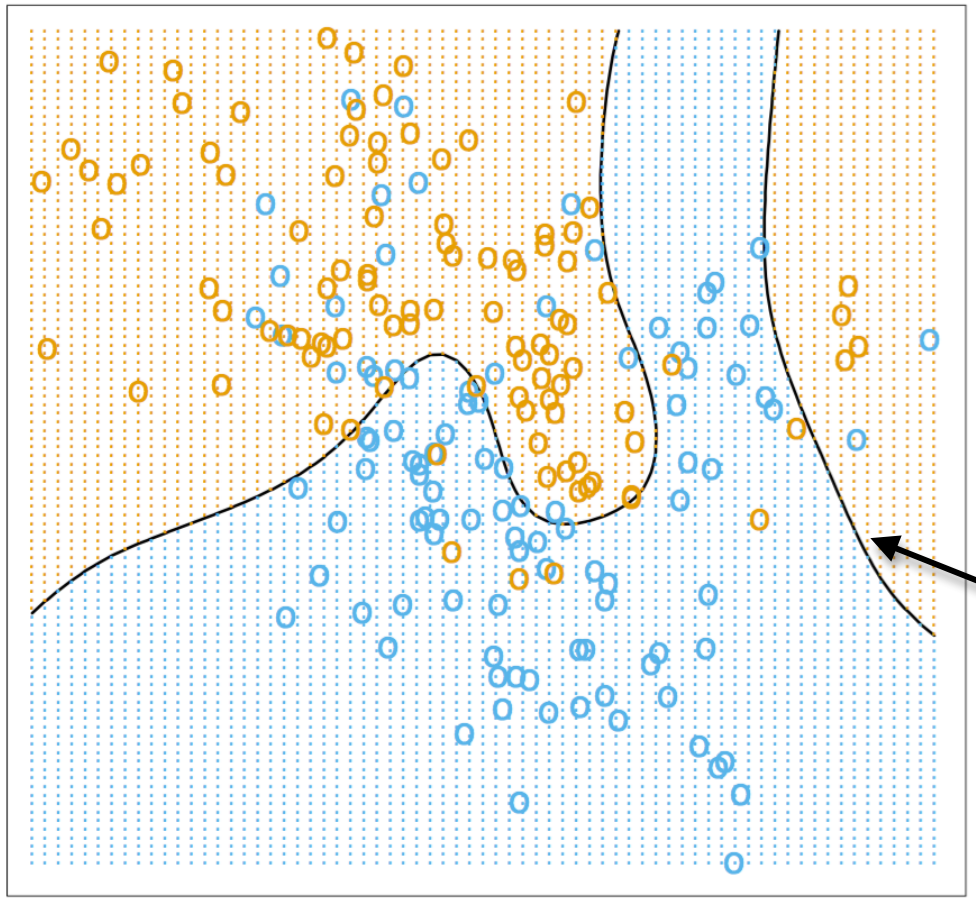
Nearest Neighbor Methods

- 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 (Does **not** mean absence of parameters!)

Some data, Bayes Classifier



Training data:

True label: +1

True label: -1

Optimal "Bayes" classifier:

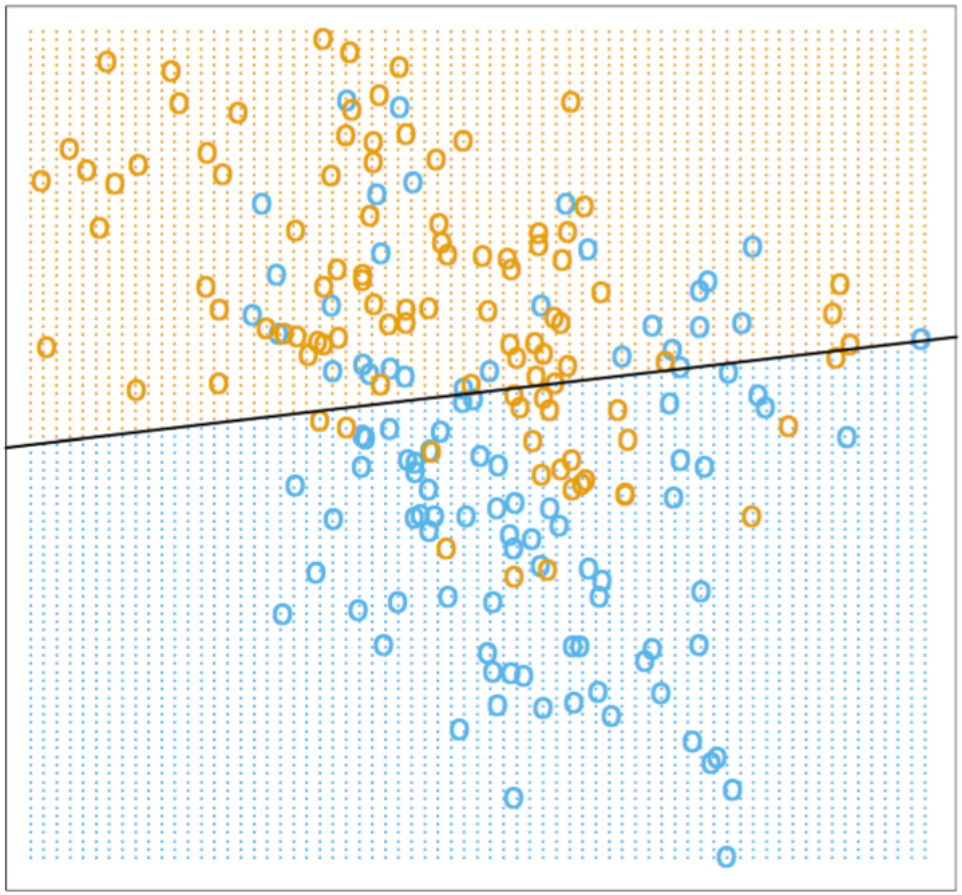
$$\mathbb{P}(Y = 1|X = x) = \frac{1}{2}$$

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

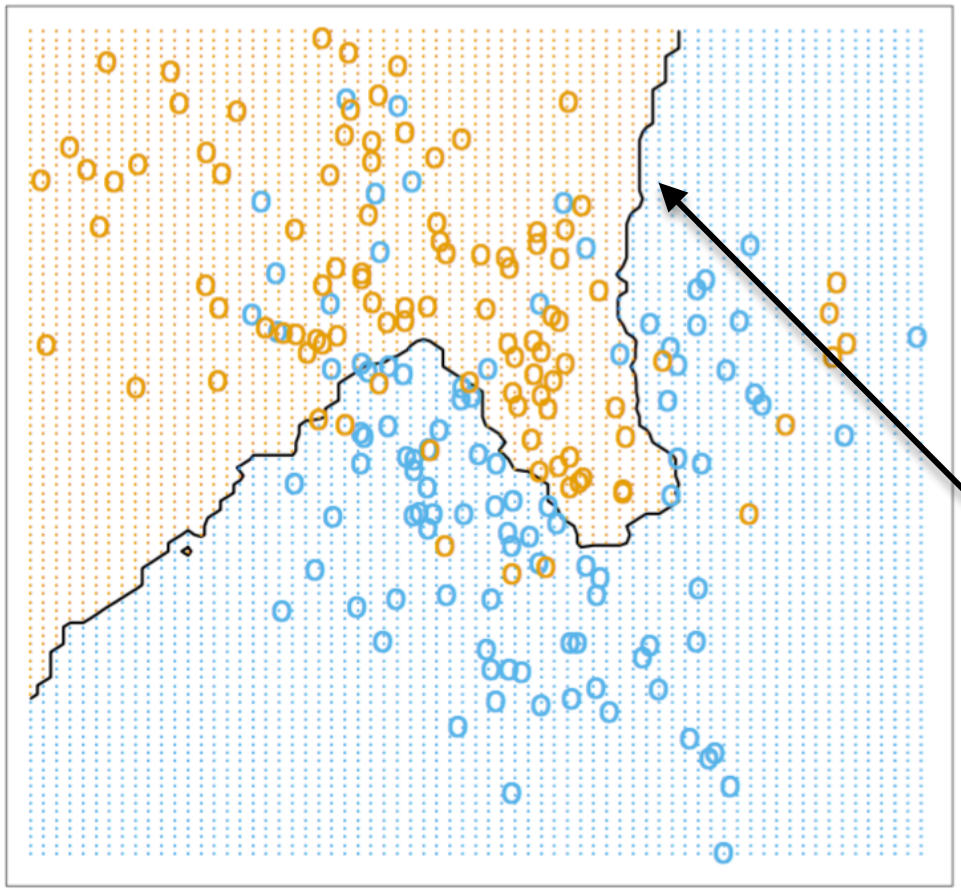
$$x^T w + b = 0$$

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)

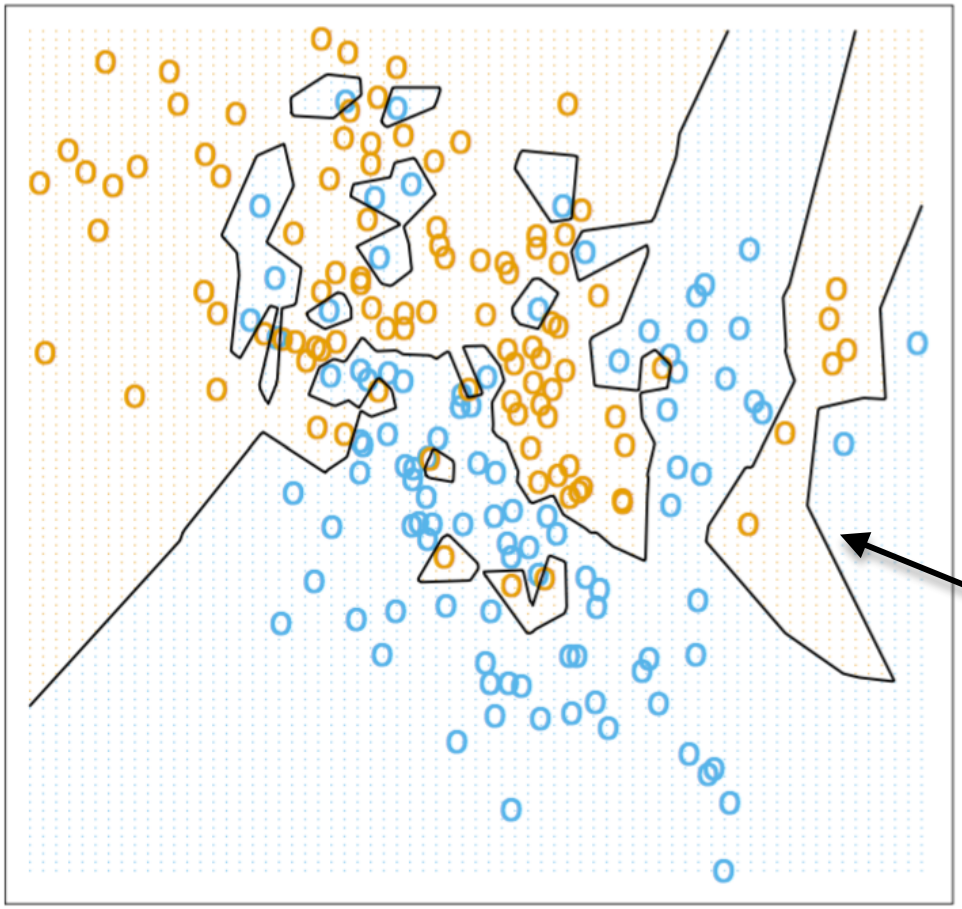
Predicted label: +1

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

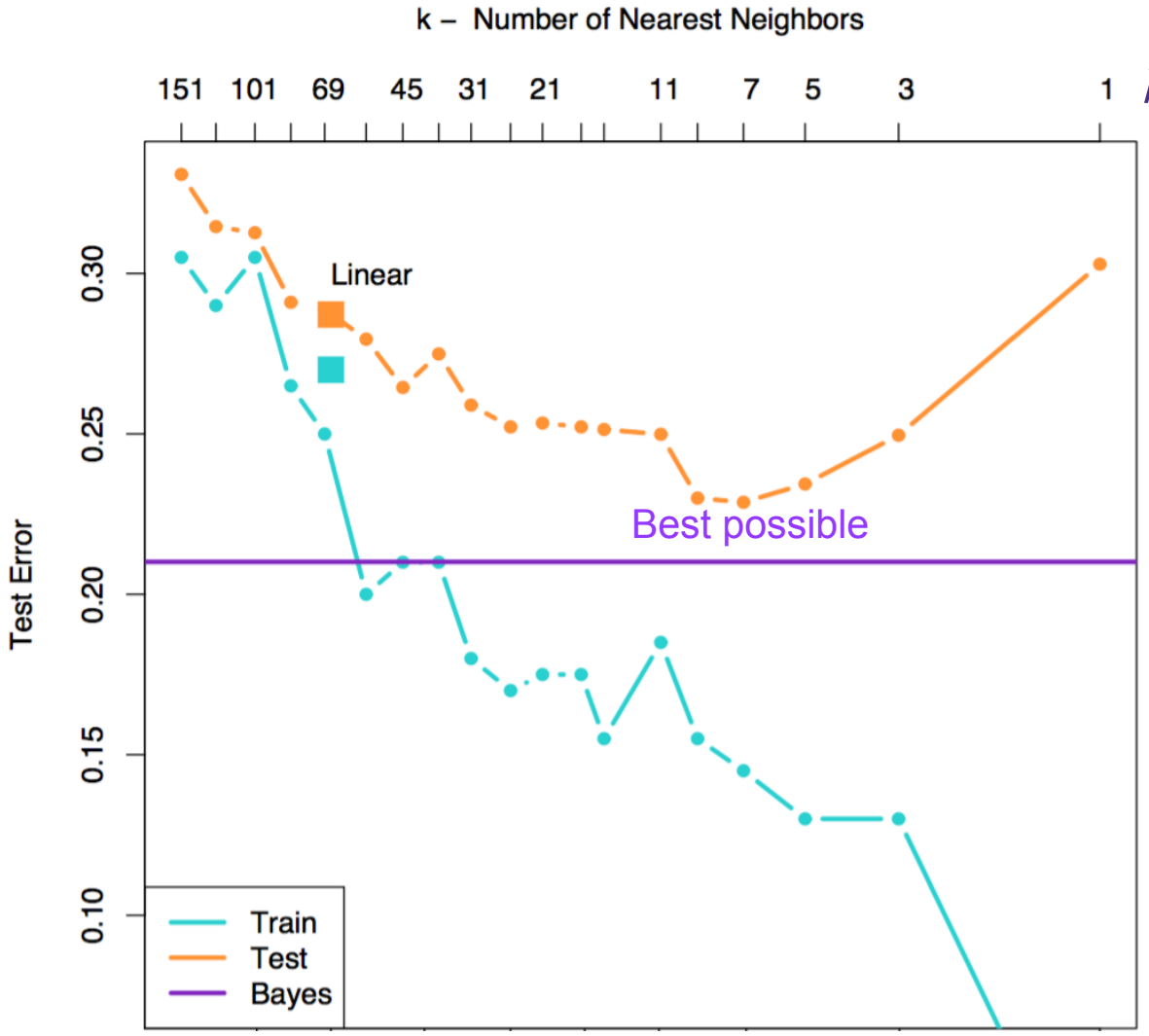
- With a small k, we tend to overfit.

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:

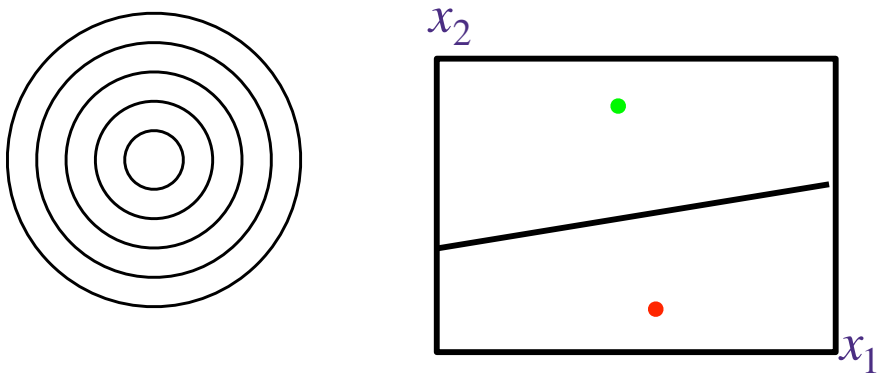
Figures from Hastie et al

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

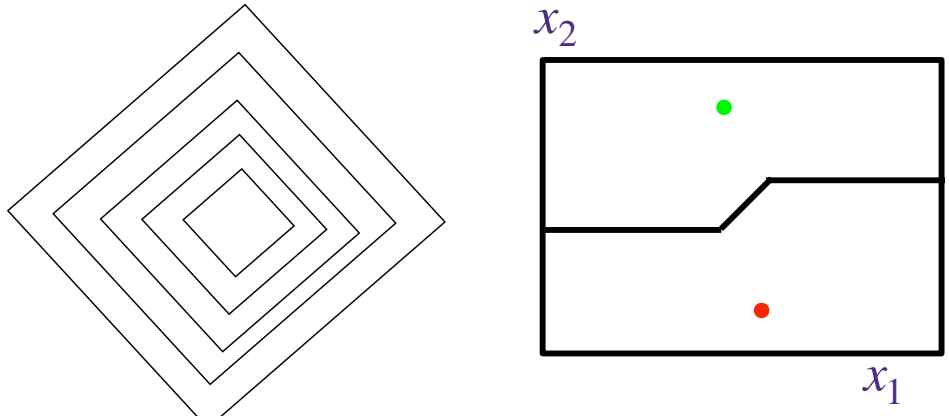
Notable distance metrics (and their level sets)

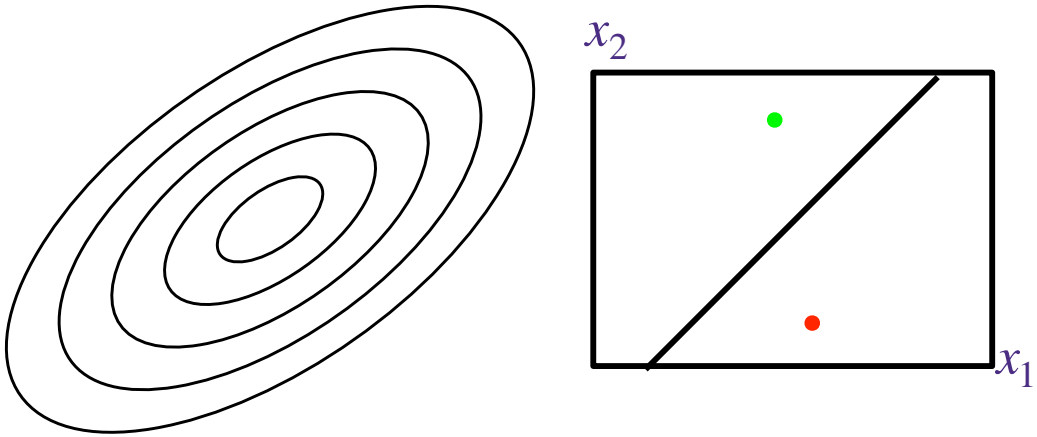
Consider 2 dimensional example with 2 data points with labels green, red,
and we show $k = 1$nearest neighbor decision boundaries for various choices of distances

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

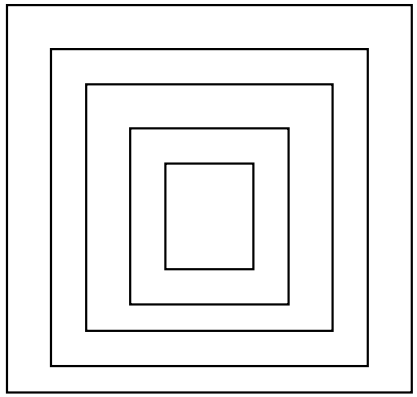


L_1 norm (taxi-cab)

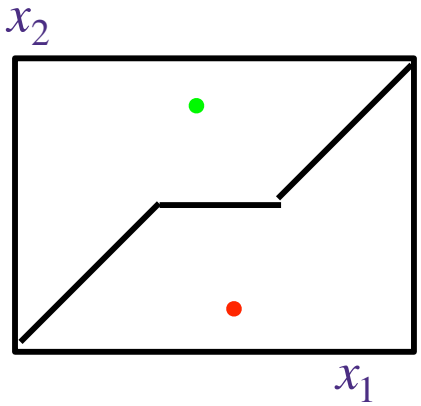




Mahalanobis norm: $d(x, y) = (x - y)^T M (x - y)$

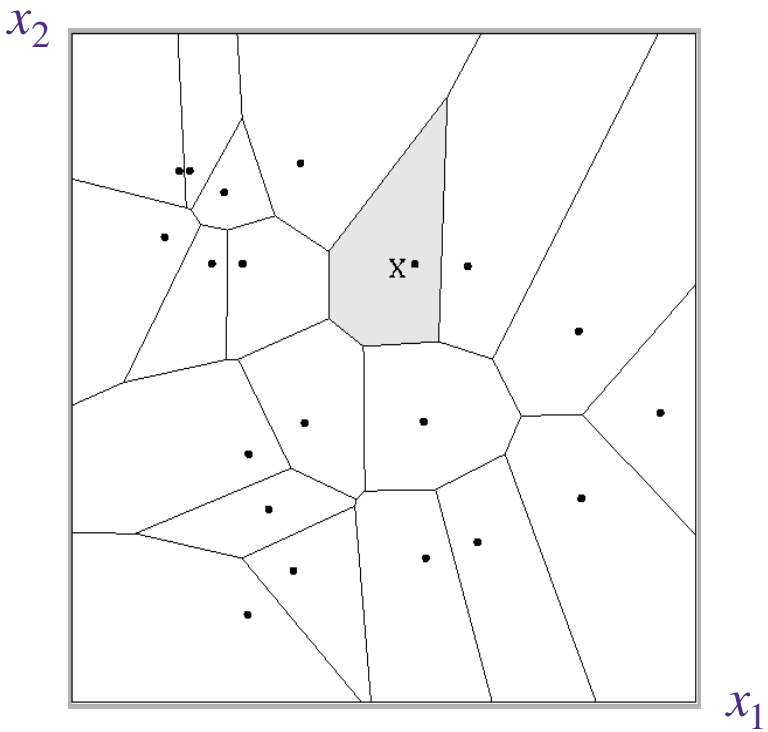


L-infinity *(max) norm*

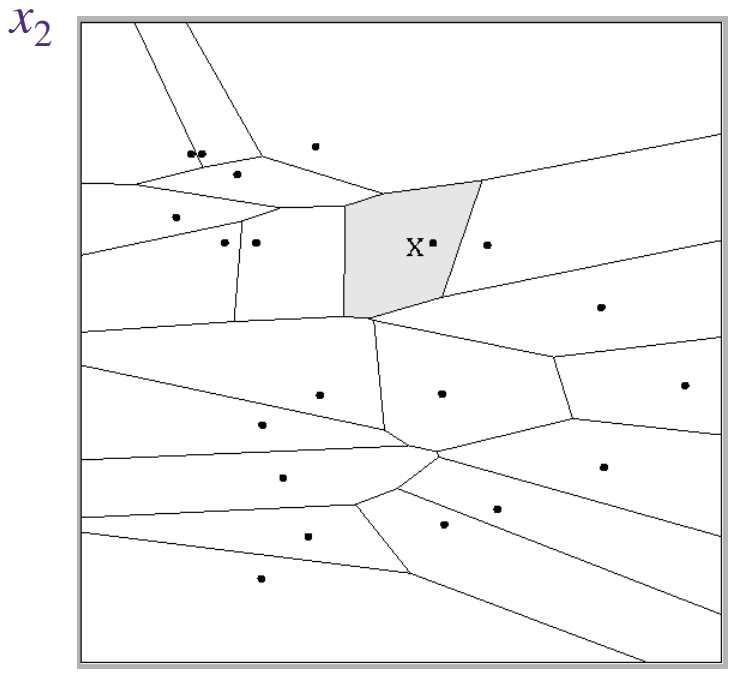


$k = 1$ nearest neighbor

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



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



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

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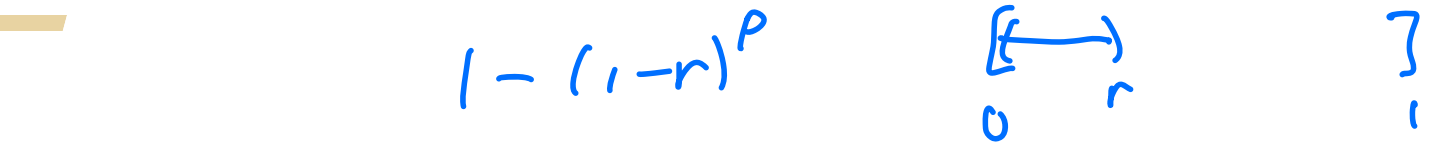
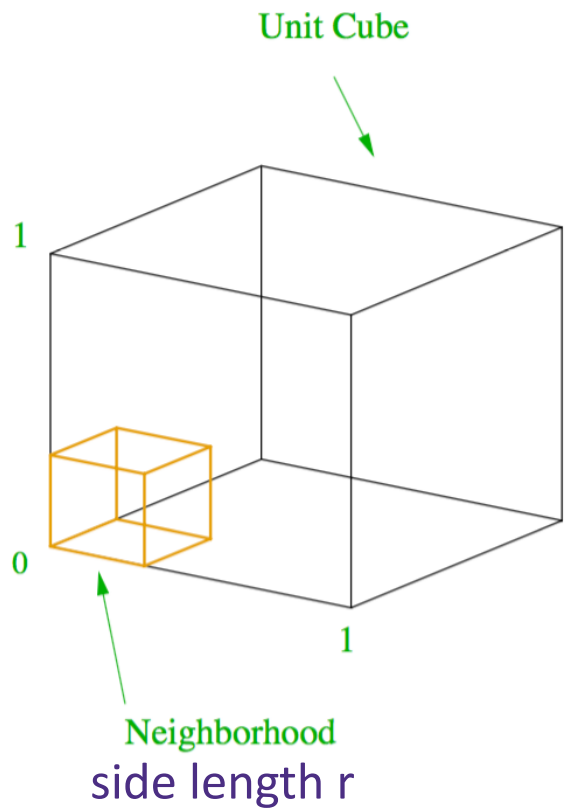
- Let x_{NN} denote the nearest neighbor at a point x
- First note that as $n \to \infty, P(y = +1 \,|\, x_{NN}) \to P(y = +1 \,|\, x)$
- Let $p^* = \min\{P(y = +1 \,|\, x), P(y = -1 \,|\, x)\}$ denote the Bayes error rate
- At a point x,
  - Case 1: nearest neighbor is $+1$, which happens with $P(y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

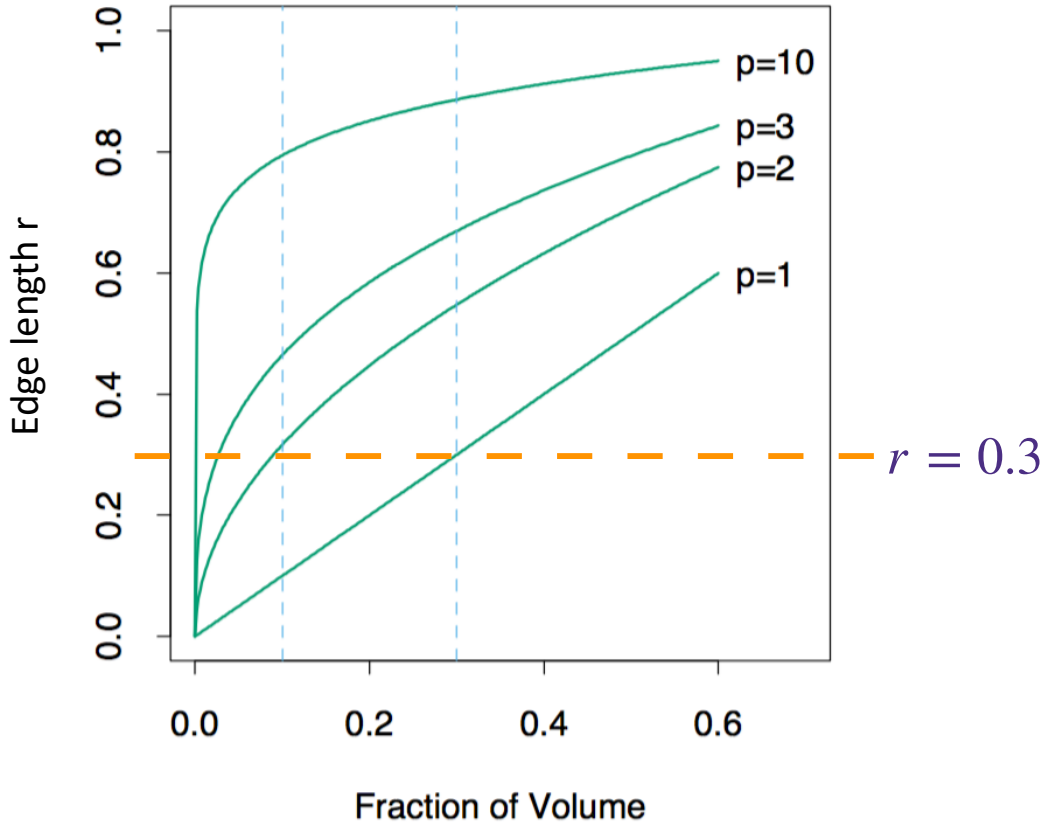
$$P(y = +1 \,|\, x)\, P(y = -1 \,|\, x) + P(y = -1 \,|\, x)\, P(y = +1 \,|\, x) \;= 2p^*(1 - p^*)$$

Curse of dimensionality Ex. 1

$1-(1-r)^p$



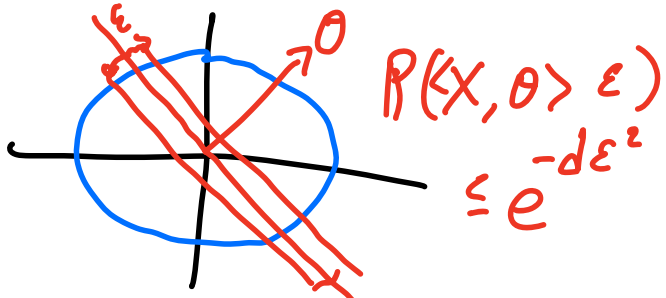




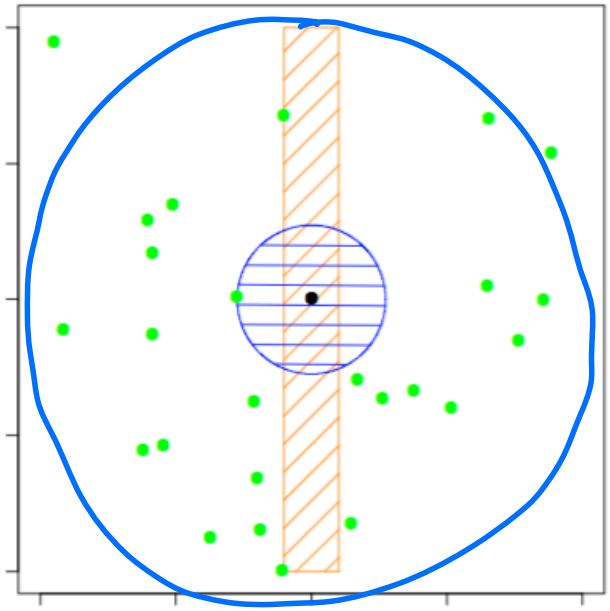
X is uniformly distributed over $[0,1]^p$. What is $\mathbb{P}(X \in [0,r]^p)$?

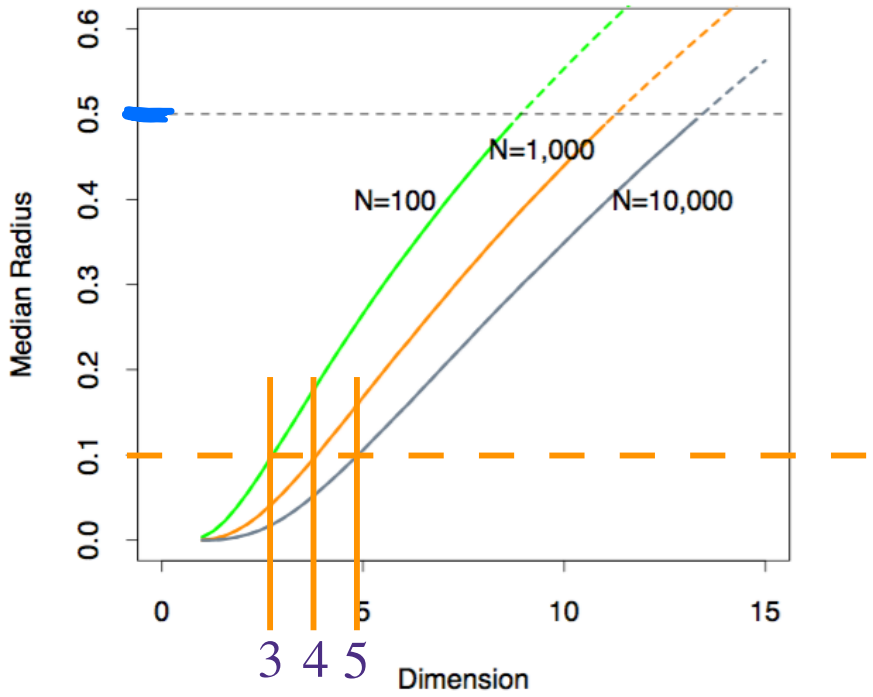
How many samples do we need so that a nearest neighbor is within a cube of side length r?

Curse of dimensionality Ex. 2



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

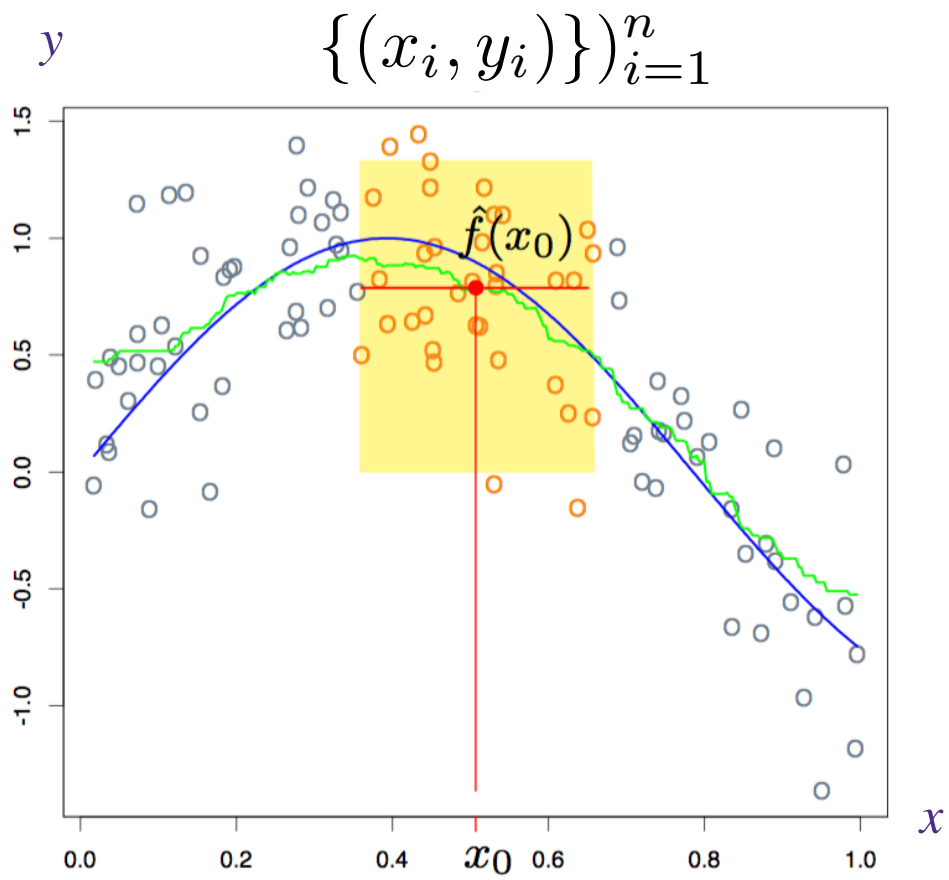




What is the median distance from a point at origin to its 1NN?

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

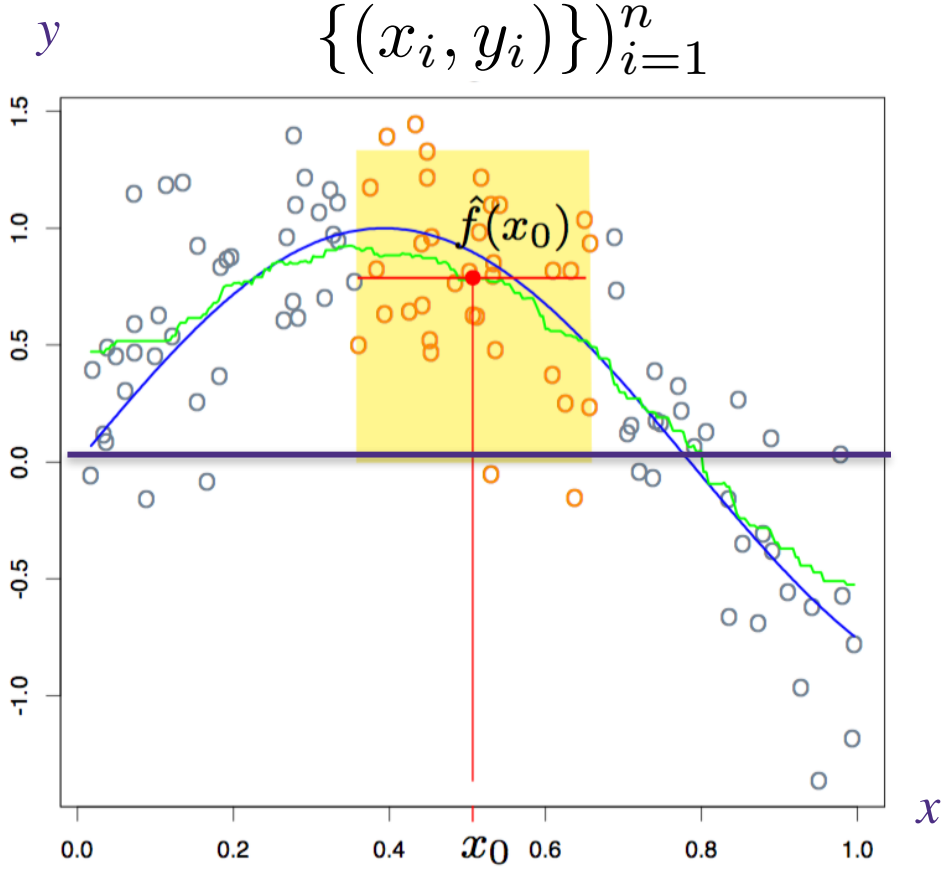
$$\hat{y} = \mathbb{E}[y \mid x]$$

- k-nearest neighbor regressor is

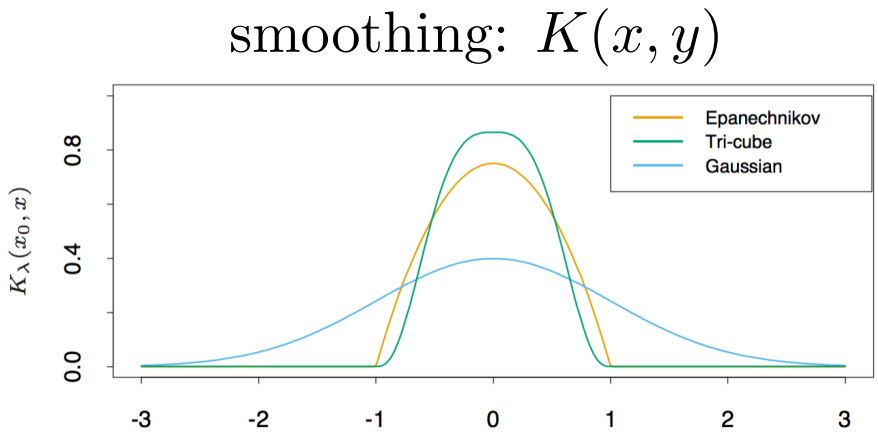
$$\hat{f}(x) = \frac{1}{k} \sum_{j \in \text{nearest neighbor}} y_j$$

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

Nearest neighbor regression



In nearest neighbor methods, the "weight" changes abruptly

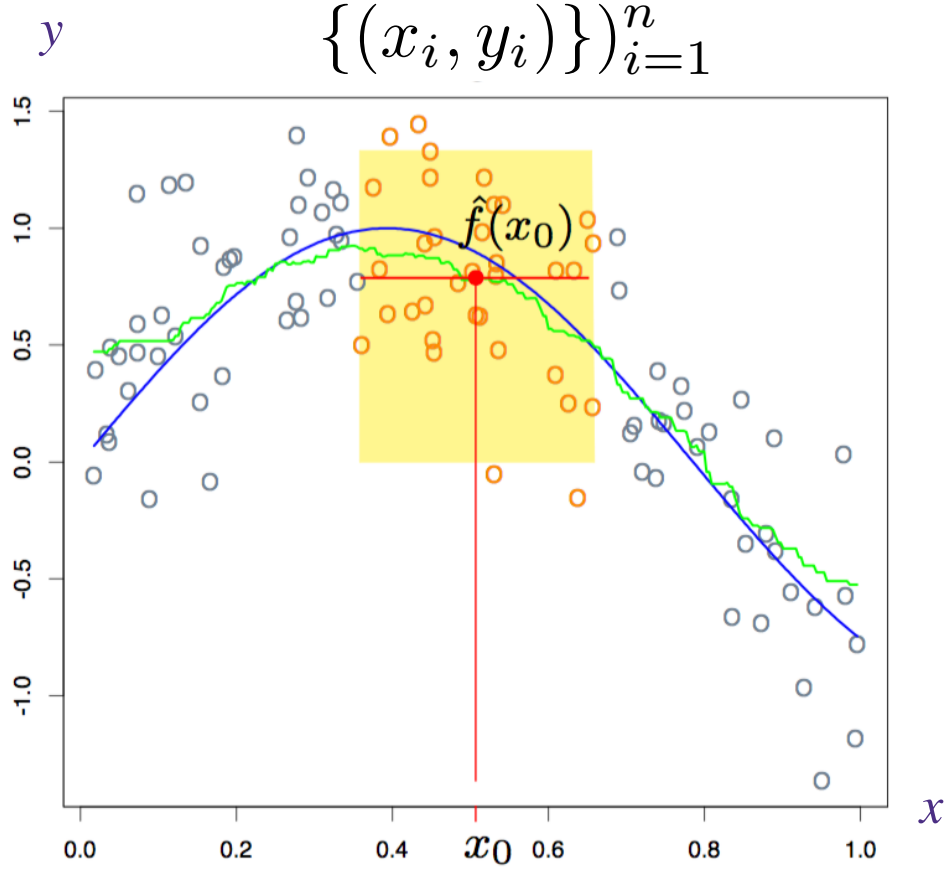


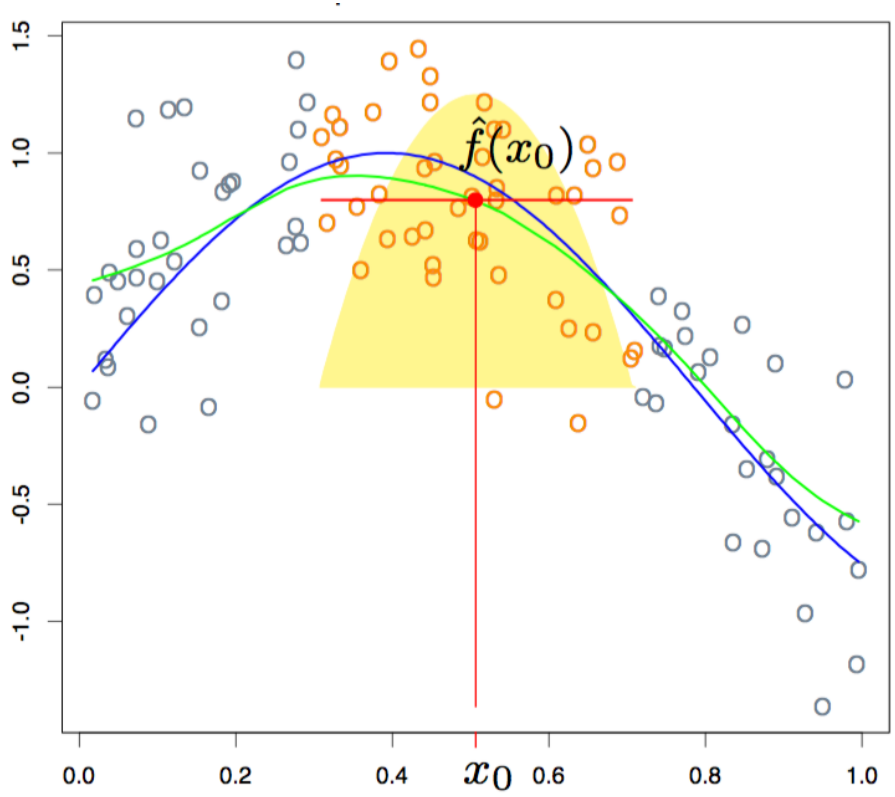
- k-nearest neighbor regressor is

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

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

Nearest neighbor regression



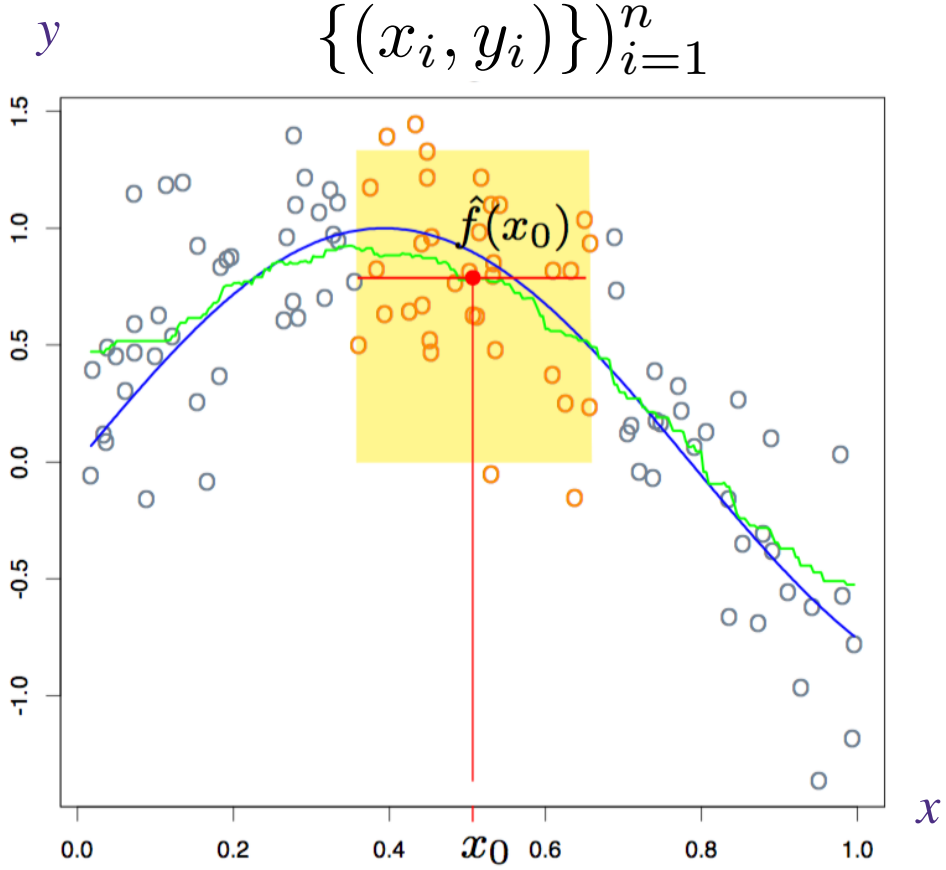


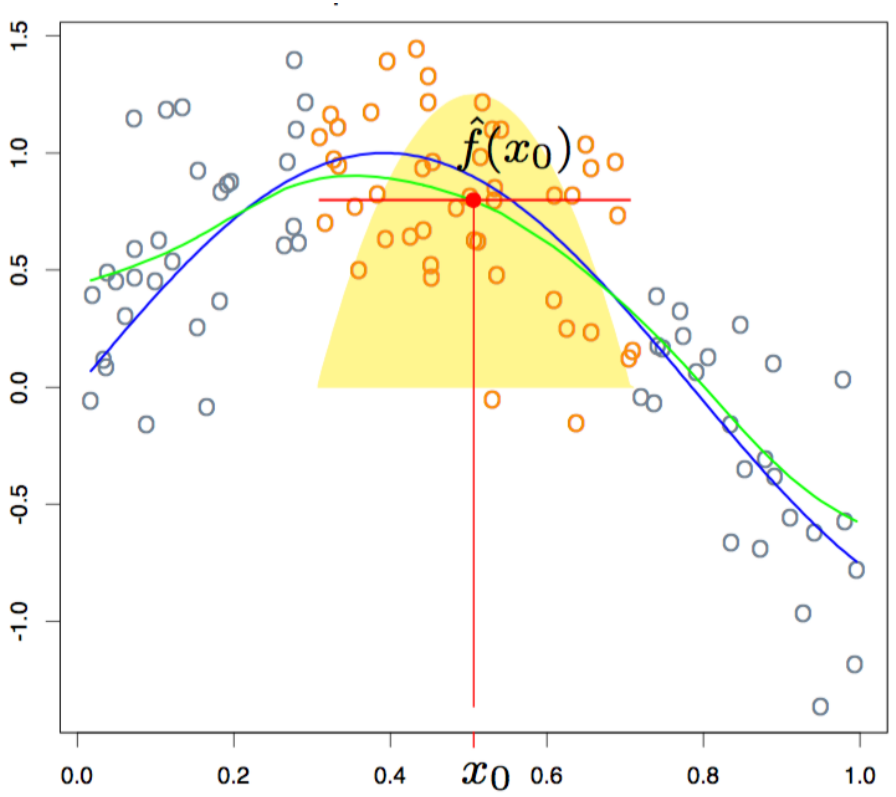
- k-nearest neighbor regressor is

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

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

Nearest neighbor regression





- k-nearest neighbor regressor is

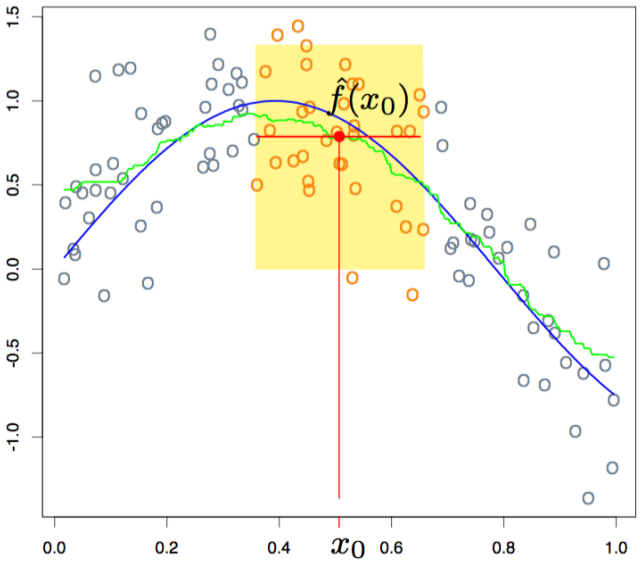
$$\hat{f}(x_0) = \frac{\sum_{i=1}^{n} y_i \times \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}{\sum_{i=1}^{n} \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}$$

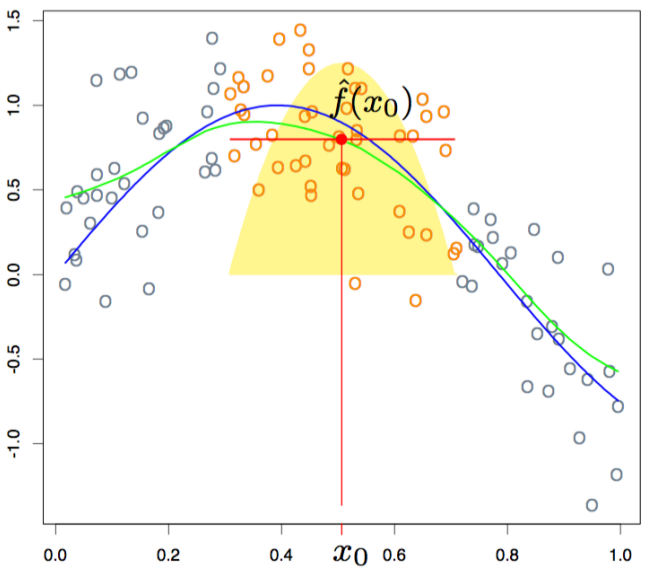
Why just average them?

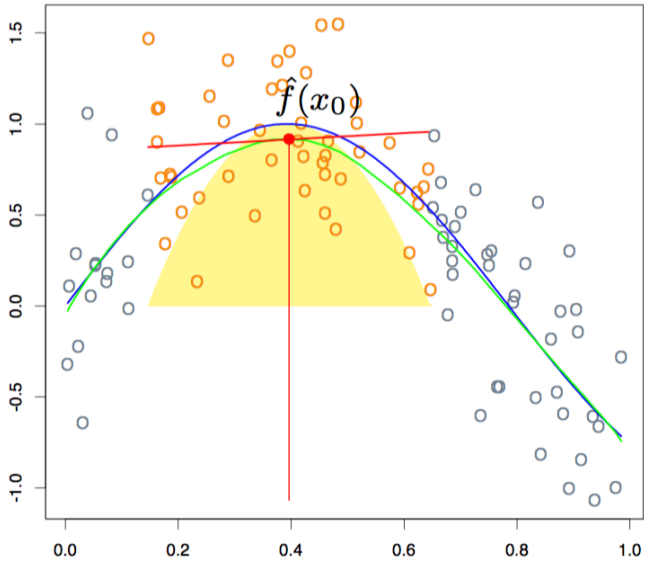
$$\widehat{f}(x_0) = \frac{\sum_{i=1}^{n} K(x_0, x_i) y_i}{\sum_{i=1}^{n} K(x_0, x_i)}$$

Nearest neighbor regression

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







- 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

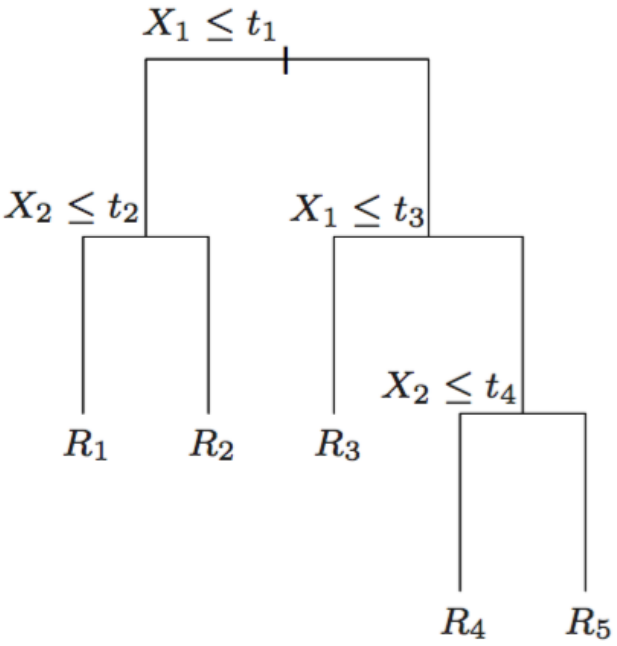
- Very simple to explain and implement
- No training! But finding nearest neighbors in large dataset at test can be computationally demanding (KD-trees help)
- You can use other forms of distance (not just Euclidean)
- Smoothing and local linear regression can improve performance (at the cost of higher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

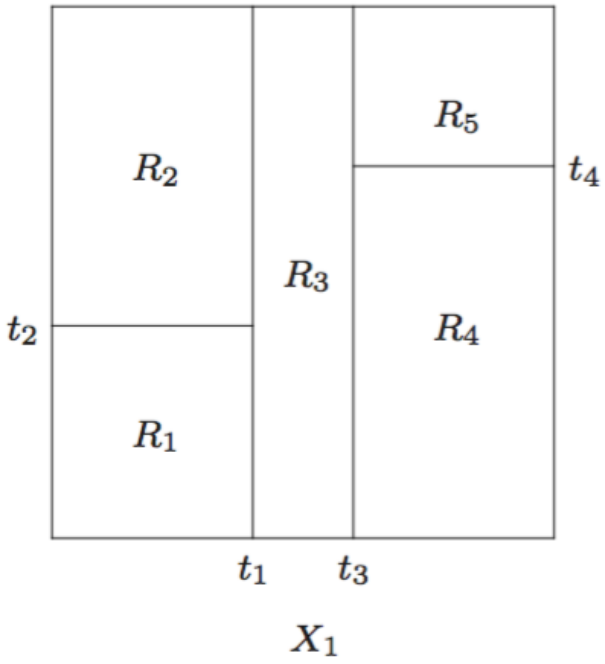
Questions?

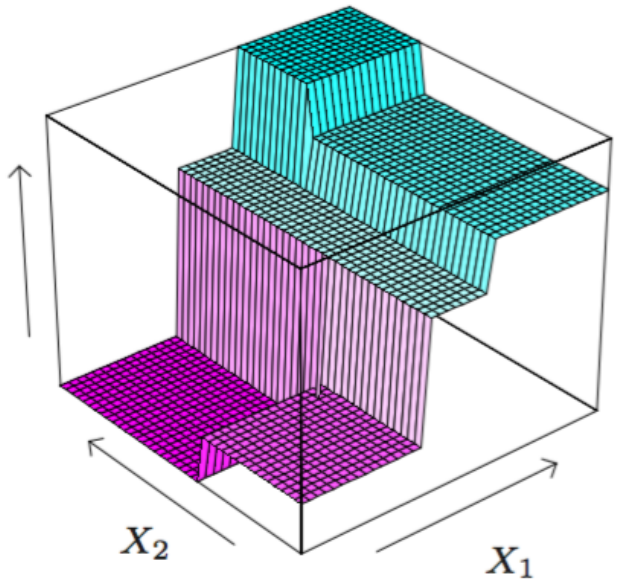
Trees

Trees

Example: binary tree with splits along axes







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

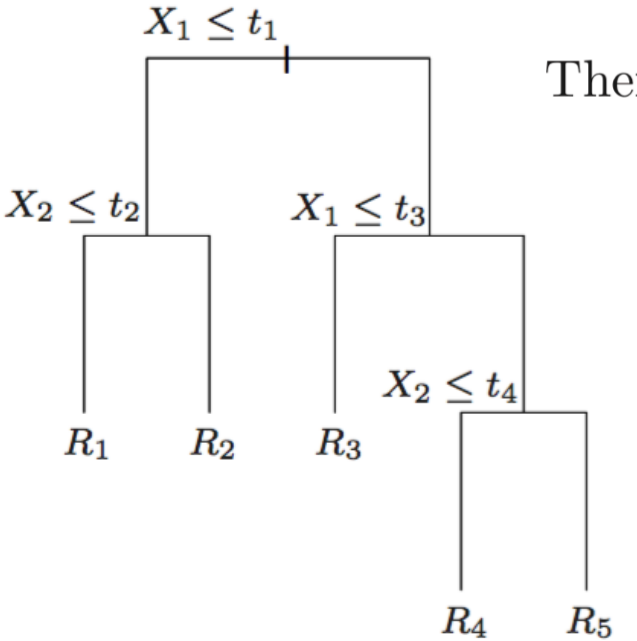
Regression Trees

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

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

Binary tree with splits along axes.

How do you build the tree / find the splits?



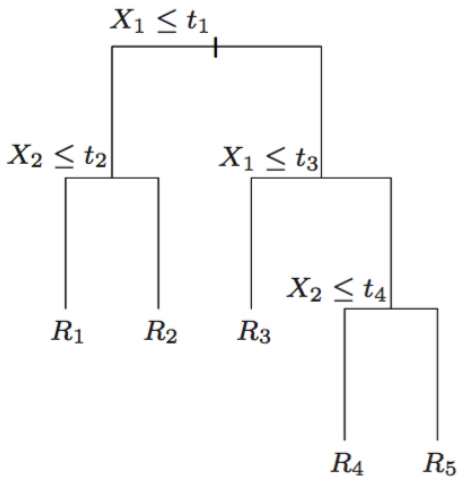
$$R_1(j,s) = \{X | X_j \le s\} \text{ and } R_2(j,s) = \{X | X_j > s\}.$$

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

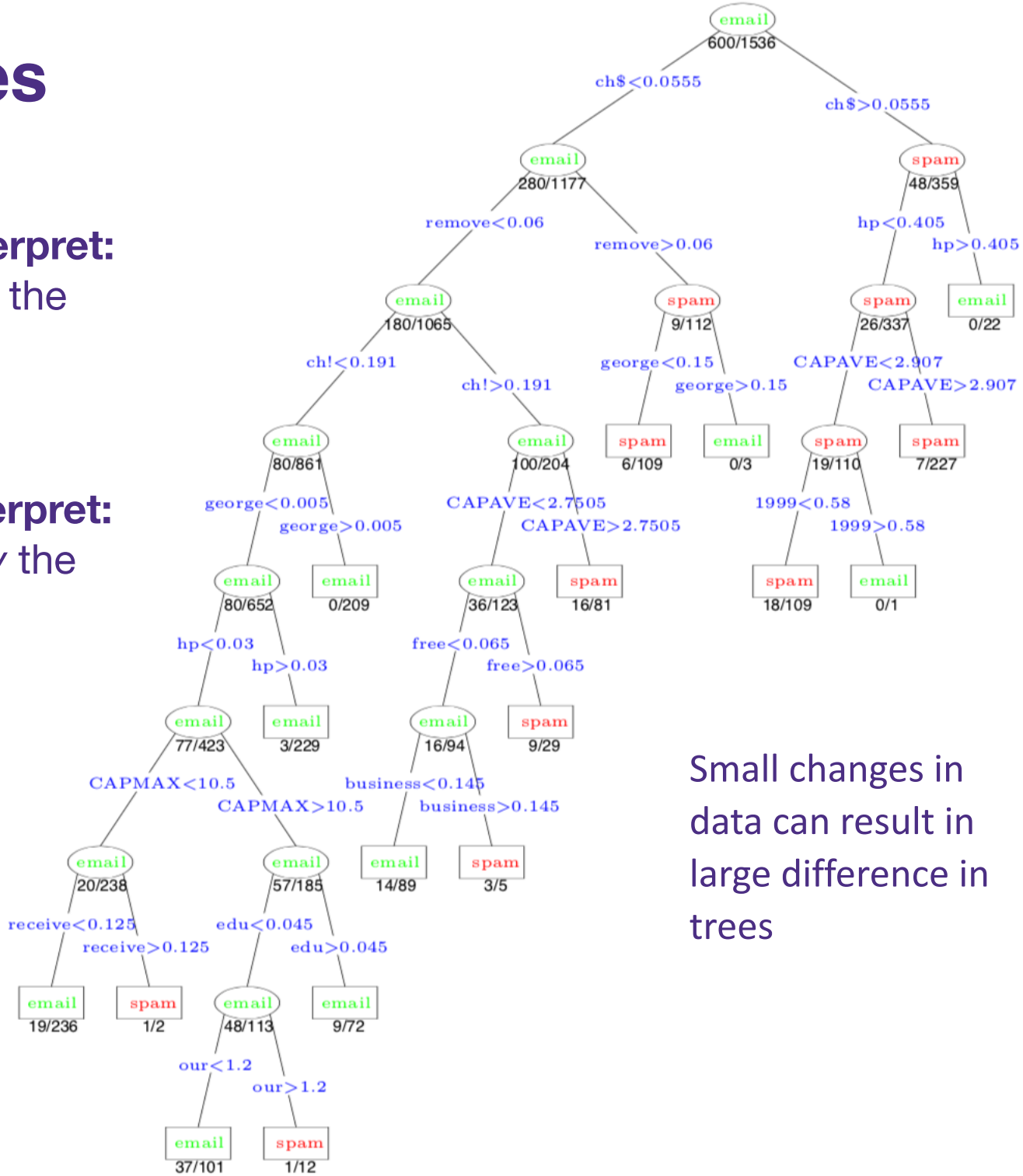


$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m).$$

Decision Trees

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

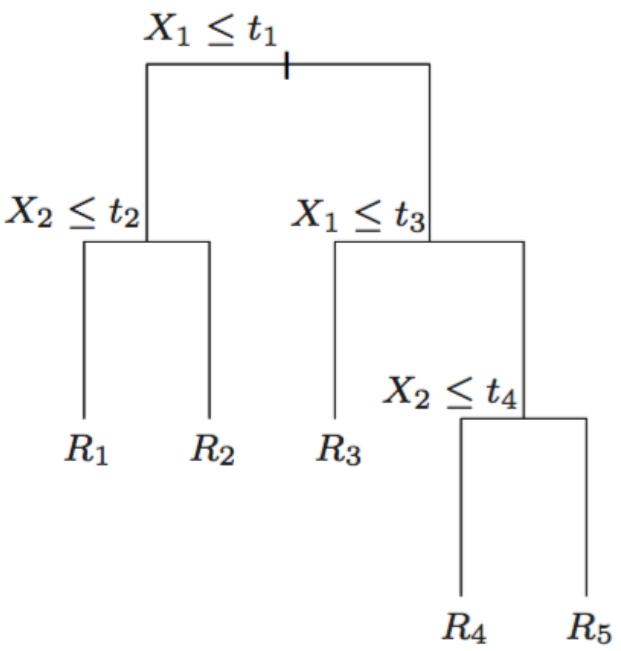
Trees are hard to interpret:
- Tough to explain *why* the classifier came to the conclusion it did



Small changes in data can result in large difference in trees

Trees

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



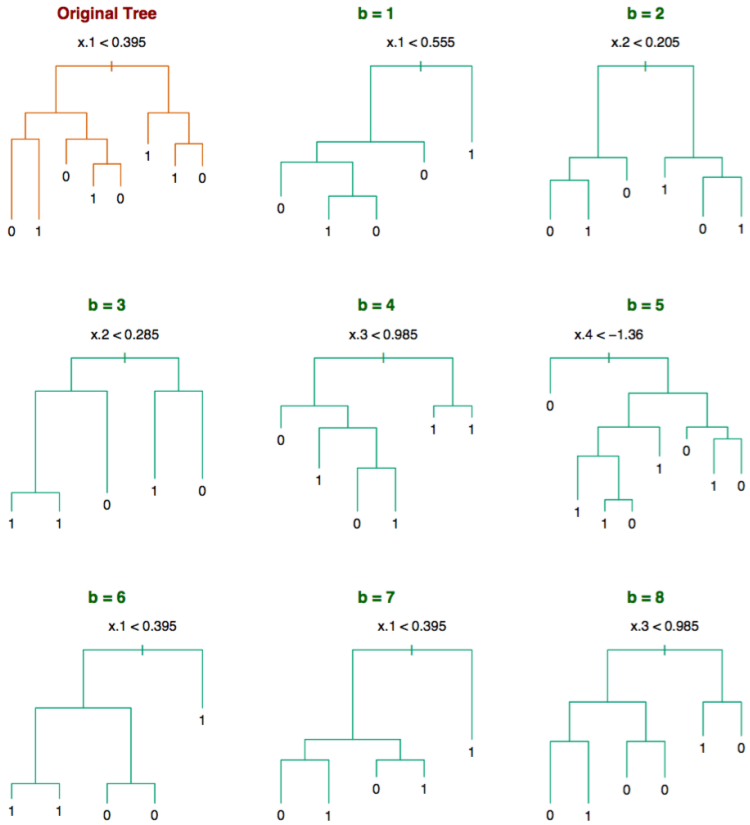
- Trees
  - **have low bias, high variance**
  - deal with categorial variables well
  - intuitive, interpretable
  - good software exists
  - Some theoretical guarantees

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.

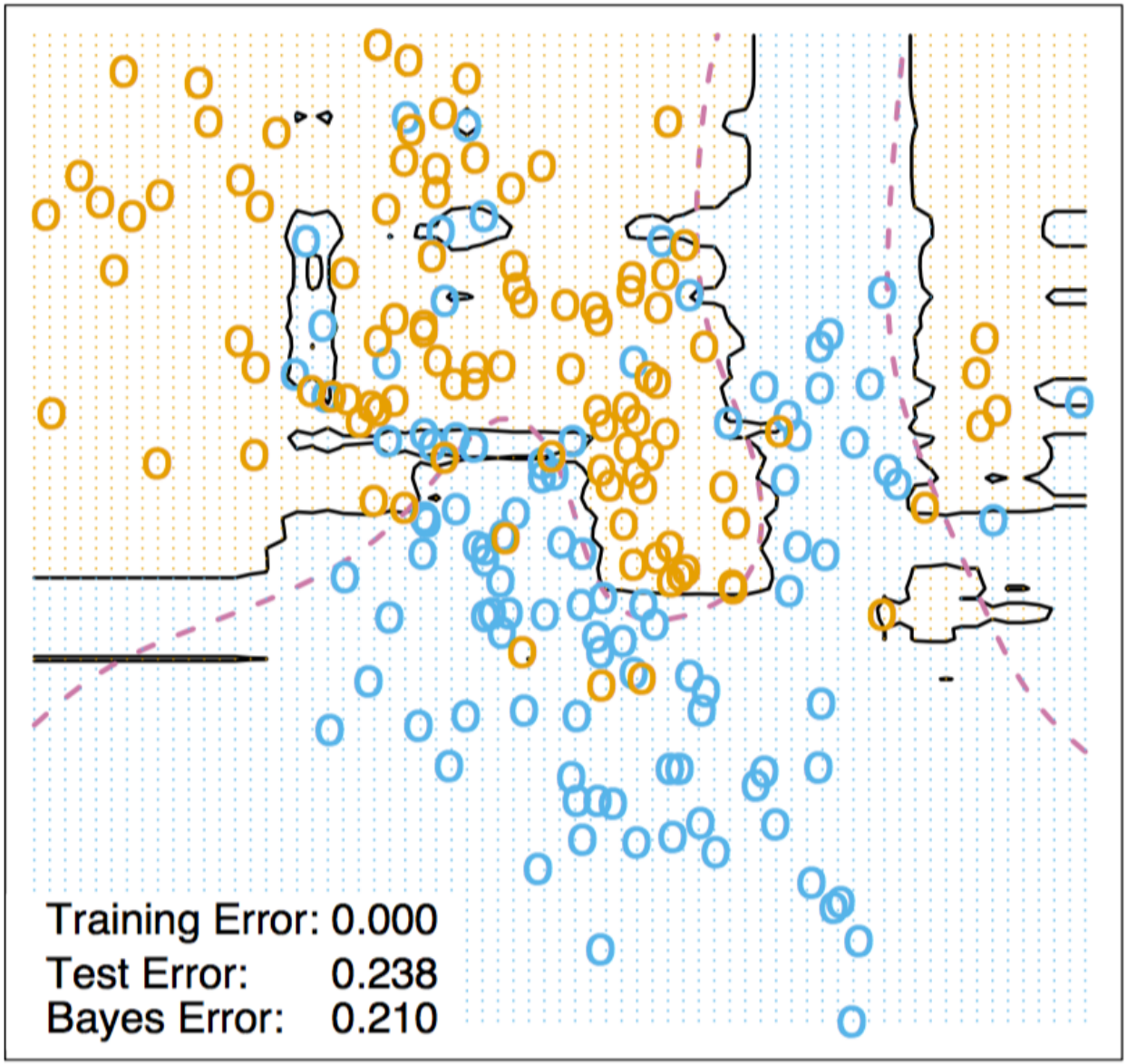
2. Output the ensemble of trees $\{T_b\}_1^B$.

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
$\mathbb{E}[Y_i] = y$, $\mathbb{E}[(Y_i - y)^2] = \sigma^2$, $\mathbb{E}[(Y_i - y)(Y_j - y)] = \rho\sigma^2$

σ^2 **Variance of individual predictor**

Assume bias = 0

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

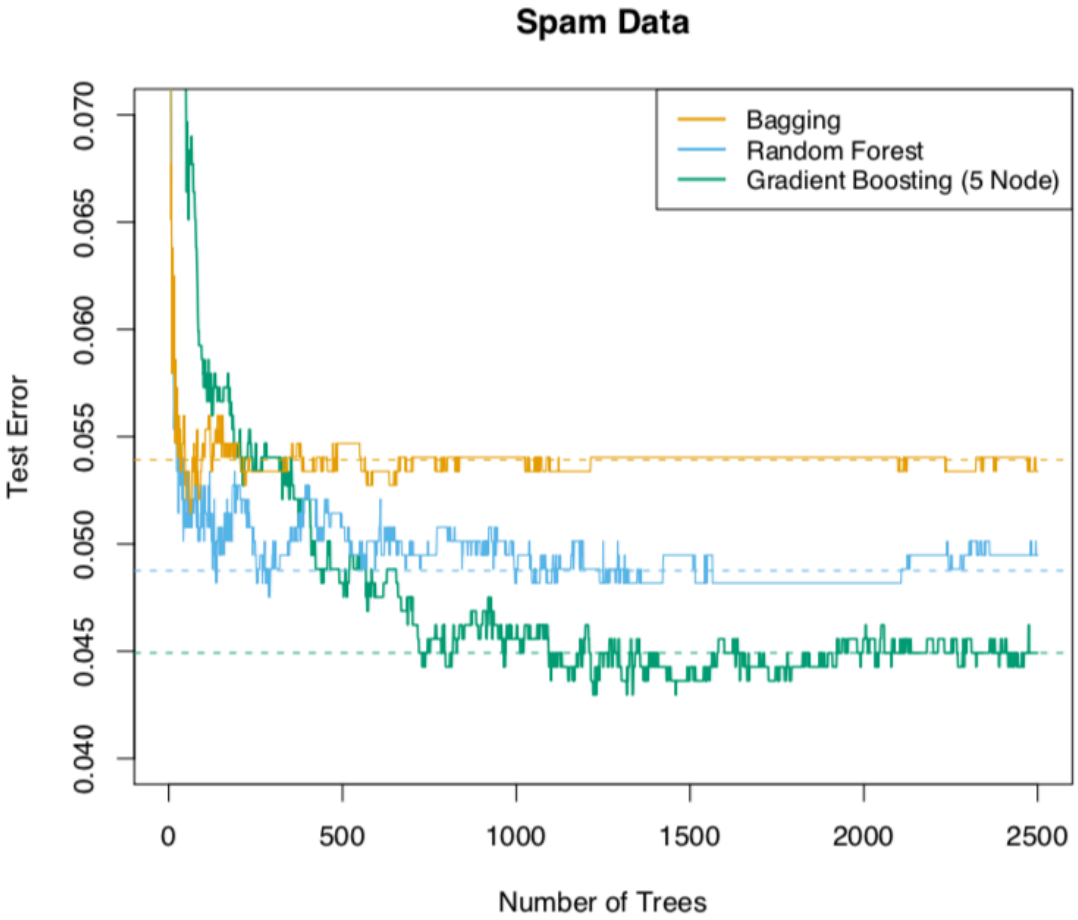
The Yi's are identically distributed but **not** independent

$$\mathbb{E}[(\frac{1}{B}\sum_{i=1}^{B} Y_i - y)^2] = \mathbb{E}\left[\frac{1}{B^2}\sum_{i=1}^{B}(Y_i - y)^2\right] + \mathbb{E}\left[\frac{1}{B^2}\sum_{i \neq j}(Y_i - y)(Y_j - y)\right]$$

$$= \frac{\sigma^2}{B} + \frac{B-1}{B}\rho\sigma^2$$

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
  - Some theoretical guarantees
  - **works well with default hyperparameters**

Boosting and Additive Models

UNIVERSITY of WASHINGTON

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”
- 2014 Tianqi Chen: “Scale it up!” XGBoost

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

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

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

is in general computationally hard

Forward Stagewise Additive models

$b(x, \gamma)$ is a function with parameters γ

Examples: $b(x, \gamma) = \dfrac{1}{1 + e^{-\gamma^T x}}$

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

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

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

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

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

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

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

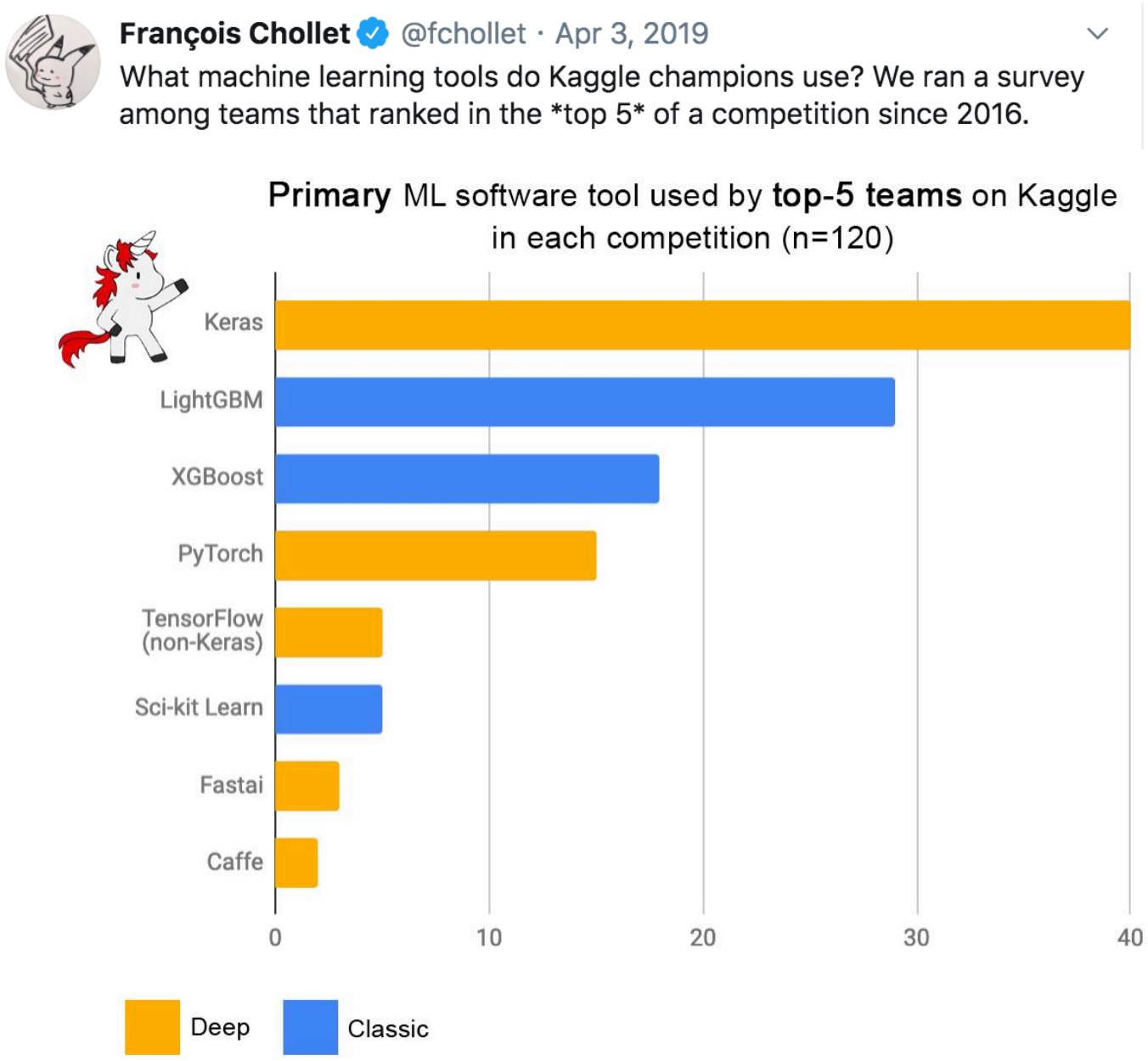
$$\begin{aligned} L(y_i, f_{m-1}(x_i) + \beta b(x_i; \gamma)) &= (y_i - f_{m-1}(x_i) - \beta b(x_i; \gamma))^2 \\ &= (r_{im} - \beta b(x_i; \gamma))^2, \qquad r_{im} = y_i - f_{m-1}(x_i) \end{aligned}$$

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