10-301/601: Introduction to Machine Learning Lecture 5 – KNNs

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5/14/25

Front Matter

- Announcements:
  - HW1 released on 5/13, due 5/16 at 11:59 PM
    - You will submit your homework to Gradescope
      1. Submit your code to the “programming” submission slot
      2. Submit a PDF with your answers to the questions “written” submission slot
         - **You must use LaTeX to typeset your responses!**

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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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

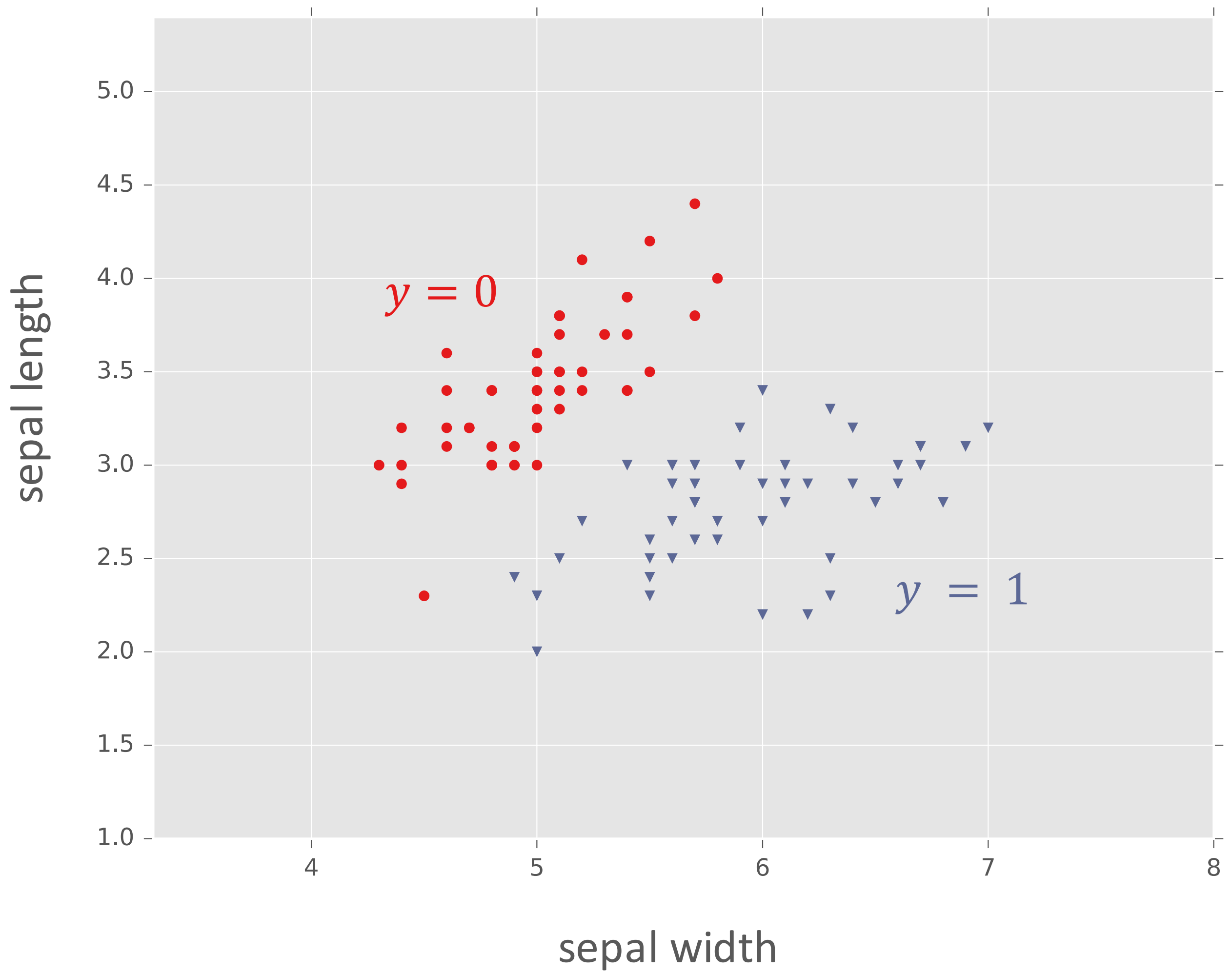
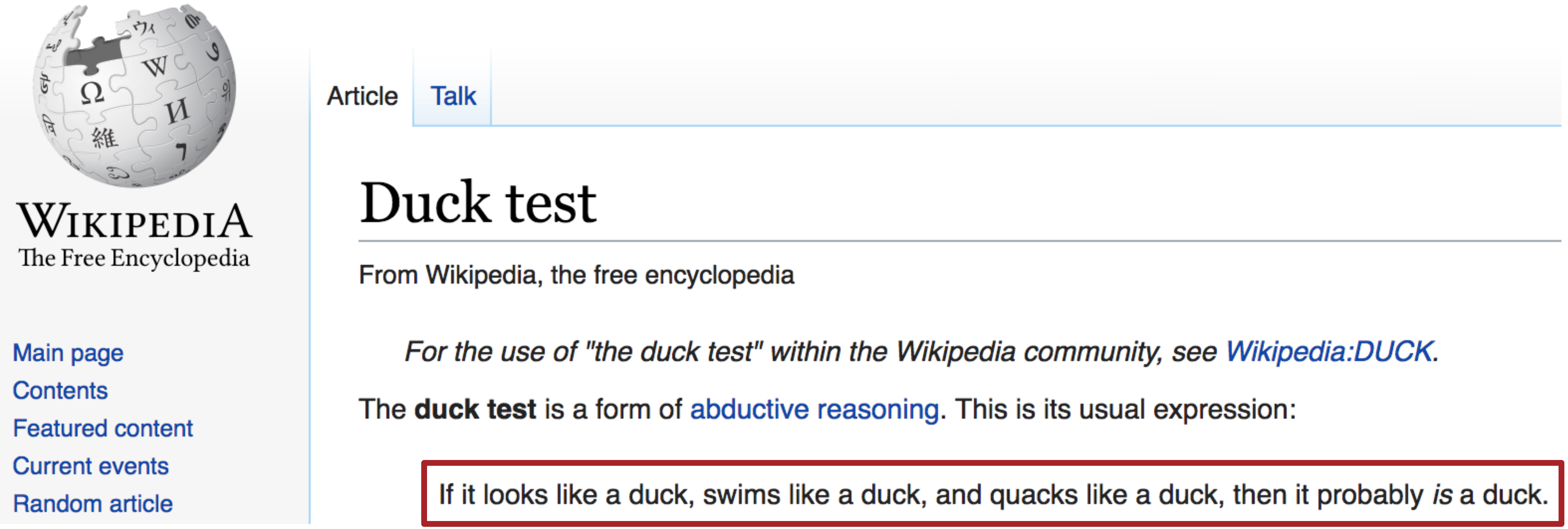


Figure courtesy of Matt Gormley



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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:

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

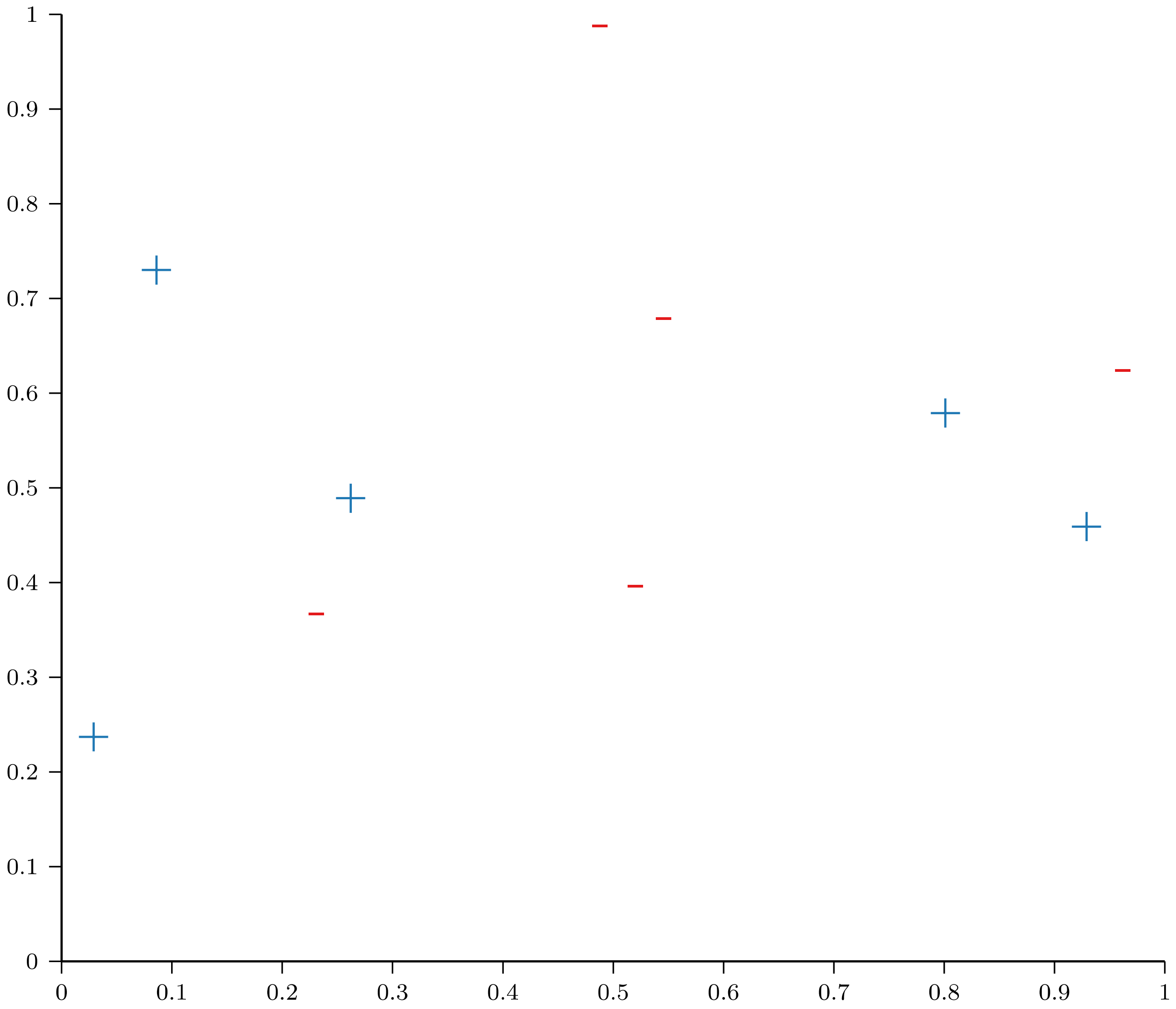
- An alternative is the Manhattan distance:

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

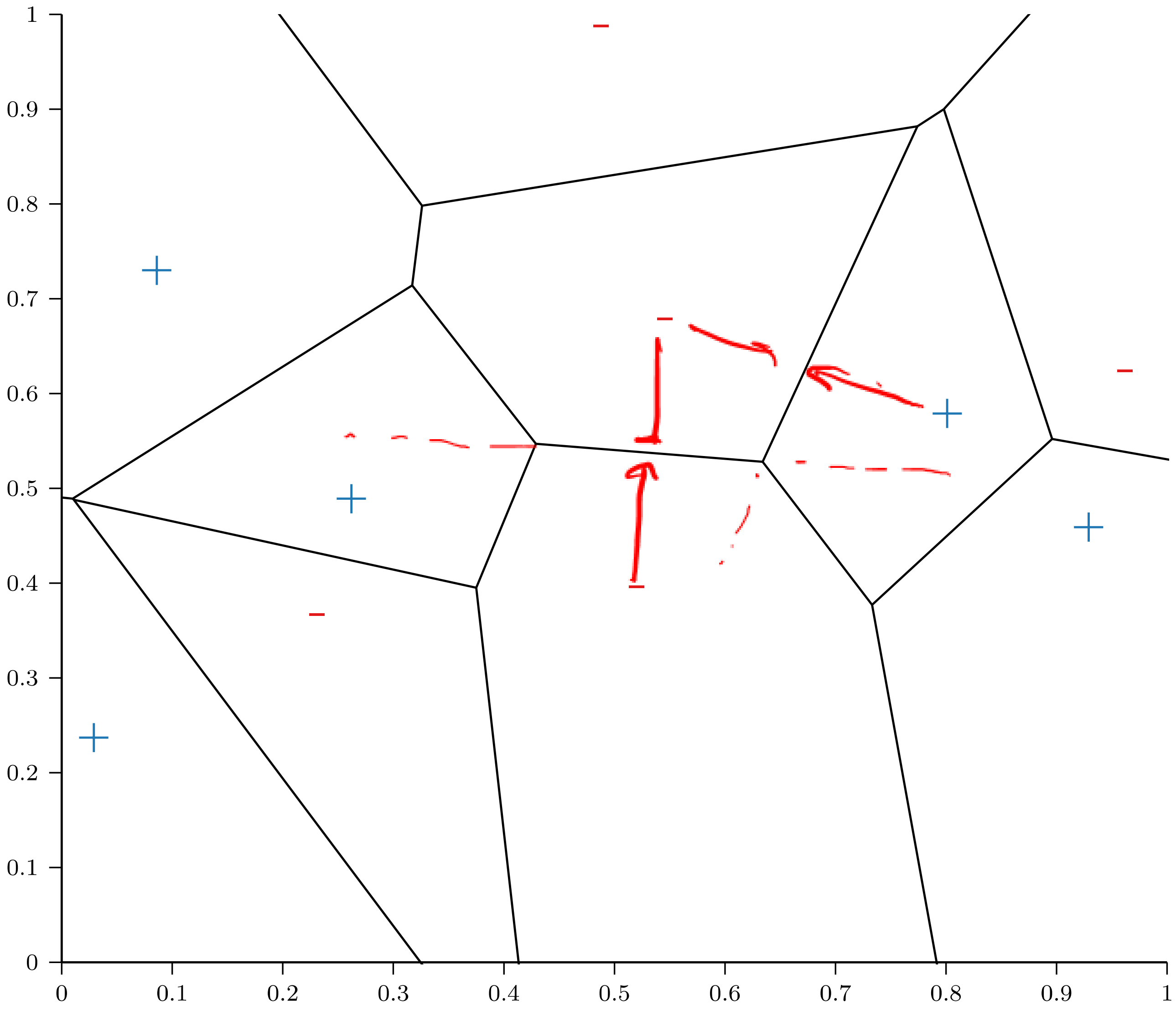
Nearest Neighbor: Pseudocode

```
def train(𝒟):
    Store D
def predict(x′):
    find the closest data point to x⃗′ in D
             x⃗(i)
    return y(i)
```

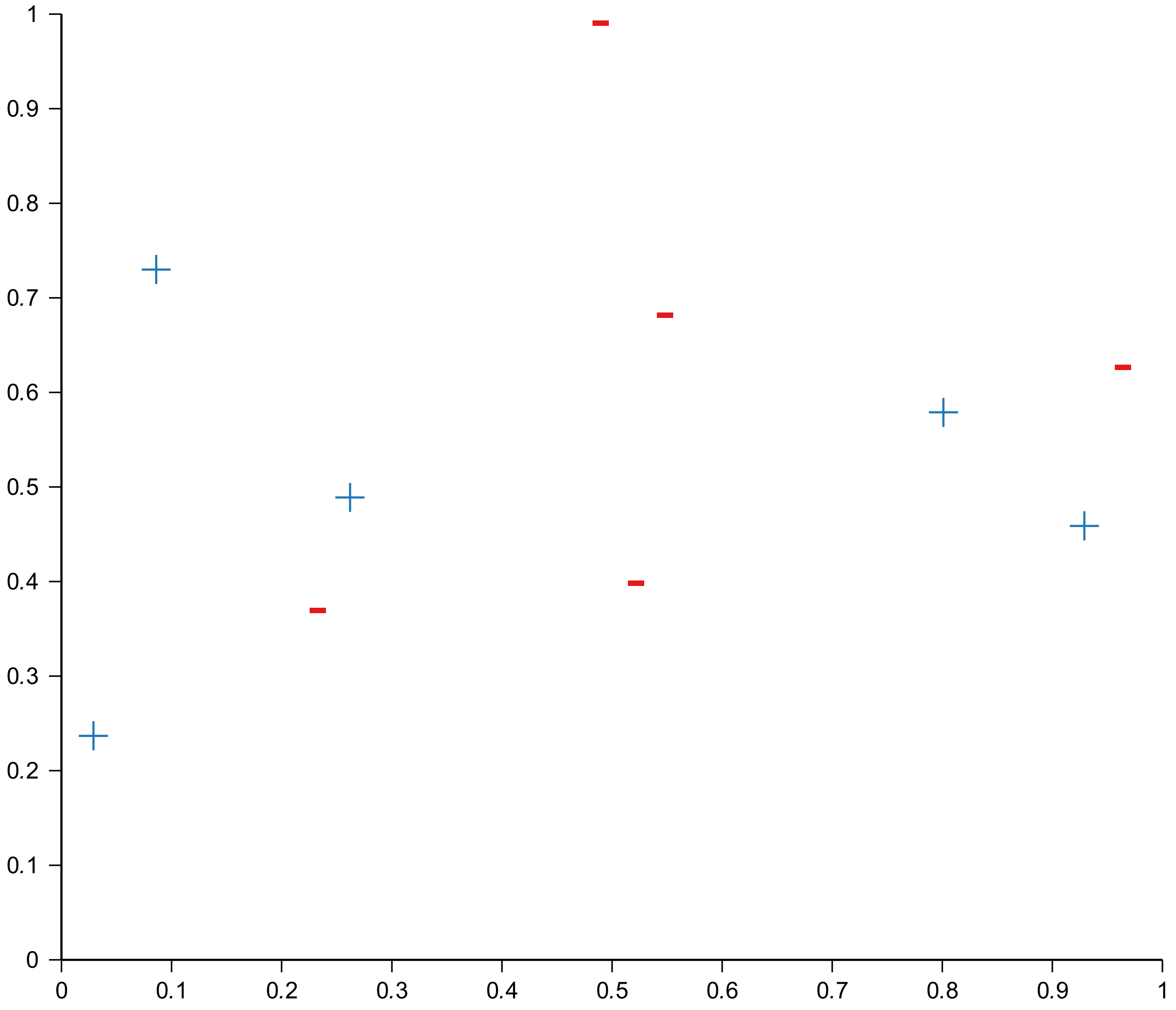
Nearest Neighbor: Example



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***

$\vdots$

- Always has zero training error…

Generalization of Nearest Neighbor (Cover and Hart, 1967)

- Claim: under certain conditions, as $N \rightarrow \infty$, 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)
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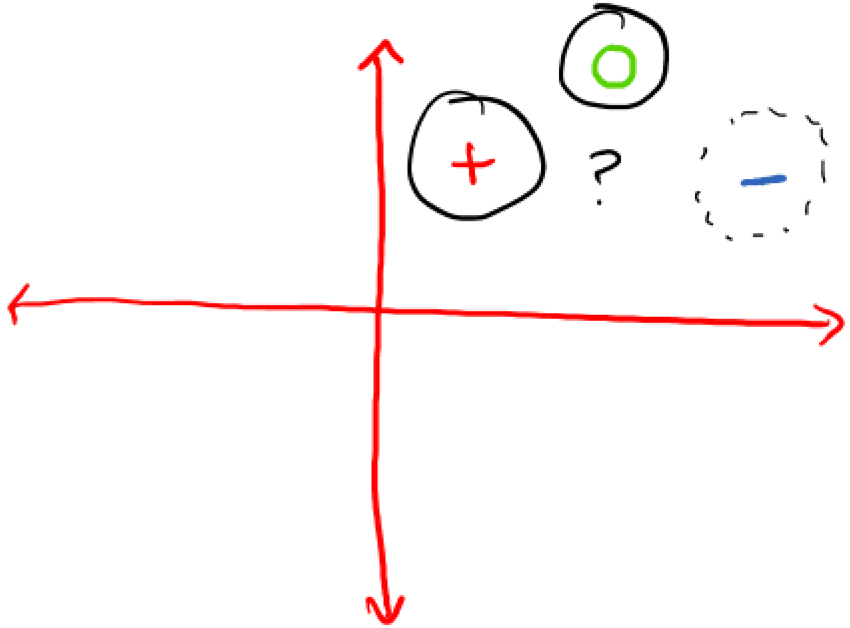
k-Nearest Neighbors (kNN)

- 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)



Lecture 5 + 6 Polls

0 surveys completed

0 surveys underway

Suppose you have a kNN model with $k > 1$ and 3 possible classes. Which of the following tie-breaking methods is *guaranteed* to break a tie in the majority vote? Select all that apply

- Weight the votes by distance
- Remove the furthest neighbor
- Add another neighbor
- Use a different distance metric
- None of the above

k-Nearest Neighbors (kNN): Pseudocode

def train($\mathcal{D}$):

    store D

def predict(x'):

    return majority_vote(labels of the k nearest neighbors to $\vec{x}'$ in D)

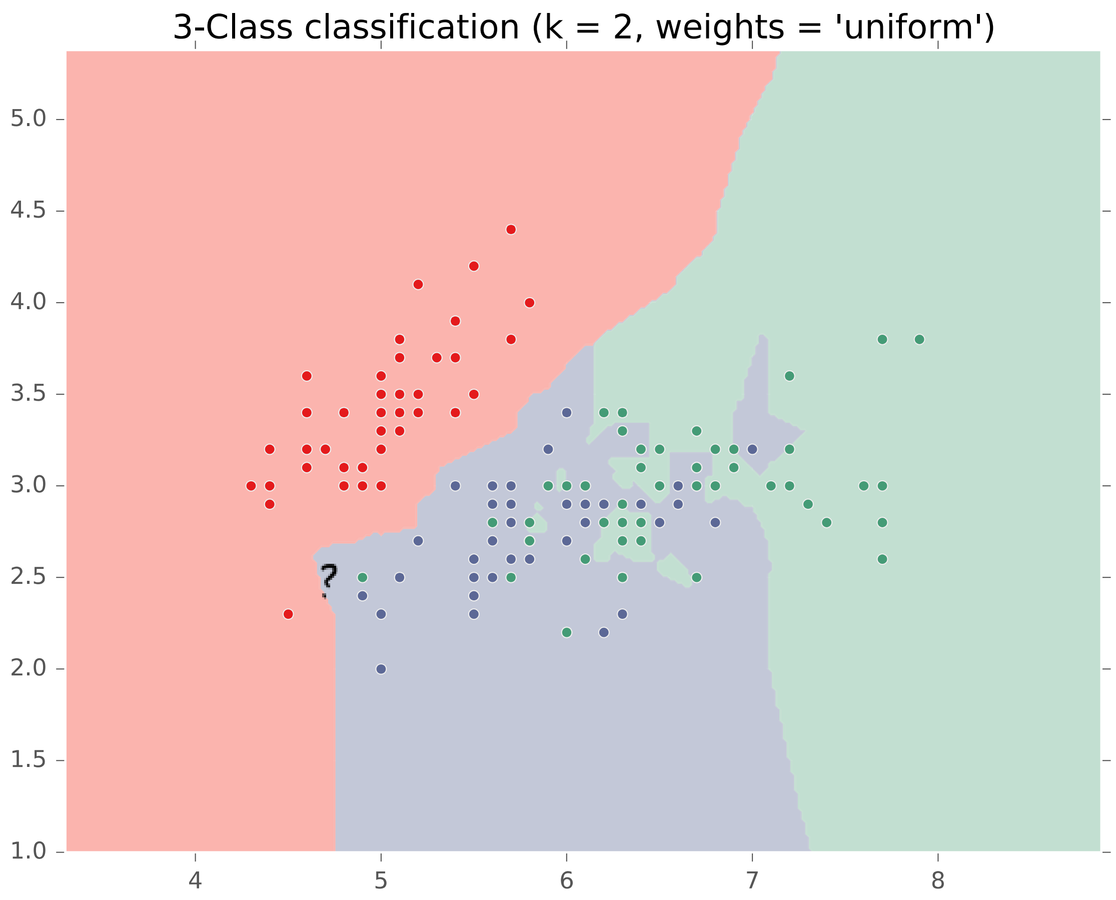
label tie-breaking

distance tie-breaking

kNN on Fisher Iris Data

Figure courtesy of Matt Gormley

kNN on Fisher Iris Data



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kNN on Fisher Iris Data

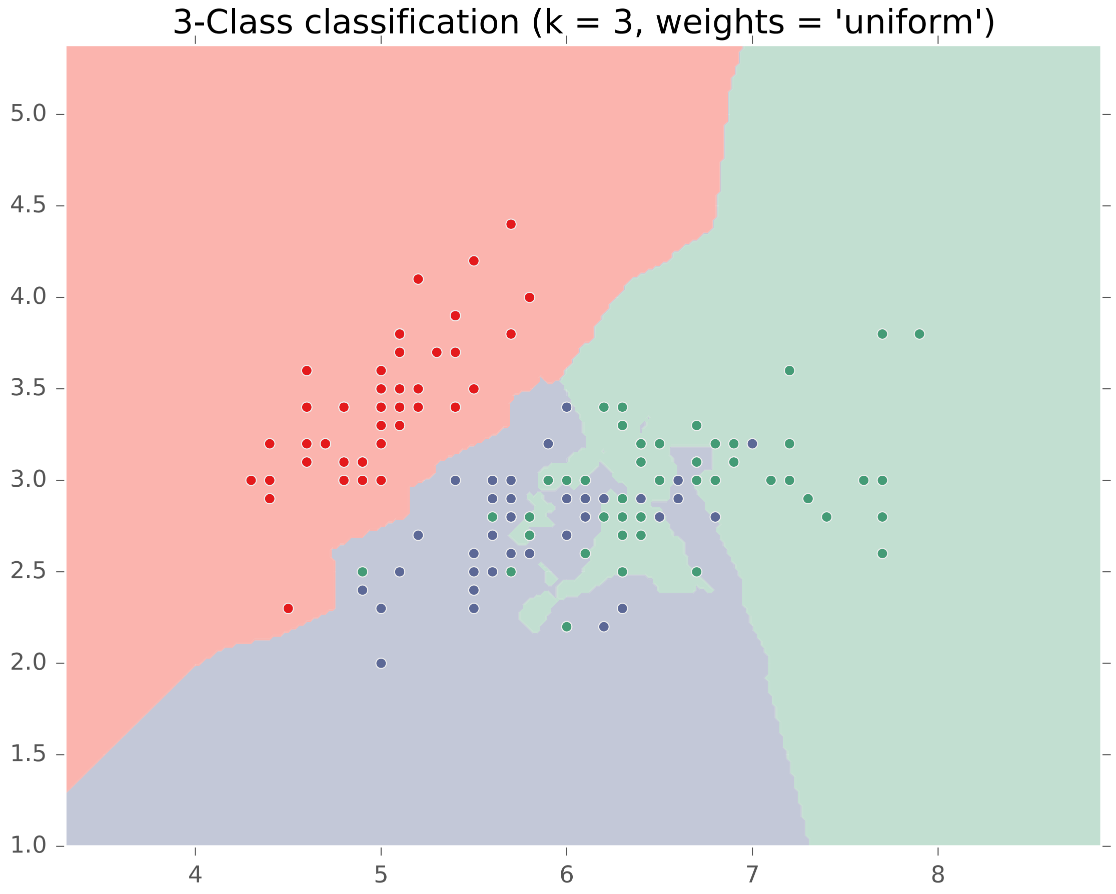

Figure courtesy of Matt Gormley

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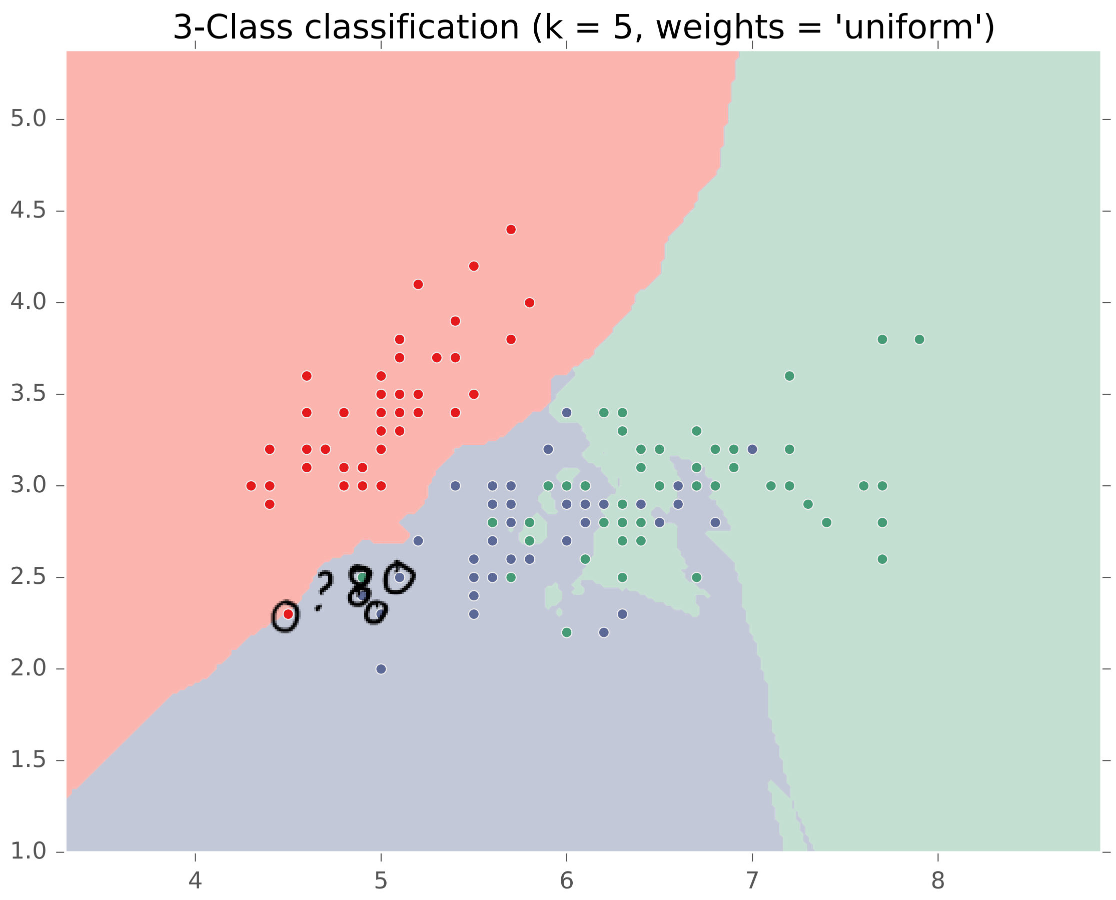


Figure courtesy of Matt Gormley

kNN on Fisher Iris Data

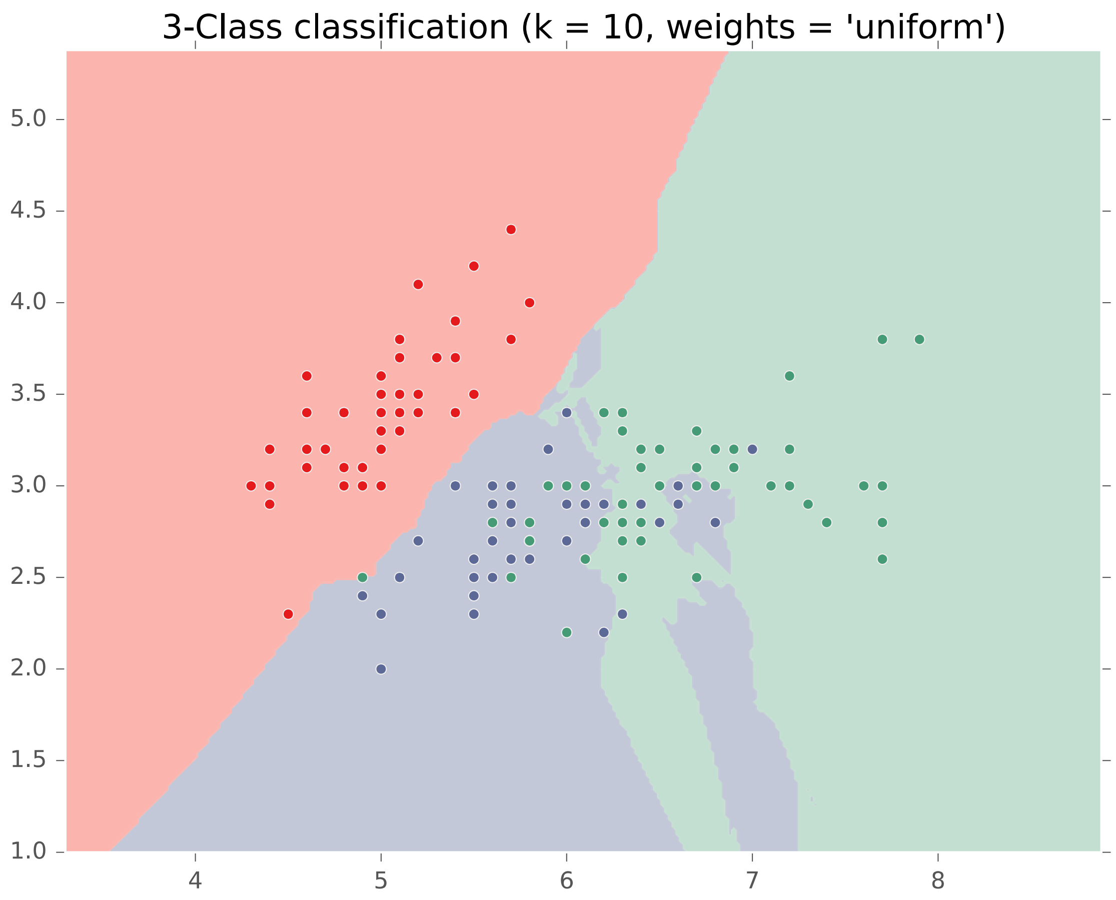


Figure courtesy of Matt Gormley

kNN on Fisher Iris Data

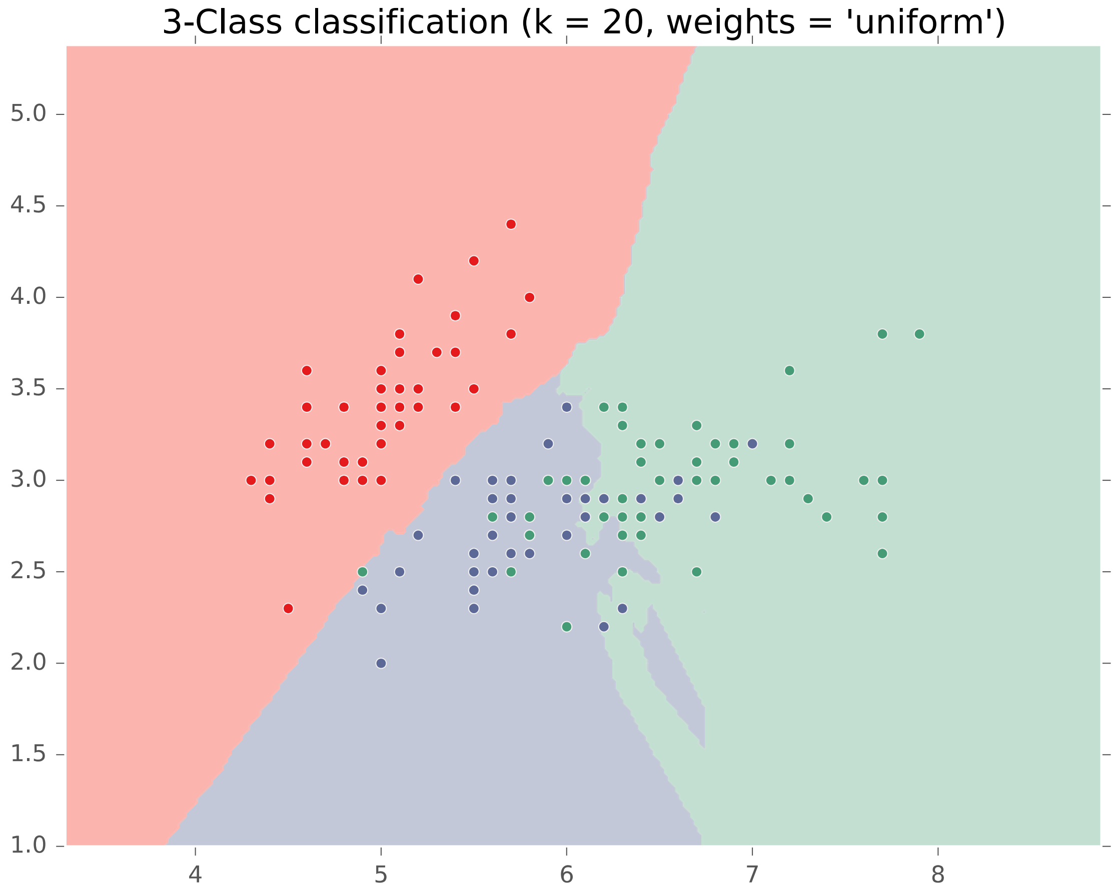
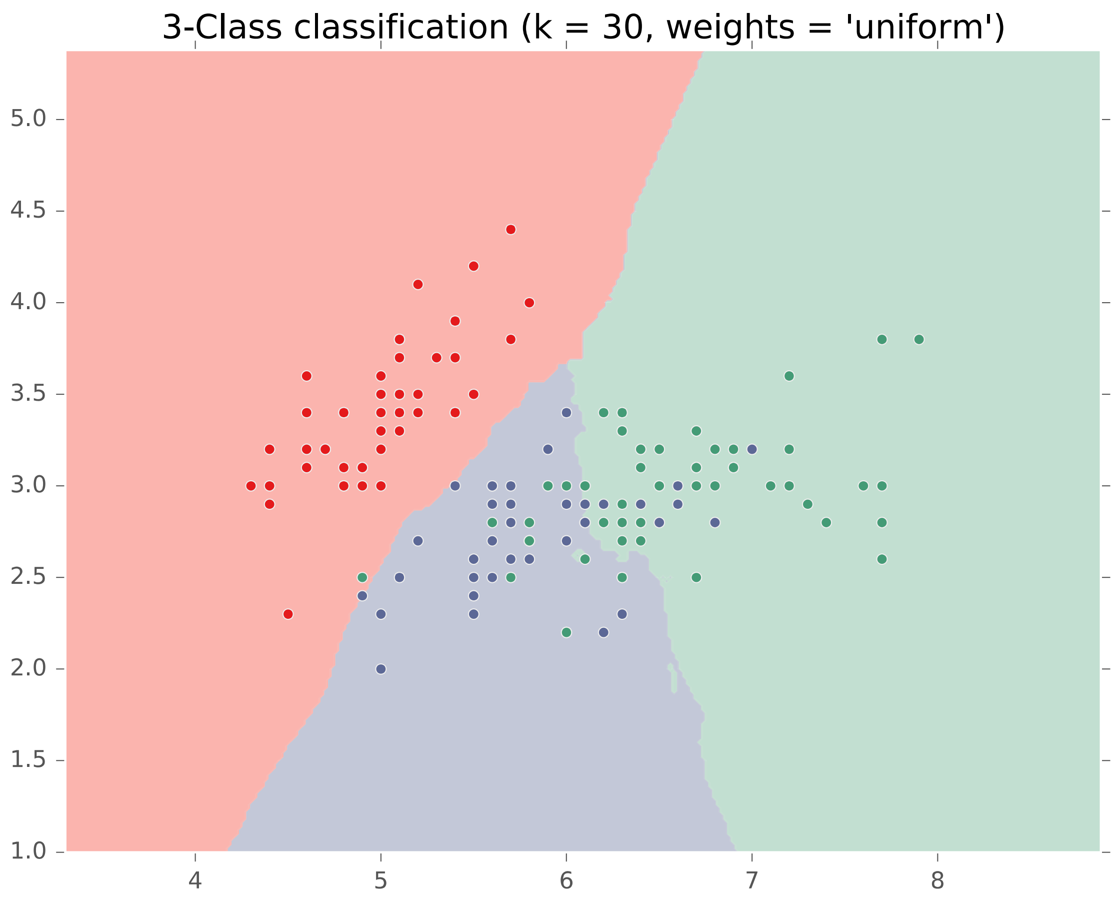


Figure courtesy of Matt Gormley

kNN on Fisher Iris Data



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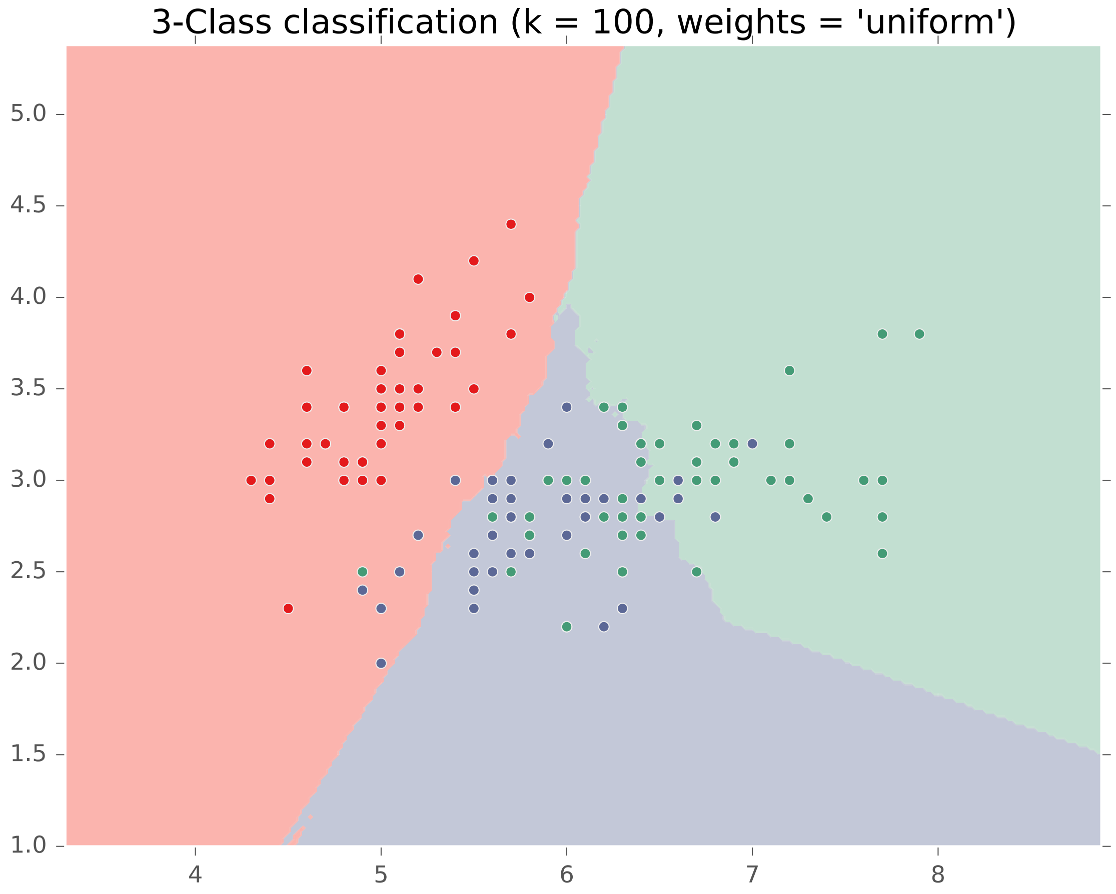

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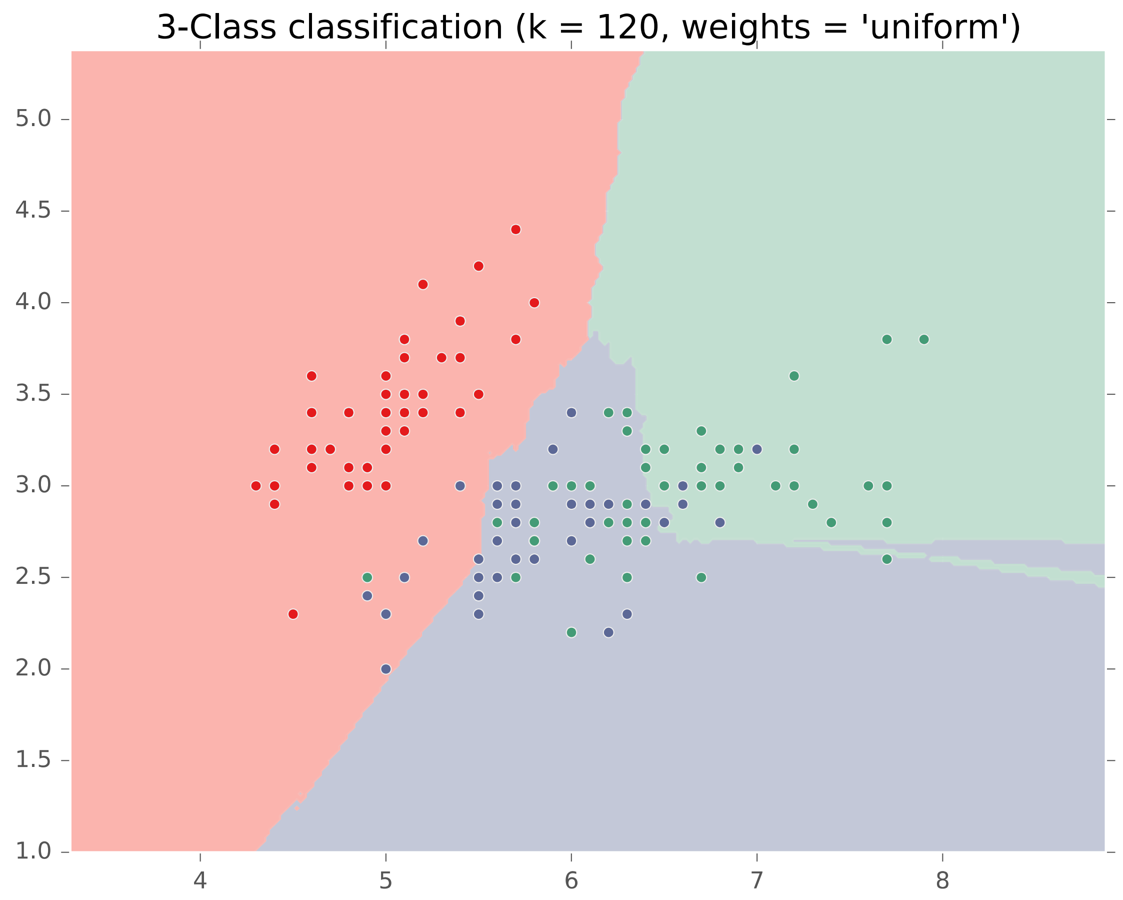

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kNN on Fisher Iris Data

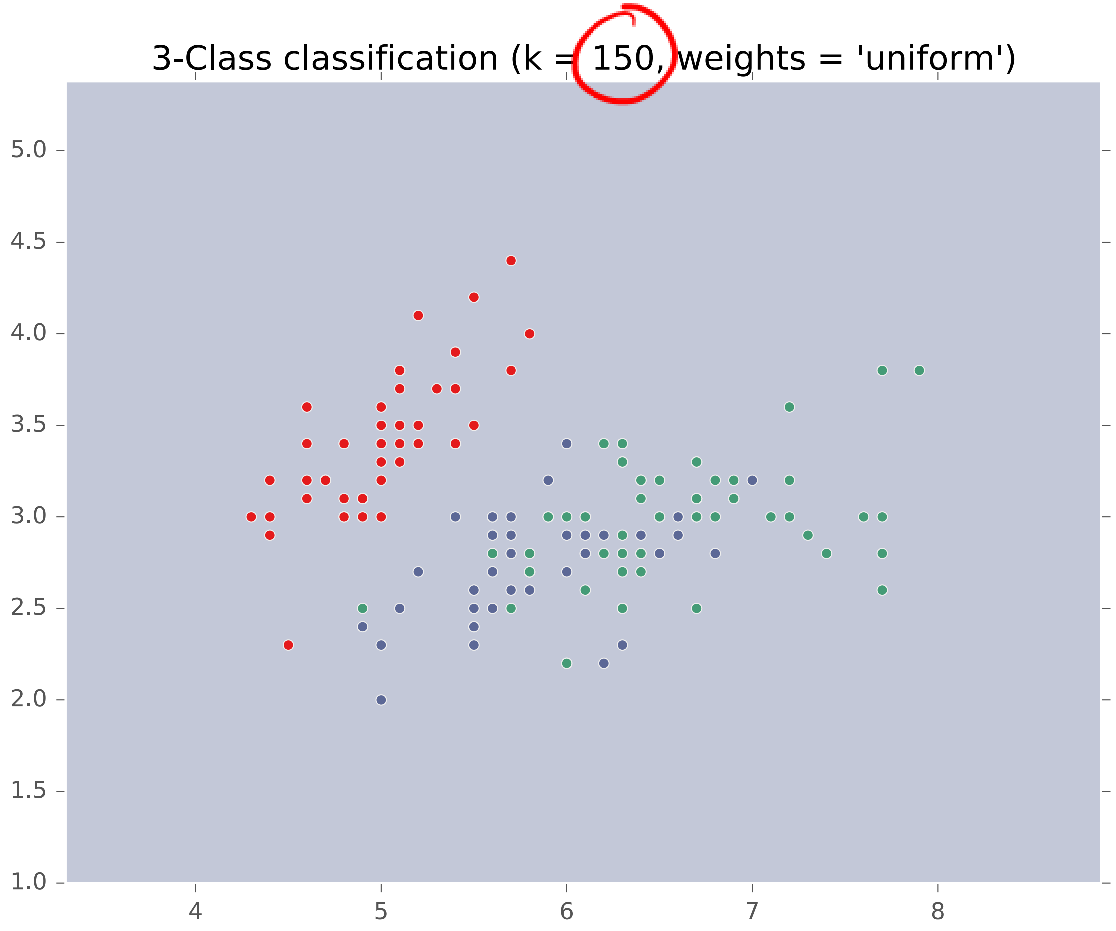

Figure courtesy of Matt Gormley

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

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:

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

kNN: Inductive Bias

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