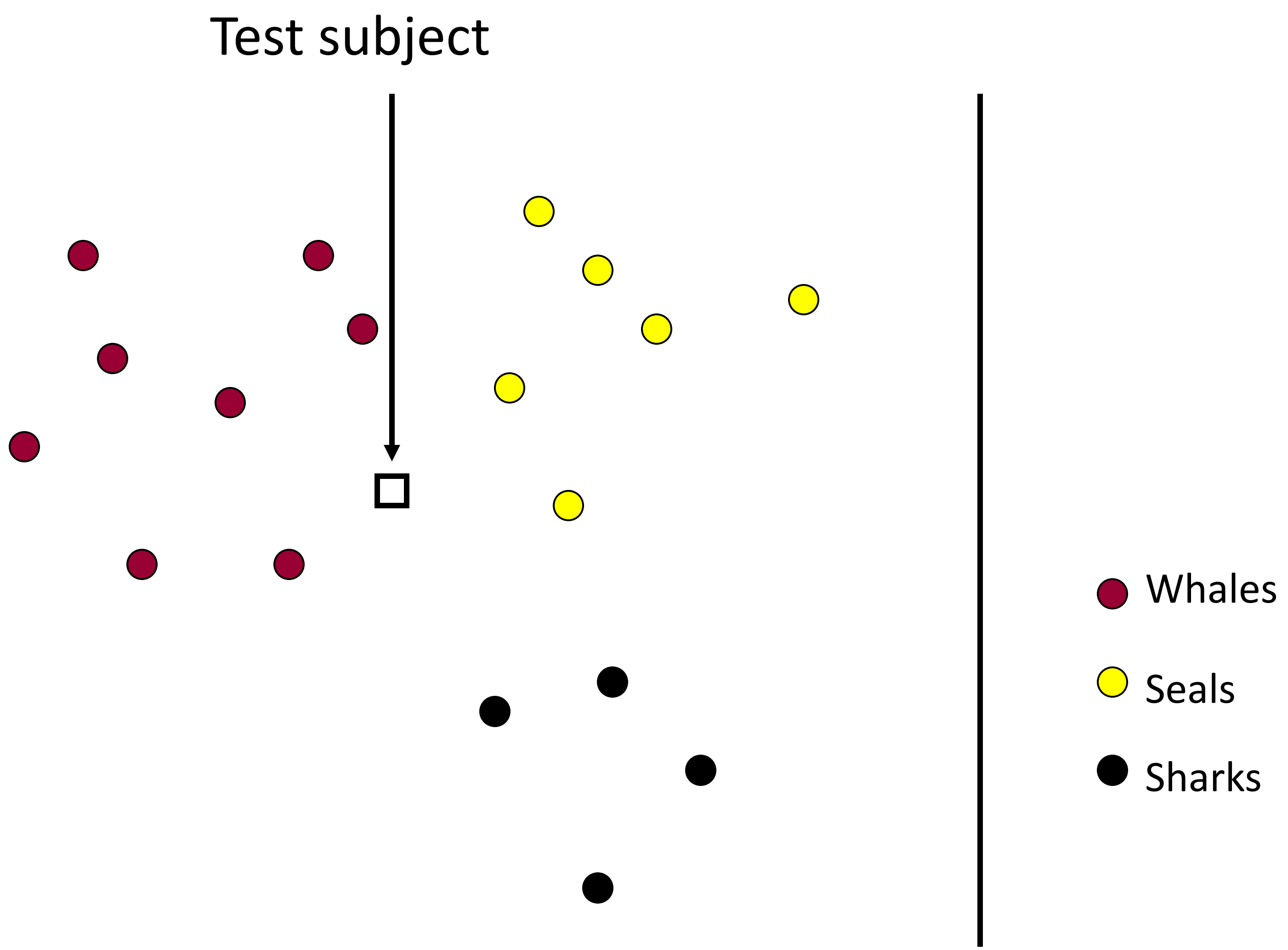
10-315
Introduction to ML

K-Nearest Neighbor

Instructor: Pat Virtue

Nearest Neighbor Classifier



Nearest Neighbor Classification

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

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

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

$$n = \operatorname*{argmin}_n d(\mathbf{x}_{test}, \mathbf{x}^{(n)})$$

2) Return the class label of that closest point

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

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

Fisher Iris Dataset

Fisher (1936) used 150 measurements of flowers from 3 different species: Iris setosa (0), Iris virginica (1), Iris versicolor (2) collected by Anderson (1936)

Species	Sepal Length	Sepal Width	Petal Length	Petal Width
0	4.3	3.0	1.1	0.1
0	4.9	3.6	1.4	0.1
0	5.3	3.7	1.5	0.2
1	4.9	2.4	3.3	1.0
1	5.7	2.8	4.1	1.3
1	6.3	3.3	4.7	1.6
1	6.7	3.0	5.0	1.7

Full dataset: https://en.wikipedia.org/wiki/Iris_flower_data_set

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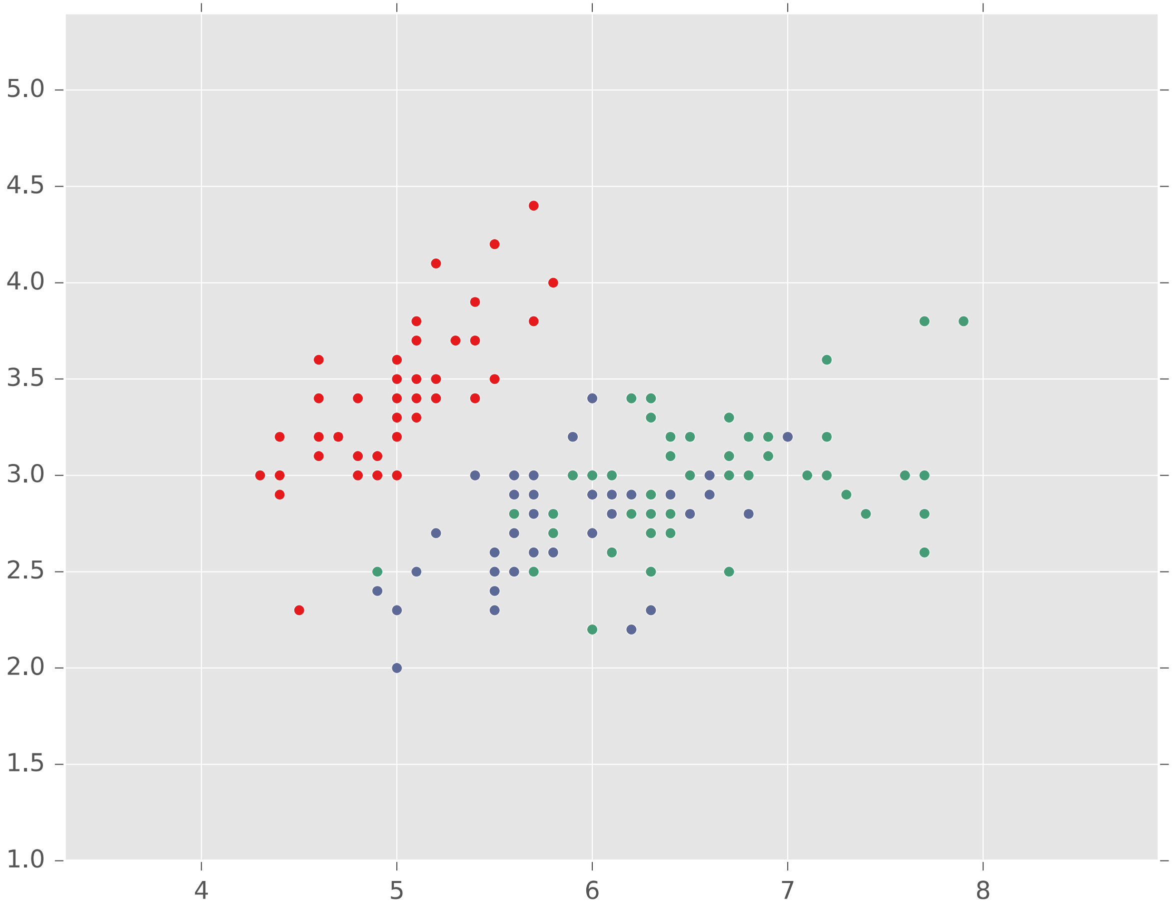
0	5.3	3.7
1	4.9	2.4
1	5.7	2.8
1	6.3	3.3
1	6.7	3.0

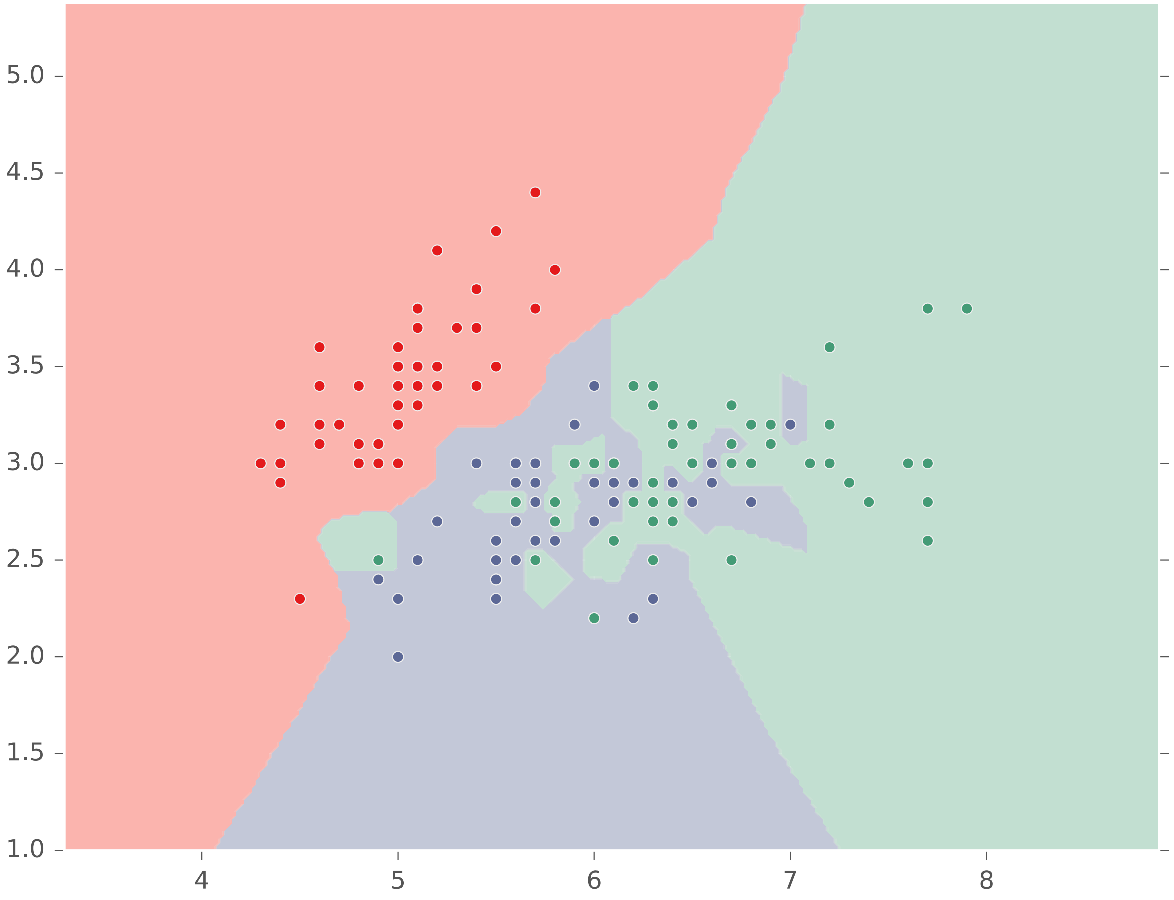
Deleted two of the four features, so that input space is 2D

Full dataset: https://en.wikipedia.org/wiki/Iris_flower_data_set

Nearest Neighbor on Fisher Iris Data

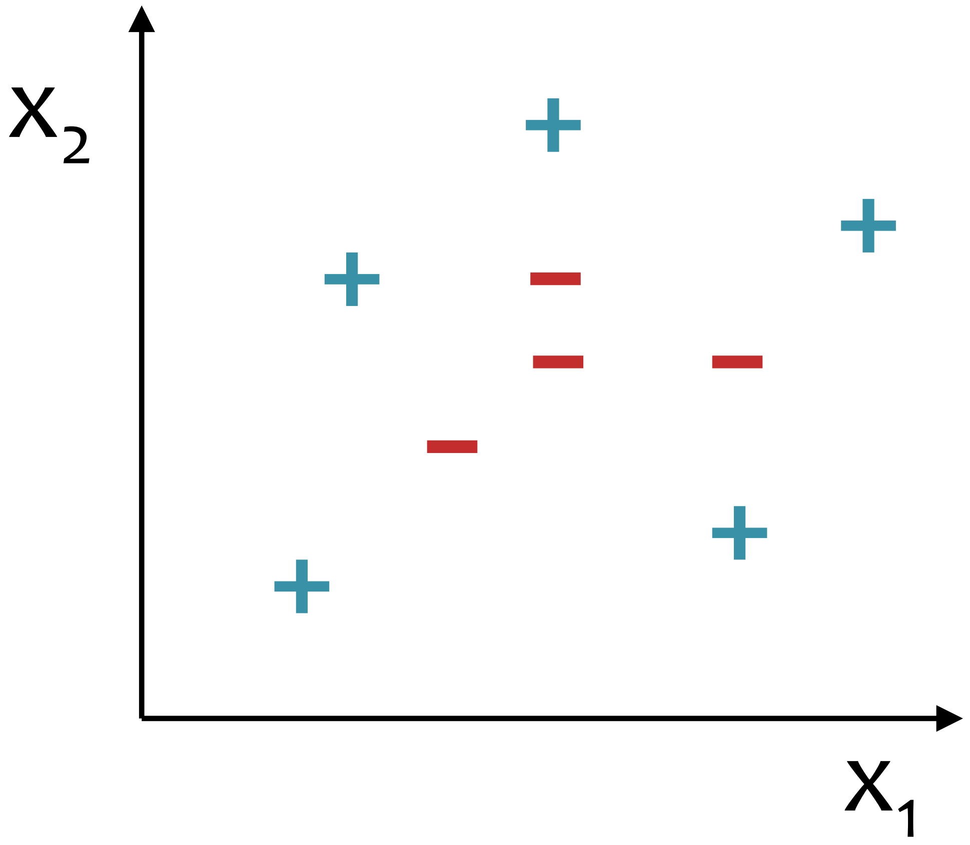


Nearest Neighbor on Fisher Iris Data

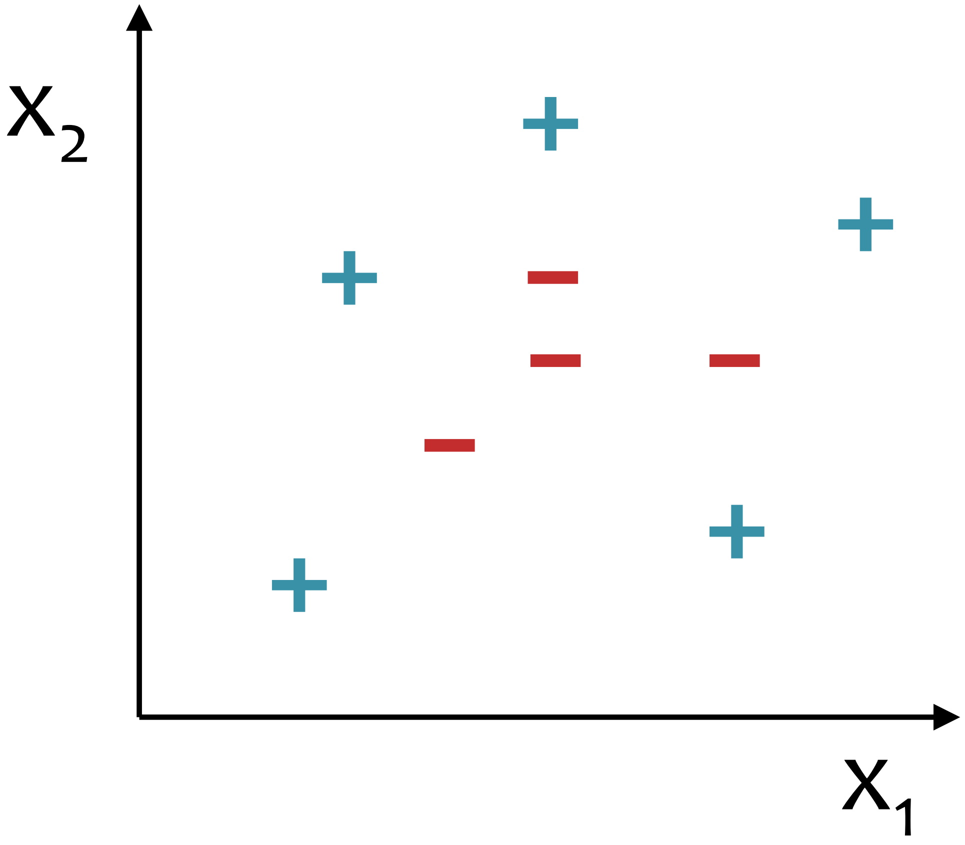


Recitation: Decision Boundaries

Decision tree

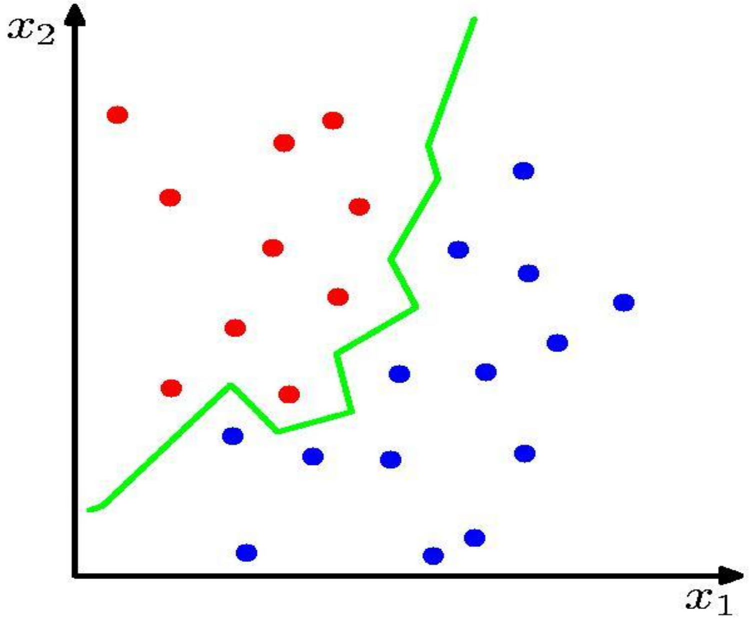


Nearest neighbor

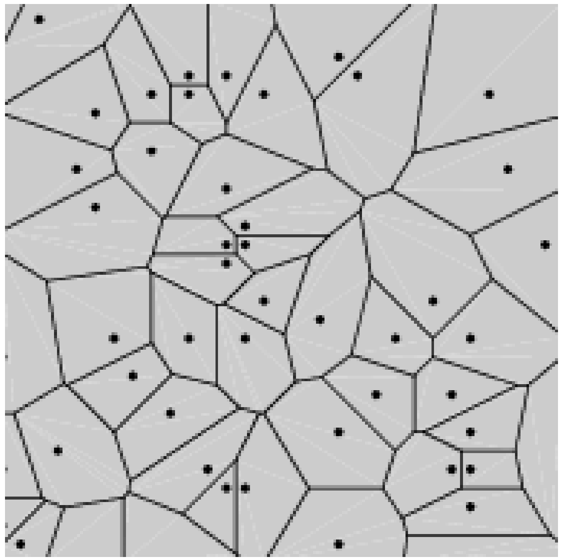


Nearest Neighbor Decision Boundary

1-nearest neighbor classifier decision boundary

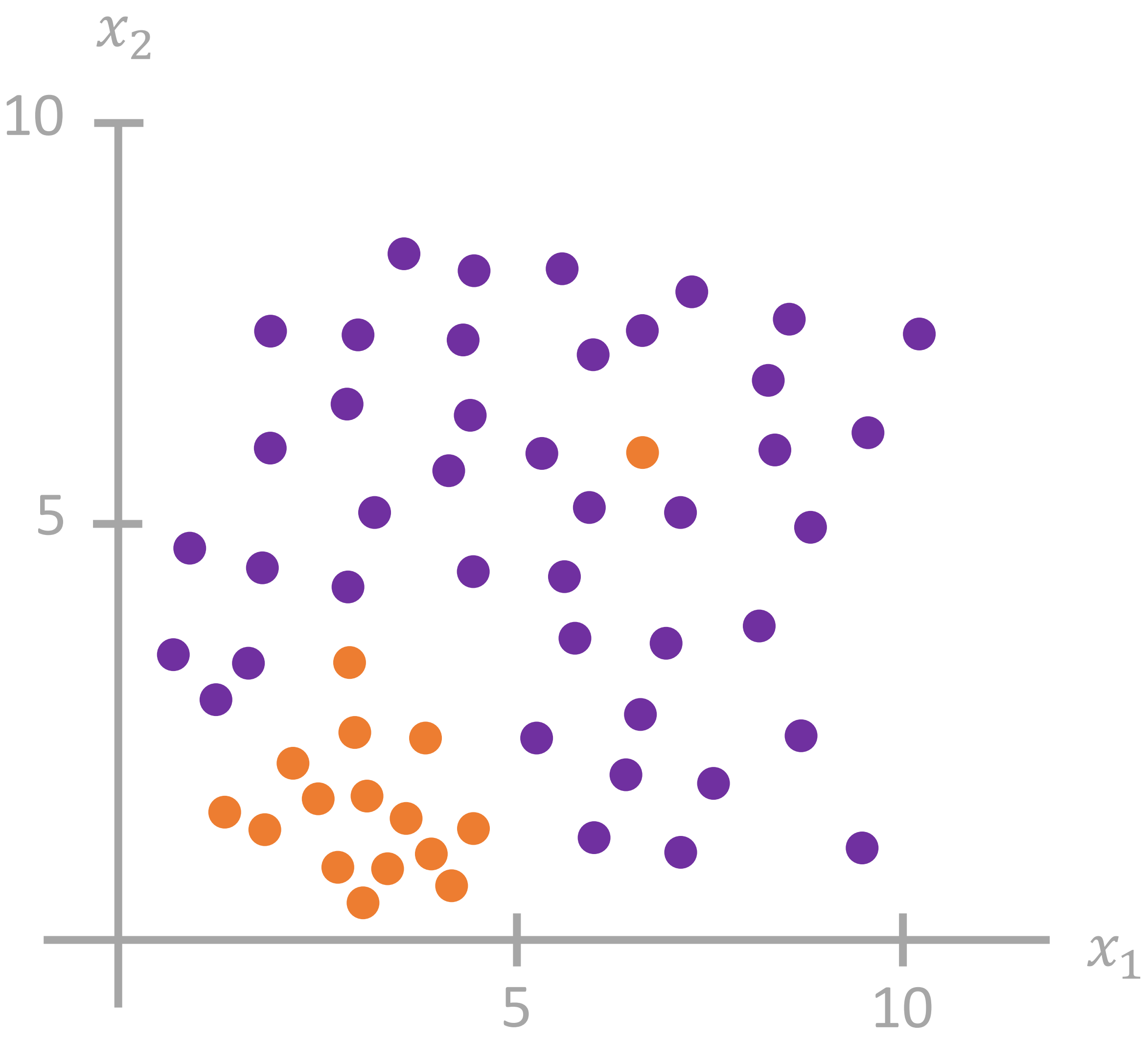


Voronoi Diagram



Nearest Neighbor Classification

Consider input features $x \in \mathbb{R}^2$.



Nearest Neighbor on Gaussian Data

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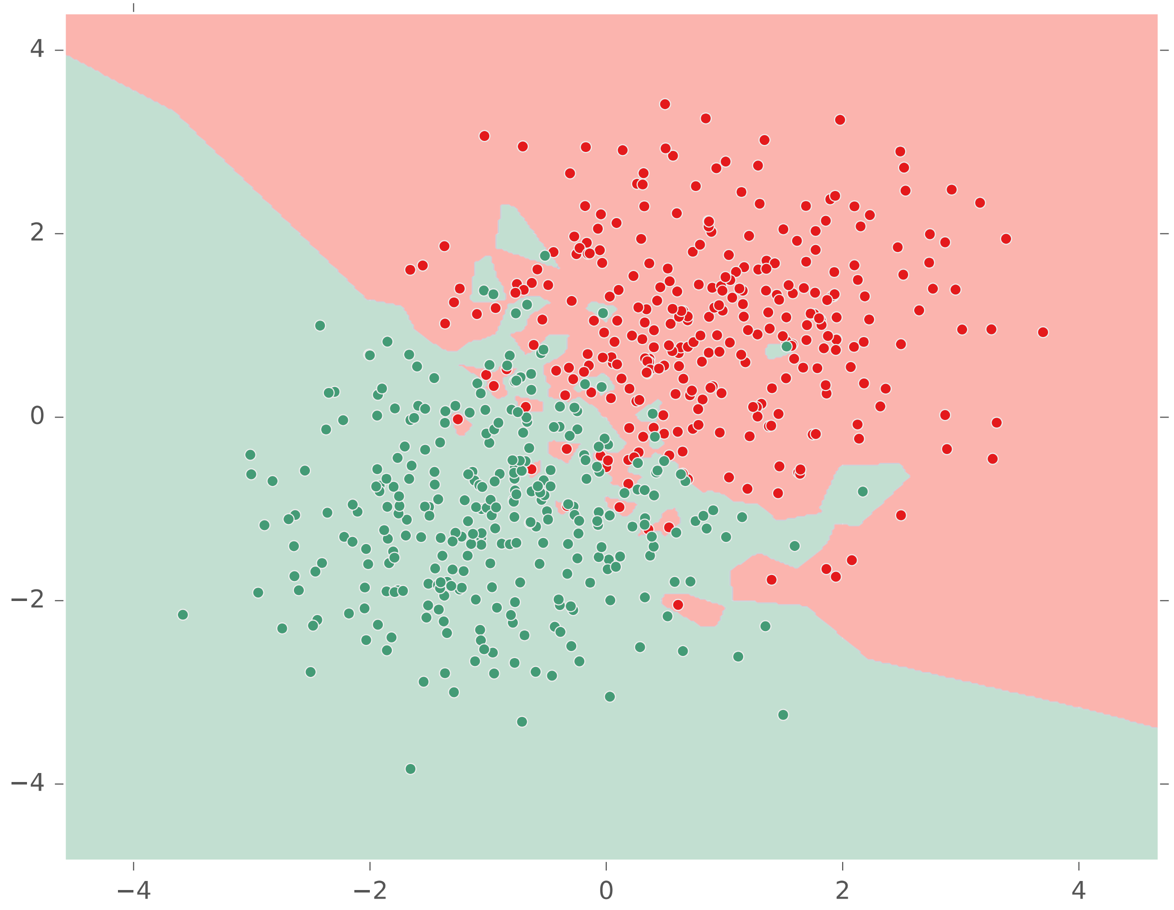
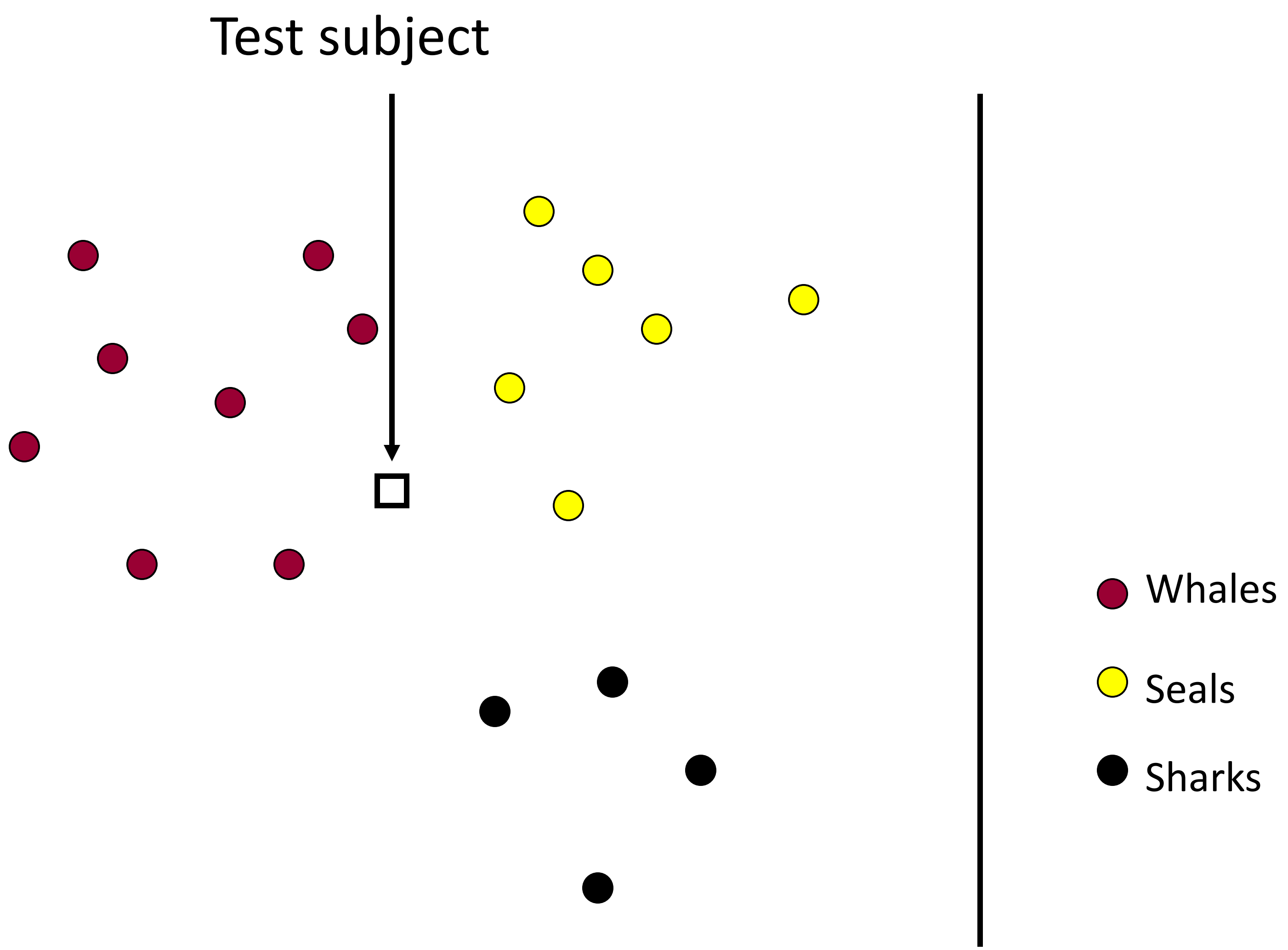
Nearest Neighbor on Gaussian Data



kNN classifier (k=5)



Nearest Neighbor Classification

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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

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

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

What is the best k?

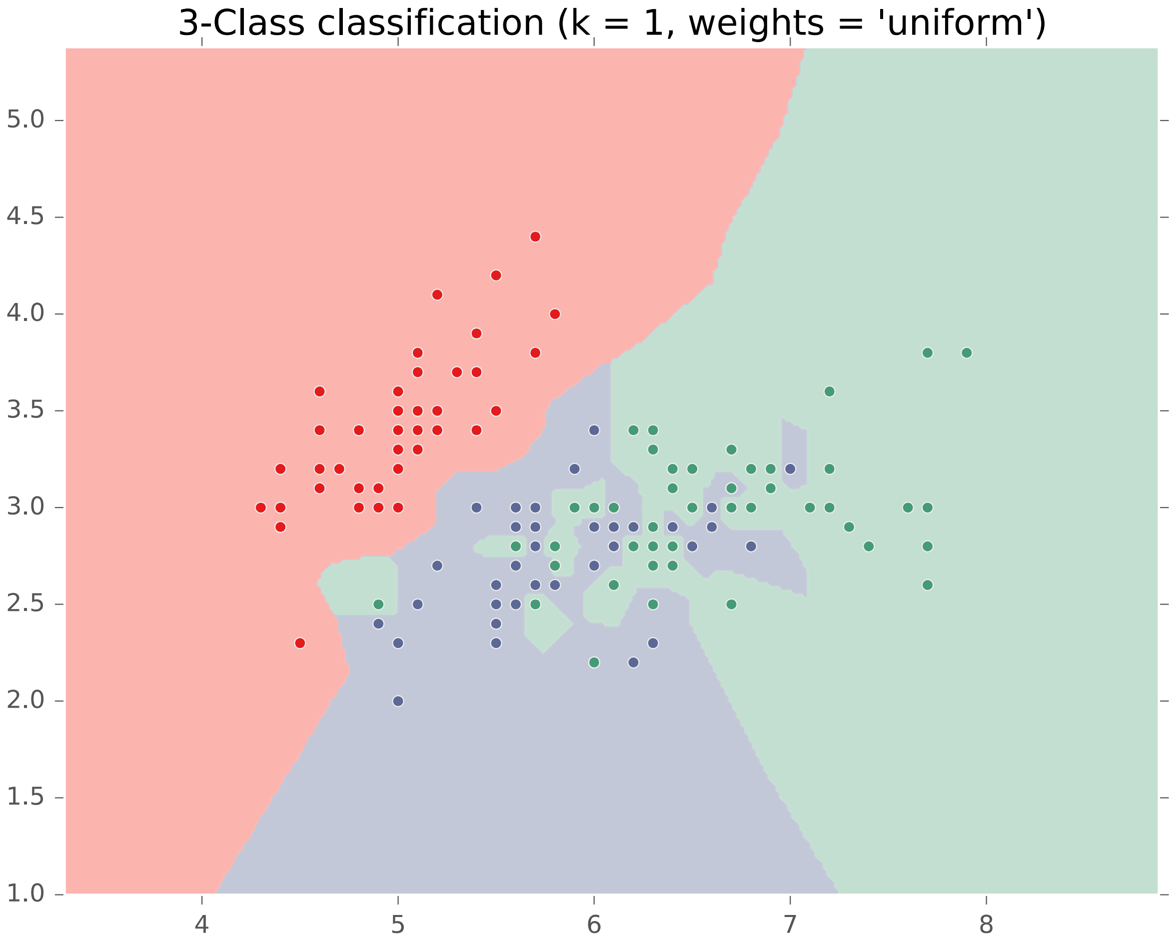
How do we choose a learner that is accurate and also generalizes to unseen data?

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

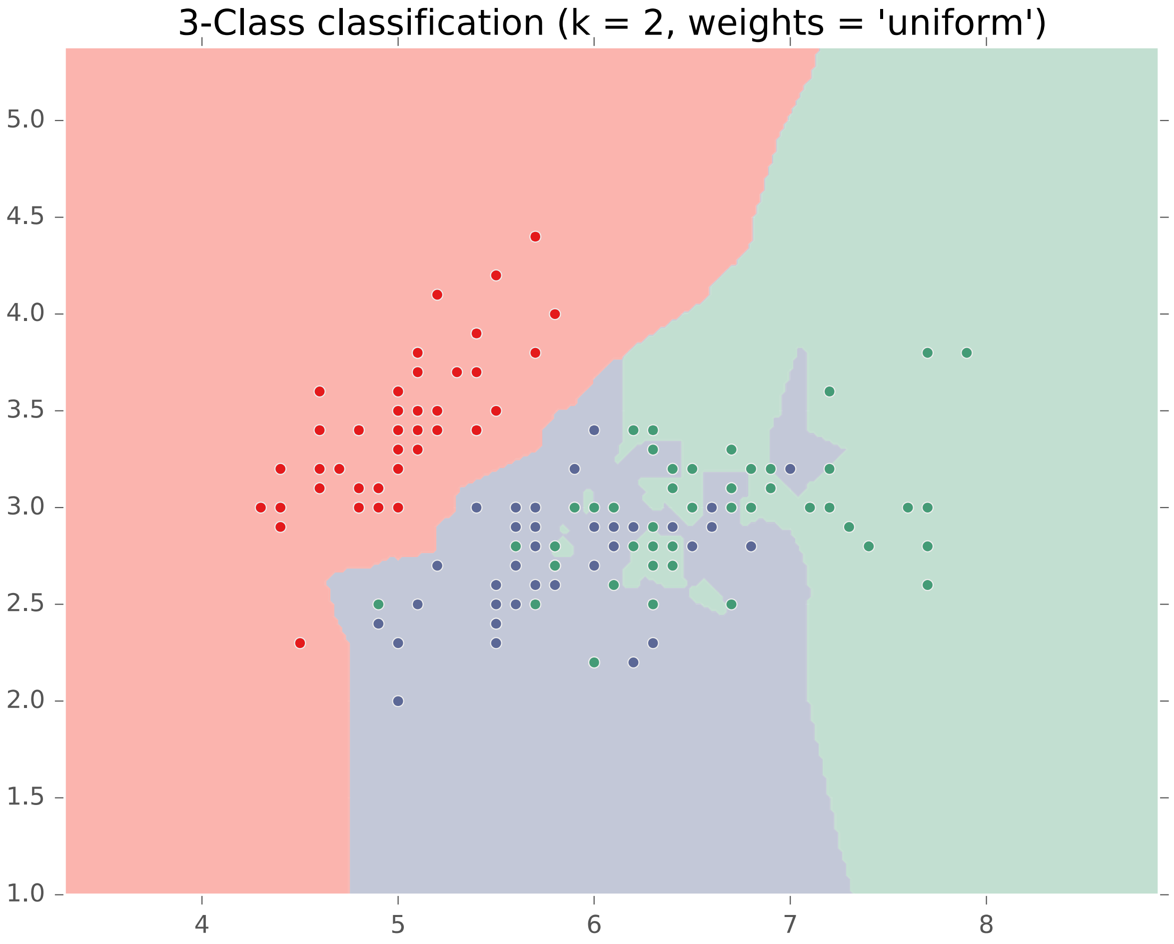
But how to choose k?

k-NN on Fisher Iris Data

Special Case: Nearest Neighbor



k-NN on Fisher Iris Data



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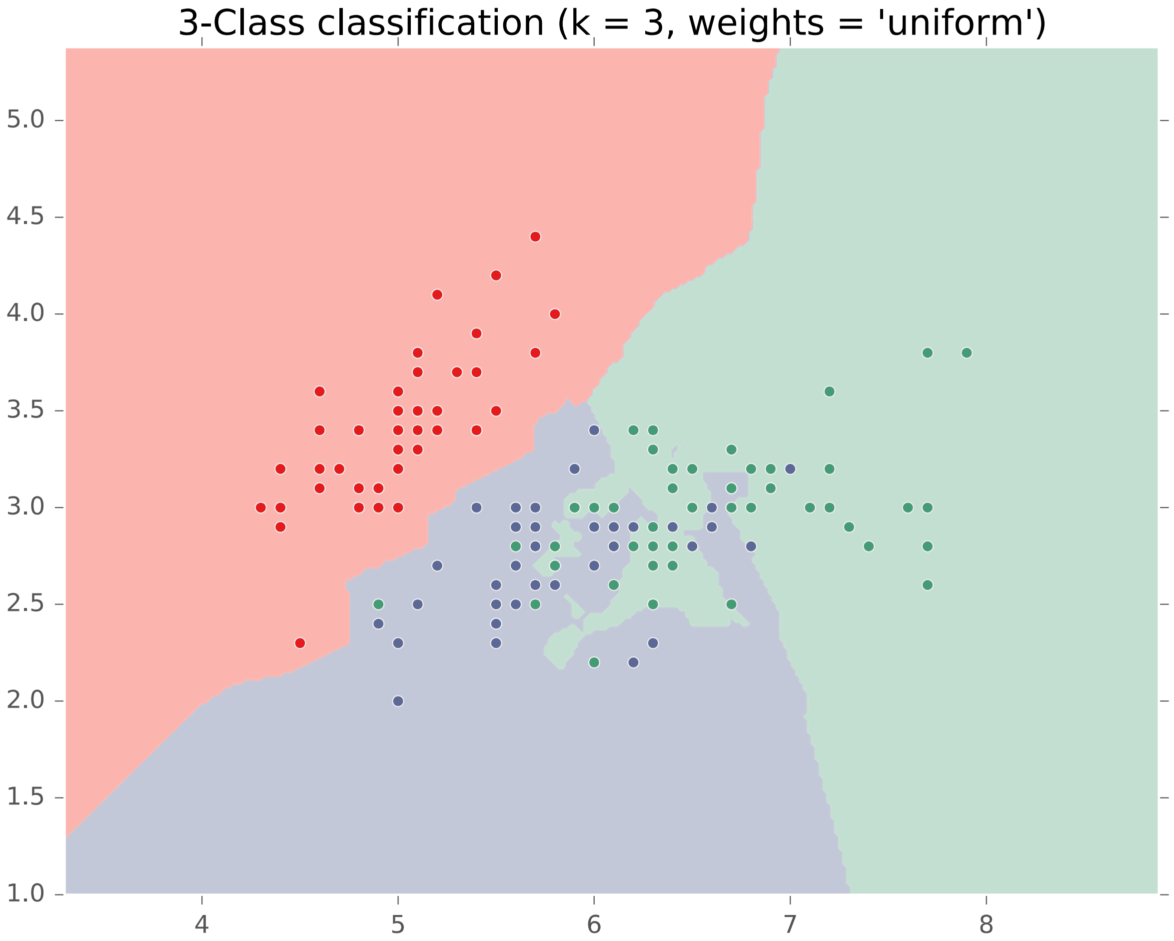
k-NN on Fisher Iris Data



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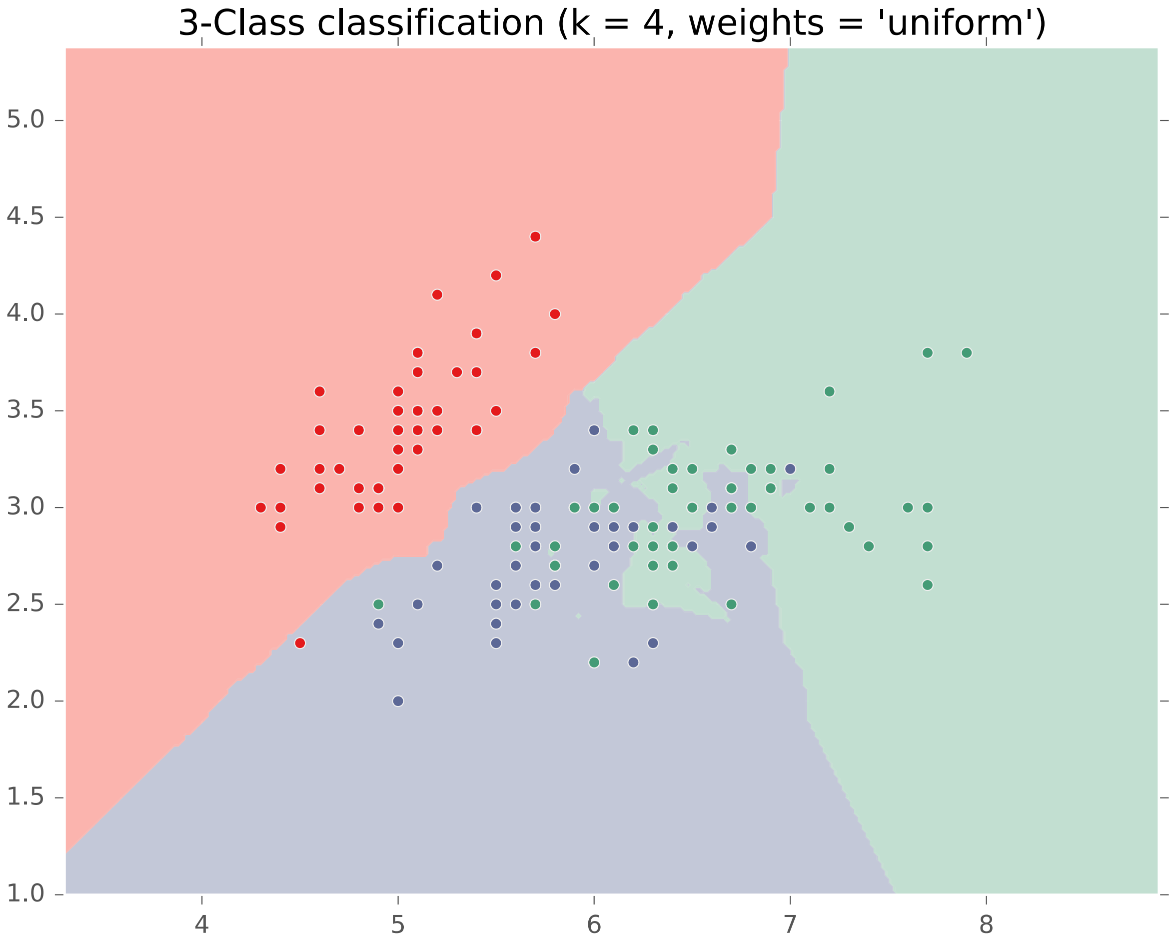
k-NN on Fisher Iris Data



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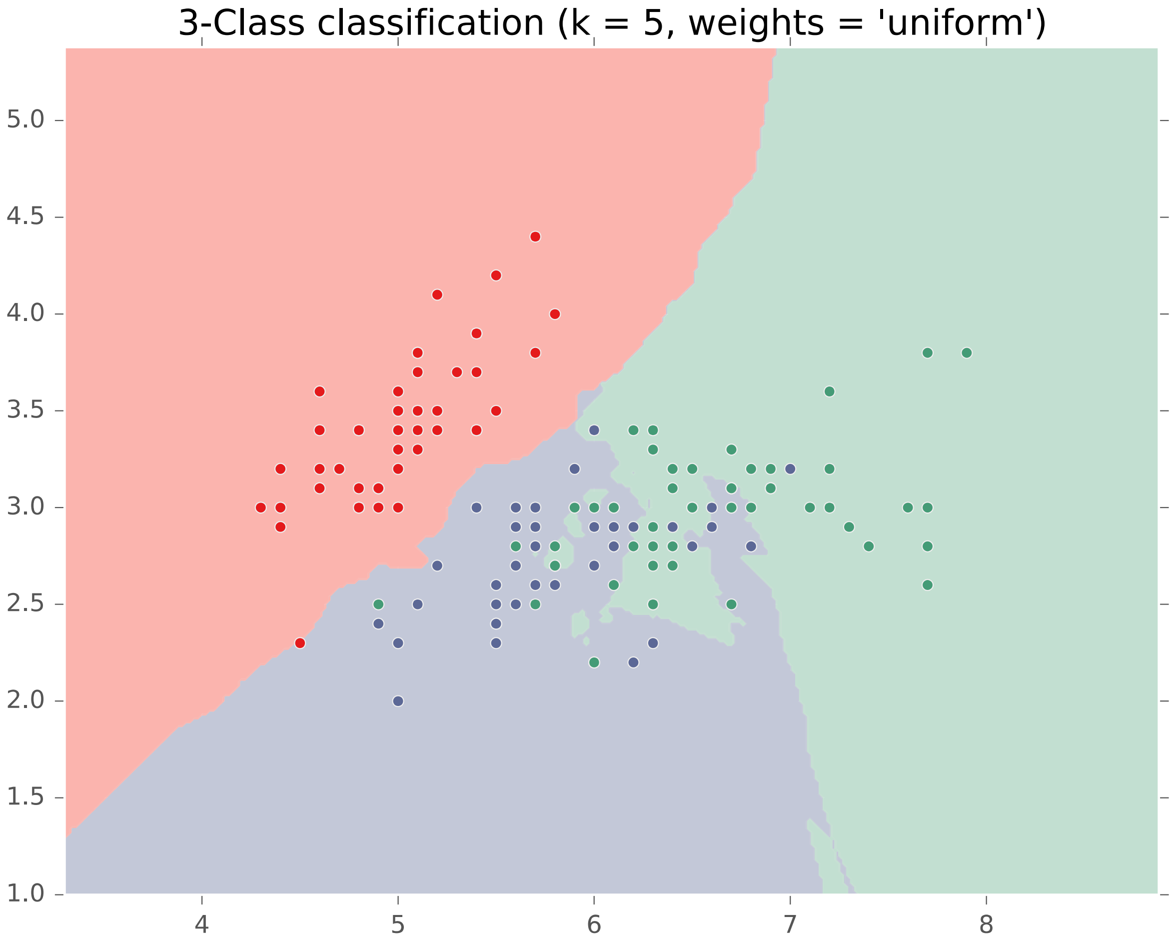
k-NN on Fisher Iris Data



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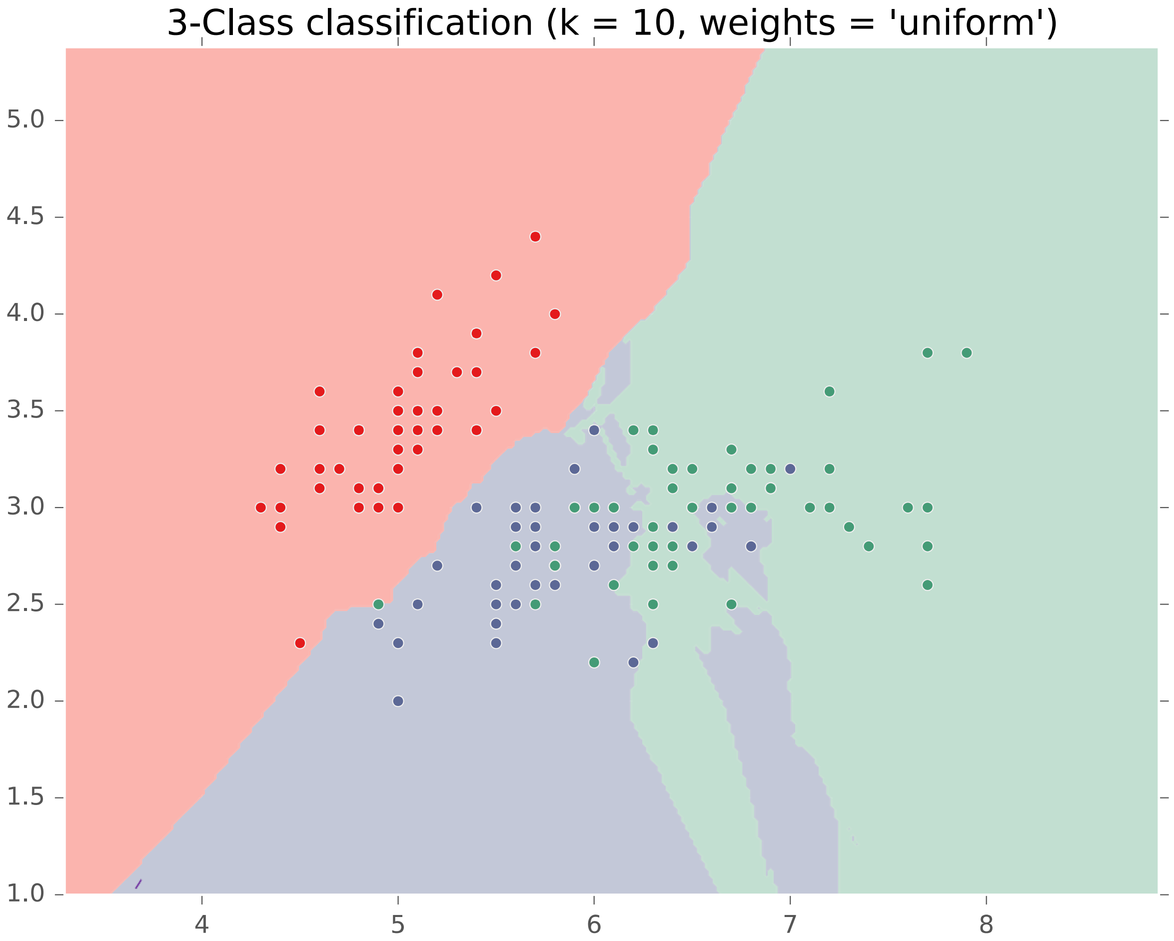
k-NN on Fisher Iris Data



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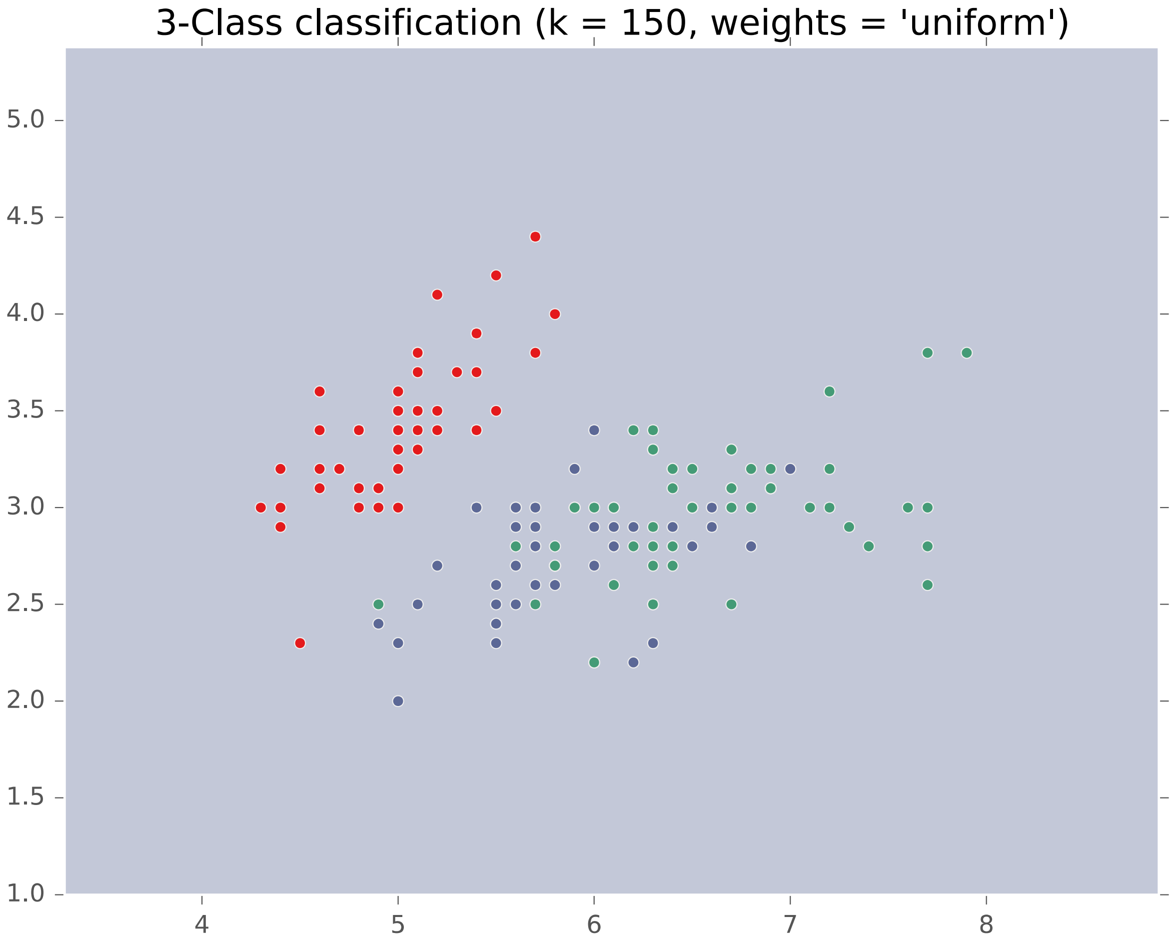
k-NN on Fisher Iris Data

Special Case: Majority Vote



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K-NN Details

Poll 1: Two questions (train) and (predict)

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)

k-NN: Details

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
Train	O(1)
Predict (one test example)	O(MN)

In practice:

- k-d trees
- stochastic approximations (very fast, and empirically often as good)

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k-NN: Details

The **inductive bias** of a machine learning algorithm is the principal by which it generalizes to unseen examples

Inductive Bias:

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

k-NN: Details

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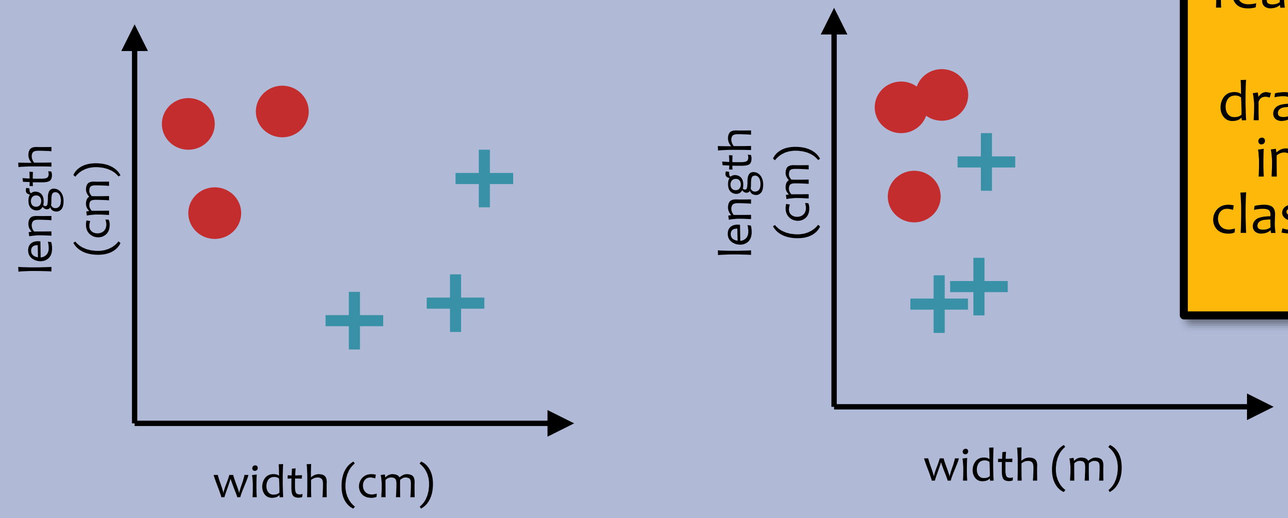
Example: two features for k-NN



big problem: feature scale could dramatically influence classification results