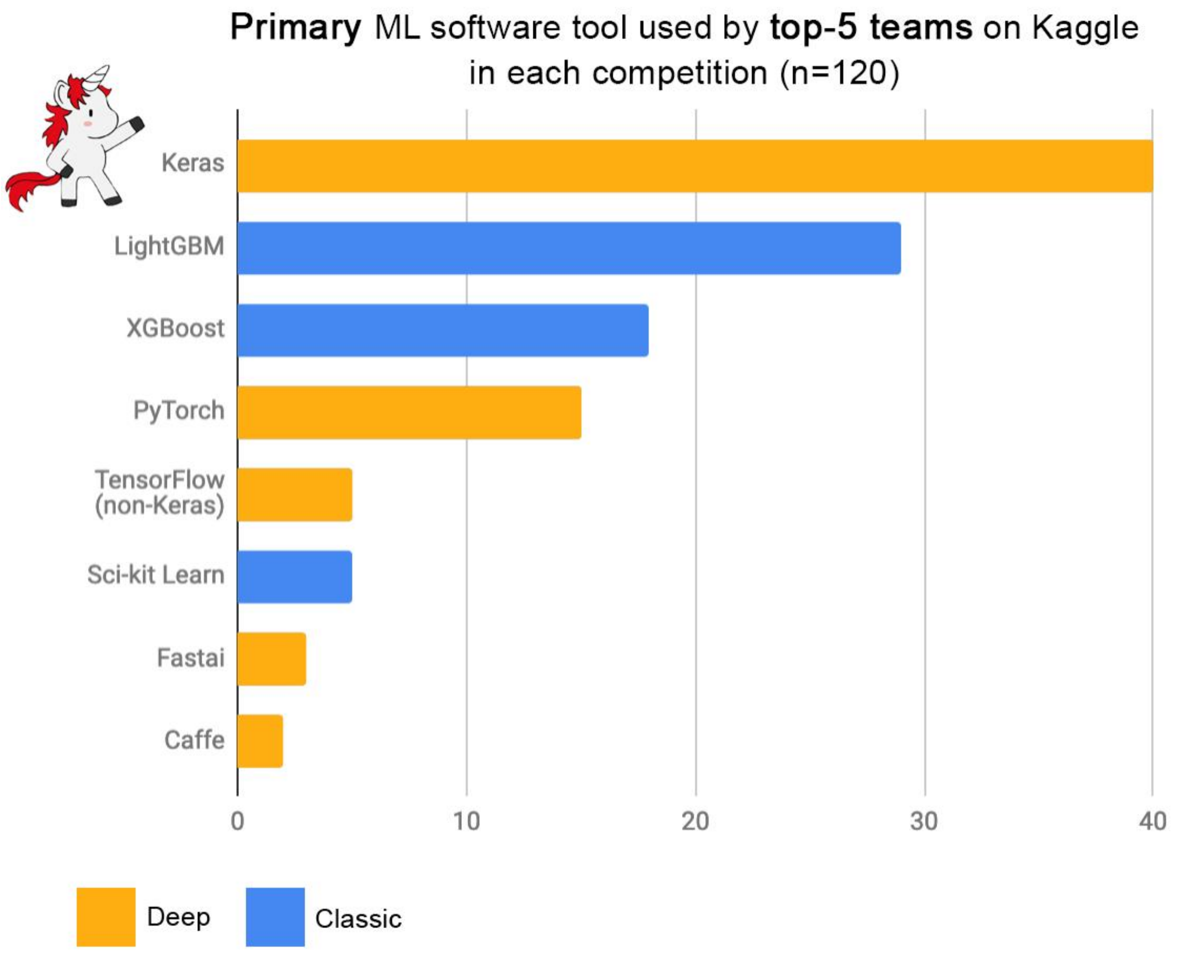
Gradient boosting

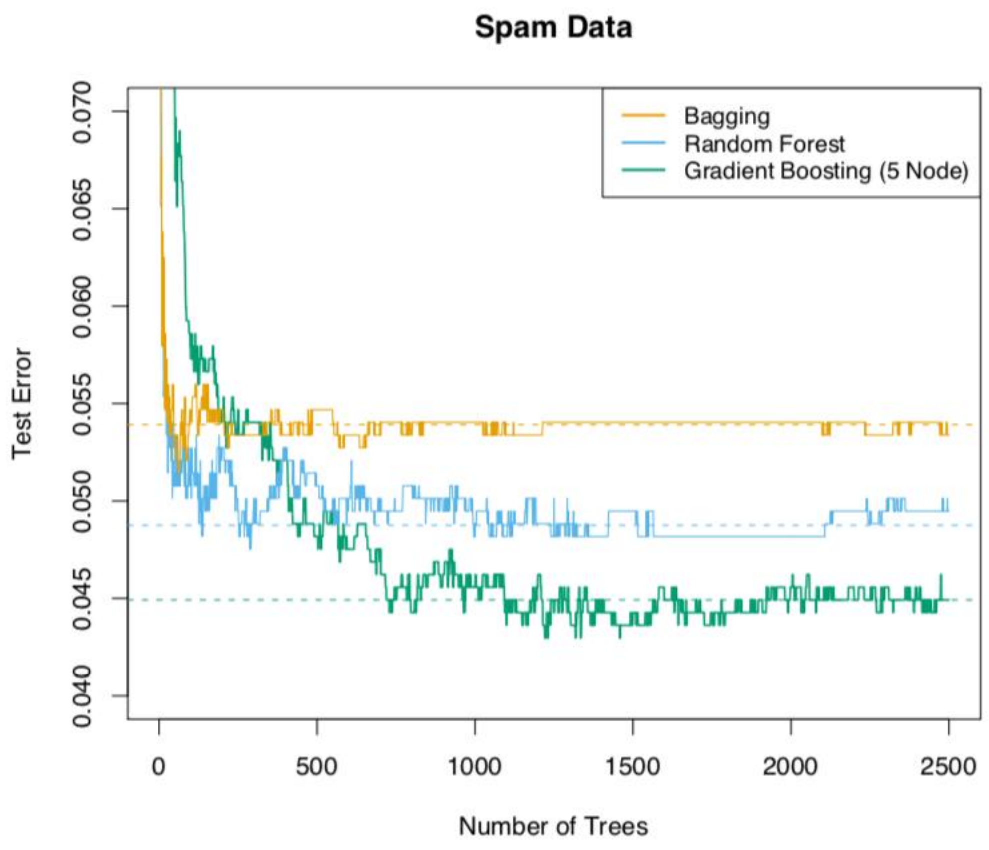
A brief history of boosting

- 1988 Kearns and Valiant: “Can weak learners be combined to create a strong learner?”
- 1990 Schapire: “Yup, in theory”
- 1995 Schapire and Freund: “Practical for 0/1 loss” -> AdaBoost
- 2001 Friedman: “Practical for arbitrary losses”
- 2014 Tianqi Chen: “Scale it up!” -> XGBoost

François Chollet @fchollet · Apr 3, 2019

What machine learning tools do Kaggle champions use? We ran a survey among teams that ranked in the *top 5* of a competition since 2016.





Bagging: Averaged trees on bootstrapped datasets using all d features

Random forest: Averaged trees on bootstrapped datasets using m randomly selected features

Boosting: Learned combinations of trees

Takeaways

- Single trees: low bias, high variance
- Ensembles: low bias, (relatively) low variance
- Bagging averages many lightly dependent models to reduce variance
  - Random forests: same but with random subset of features
- Boosting learns a linear combination of high bias, highly dependent classifiers to reduce error
- Gradient boosted trees are commonly used for categorical data

Bonus: Non-parametric methods today

- Are neural networks non-parametric?
    - Technically no, but…

Retrieval-augmented generation and search agents

What's the state-of-the-art in immunotherapy for cervical cancer?

… Pembrolizumab can extend progression-free and overall survival in patients with persistent, recurrent, or metastatic PD-L1-positive cervical cancer [1] and locally advanced cervical cancer [2]…

[1] Colombo et al., KEYNOTE-826, 2021
[2] Lorusso et al., KEYNOTE-A18, 2024

Attribution

Up-to-date

Credible sources

Next token prediction

Enter text:

One, two,

One 3198 | , 11 | two 734 | , 11

3198 11 734 11

Prediction

#	probs	next token ID	predicted next token
0	39.71%	1115	three
1	16.97%	290	and
2	7.55%	734	two
3	3.76%	1440	four
4	2.76%	393	or
5	2.18%	1936	five
6	1.57%	530	one
7	1.43%	345	you
8	1.15%	257	a
9	0.84%	3598	seven

https://huggingface.co/blog/alonsosilva/nexttokenprediction

Next token prediction

Enter text:

One, two, three

One	,	two	,	three
3198	11	734	11	1115

3198 11 734 11 1115

Prediction

#	probs	next token ID	predicted next token
0	54.42%	11	,
1	5.45%	1399	...
2	4.82%	13	.
3	4.51%	290	and
4	2.72%	986	...
5	2.51%	25	:
6	1.50%	393	or
7	1.23%	3926	...
8	0.85%	553	,"
9	0.84%	960	—

https://huggingface.co/blog/alonsosilva/nexttokenprediction

Next token prediction

Enter text:

One, two, three,

One , two , three ,

3198 11 734 11 1115 11

3198 11 734 11 1115 11

Prediction

#	probs	next token ID	predicted next token
0	46.44%	1440	four
1	7.48%	290	and
2	7.31%	1936	five
3	2.66%	393	or
4	2.54%	2237	six
5	2.09%	1115	three
6	1.86%	3863	maybe
7	1.62%	345	you
8	1.23%	257	a
9	0.92%	530	one

https://huggingface.co/blog/alonsosilva/nexttokenprediction

Next token prediction

Enter text:

One, two, three, four

One `3198` , `11` two `734` , `11` three `1115` , `11` four `1440`

3198 11 734 11 1115 11 1440

Prediction

#	probs	next token ID	predicted next token
0	50.14%	11	,
1	6.66%	13	.
2	5.91%	1399	...
3	3.15%	25	:
4	2.63%	290	and
5	2.58%	986	...
6	1.42%	3926	...
7	1.17%	553	,"
8	1.09%	960	—
9	1.08%	526	."

https://huggingface.co/blog/alonsosilva/nexttokenprediction

Conditioning on retrieved context

Retrieving the right documents

Takeaways

- Retrieval-augmented language models are nonparametric models
- Compare and contrast with k-NN
- Many design choices
  - How to find documents?
  - How to incorporate retrieved documents into generation?
  - Multimodal retrieval?
- Highly active research area