10-301/601: Introduction to Machine Learning Lecture 4 –KNNs

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5/22/23

Front Matter

- Announcements:
  - PA1 released 5/18, due 5/25 at 11:59 PM
  - Quiz 1: Decision Trees on 5/19 (tomorrow!)
    - The quiz will begin promptly at 11 AM, please show up on time!
    - Closed book, closed notes, no calculators.
- Recommended Readings:
  - Daumé III, Chapter 2: Geometry and Nearest Neighbors

Real-valued Features

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

Source: 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

Source: https://en.wikipedia.org/wiki/Iris_flower_data_set

Fisher Iris Dataset

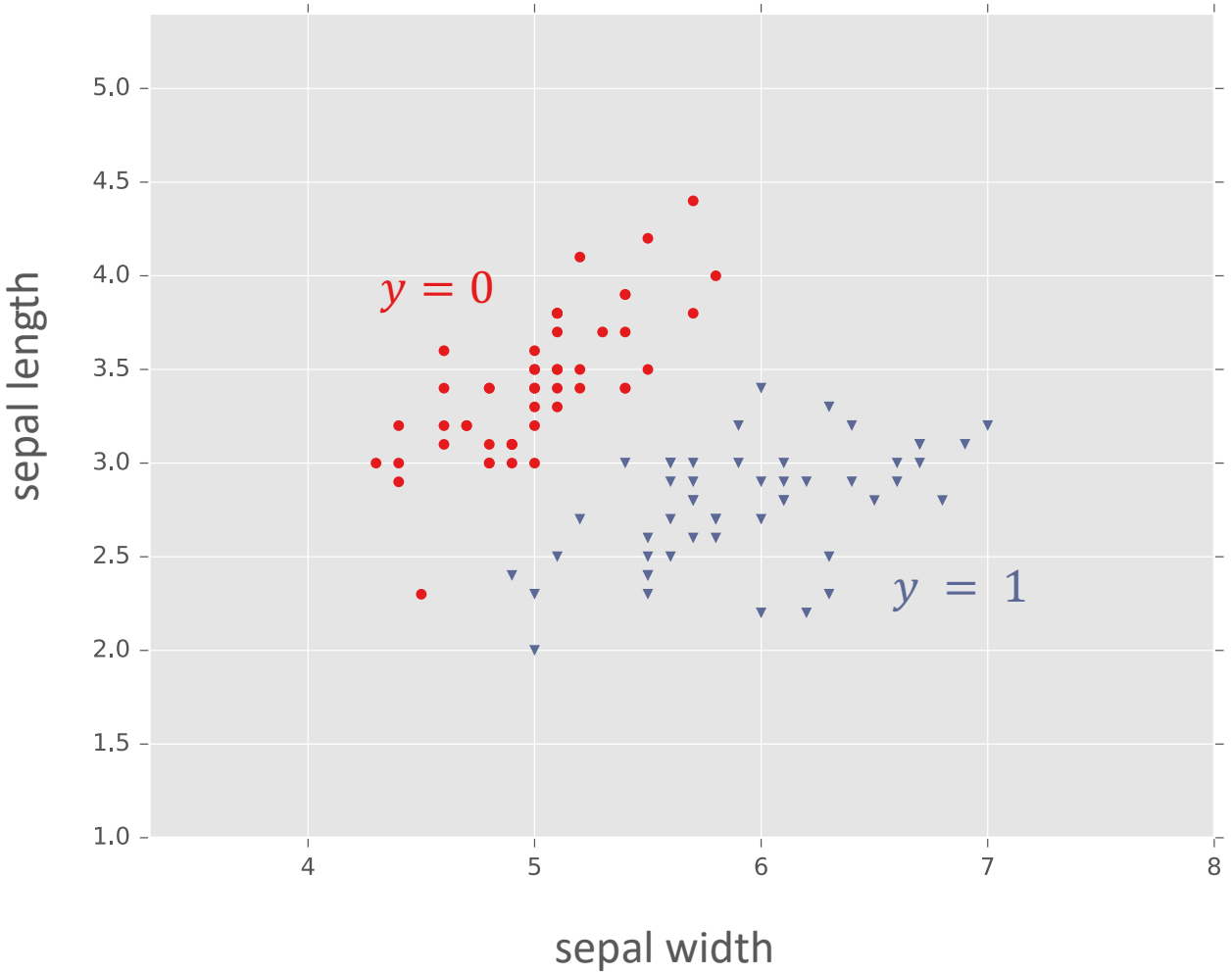

Figure courtesy of Matt Gormley

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Duck test

From Wikipedia, the free encyclopedia

For the use of "the duck test" within the Wikipedia community, see Wikipedia:DUCK.

The **duck test** is a form of abductive reasoning. This is its usual expression:

> If it looks like a duck, swims like a duck, and quacks like a duck, then it probably *is* a duck.

The Duck Test

Source: https://en.wikipedia.org/wiki/Duck_test

The Duck Test for Machine Learning

- Classify a point as the label of the “most similar” training point
- Idea: given real-valued features, we can use a distance metric to determine how similar two data points are
- A common choice is Euclidean distance:

$$d(\boldsymbol{x}, \boldsymbol{x}') = \|\boldsymbol{x} - \boldsymbol{x}'\|_2 = \sqrt{\sum_{d=1}^{D} (x_d - x'_d)^2}$$

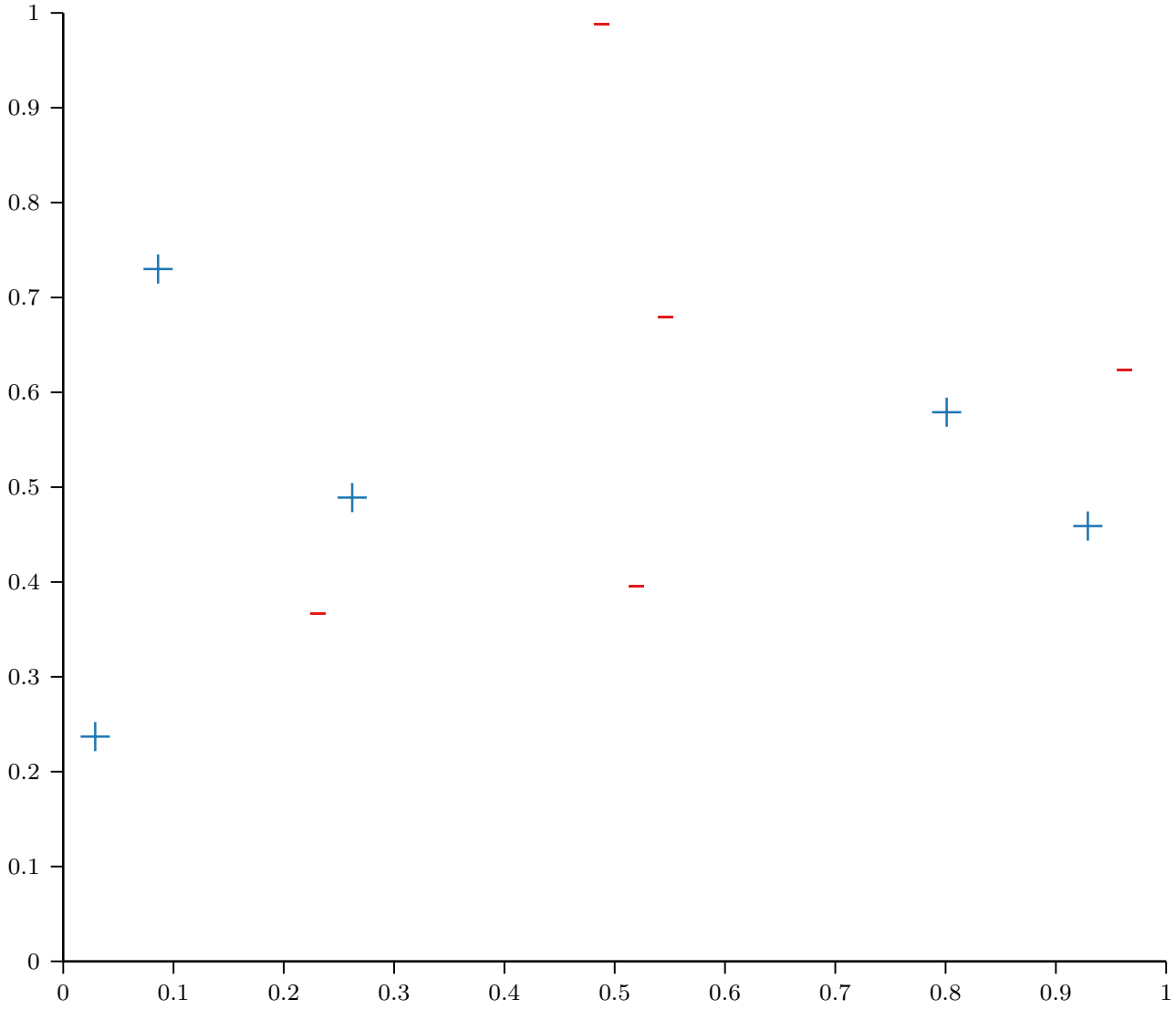
- An alternative is the Manhattan distance:

$$d(\boldsymbol{x}, \boldsymbol{x}') = \|\boldsymbol{x} - \boldsymbol{x}'\|_1 = \sum_{d=1}^{D} |x_d - x'_d|$$

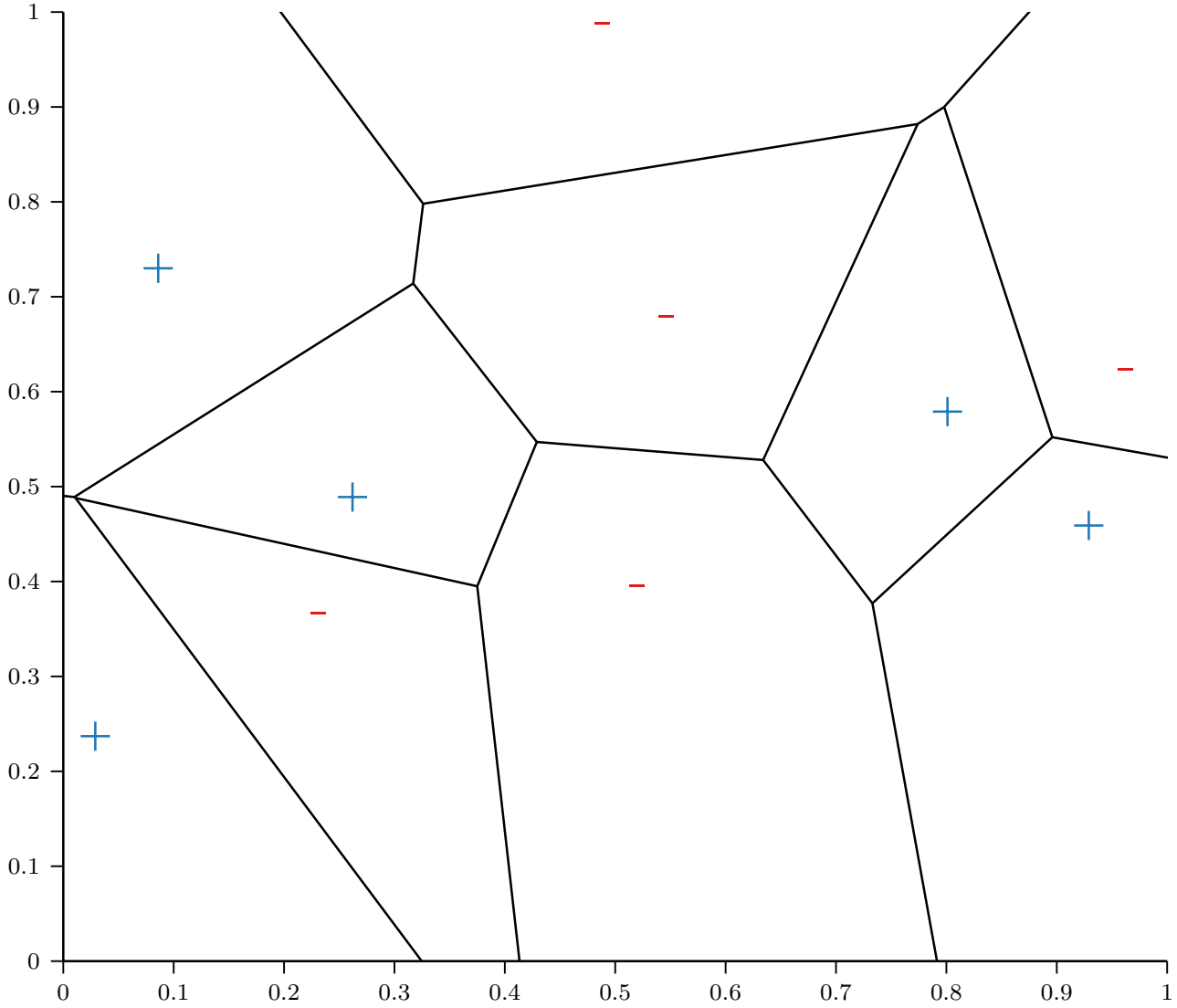
Nearest Neighbor: Pseudocode

```
def train(𝒟):
        store 𝒟
def predict(𝒙′):
        find the nearest neighbor to 𝒙′ in 𝒟, 𝒙^(i)
        return 𝑦^(i)
```

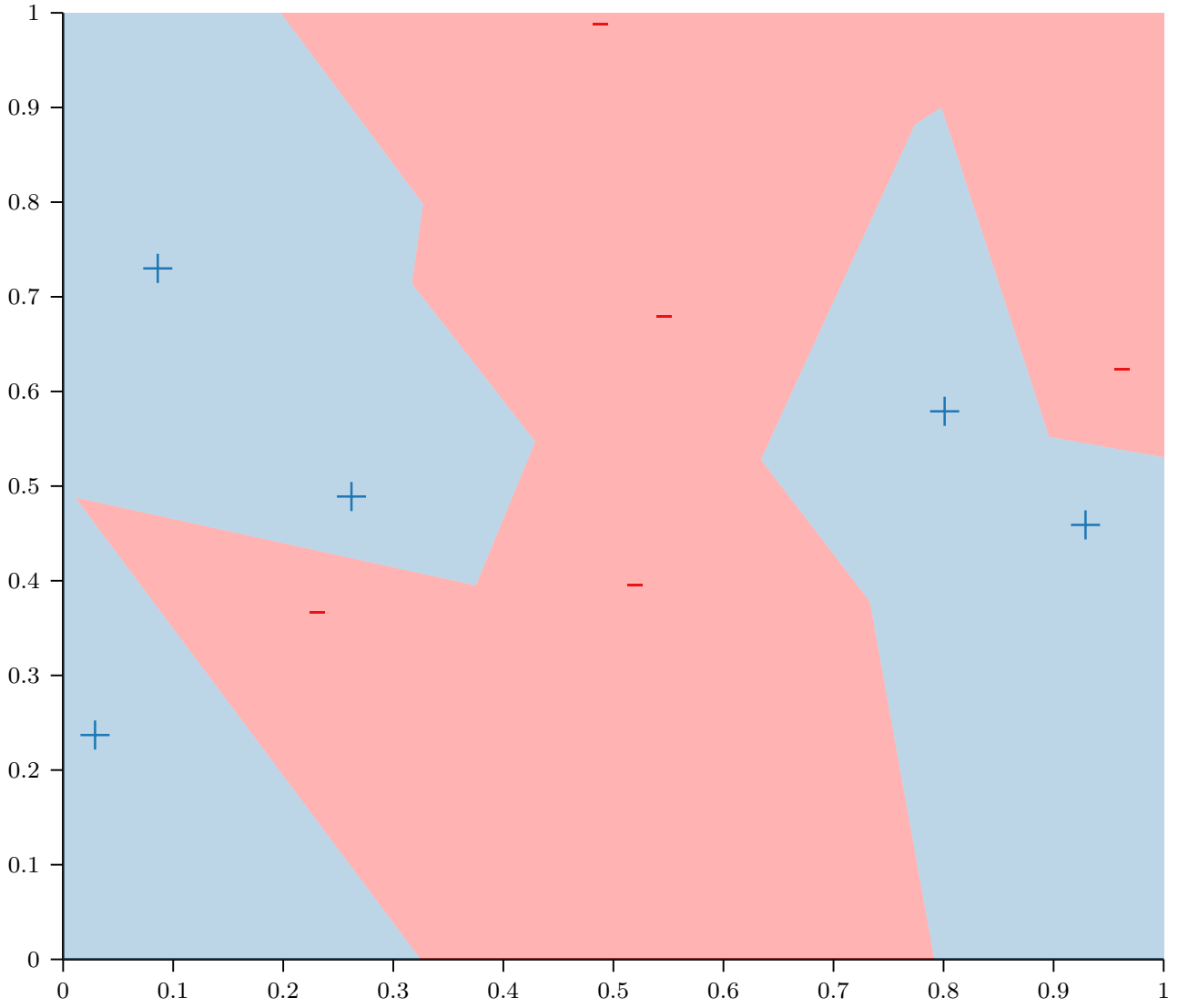
Nearest Neighbor: Example



Nearest Neighbor: Example



Nearest Neighbor: Example



The Nearest Neighbor Model

- Requires no training!
- Always has zero training error!
  - ***A data point is always its own nearest neighbor***

⋮

- Always has zero training error…

Generalization of Nearest Neighbor (Cover and Hart, 1967)

- Claim: under certain conditions, as $n \to \infty$, with high probability, the true error rate of the nearest neighbor model $\leq 2 * $ the Bayes error rate (the optimal classifier)
- Interpretation: "In this sense, it may be said that half the classification information in an infinite sample set is contained in the nearest neighbor."

Source: https://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=1053964

But why limit ourselves to just one neighbor?

- Claim: under certain conditions, as $n \to \infty$, with high probability, the true error rate of the nearest neighbor model $\leq 2 * $ the Bayes error rate (the optimal classifier)
- Interpretation: “In this sense, it may be said that half the classification information in an infinite sample set is contained in the nearest neighbor.”

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k-Nearest Neighbors (kNN)

- Classify a point as the most common label among the labels of the k nearest training points
- Tie-breaking (in case of even k and/or more than 2 classes)
  - Weight votes by distance
  - Remove furthest neighbor
  - Add next closest neighbor
  - Use a different distance metric

k-Nearest Neighbors (kNN): Pseudocode

```
def train(𝒟):
    store 𝒟
def predict(𝒙′):
    return majority_vote(labels of the k
    nearest neighbors to 𝒙′ in 𝒟)
```

kNN on Fisher Iris Data

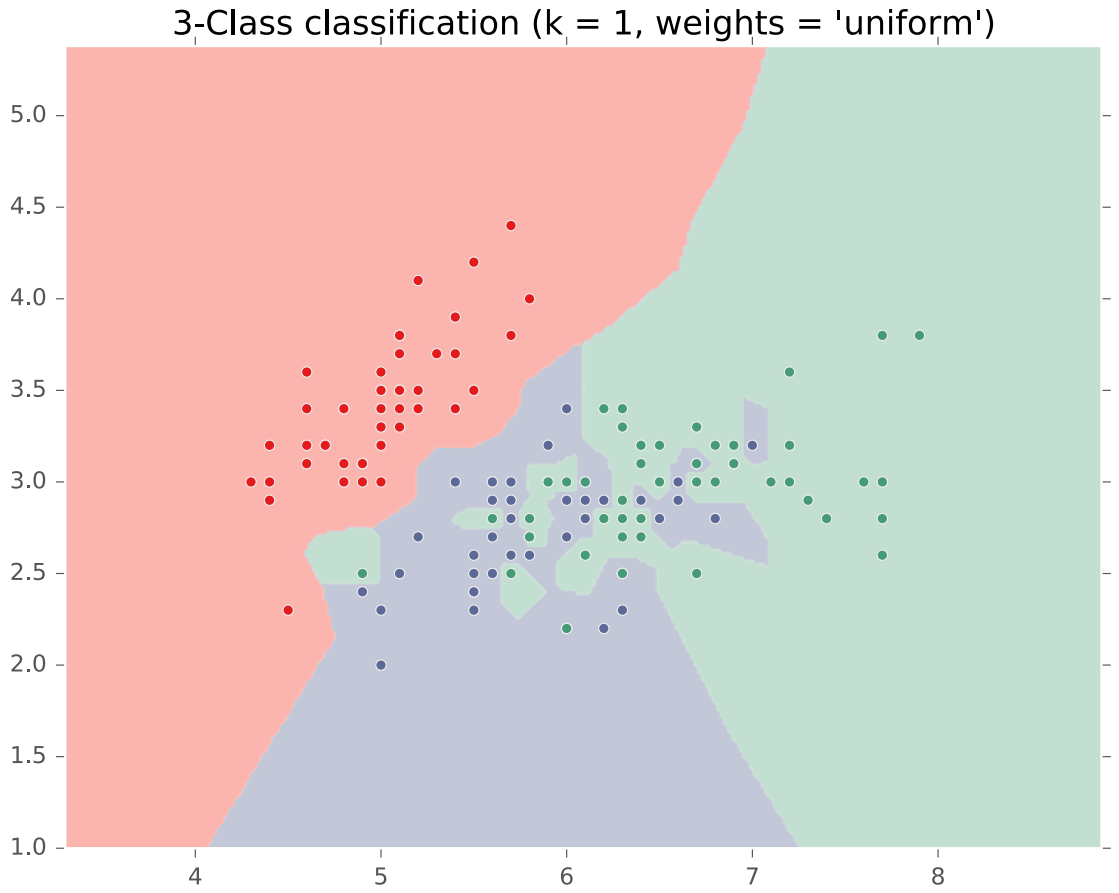

Figure courtesy of Matt Gormley

kNN on Fisher Iris Data

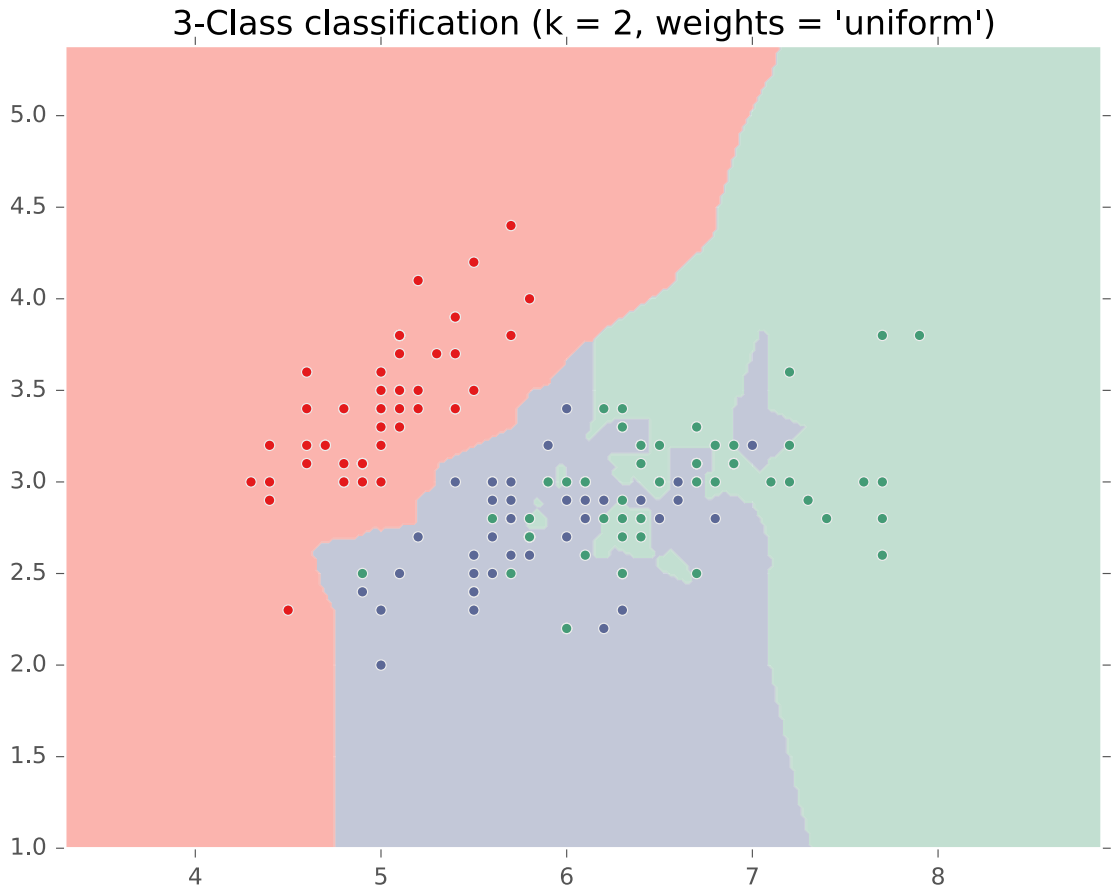

Figure courtesy of Matt Gormley

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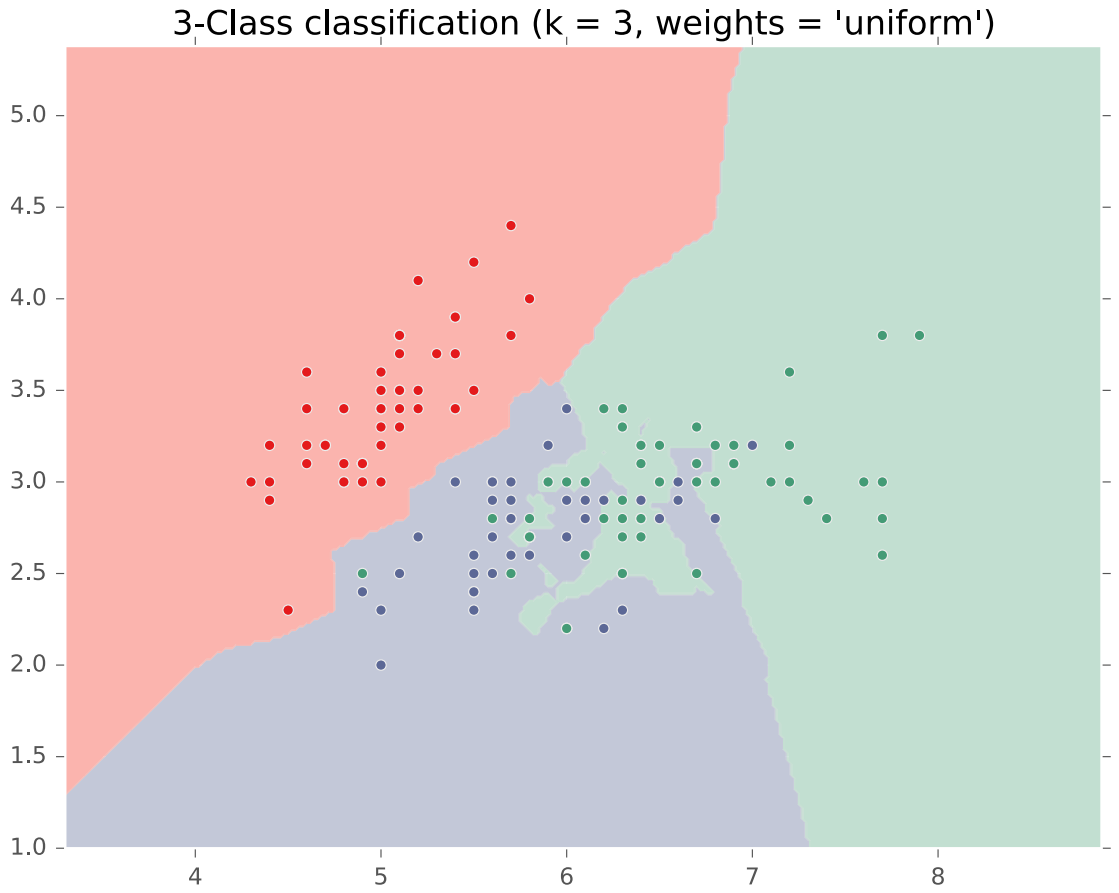

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kNN on Fisher Iris Data

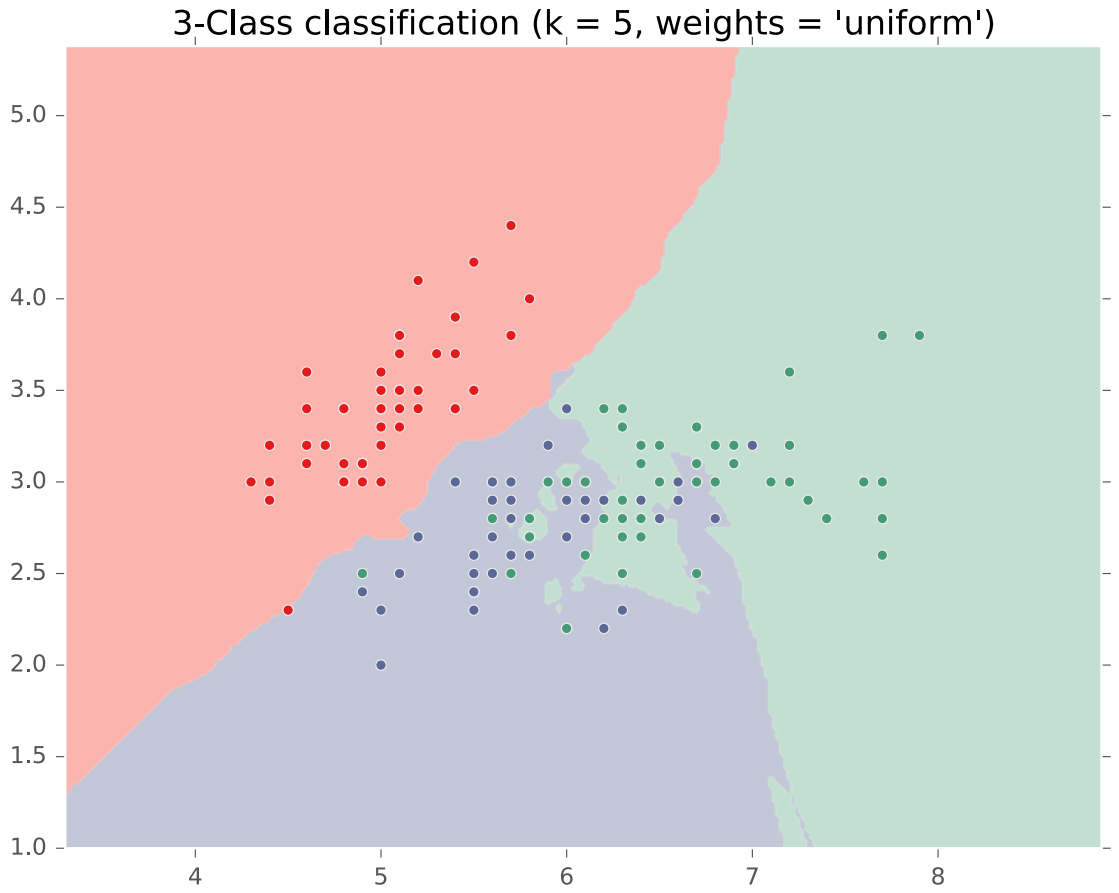
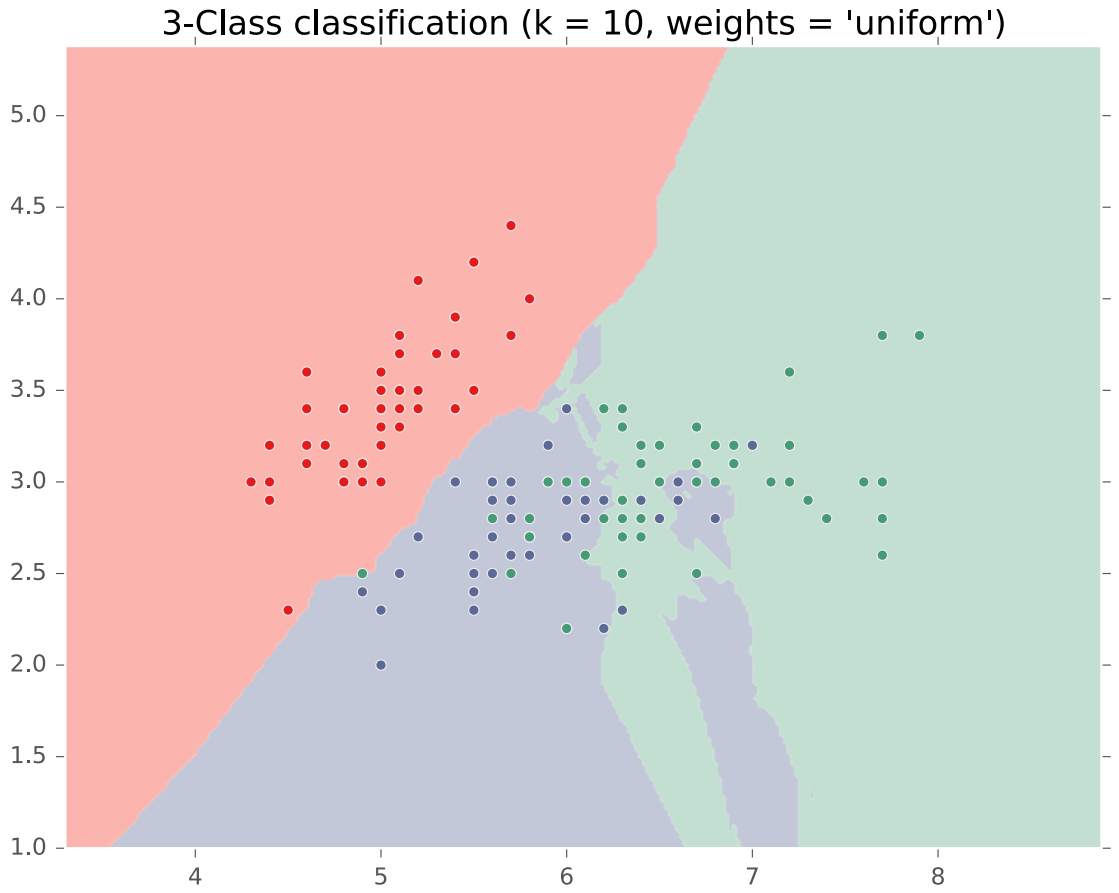


Figure courtesy of Matt Gormley

kNN on Fisher Iris Data



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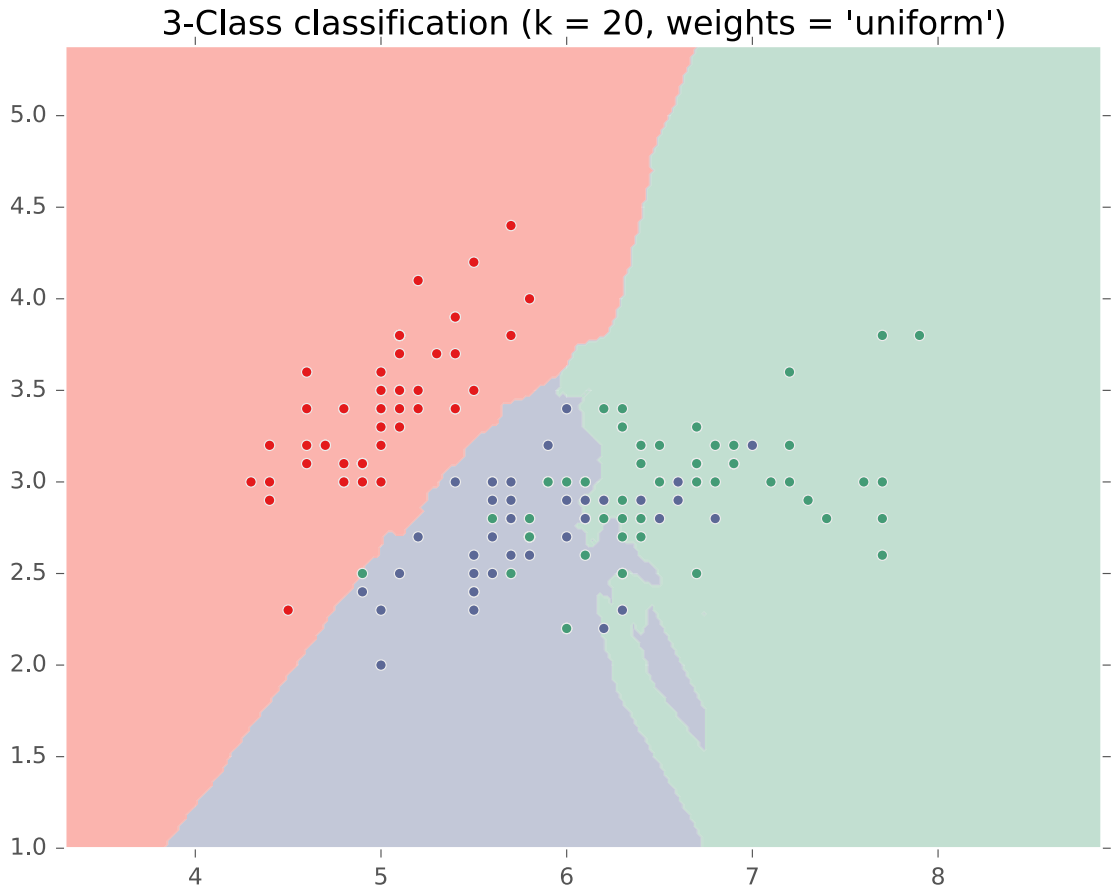

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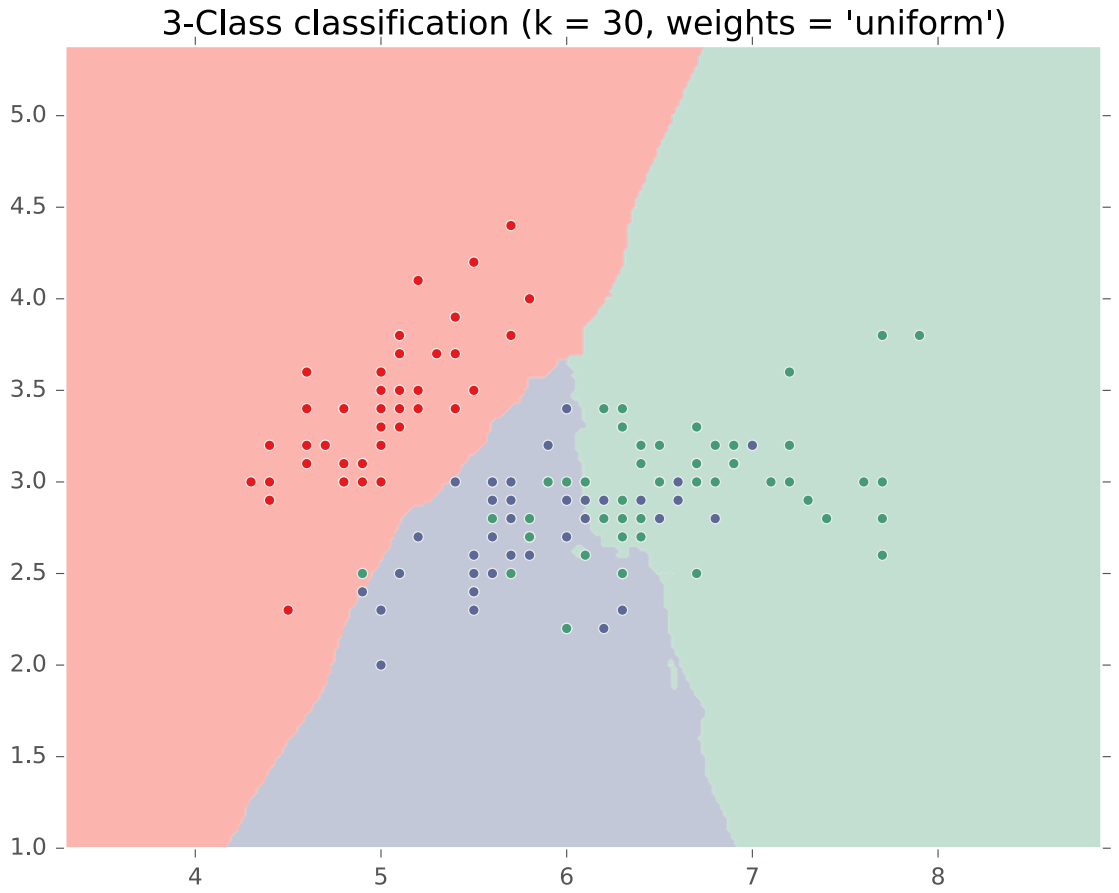

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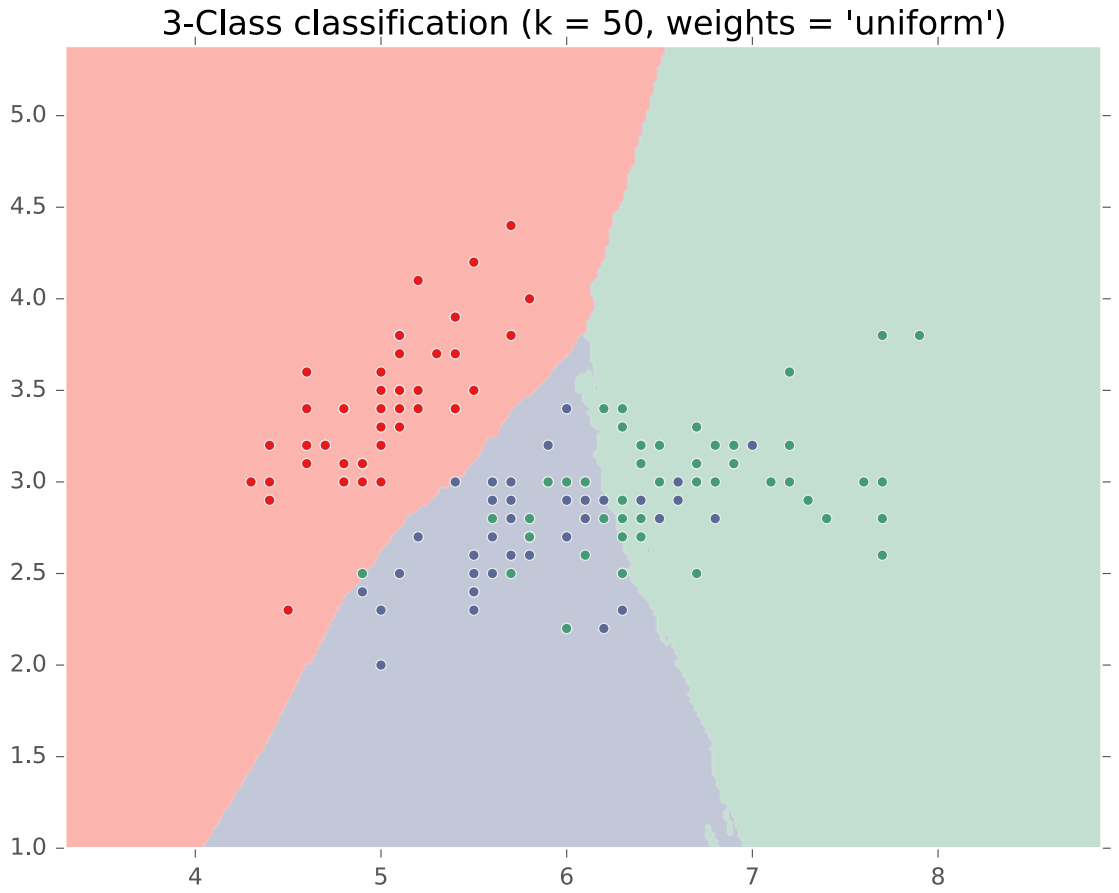

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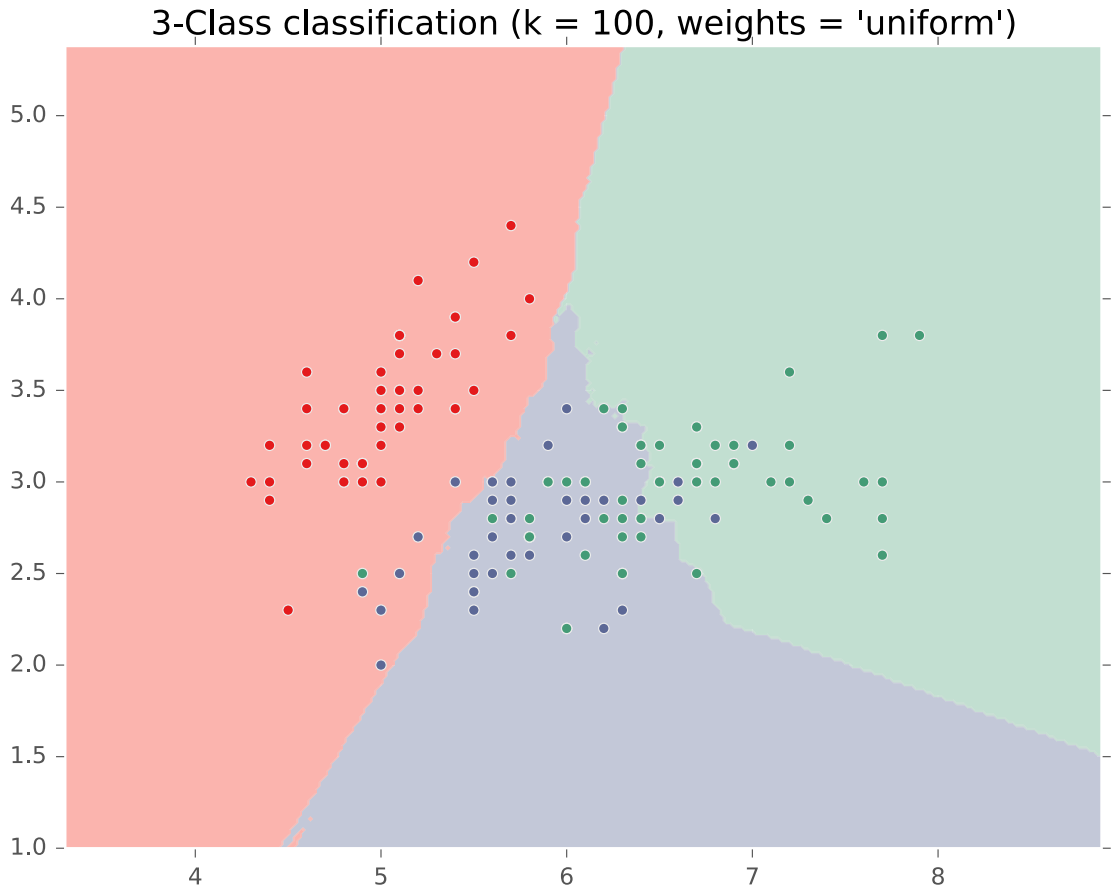

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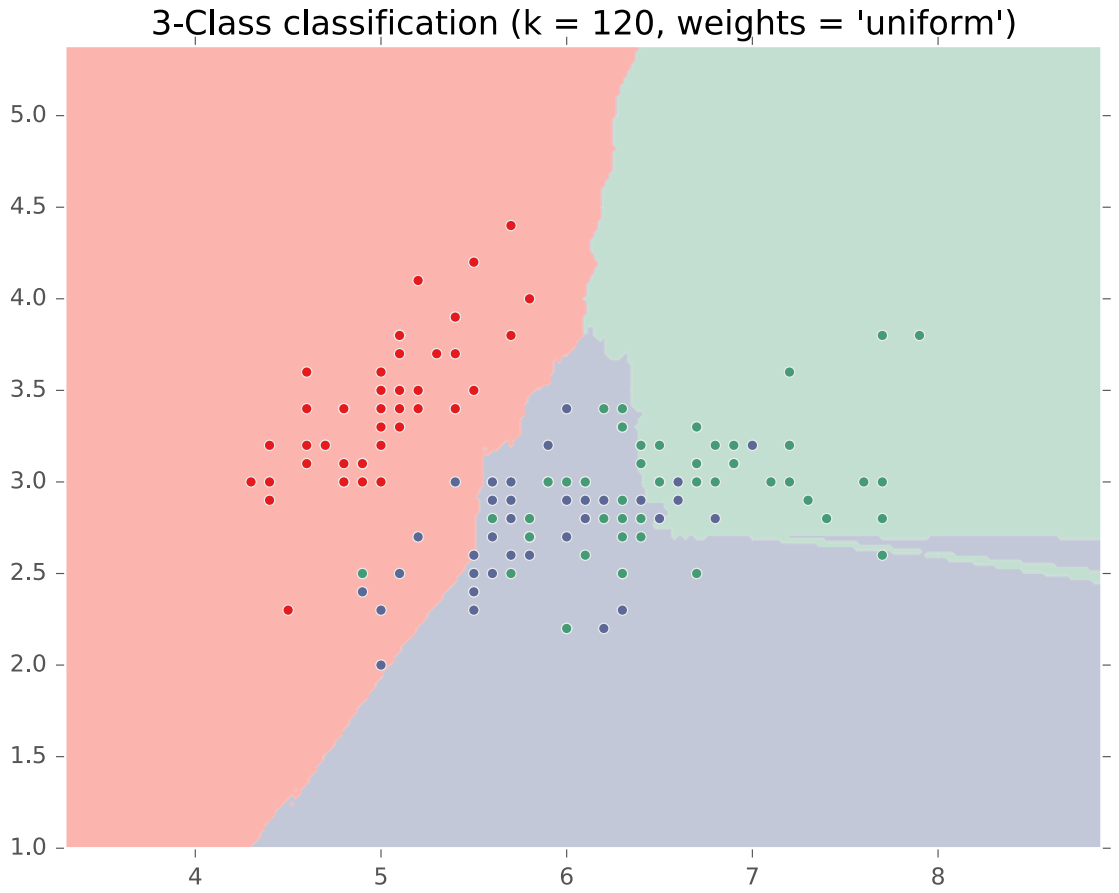

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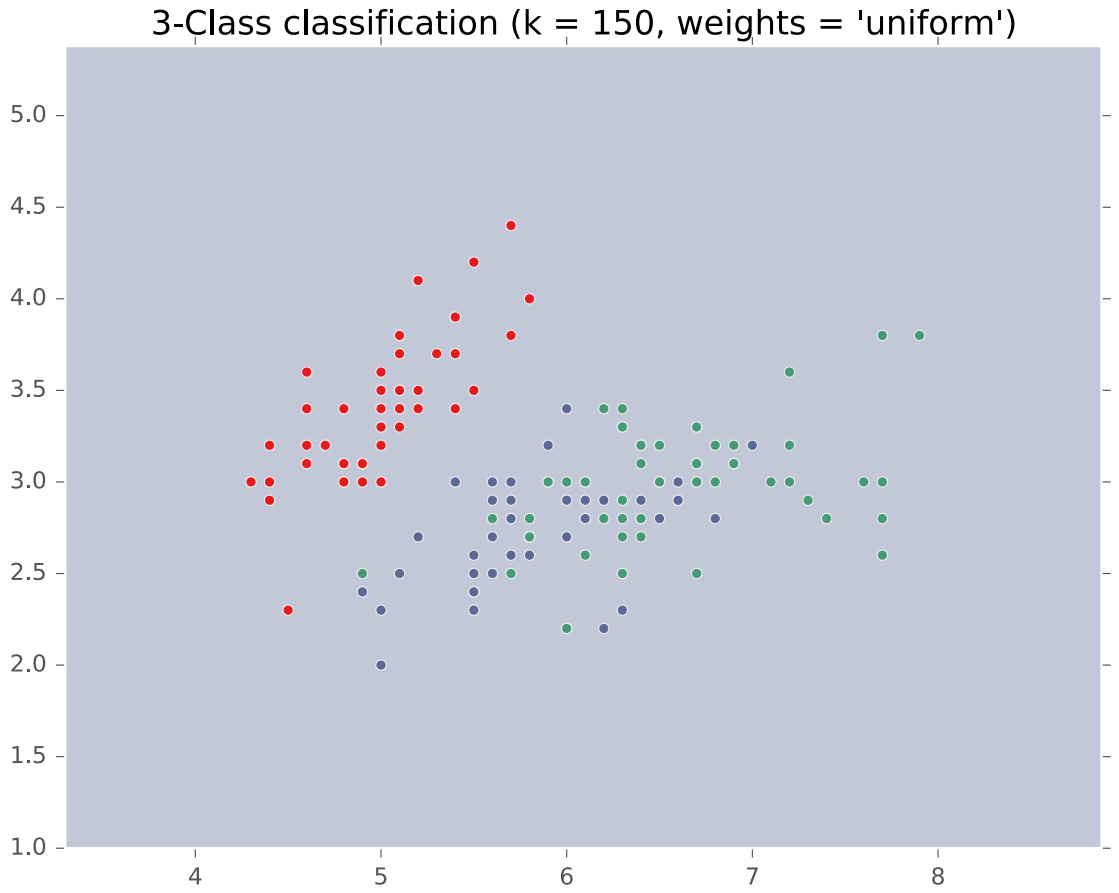


Figure courtesy of Matt Gormley

Setting k

- When $k = 1$:
  - many, complicated decision boundaries
  - may overfit
- When $k = N$:
  - no decision boundaries; always predicts the most common label in the training data
  - may underfit
- k controls the complexity of the hypothesis set $\Longrightarrow$ k affects how well the learned hypothesis will generalize

Setting k

- Theorem:
  - If k is some function of N s.t. $k(N) \to \infty$ and $\frac{k(N)}{N} \to 0$ as $N \to \infty$ …
  - … then (under certain assumptions) the true error of a kNN model → the Bayes error rate
- Practical heuristics:
  - $k = \lfloor \sqrt{N} \rfloor$
  - $k = 3$
- Can also set k through (cross-)validation (stay tuned)

Aside: kNN and Categorical Features

- kNNs are compatible with categorical features, either by:
  1. Converting categorical features into binary ones:

Cholesterol
Normal
Normal
Abnormal

→

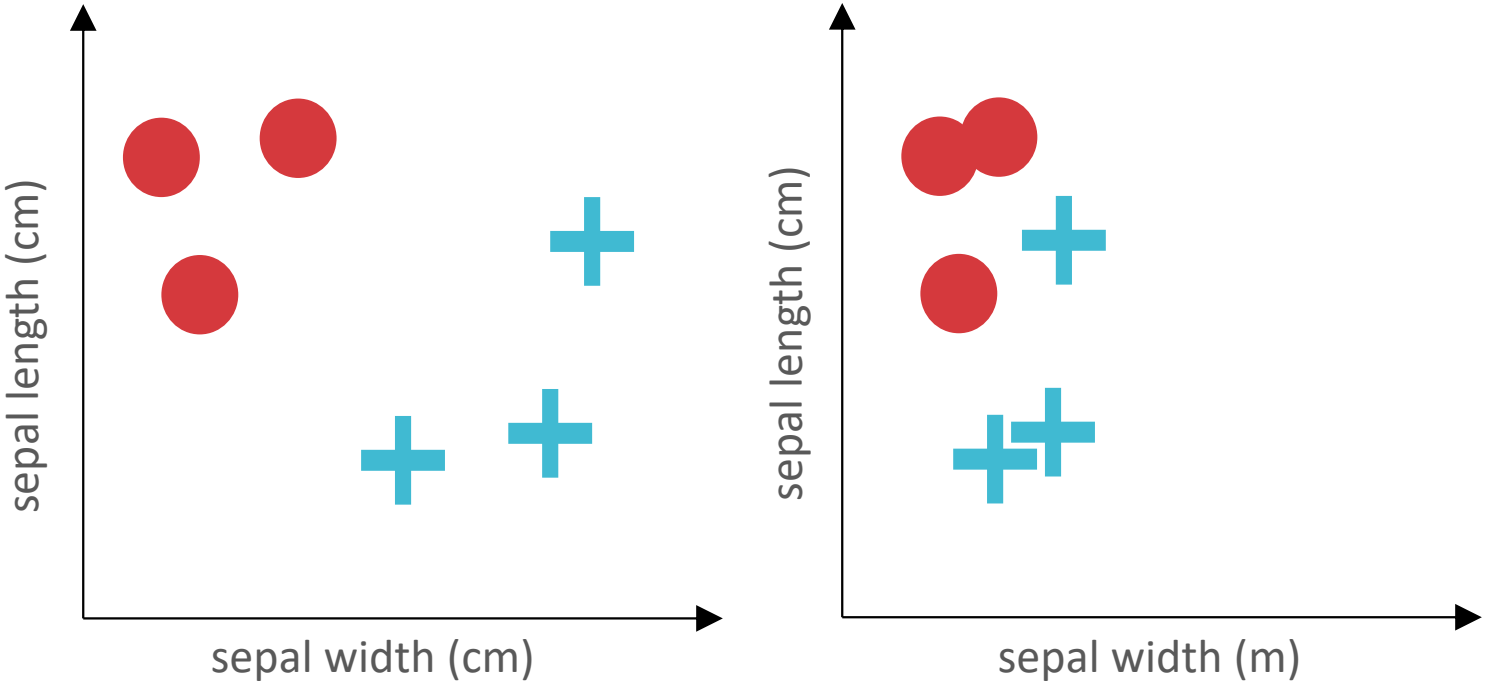
Normal Cholesterol?	Abnormal Cholesterol?
1	0
1	0
0	1

  2. Using a distance metric that works over categorical features e.g., the Hamming distance:

$$d(\boldsymbol{x}, \boldsymbol{x}') = \sum_{d=1}^{D} \mathbb{1}(x_d = x'_d)$$

kNN: Inductive Bias

- Similar points should have similar labels and *all features are equivalently important for determining similarity*



- Feature scale can dramatically influence results!

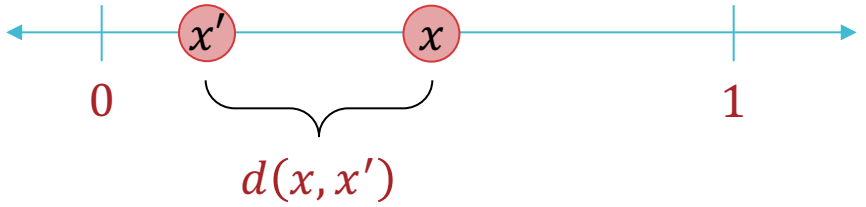
Figure courtesy of Matt Gormley

Curse of Dimensionality

- The fundamental assumption of kNN is that "similar" points or points close to one another should have the same label
- The closer two points are, the more confident we can be that they will have the same label
- As the dimensionality of the input grows, the less likely it is that two random points will be close
- As the dimensionality of the input grows, it takes more points to "cover" the input space

Curse of Dimensionality

- Suppose you independently draw two one-dimensional points between 0 and 1 uniformly at random:



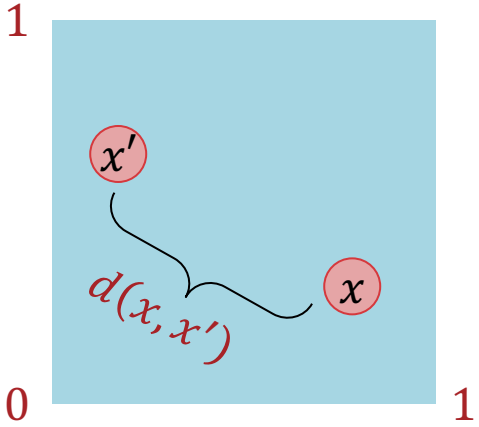
- $\mathbb{E}[d(x, x')] = \mathbb{E}[(x - x')^2]$

$$= \mathbb{E}[x^2] - 2\mathbb{E}[x]\mathbb{E}[x'] + \mathbb{E}[x'^2]$$

$$= 2\mathbb{E}[x^2] - 2\mathbb{E}[x]^2 = 2\left(\frac{1}{3}\right) - 2\left(\frac{1}{2}\right)^2 = \frac{1}{6}$$

Curse of Dimensionality

- Suppose you independently draw two two-dimensional points in the unit square uniformly at random:



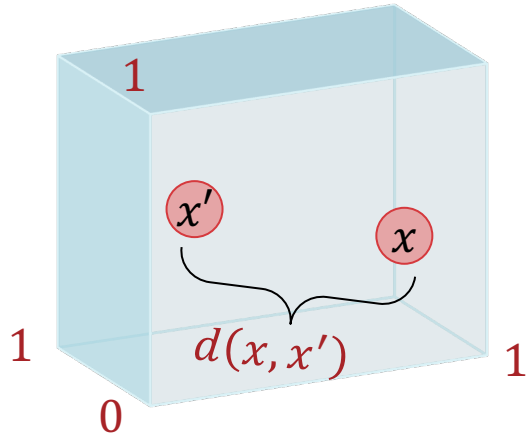
- $\mathbb{E}[d(x, x')] = \mathbb{E}[(x_1 - x_1')^2 + (x_2 - x_2')^2]$

$$= 2\mathbb{E}[(x_1 - x_1')^2]$$

$$= 2\left(\frac{1}{6}\right) = \frac{1}{3}$$

Curse of Dimensionality

- Suppose you independently draw two three-dimensional points in the unit cube uniformly at random:



- $\mathbb{E}[d(x, x')] = \mathbb{E}[(x_1 - x_1')^2 + (x_2 - x_2')^2 + (x_3 - x_3')^2]$

$$= 3\mathbb{E}[(x_1 - x_1')^2]$$

$$= 3\left(\frac{1}{6}\right) = \frac{1}{2}$$

Curse of Dimensionality

- Assume all dimensions of the input are independent and identically distributed.
- Given $N + 1$ data points, $\mathcal{D} = \left\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(N)}\right\}$ and $\boldsymbol{x}^*$, let

$$d_+ = \max_{\boldsymbol{x} \in \mathcal{D}} d(\boldsymbol{x}, \boldsymbol{x}^*) \text{ and } d_- = \min_{\boldsymbol{x} \in \mathcal{D}} d(\boldsymbol{x}, \boldsymbol{x}^*)$$

- Then

$$\lim_{D \to \infty} \mathbb{E}\left[\frac{d_+ - d_-}{d_-}\right] \to 0$$

Curing the Curse of Dimensionality

- More data
- Fewer dimensions
- Blessing of non-uniformity: data from the real world is rarely uniformly distributed across the input space

kNN: Pros and Cons

- Pros:
  - Intuitive / explainable
  - No training / retraining
  - Provably near-optimal in terms of true error rate
- Cons:
  - Computationally expensive
    - Always needs to store all data: $O(ND)$
    - Finding the k closest points in D dimensions: $O(ND + N\log(k))$
      - Can be sped up through clever use of data structures (trades off training and test costs)
      - Can be approximated using stochastic methods
  - Affected by feature scale
  - Suffers from the curse of dimensionality

Key Takeaways

- Real-valued features and decision boundaries
- Nearest neighbor model and generalization guarantees
- kNN "training" and prediction
- Effect of k on model complexity
- kNN inductive bias
- Curse of dimensionality