As you login

1. Rename yourself in Zoom to *pre*-pend your house number
   - e.g. “0 – Pat Virtue”
2. Open Piazza (getting ready for polls)
3. Download preview slides from course website
4. Grab something to write with/on ☺

Announcements

Assignments

- HW1 Feedback
- HW2
  - Due Mon, 9/21, 11:59 pm
  - Start now! OH will be *super* crowded as the deadline gets closer

Breakout rooms

- Video on
- Unmute
- Introduce yourself if you haven’t already met

Introduction to Machine Learning

Nearest Neighbor and Model Selection

Instructor: Pat Virtue

Plan

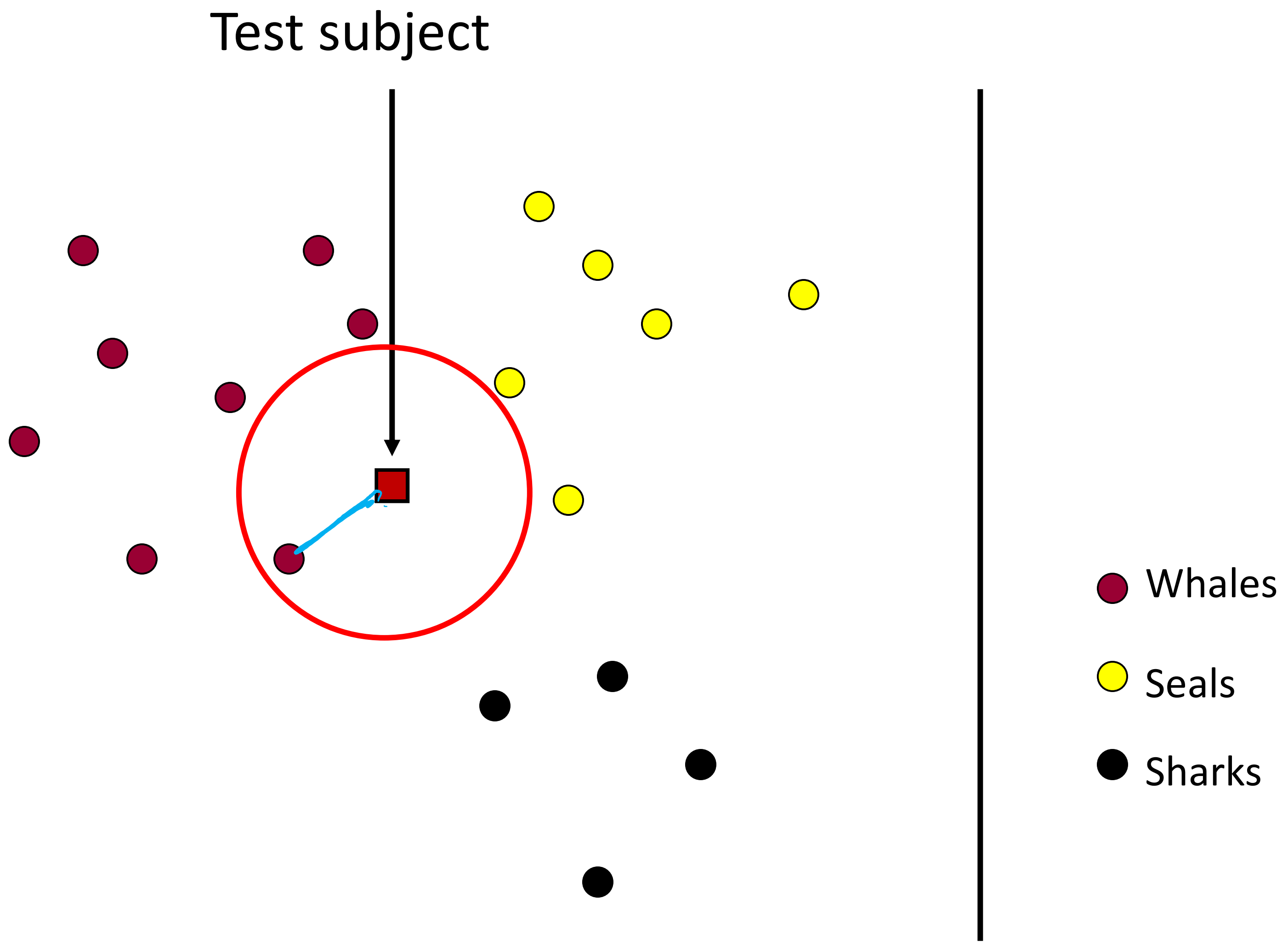
Last time

- Decision trees
  - Continuous features, Overfitting
- Nearest neighbor methods

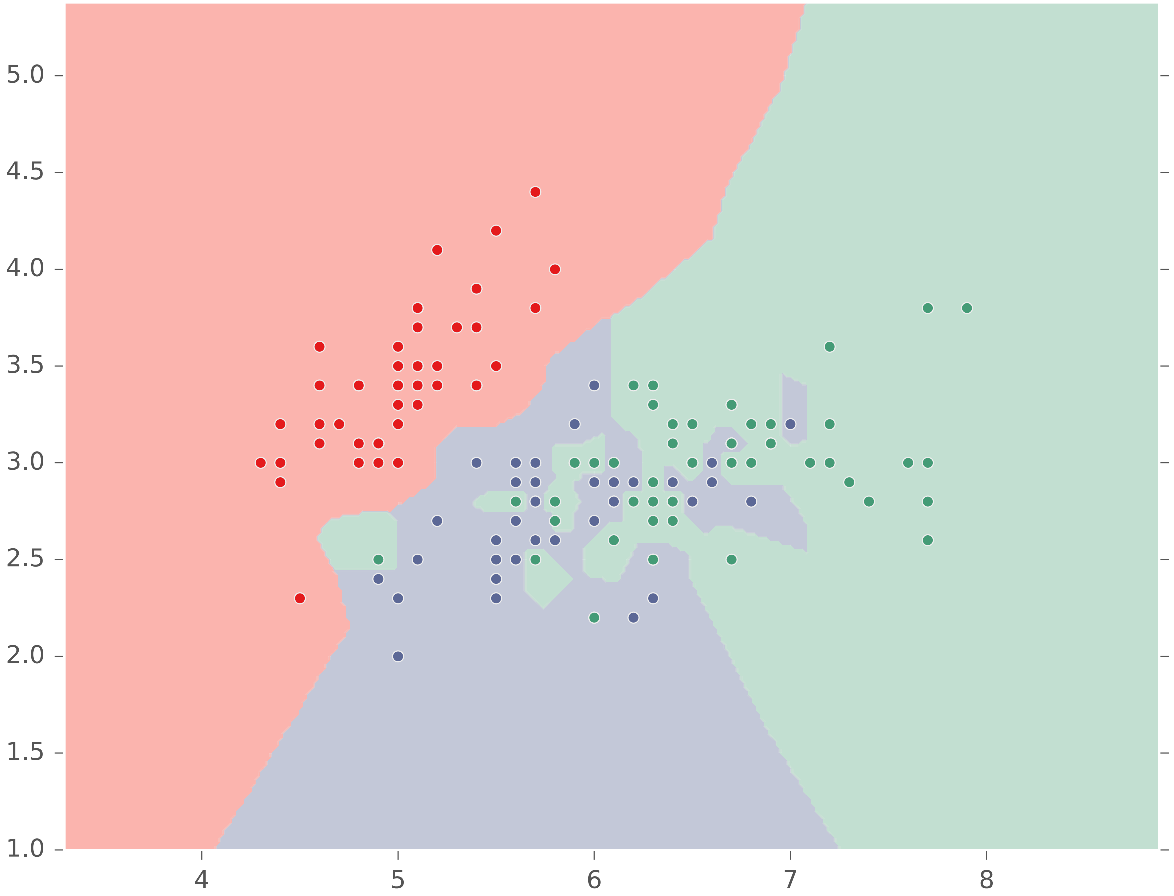
Today

- K-nearest neighbor
- Nearest neighbor remarks
- Model selection / hyperparameter optimization
  - Validation methods

Nearest Neighbor Classifier



Nearest Neighbor on Fisher Iris Data



Piazza Poll 1

Which methods can achieve zero training error on this dataset?

A. Decision trees

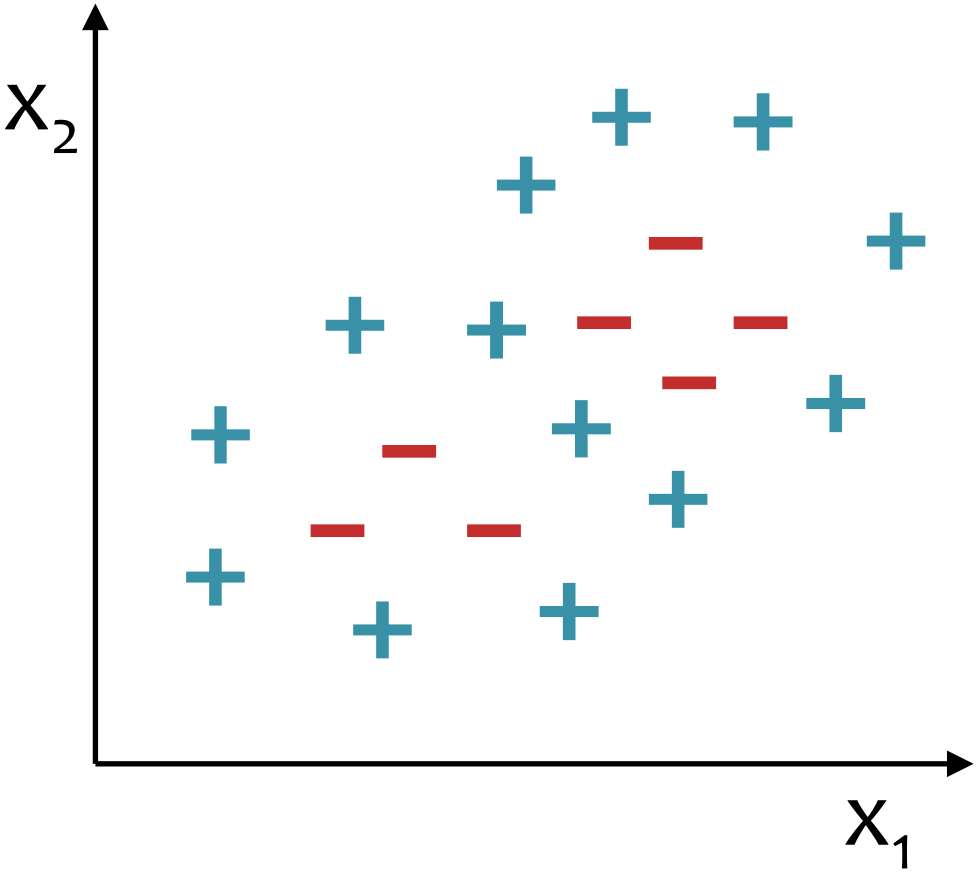
B. 1-Nearest Neighbor

C. Both

D. Neither

If zero error, draw the decision boundary.

Otherwise, why not?



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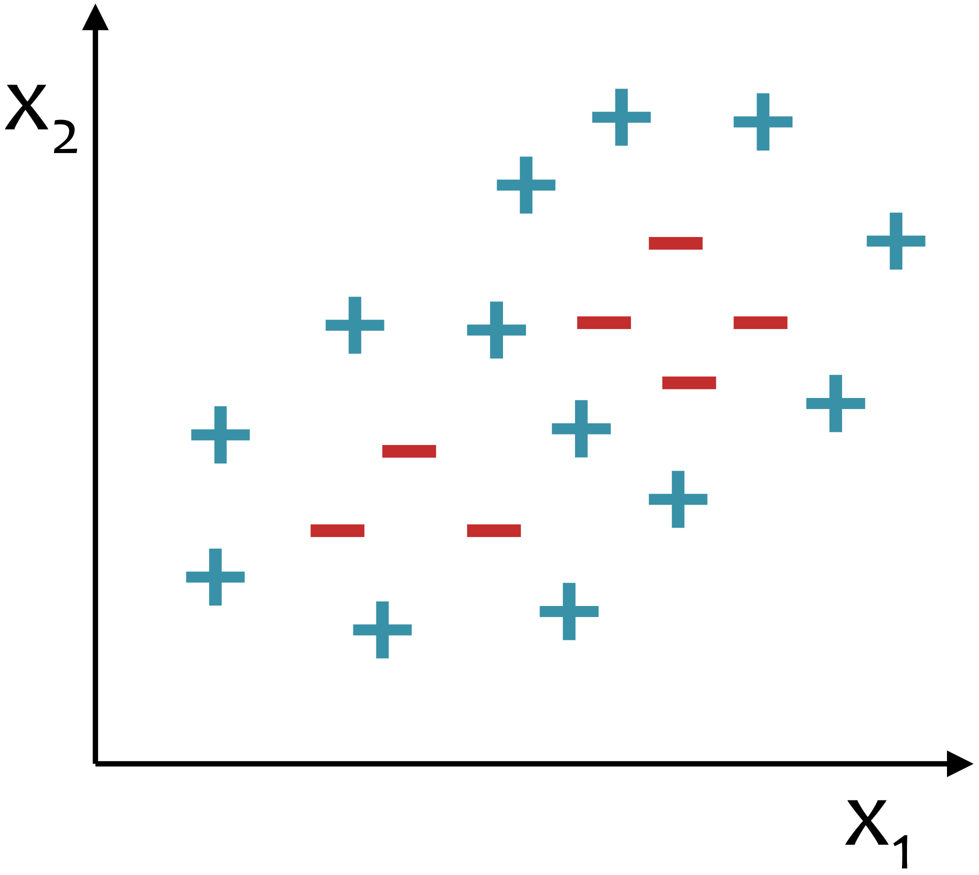

Piazza Poll 1

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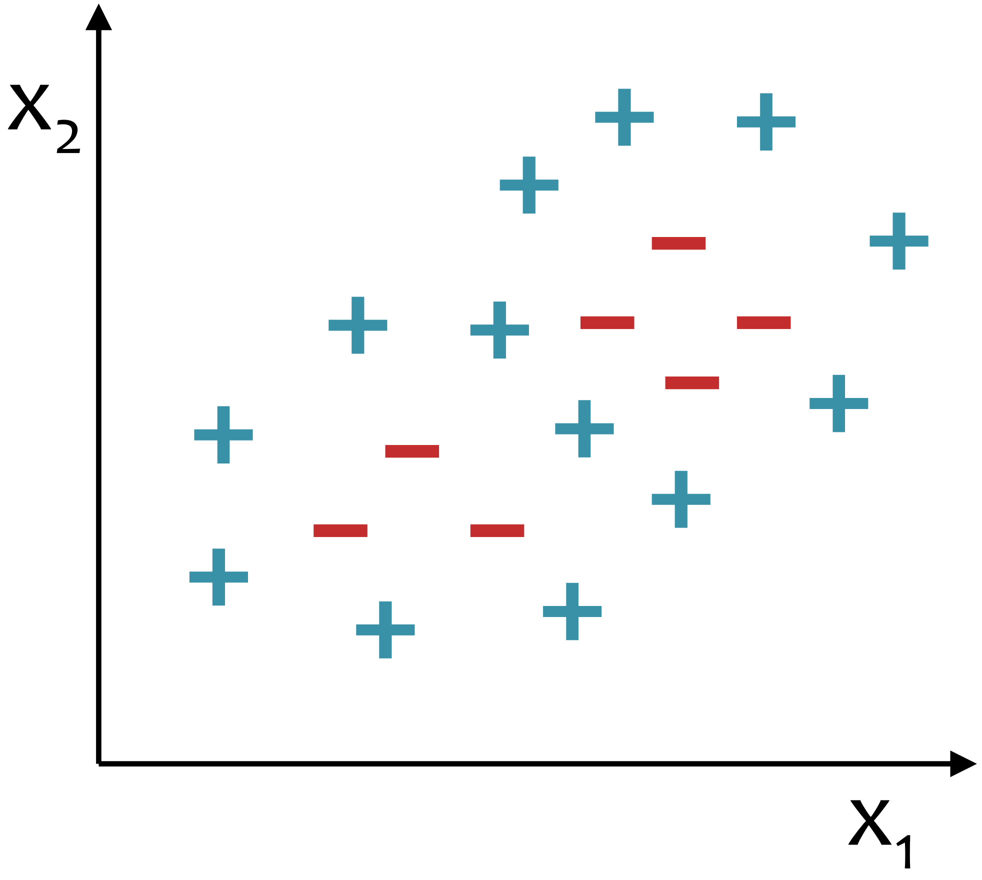
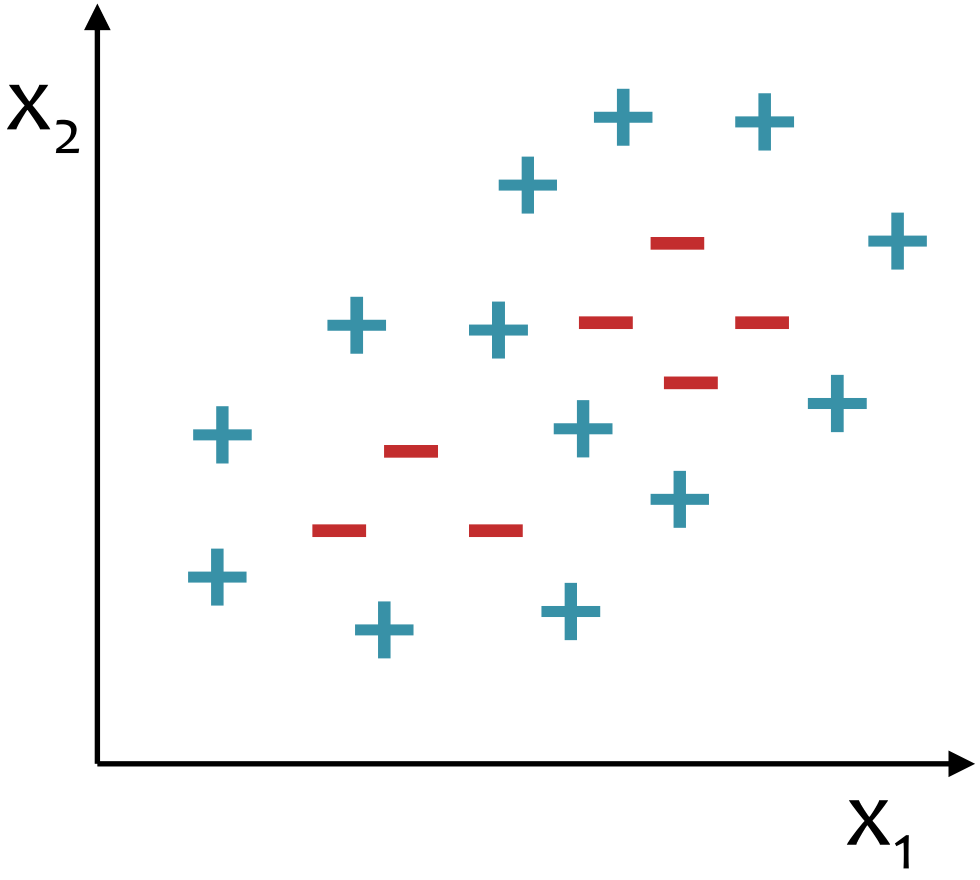
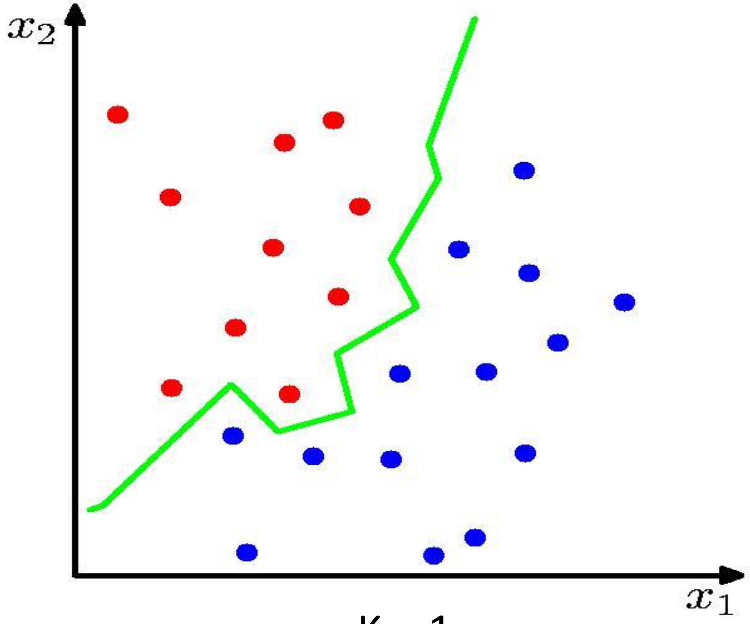




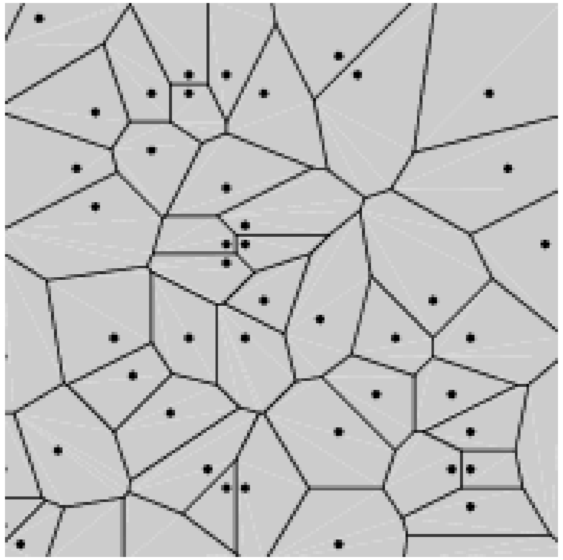
Nearest Neighbor Decision Boundary

1-nearest neighbor classifier decision boundary



K = 1

Voronoi Diagram



Piazza Poll 2

1-nearest neighbor will likely:

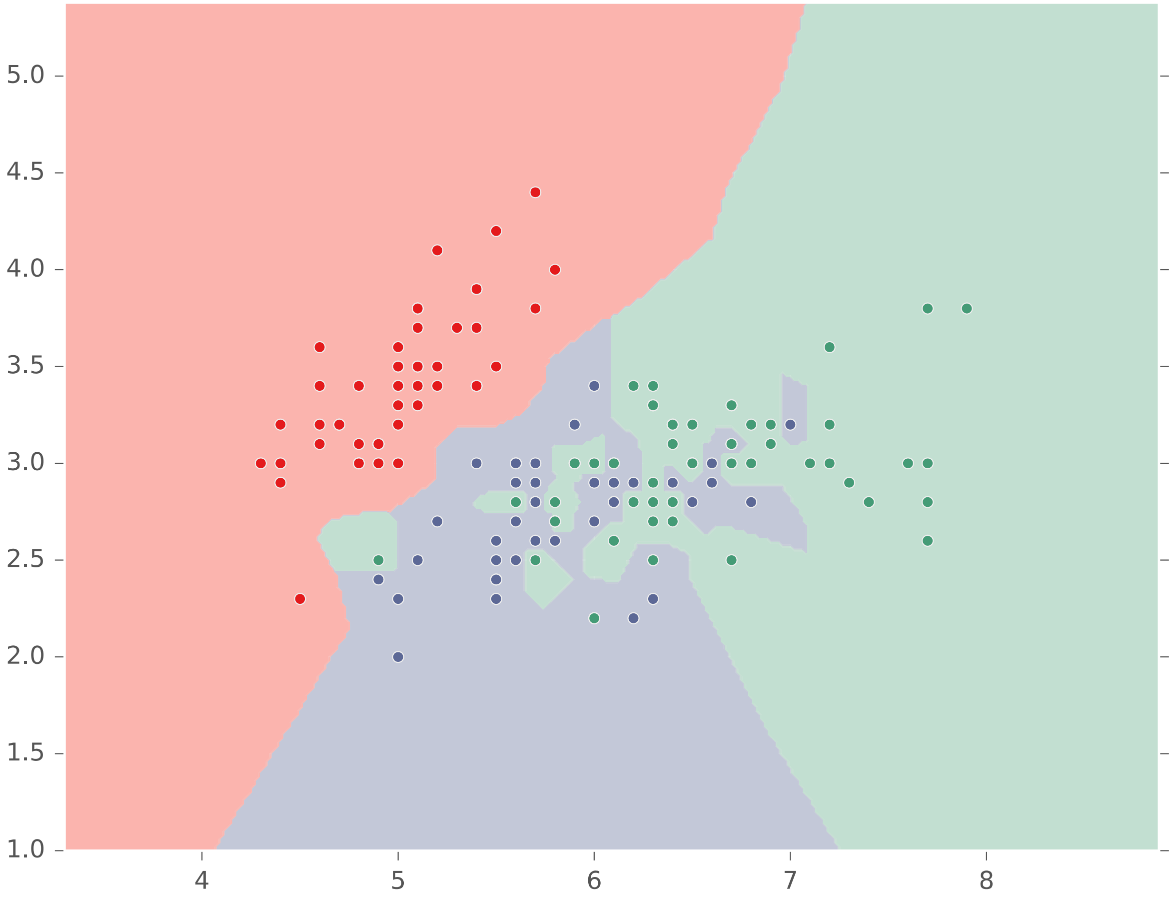
A. Overfit
B. Underfit
C. Neither (it’s a great learner!)

Piazza Poll 2

1-Nearest neighbor will likely:

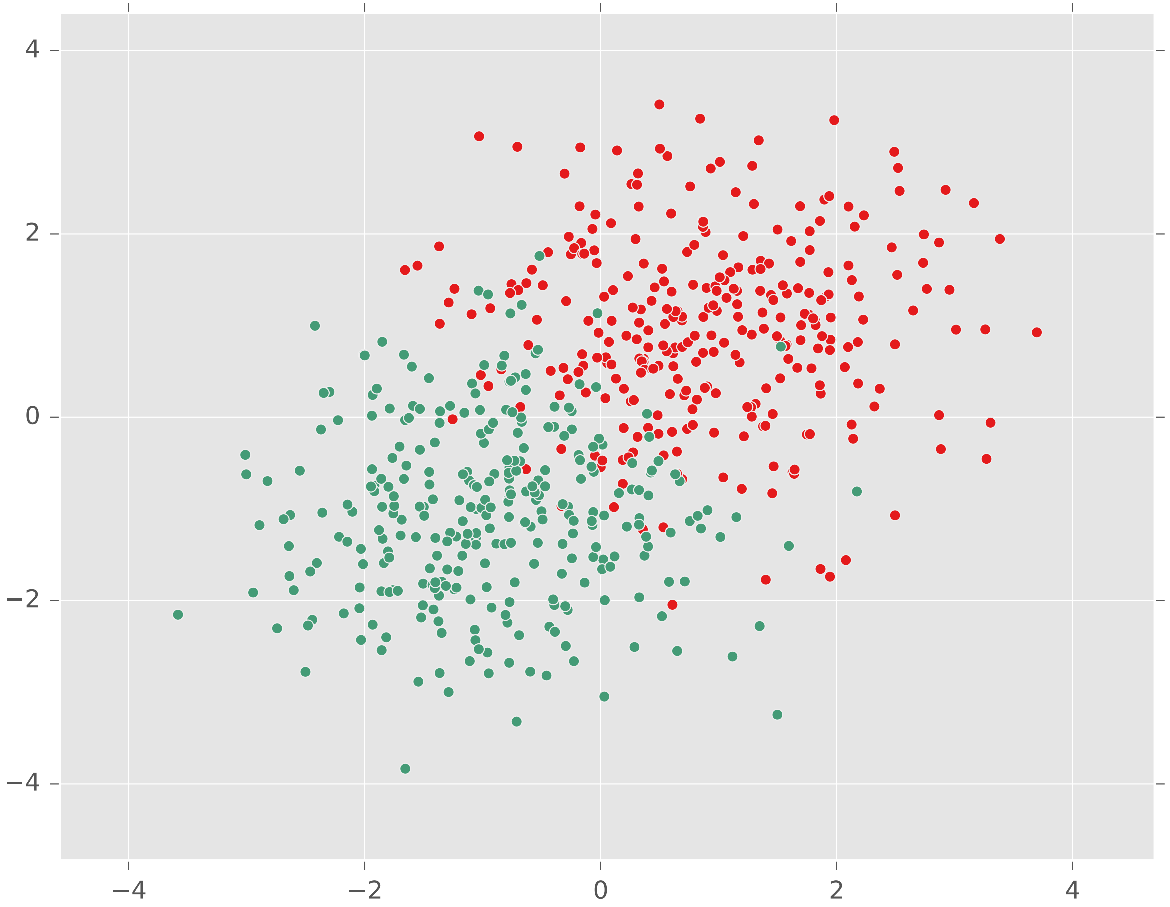
A. Overfit
B. Underfit
C. Neither (it’s a great learner!)

Nearest Neighbor on Fisher Iris Data



Slide credit: CMU MLD Matt Gormley

Nearest Neighbor on Gaussian Data



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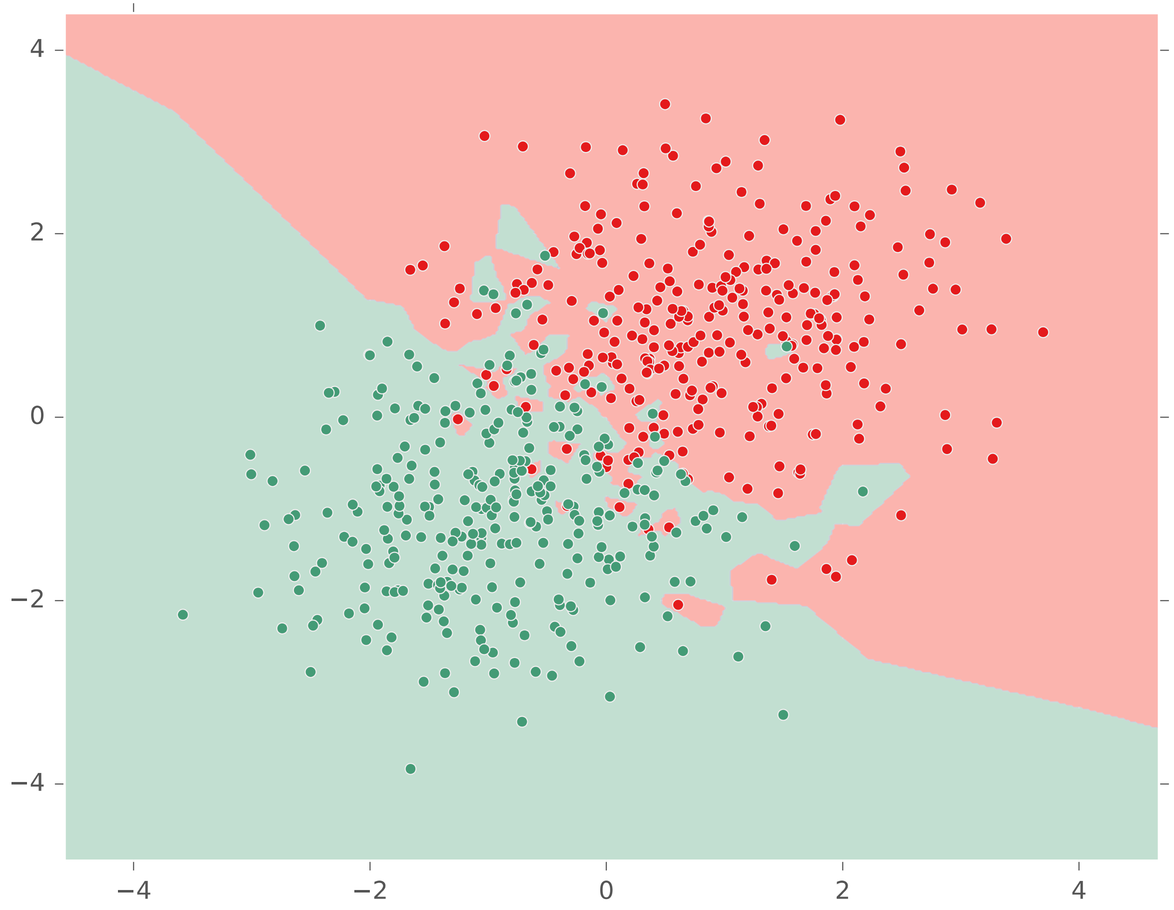
Nearest Neighbor on Gaussian Data



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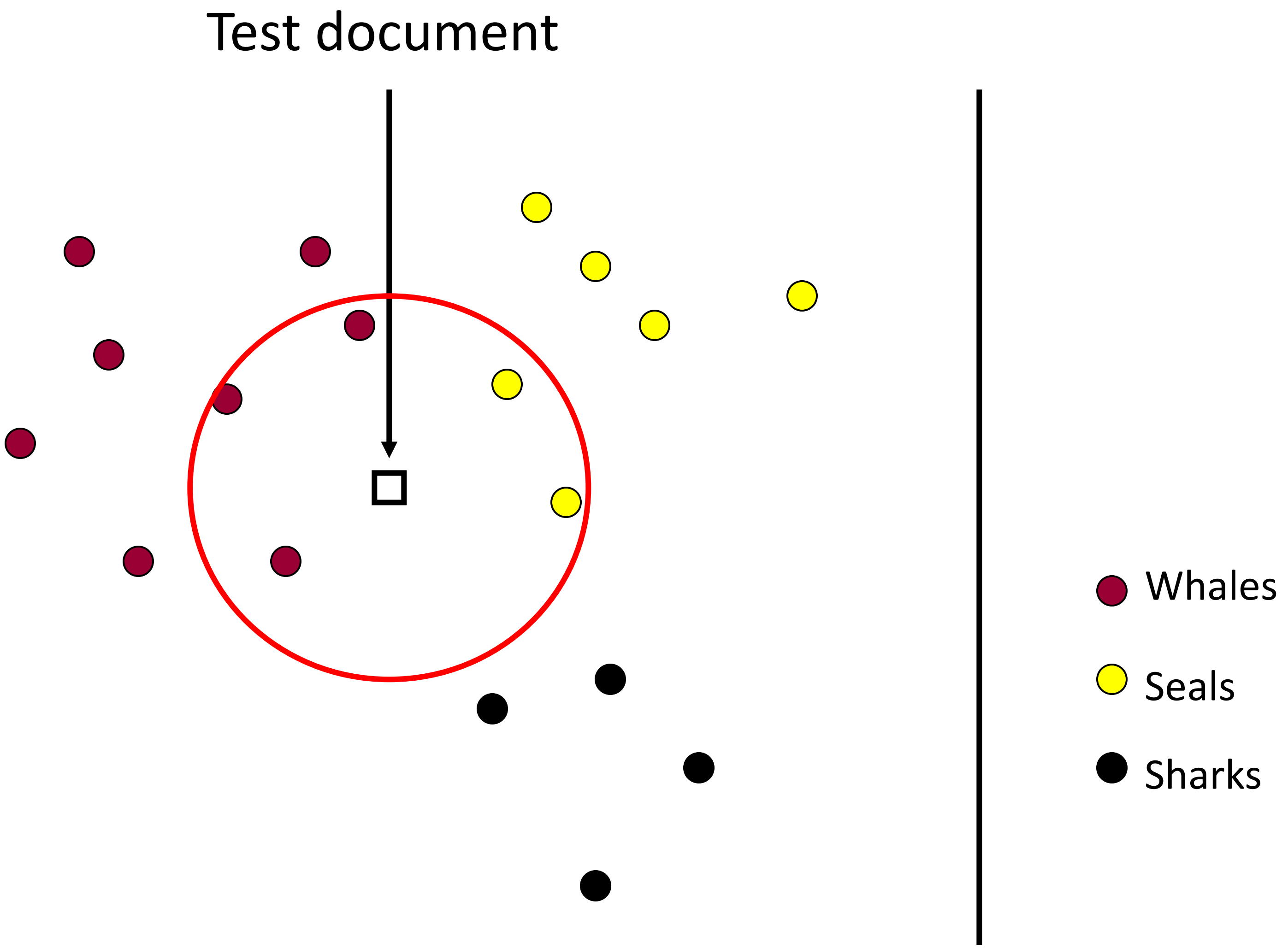
kNN classifier (k=5)



Nearest Neighbor Classification

train(D)
store D

Given a training dataset $\mathcal{D} = \{y^{(n)}, \boldsymbol{x}^{(n)}\}_{n=1}^{N}$, $y \in \{1, \ldots, C\}$, $\boldsymbol{x} \in \mathbb{R}^M$

and a test input $\boldsymbol{x}_{test}$, predict the class label, $\hat{y}_{test}$:

$h(\vec{x}_{test})$

1) Find the closest point in the training data to $\boldsymbol{x}_{test}$

$$n = \underset{n}{\operatorname{argmin}}\, d(\boldsymbol{x}_{test}, \boldsymbol{x}^{(n)})$$

2) Return the class label of that closest point

$$\hat{y}_{test} = y^{(n)}$$

Need distance function! What should $d(\boldsymbol{x}, \boldsymbol{z})$ be?

$$d(\vec{x}, \vec{z}) = \|\vec{x} - \vec{z}\|_2 = \left(\sum_{i=1}^{M} (x_i - z_i)^2\right)^{1/2}$$

ℓ_2

$$d(\vec{x}, \vec{z}) = \|\vec{x} - \vec{z}\|_1 = \sum_{i=1}^{M} |x_i - z_i|$$

ℓ_1

k-Nearest Neighbor Classification

Given a training dataset $\mathcal{D} = \{y^{(n)}, \boldsymbol{x}^{(n)}\}_{n=1}^{N}$, $y \in \{1, \dots, C\}$, $\boldsymbol{x} \in \mathbb{R}^M$

and a test input $\boldsymbol{x}_{test}$, predict the class label, $\hat{y}_{test}$:

1) Find the closest k points in the training data to $\boldsymbol{x}_{test}$

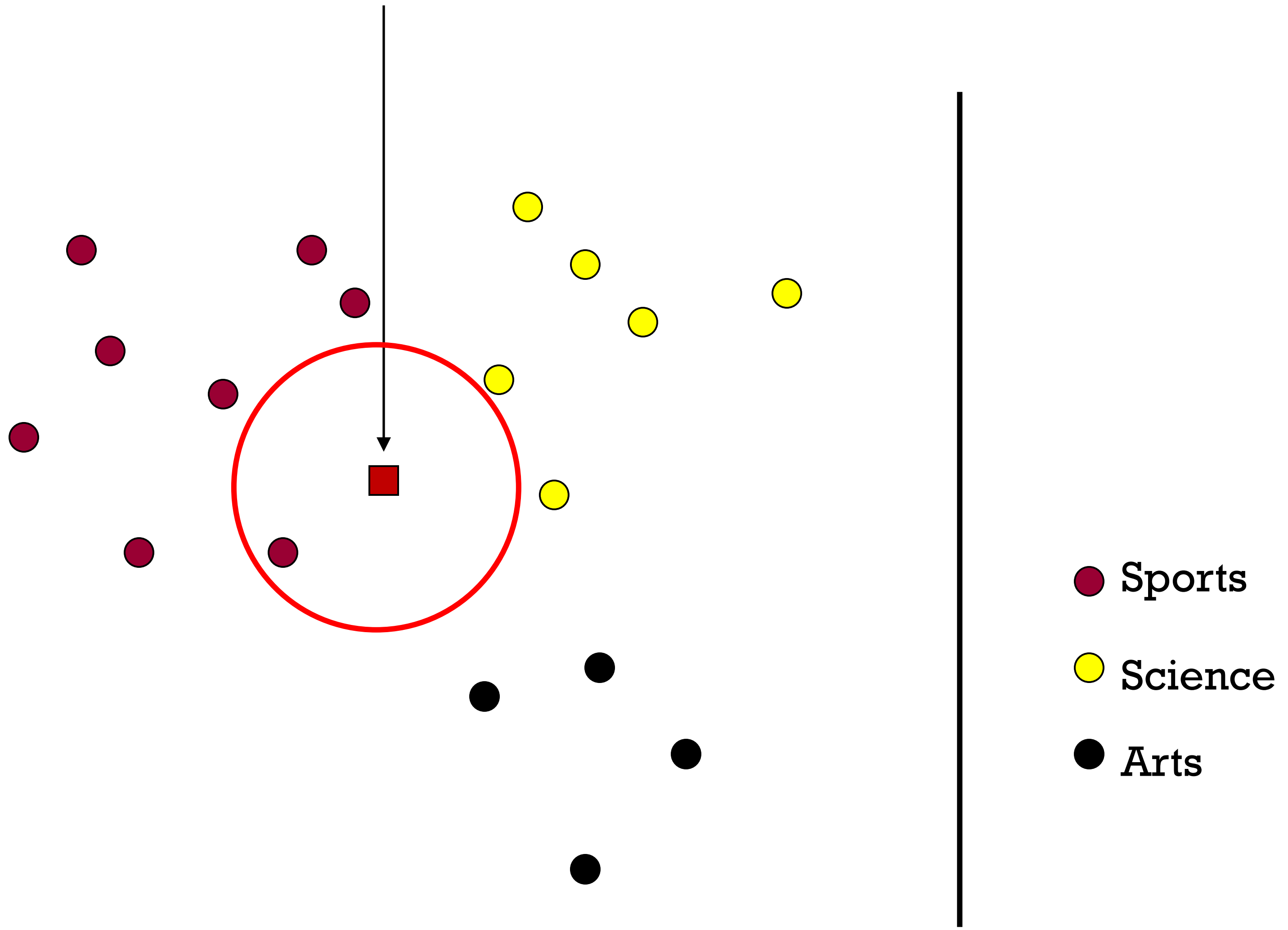
$$\mathcal{N}_k(\boldsymbol{x}_{test}, \mathcal{D})$$

2) Return the class label of that closest point

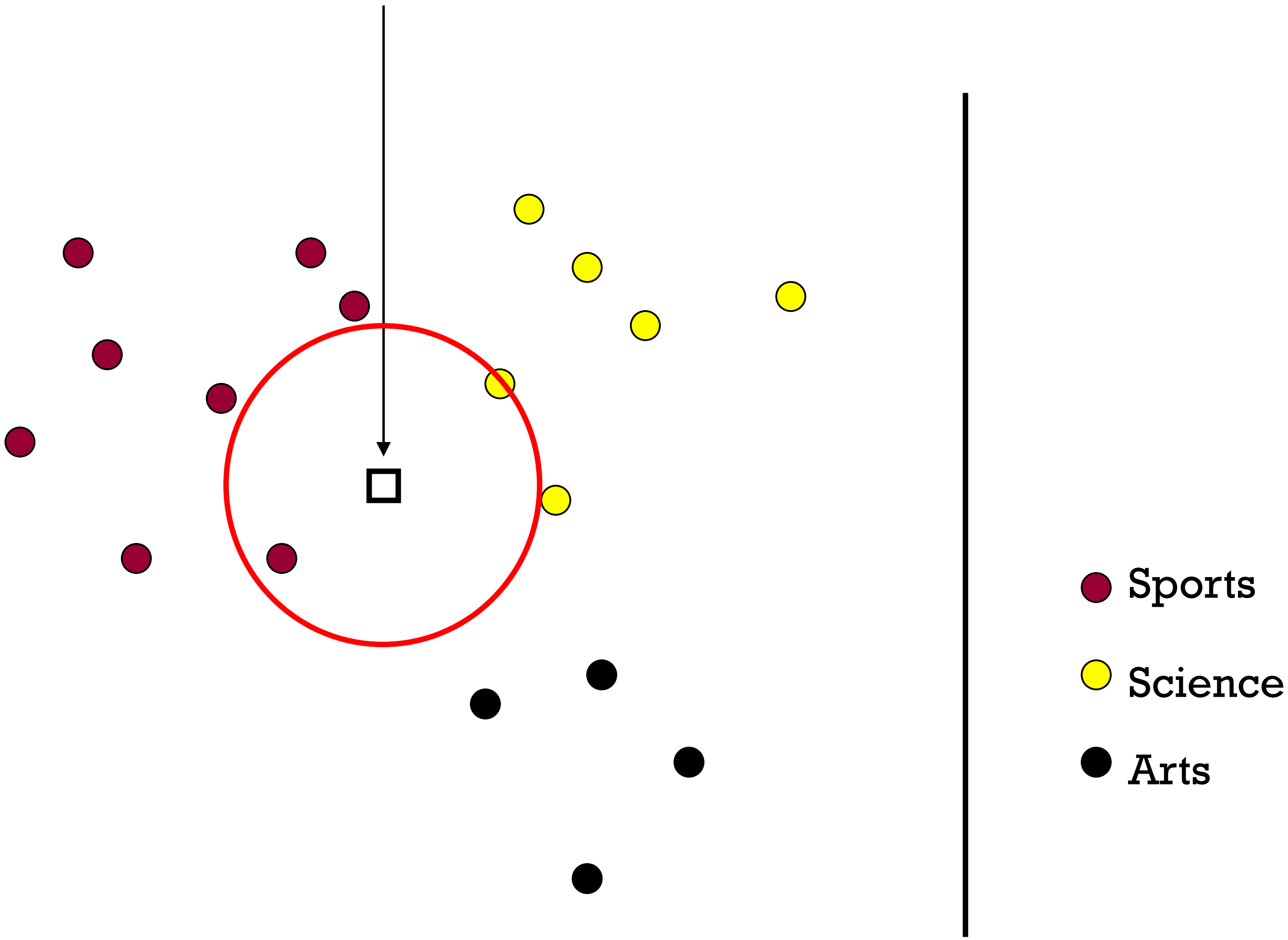
$$\begin{aligned}
\hat{y}_{test} &= \operatorname*{argmax}_c p(Y = c \mid \boldsymbol{x}_{test}, \mathcal{D}, k) \\
&= \operatorname*{argmax}_c \frac{1}{k} \sum_{i \in \mathcal{N}_k(\boldsymbol{x}_{test}, \mathcal{D})} \mathbb{I}(y^{(i)} = c) \\
&= \operatorname*{argmax}_c \frac{k_c}{k},
\end{aligned}$$

where k_c is the number of the k-neighbors with class label c

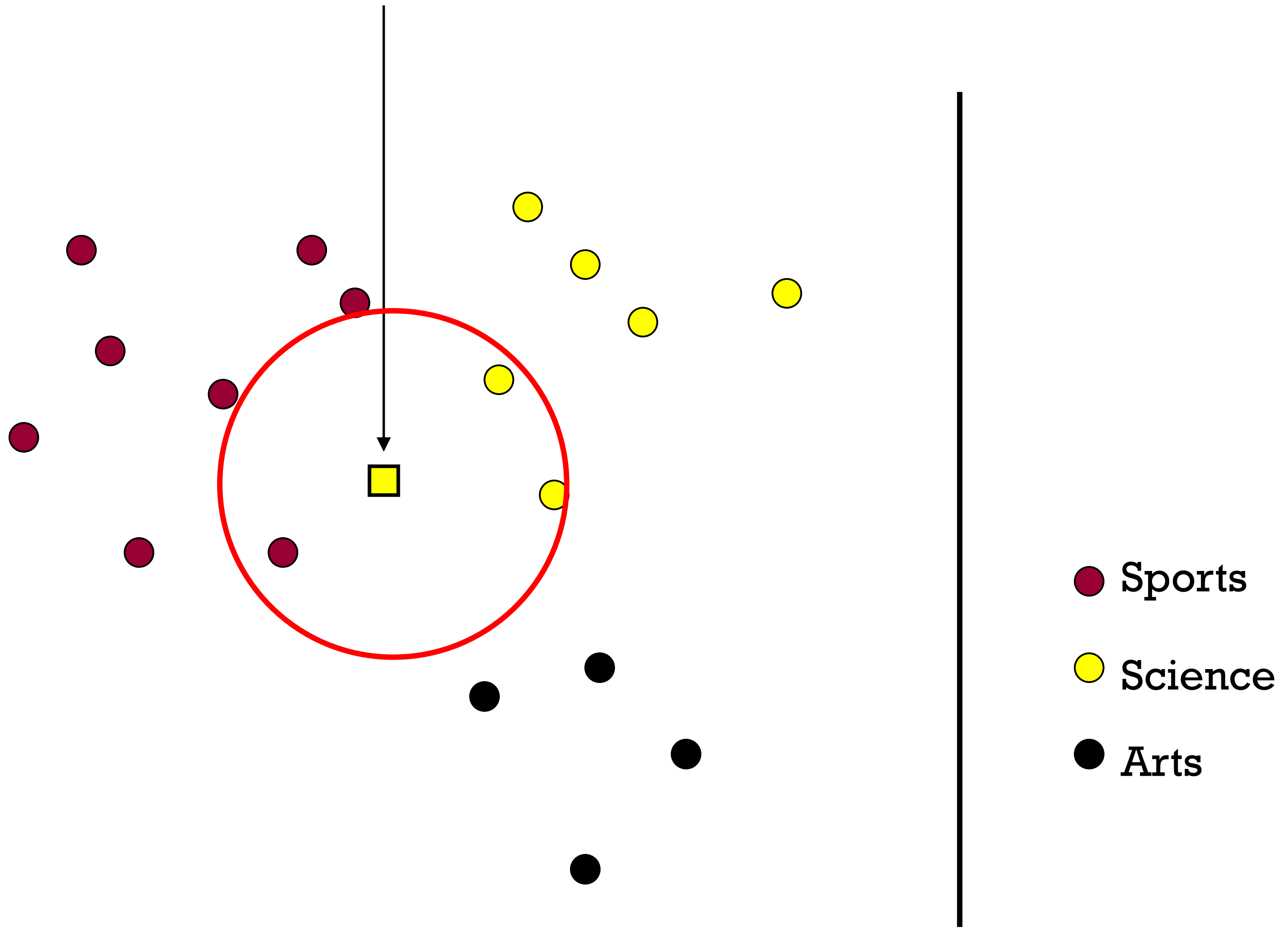
1-Nearest Neighbor (kNN) classifier



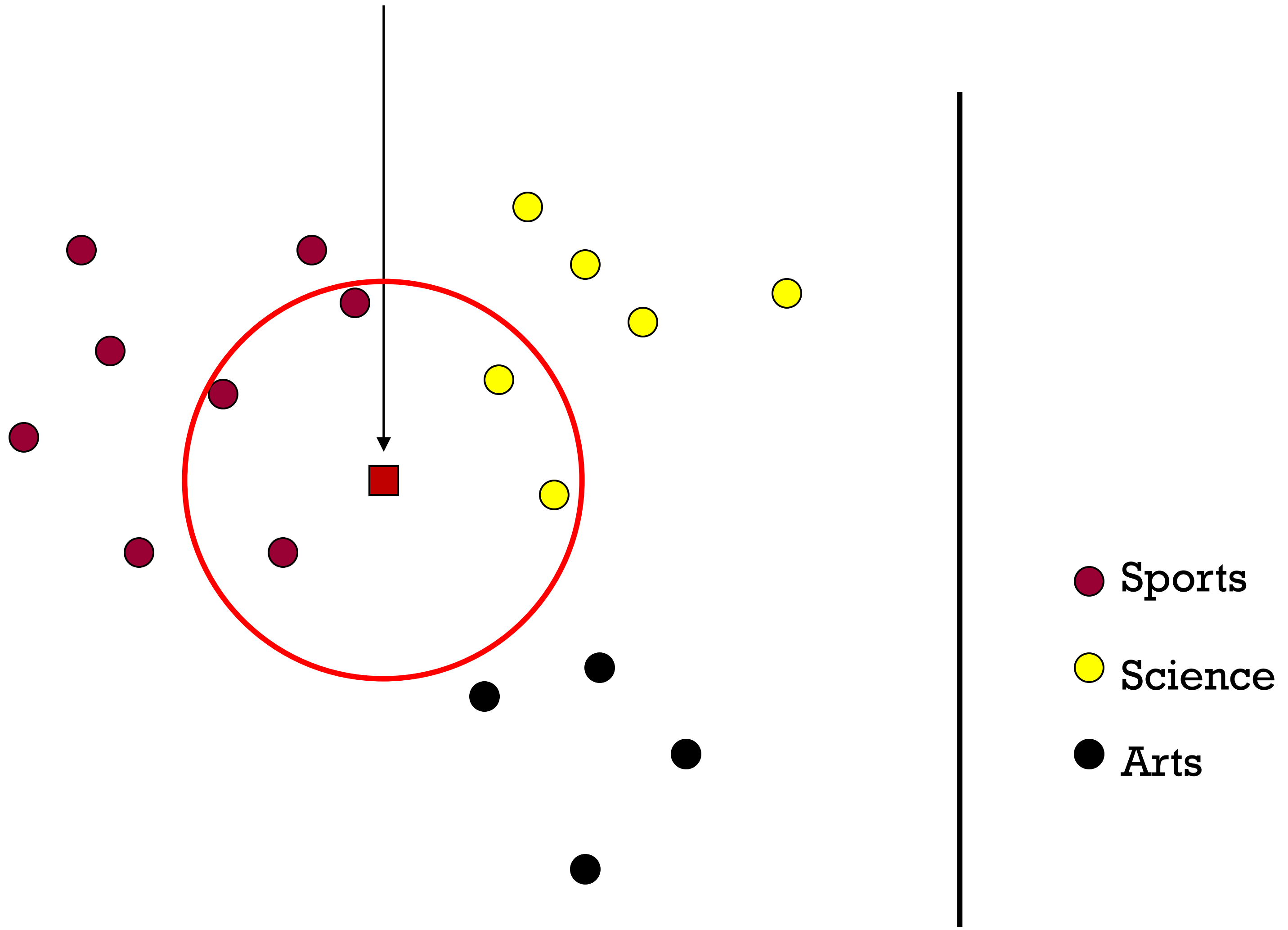
2-Nearest Neighbor (kNN) classifier



3-Nearest Neighbor (kNN) classifier



5-Nearest Neighbor (kNN) classifier



What is the best k?

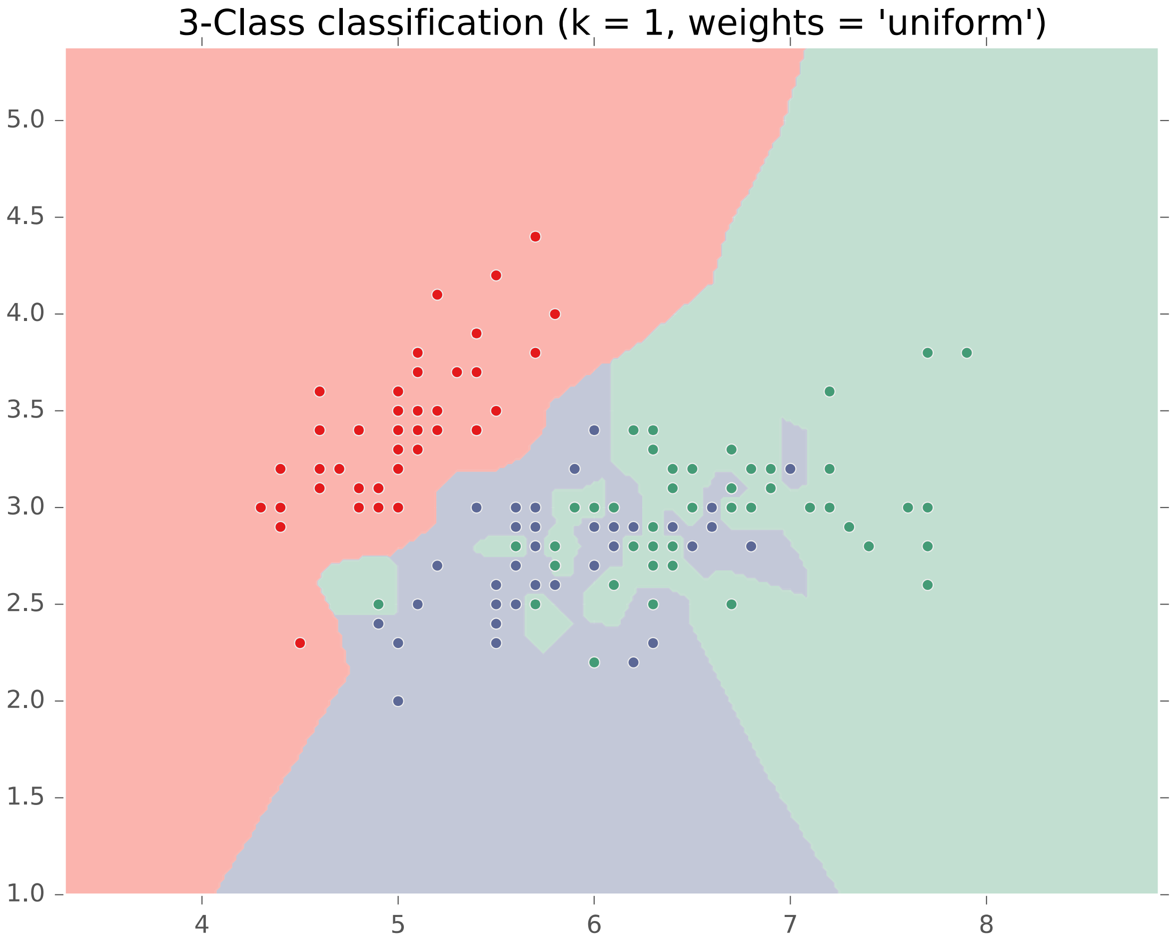
How do we choose a learner that is accurate and also generalizes to unseen data?

- Larger k → predicted label is more stable
- Smaller k → predicted label is more affected by individual training points

But how to choose k?

k-NN on Fisher Iris Data

Special Case: Nearest Neighbor



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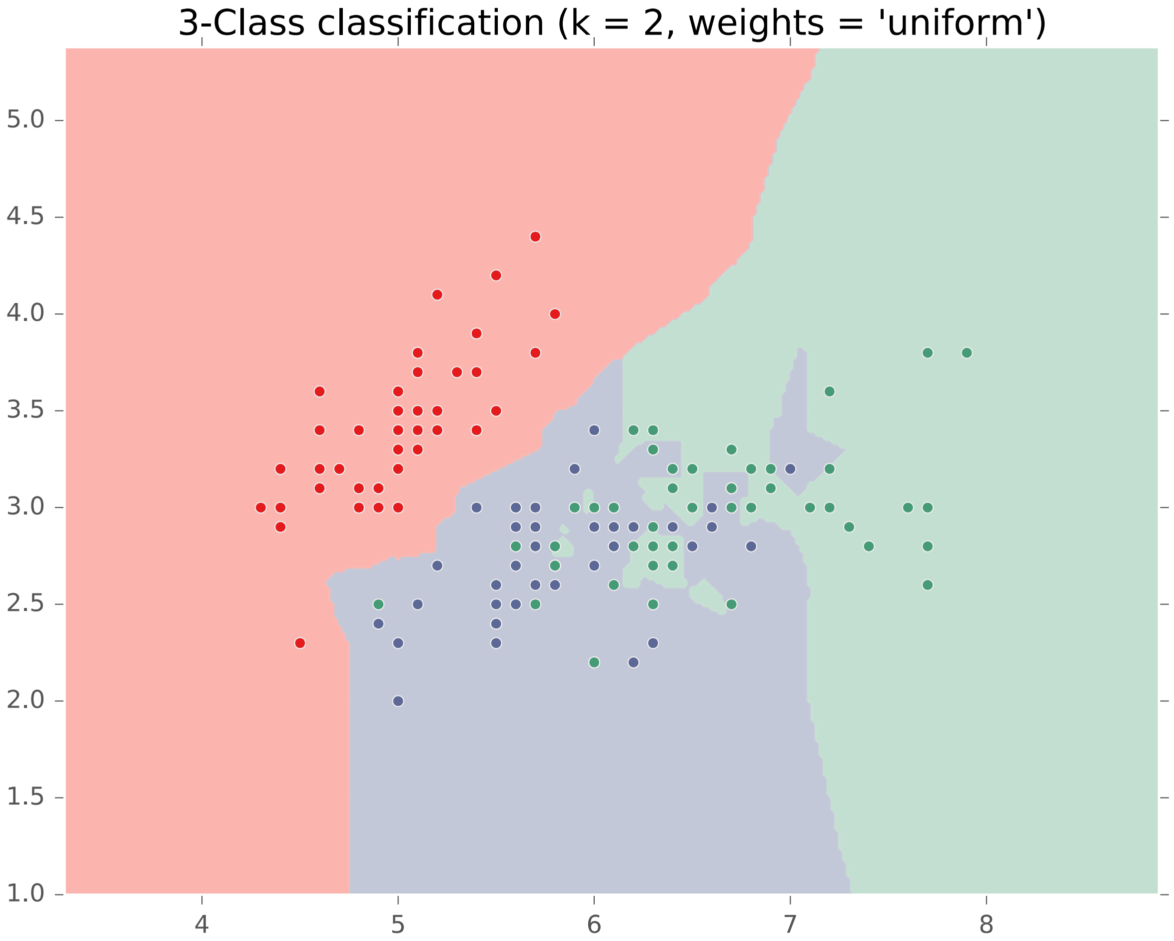

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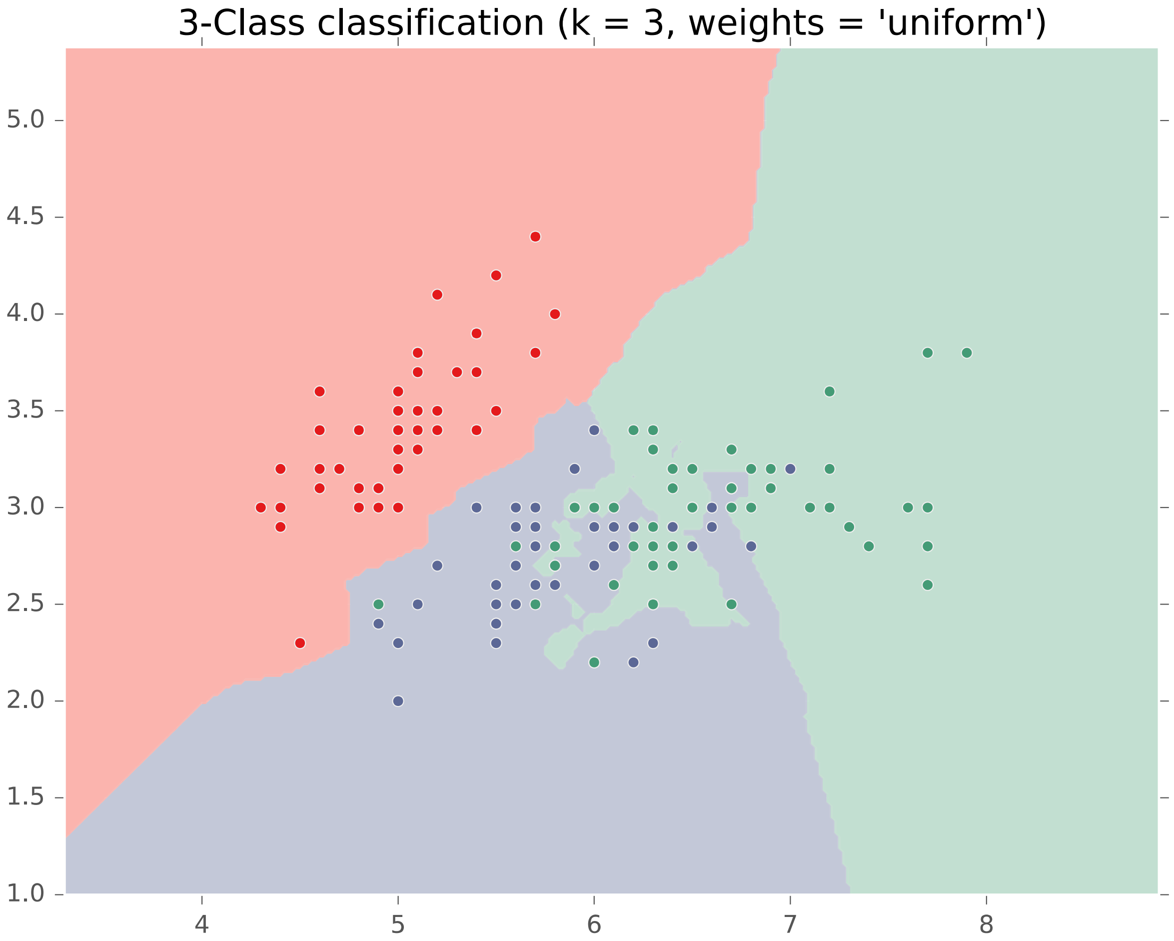

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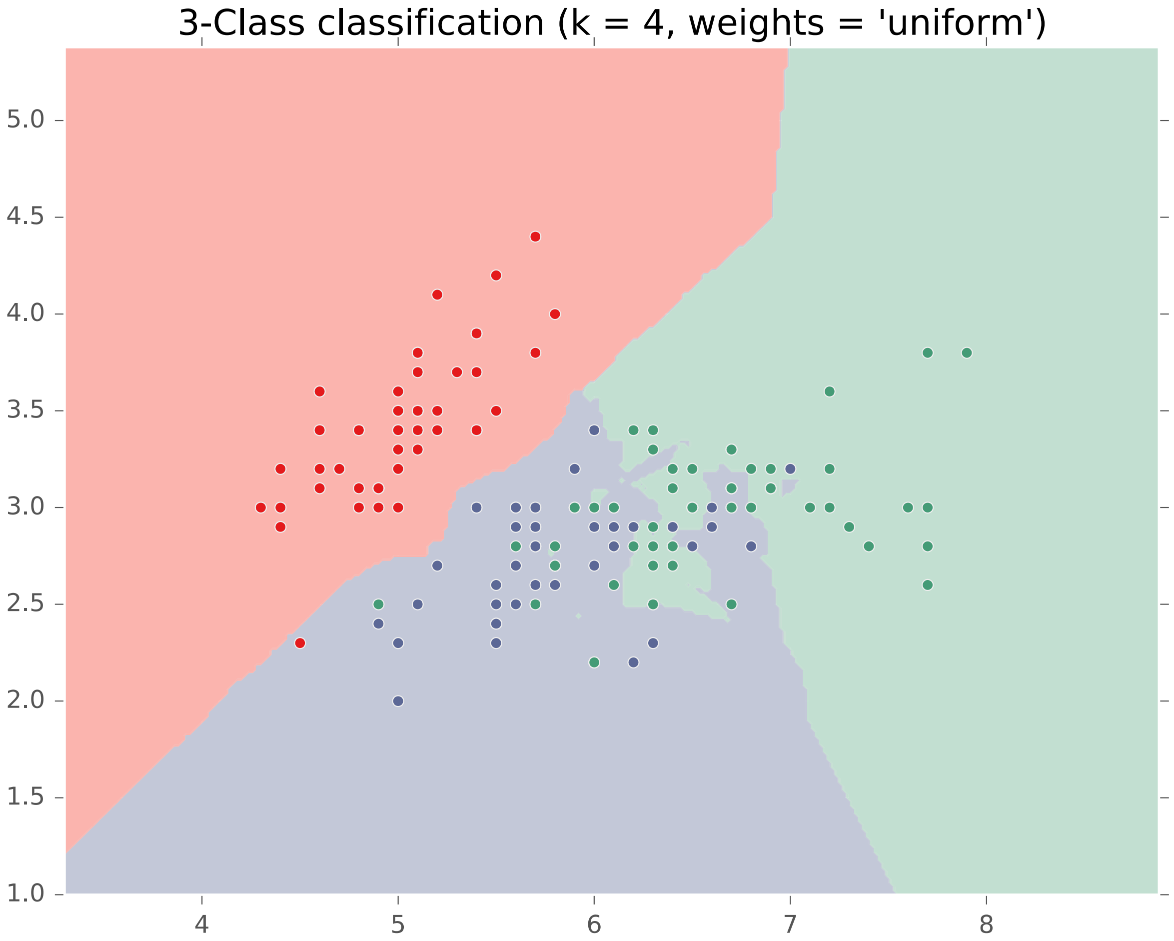

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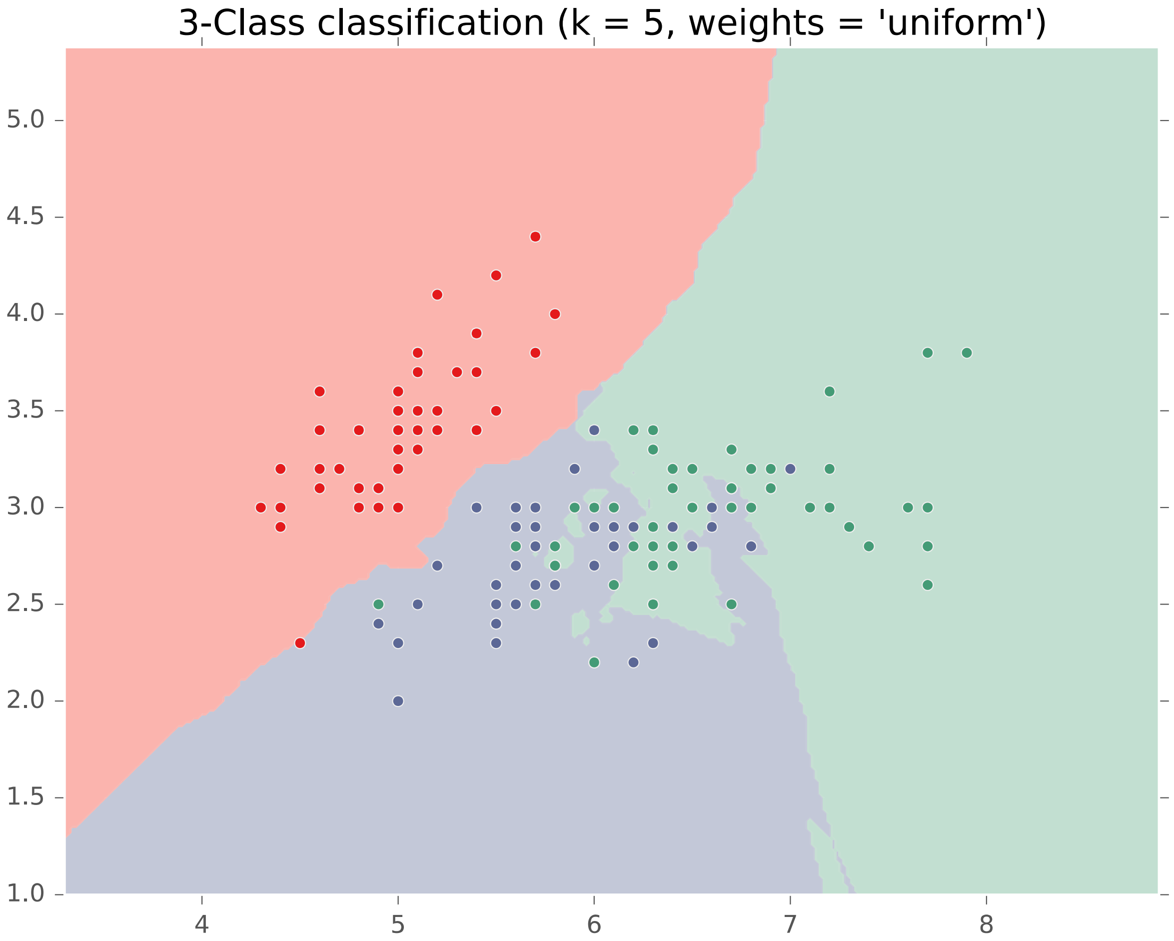

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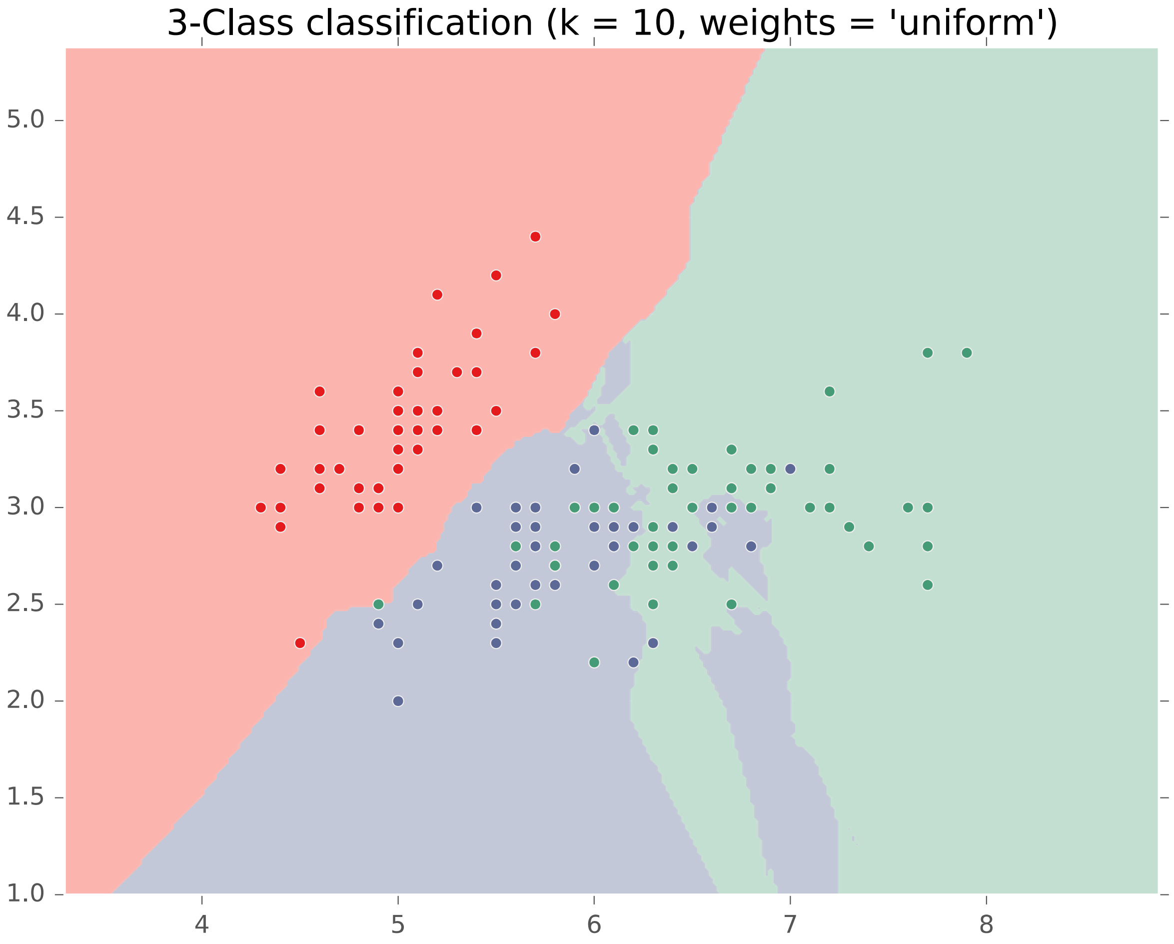

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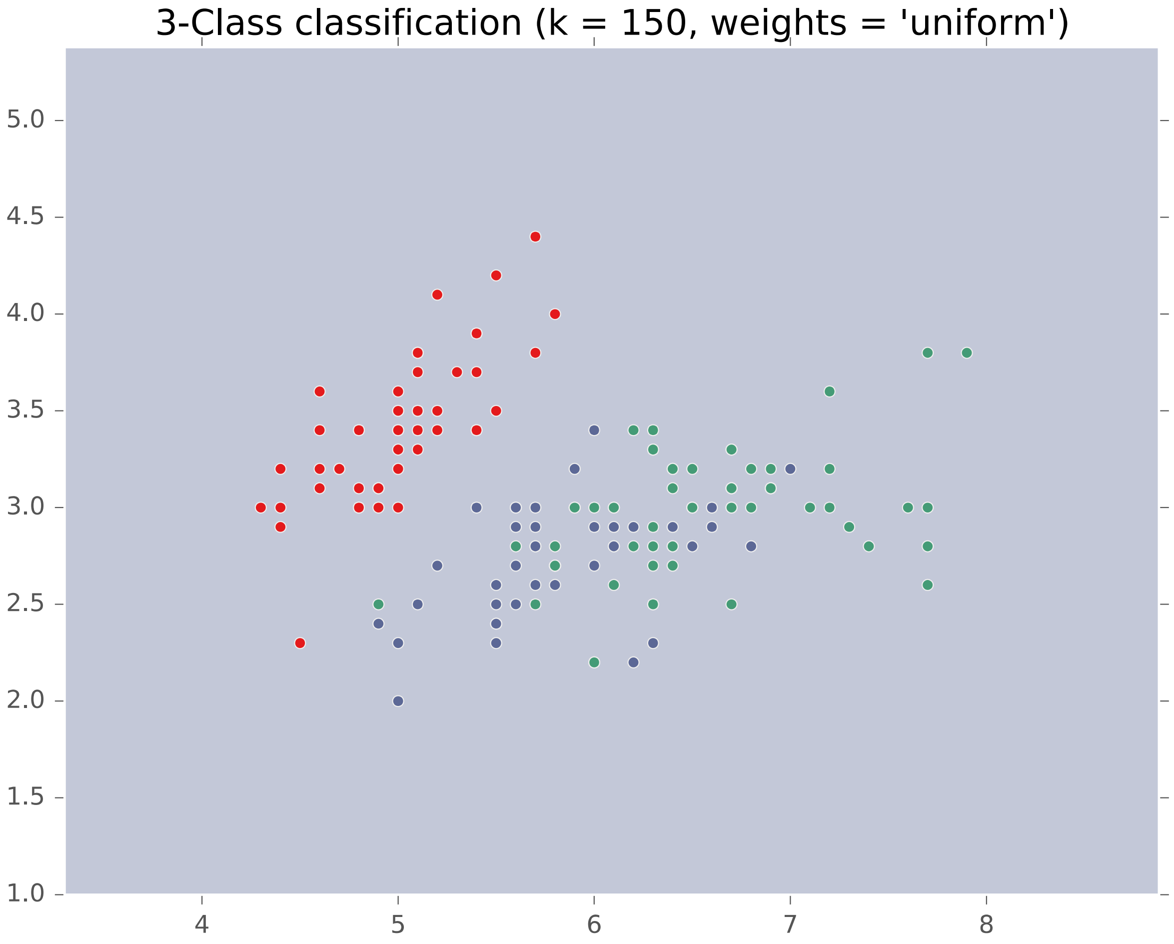
k-NN on Fisher Iris Data

Special Case: Majority Vote



k-NN: Remarks

Inductive Bias:

1. Close points should have similar labels
2. All dimensions are created equally!

k-NN: Remarks

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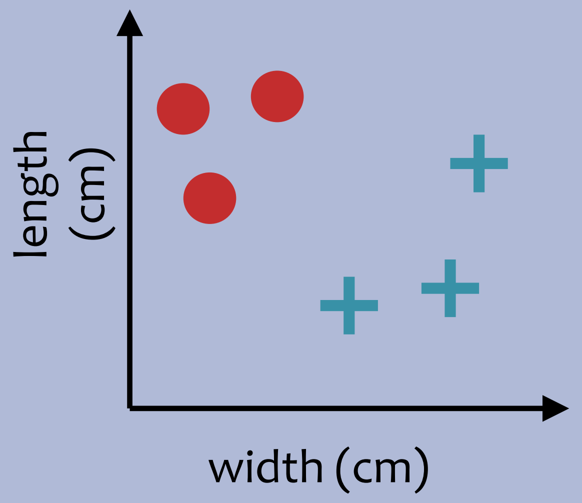
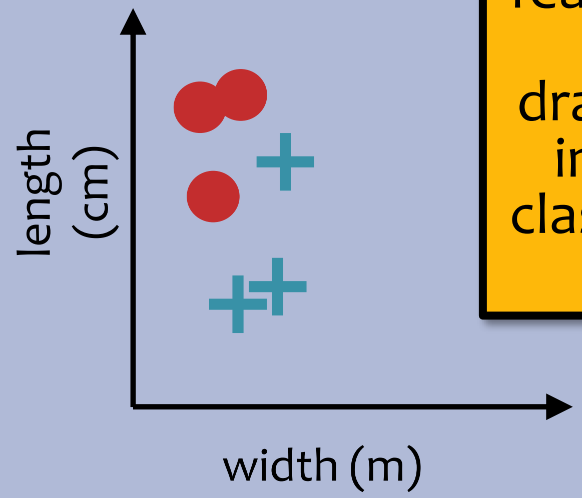
Example: two features for k-NN





big problem: feature scale could dramatically influence classification results

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k-NN: Remarks

Computational Efficiency:

- Suppose we have N training examples, and each one has M features
- Computational complexity for the special case where k=1:

Piazza Poll 3 (train) and Poll 4 (test)

Suppose we have N training examples, and each one has M features
Computational complexity for the special case where k=1:

A. O(1)
B. O(log N)
C. O(log M)
D. O(log NM)
E. O(N)
F. O(M)
G. O(NM)
H. O(N^2)
I. O(N^2M)

Piazza Poll 3 (train) and Poll 4 (test)

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k-NN: Remarks

Computational Efficiency:

- Suppose we have N training examples, and each one has M features
- Computational complexity for the special case where k=1:

Task	Naive	k-d Tree
Train	O(1)	~ O(M N log N)
Predict (one test example)	O(MN)	~ $O(2^M \log N)$ on average

Problem: Very fast for small M, but very slow for large M

In practice: use stochastic approximations (very fast, and empirically often as good)

k-NN Learning Objectives

You should be able to…

- Describe a dataset as points in a high dimensional space
- Implement k-Nearest Neighbors with O(N) prediction
- Describe the inductive bias of a k-NN classifier and relate it to feature scale
- Sketch the decision boundary for a learning algorithm (compare k-NN and DT)

MODEL SELECTION

Model Selection

WARNING:

- In some sense, our discussion of model selection is premature.
- The models we have considered thus far are fairly simple.
- The models and the many decisions available to the data scientist wielding them will grow to be much more complex than what we've seen so far.

Model Selection

Statistics

- *Def*: a **model** defines the data generation process (i.e. a set or family of parametric probability distributions)
- *Def*: **model parameters** are the values that give rise to a particular probability distribution in the model family
- *Def*: **learning** (aka. estimation) is the process of finding the parameters that best fit the data
- *Def*: **hyperparameters** are the parameters of a prior distribution over parameters

Machine Learning

- *Def*: (loosely) a **model** defines the hypothesis space over which learning performs its search
- *Def*: **model parameters** are the numeric values or structure selected by the learning algorithm that give rise to a hypothesis
- *Def*: the **learning algorithm** defines the data-driven search over the hypothesis space (i.e. search for good parameters)
- *Def*: **hyperparameters** are the tunable aspects of the model, that the learning algorithm does *not* select

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Model Selection

Example: Decision Tree

- model = set of all possible trees, possibly restricted by some hyperparameters (e.g. max depth)
- parameters = structure of a specific decision tree
- learning algorithm = ID3, CART, etc.
- hyperparameters = max-depth, threshold for splitting criterion, etc.

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Model Selection

Example: k-Nearest Neighbors

- model = set of all possible nearest neighbors classifiers
- parameters = none
  (KNN is an instance-based or non-parametric method)
- learning algorithm = for naïve setting, just storing the data
- hyperparameters = k, the number of neighbors to consider

Machine Learning

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If "learning" is all about picking the best **parameters** how do we pick the best **hyperparameters?**

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Model Selection

- Two *very* similar definitions:
  - *Def*: **model selection** is the process by which we choose the "best" model from among a set of candidates
  - *Def*: **hyperparameter optimization** is the process by which we choose the "best" hyperparameters from among a set of candidates **(could be called a special case of model selection)**

- **Both** assume access to a function capable of measuring the quality of a model

- **Both** are typically done "outside" the main training algorithm --- typically training is treated as a black box

Experimental Design

	Input	Output	Notes
Training	• training dataset • hyperparameters	• best model parameters	We pick the best model parameters by learning on the training dataset for a fixed set of hyperparameters
Hyperparameter Optimization	• training dataset • validation dataset	• best hyperparameters	We pick the best hyperparameters by learning on the training data and evaluating error on the validation error
Testing	• test dataset • hypothesis (i.e. fixed model parameters)	• test error	We evaluate a hypothesis corresponding to a decision rule with fixed model parameters on a test dataset to obtain test error

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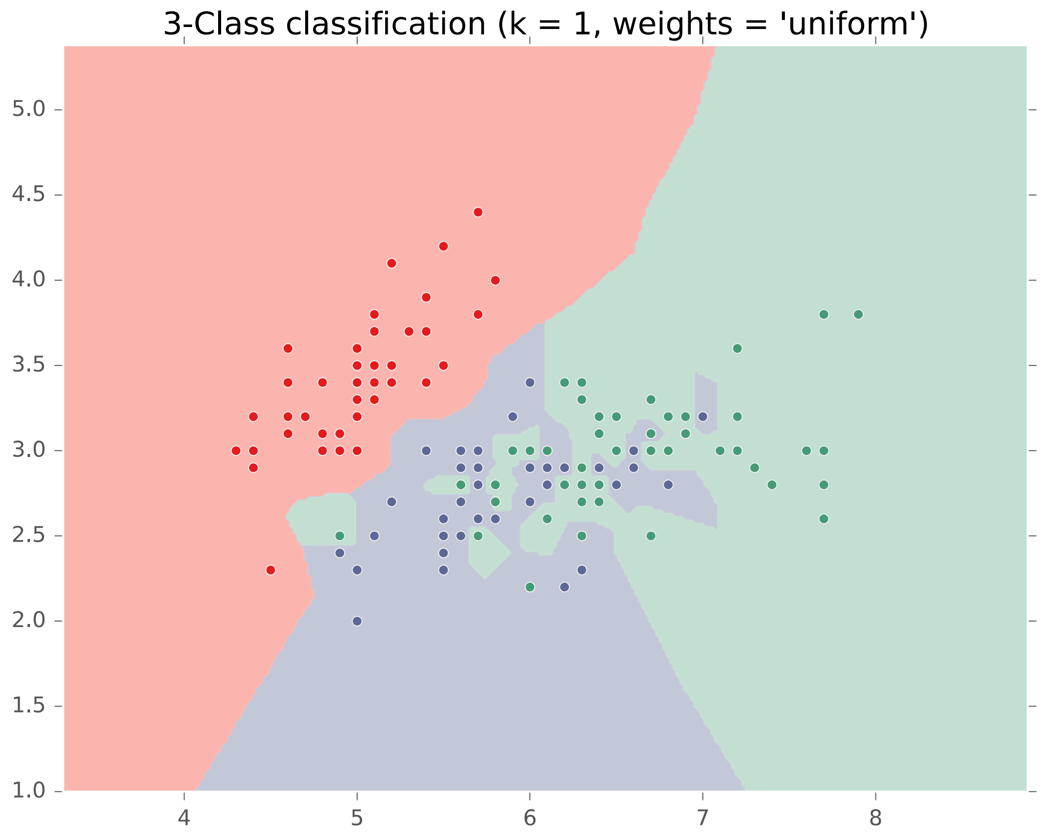
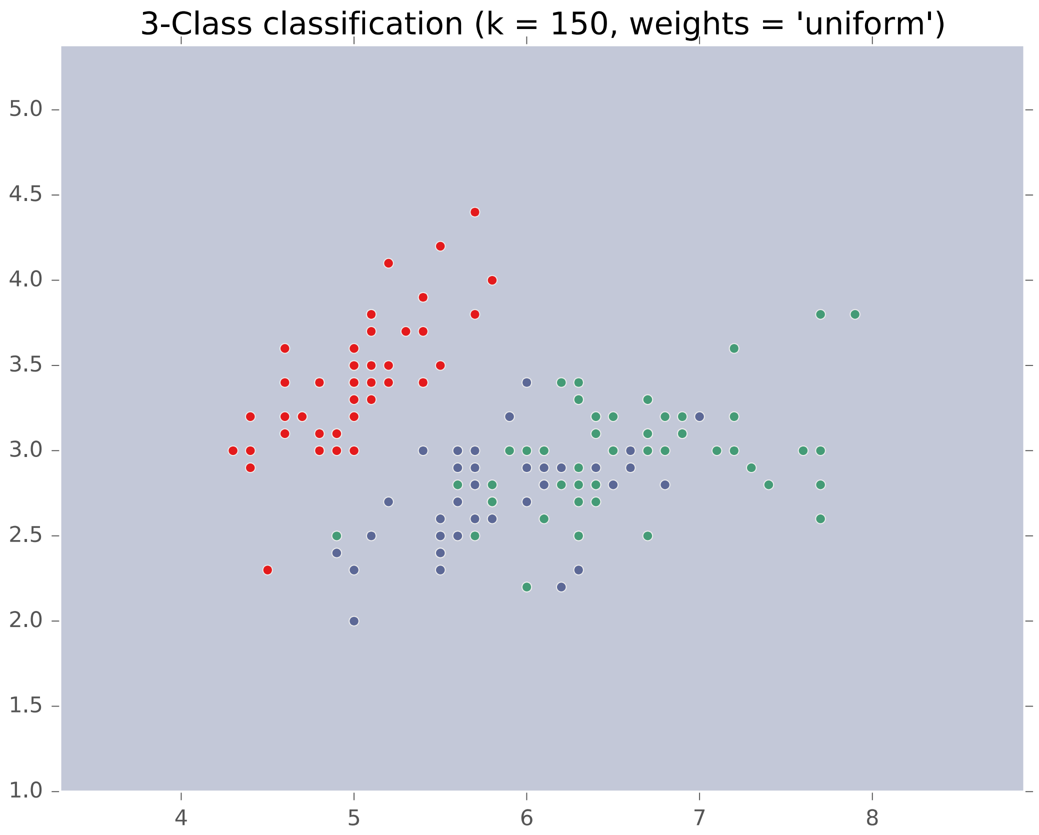
Special Cases of k-NN

k=1: Nearest Neighbor



k=N: Majority Vote



Example of Hyperparameter Optimization

Choosing k for k-NN

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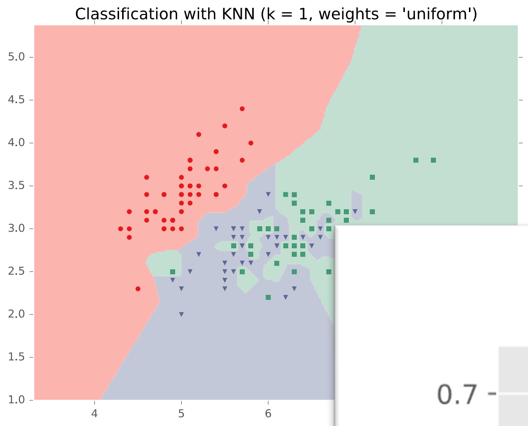
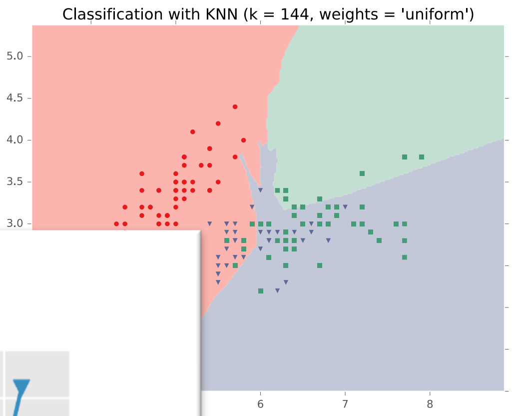
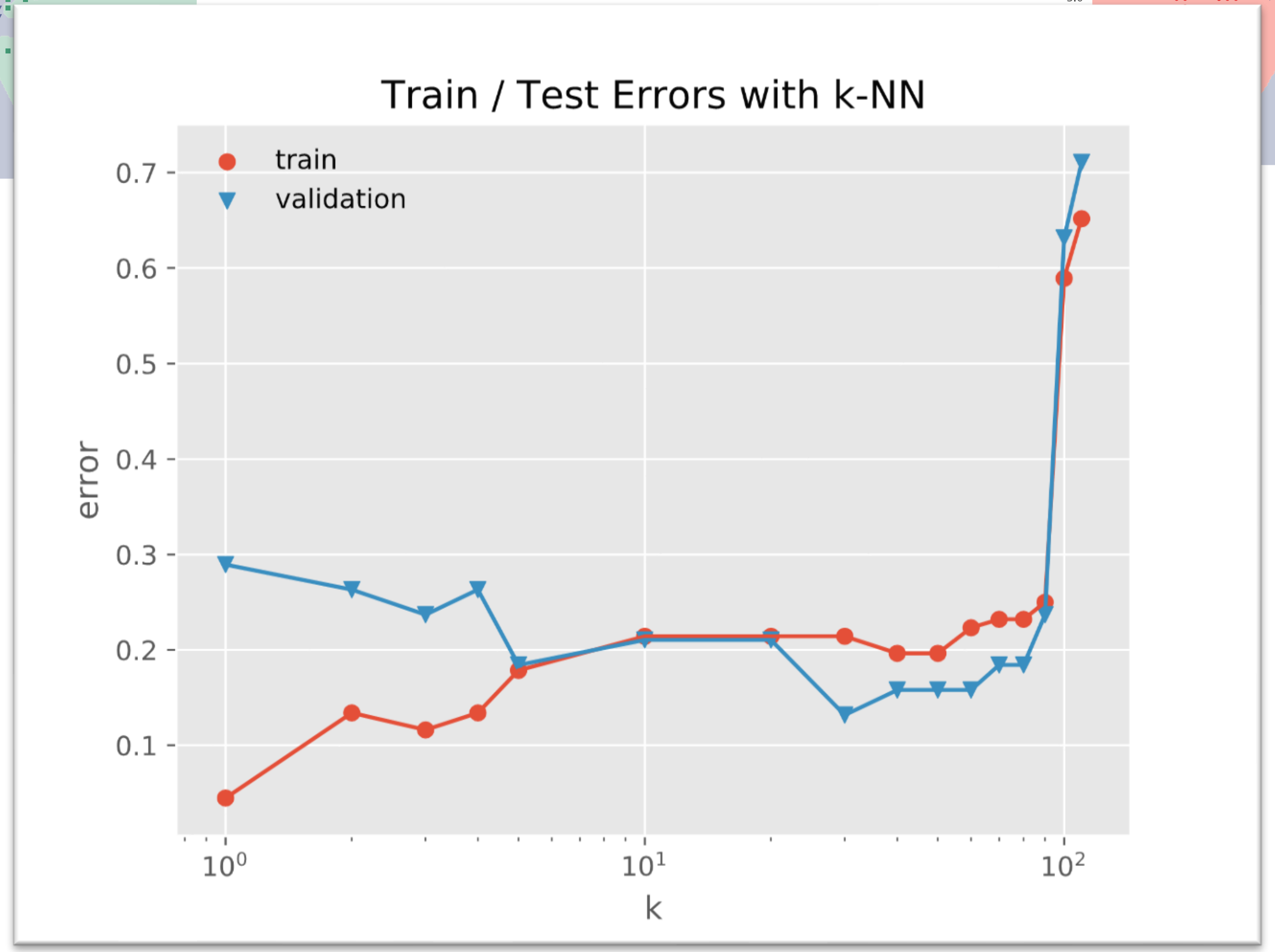


k-NN: Choosing k

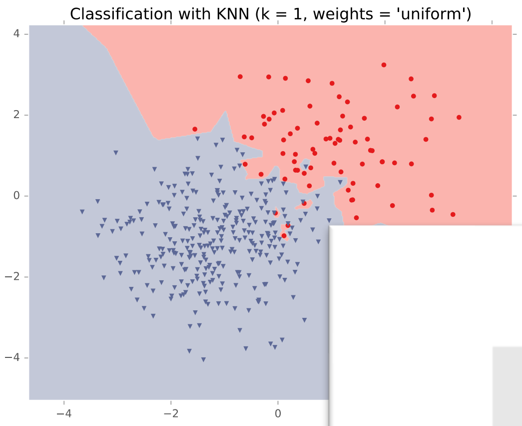


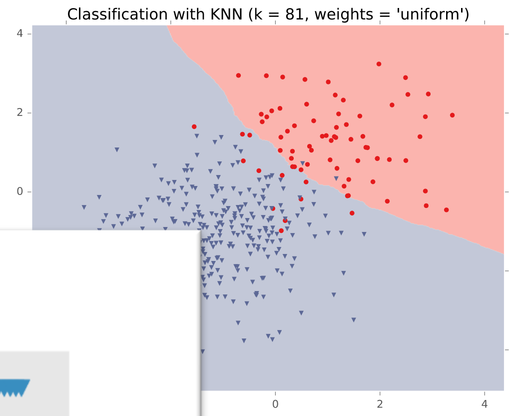


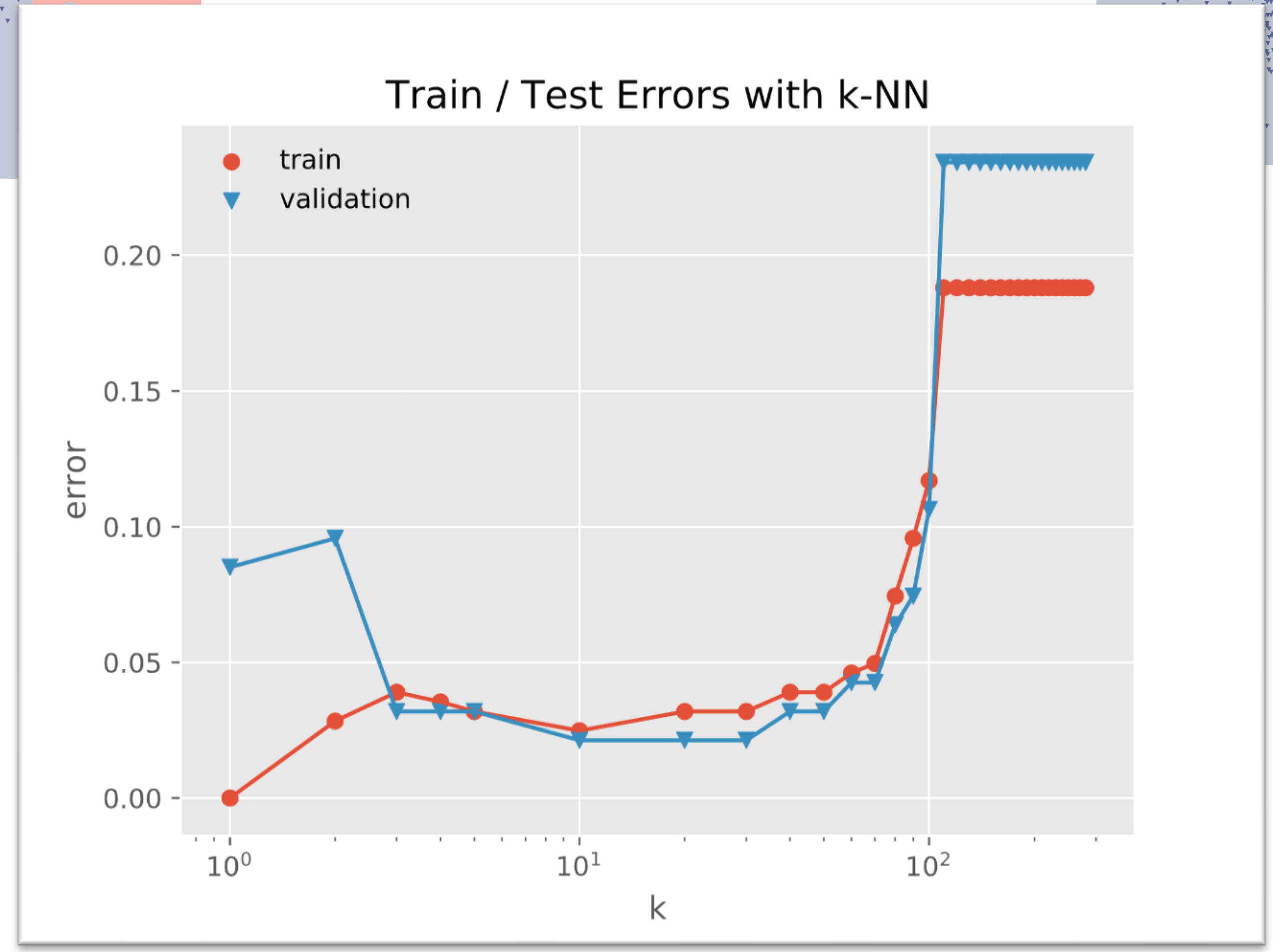
Fisher Iris Data: varying the value of k

Slide credit: CMU MLD Matt Gormley

k-NN: Choosing k







Gaussian Data: varying the value of k

Slide credit: CMU MLD Matt Gormley

Validation

Why do we need validation?

- Choose hyperparameters
- Choose technique
- Help make any choices beyond our parameters

But now, we have another choice to make!

- How do we split training and validation?

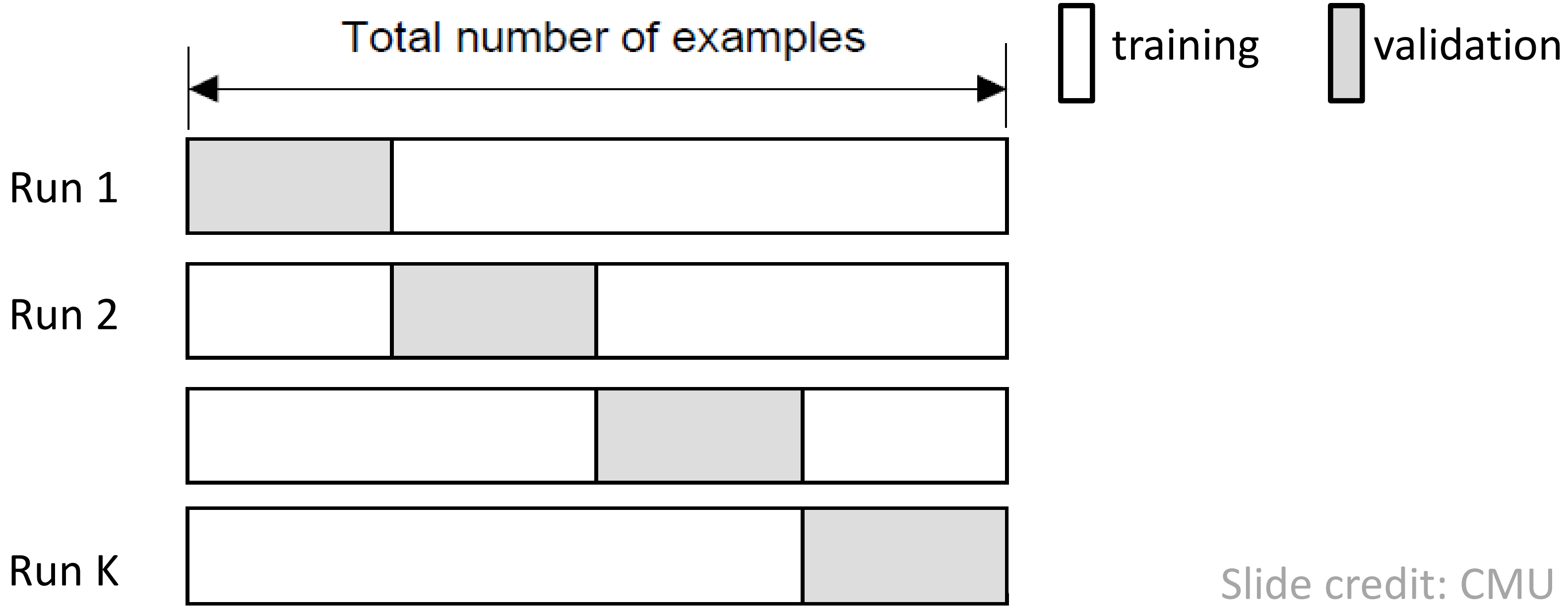
Trade-offs

- More held-out data, better meaning behind validation numbers
- More held-out data, less data to train on!

Cross-validation

K-fold cross-validation

Create K-fold partition of the dataset.
Do K runs: train using K-1 partitions and calculate validation error on remaining partition (rotating validation partition on each run).
Report average validation error

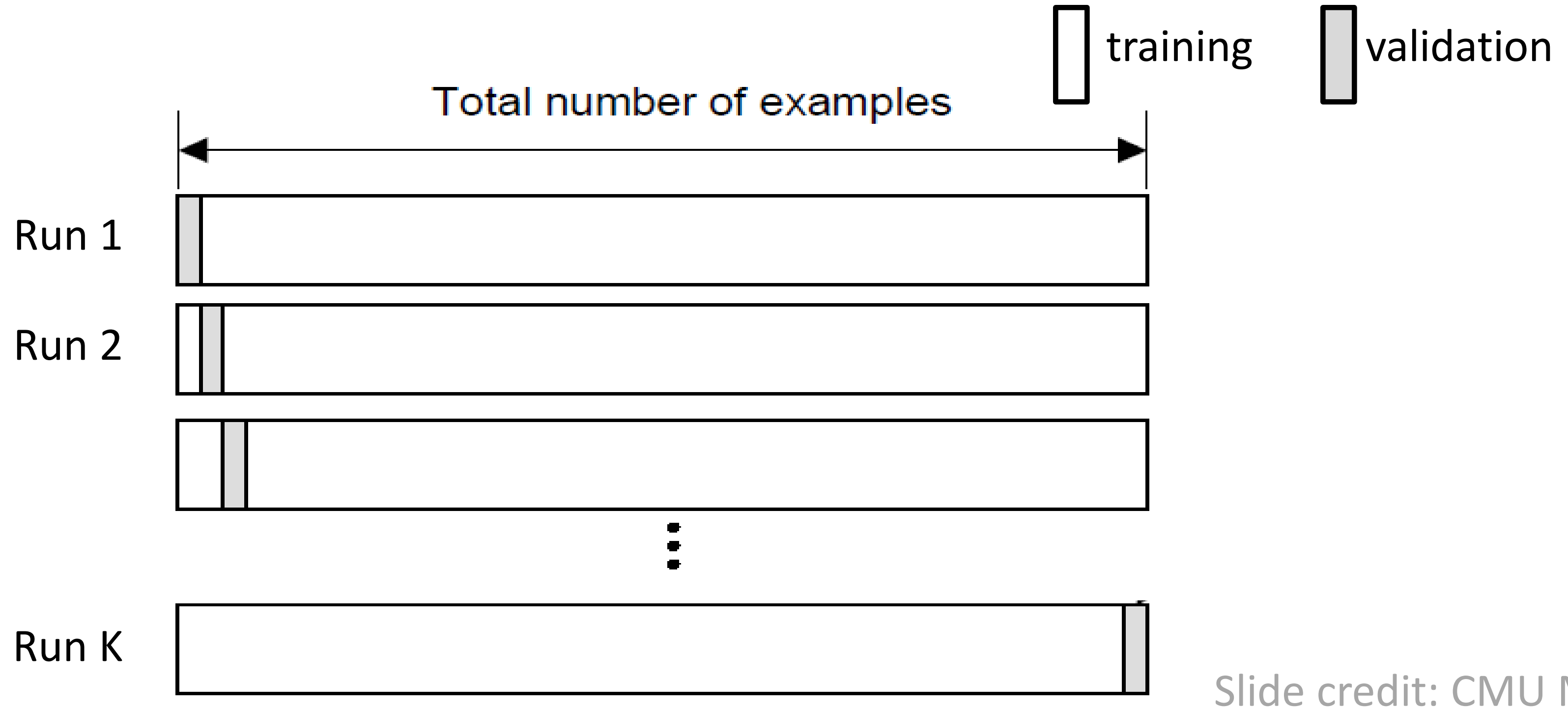


Slide credit: CMU MLD Aarti Singh

Cross-validation

Leave-one-out (LOO) cross-validation

Special case of K-fold with K=N partitions
Equivalently, train on N-1 samples and validate on only one sample per run for N runs



Slide credit: CMU MLD Aarti Singh

Cross-validation

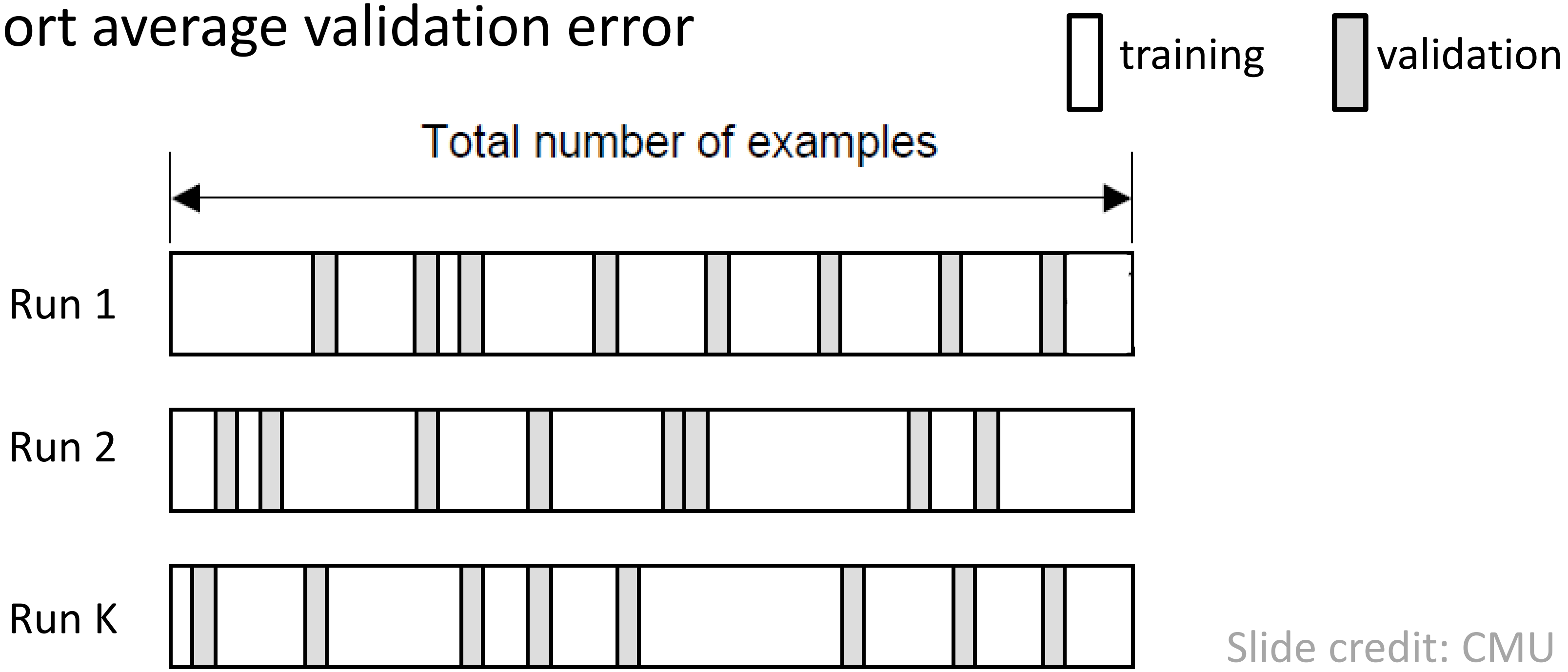
Random subsampling

Randomly subsample a fixed fraction αN (0< α <1) of the dataset for validation.

Compute validation error with remaining data as training data.

Repeat K times

Report average validation error



Slide credit: CMU MLD Aarti Singh

Practical Issues in Cross-validation

How to decide the values for K and α ?

- Large K
  - \+ Validation error can approximate test error well
  - \- Observed validation error will be unstable (few validation pts)
  - \- The computational time will be very large as well (many experiments)

- Small K
  - \+ The # experiments and, therefore, computation time are reduced
  - \+ Observed validation error will be stable (many validation pts)
  - \- Validation error cannot approximate test error well

Common choice: $K = 10$, $\alpha = 0.1$ ☺

Model Selection

WARNING (again):

- This section is only scratching the surface!
- Lots of methods for hyperparameter optimization: (to talk about later)
  - Grid search
  - Random search
  - Bayesian optimization
  - Graduate-student descent
  - …

Main Takeaway:

- Model selection / hyperparameter optimization is just another form of learning

Model Selection Learning Objectives

You should be able to…

- Plan an experiment that uses training, validation, and test datasets to predict the performance of a classifier on unseen data (without cheating)
- Explain the difference between (1) training error, (2) validation error, (3) cross-validation error, (4) test error, and (5) true error
- For a given learning technique, identify the model, learning algorithm, parameters, and hyperparamters