Machine Learning Department
School of Computer Science
Carnegie Mellon University

k-Nearest Neighbors

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Model Selection

Matt Gormley
Lecture 5
Feb. 1, 2023

Reminders

- Homework 2: Decision Trees
  - Out: Wed, Jan. 25
  - Due: Fri, Feb. 3 at 11:59pm
- Schedule Note:
  - Fri, Feb. 3: Lecture 6: Perceptron
  - Wed, Feb. 8: Recitation: HW3

Moss: Code Plagiarism Detection

What is Moss?

- Moss (Measure Of Software Similarity): is an automatic system for determining the similarity of programs. To date, the main application of Moss has been in detecting plagiarism in programming classes.
- Moss reports:
  - The Andrew IDs associated with the file submissions
  - The number of lines matched
  - The percent lines matched
  - Color coded submissions where similarities are found

What is Moss?

At first glance, the submissions may look different

```python
# Python program to find ordered words
import requests

# Scrapes the words from the URL below and stores
# them in a list
def getWords():

# contains about 2500 words
    url = "http://www.puzzlers.org/pub/wordlists/unixdict.txt"
    fetchData = requests.get(url)

# extracts the content of the webpage
    wordList = fetchData.content

# decodes the UTF-8 encoded text and splits the
# string to turn it into a list of words
    wordList = wordList.decode("utf-8").split()

    return wordList


# function to determine whether a word is ordered or not
def isOrdered():

# fetching the wordList
    collection = getWords()

# since the first few of the elements of the
# dictionary are numbers, getting rid of those
# numbers by slicing off the first 17 elements
    collection = collection[16:]
    word = ''

    for word in collection:
        result = 'Word is ordered'
        i = 0
        l = len(word) - 1

        if (len(word) < 3): # skips the 1 and 2 lettered strings
            continue

        # traverses through all characters of the word in pairs
        while i < l:
            if (ord(word[i]) > ord(word[i+1])):
                result = 'Word is not ordered'
                break
            else:
                i += 1

    # only printing the ordered words
        if (result == 'Word is ordered'):
            print(word,': ',result)


# execute isOrdered() function
if __name__ == '__main__':
    isOrdered()
```

```python
import requests

def Ordered():
    coll = getWs()
    coll = coll[16:]
    word = ''
    for word in coll:
        r = 'Word is ordered'
        a = 0
        length = len(word) - 1
        if (len(word) < 3):
            continue
        while a < length:
            if (ord(word[a]) > ord(word[a+1])):
                r = 'Word is not ordered'
                break
            else:
                a += 1
        if (r == 'Word is ordered'):
            print(word,': ',r)

def getWs():
    url = "http://www.puzzlers.org/pub/wordlists/unixdict.txt"
    fetch = requests.get(url)
    words = fetch.content
    words = words.decode("utf-8").split()
    return words

if __name__ == '__main__':
    Ordered()
```

What is Moss?

Moss can quickly find the similarities

```
>>>> file: bedmunds@andrew.cmu.edu_1_handin.c
# Python program to find ordered words
import requests

# Scrapes the words from the URL below and stores
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# contains about 2500 words
    url = "http://www.puzzlers.org/pub/wordlists/unixdict.txt"
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                break
            else:
                i += 1

    # only printing the ordered words
        if (result == 'Word is ordered'):
            print(word,': ',result)


# execute isOrdered() function
if __name__ == '__main__':
    isOrdered()
```

```
>>>> file: dpbird@andrew.cmu.edu_1_handin.c

import requests

def Ordered():
    coll = getWs()
    coll = coll[16:]
    word = ''
    for word in coll:
        r = 'Word is ordered'
        a = 0
        length = len(word) - 1
        if (len(word) < 3):
            continue
        while a < length:
            if (ord(word[a]) > ord(word[a+1])):
                r = 'Word is not ordered'
                break
            else:
                a += 1
        if (r == 'Word is ordered'):
            print(word,': ',r)


def getWs():
    url = "http://www.puzzlers.org/pub/wordlists/unixdict.txt"
    fetch = requests.get(url)
    words = fetch.content
    words = words.decode("utf-8").split()
    return words

if __name__ == '__main__':
    Ordered()
```

Q&A

Q: I'm now terrified to collaborate with anyone ever again. Can you remind me of what sort of collaboration is allowed?

A: Yes!

You should collaborate as follows: (1) sketch out pseudocode on an impermanent surface, e.g., a whiteboard (2) erase said surface and part ways with your collaborator and (3) implement your own code from scratch.

K-NEAREST NEIGHBORS

Classification & KNN

Whiteboard:

- Binary classification
- 2D examples
- Decision rules / hypotheses

Nearest Neighbor: Algorithm

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

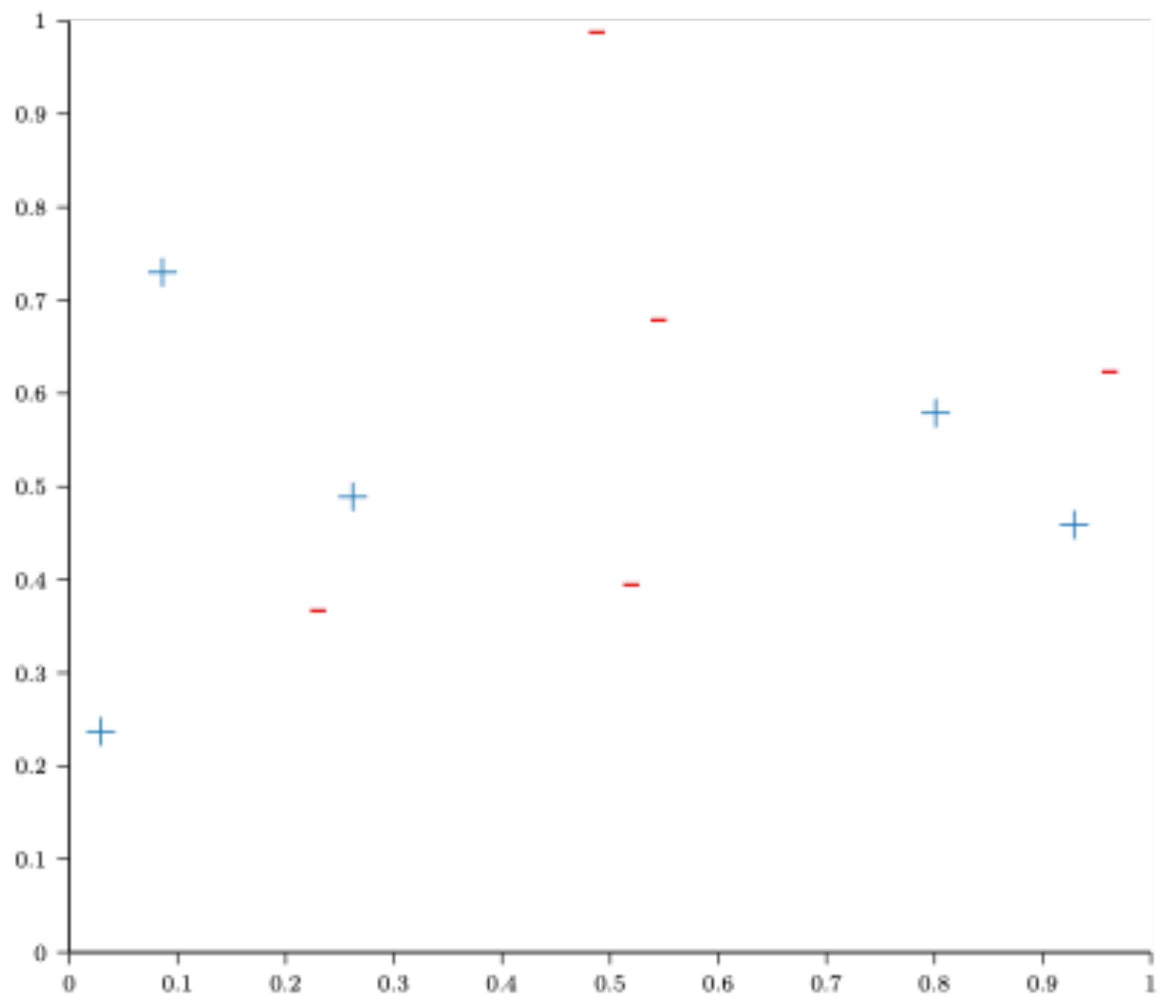
Store $\mathcal{D}$

def h($\boldsymbol{x}'$**):**

Let $\boldsymbol{x}^{(i)}$ = the point in $\mathcal{D}$ that is nearest to $\boldsymbol{x}'$

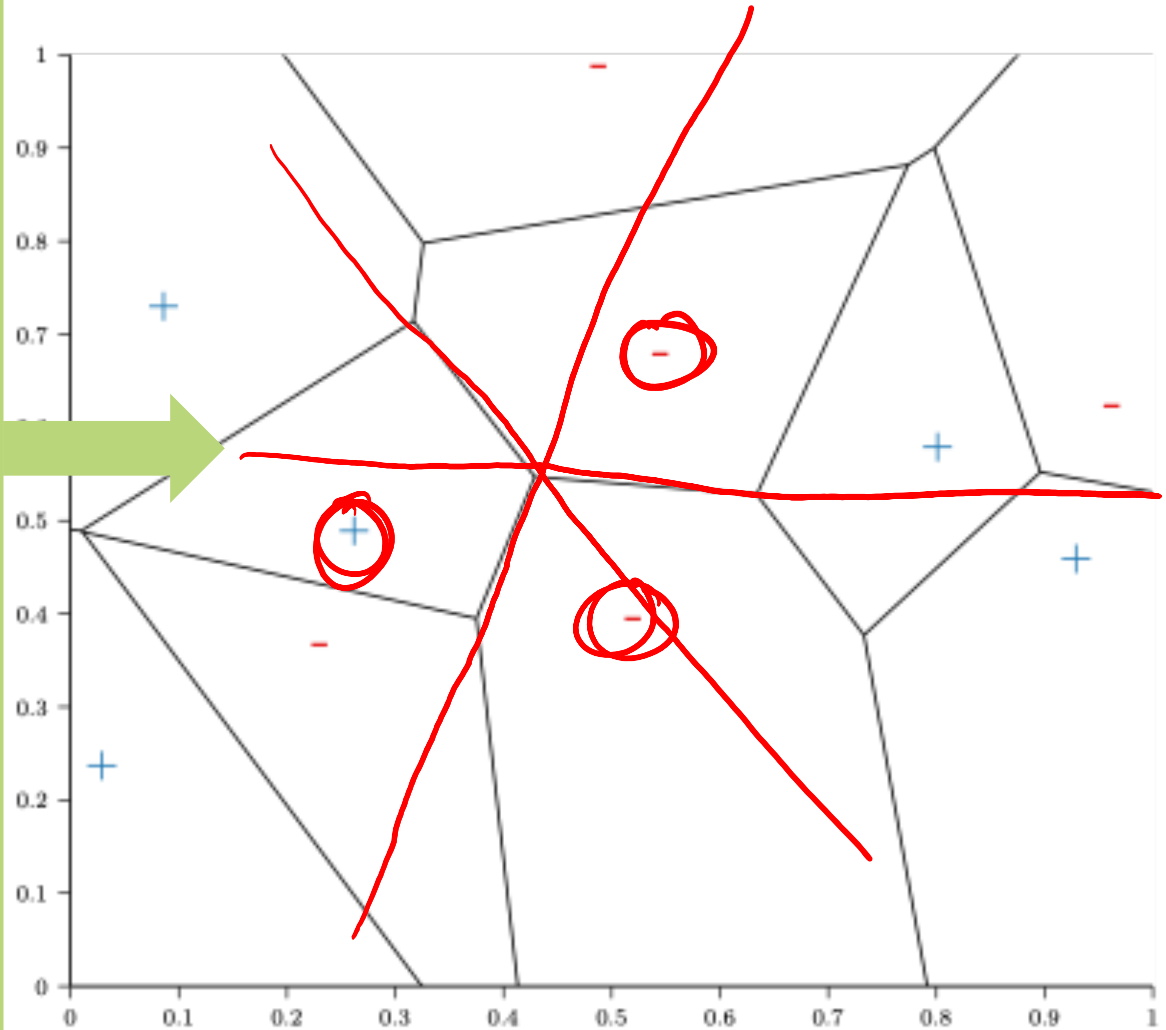
return $y^{(i)}$

Nearest Neighbor: Example

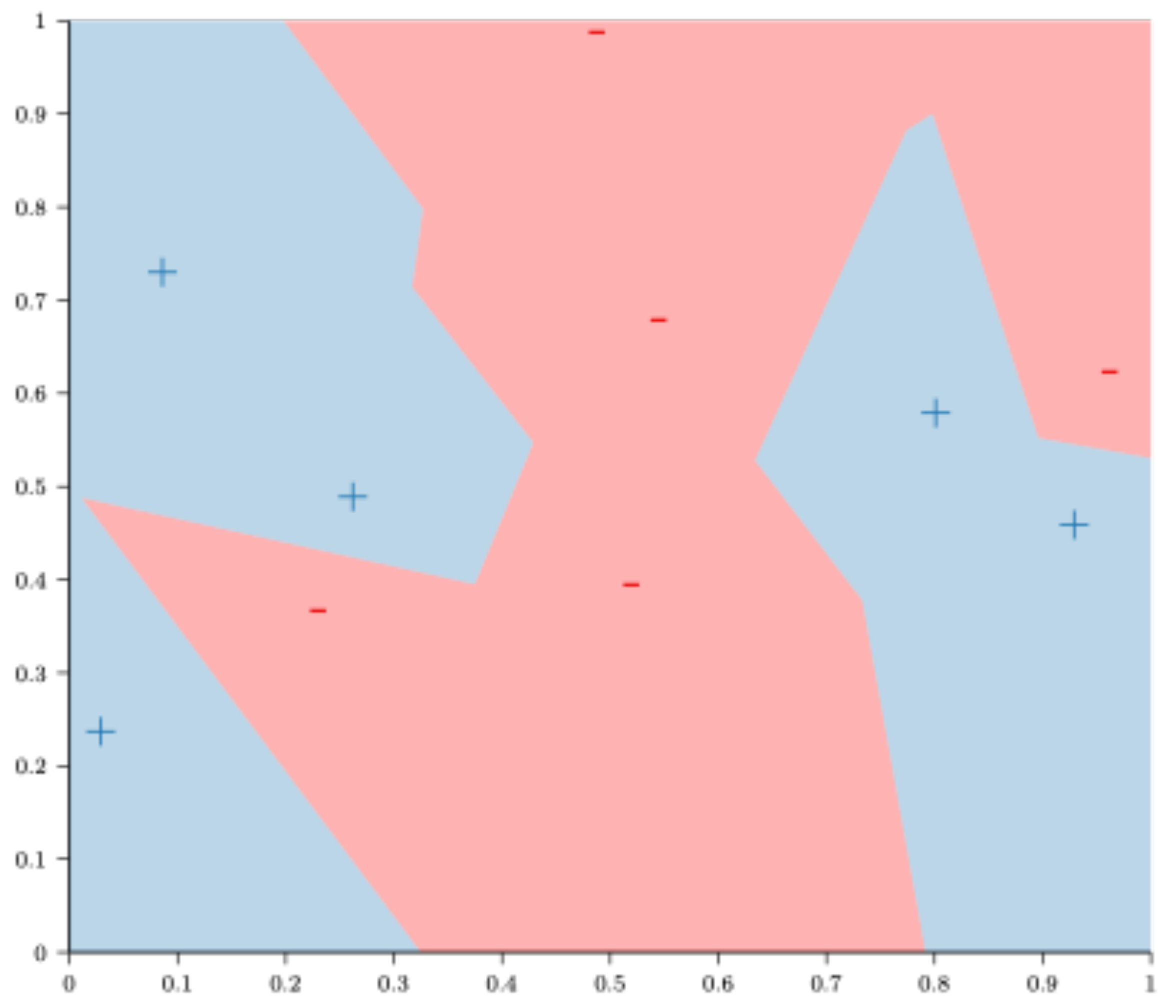


Nearest Neighbor: Example

- This is a **Voronoi diagram**
- Each **cell** contain one of our training examples
- **All points within a cell** are **closer** to that training example, than to any other training example
- **Points on the Voronoi line segments** are **equidistant** to one or more training examples



Nearest Neighbor: Example



The Nearest Neighbor Model

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

k-Nearest Neighbors: Algorithm

def set_hyperparameters(k, d)**:**
    Store k
    Store d(·, ·)

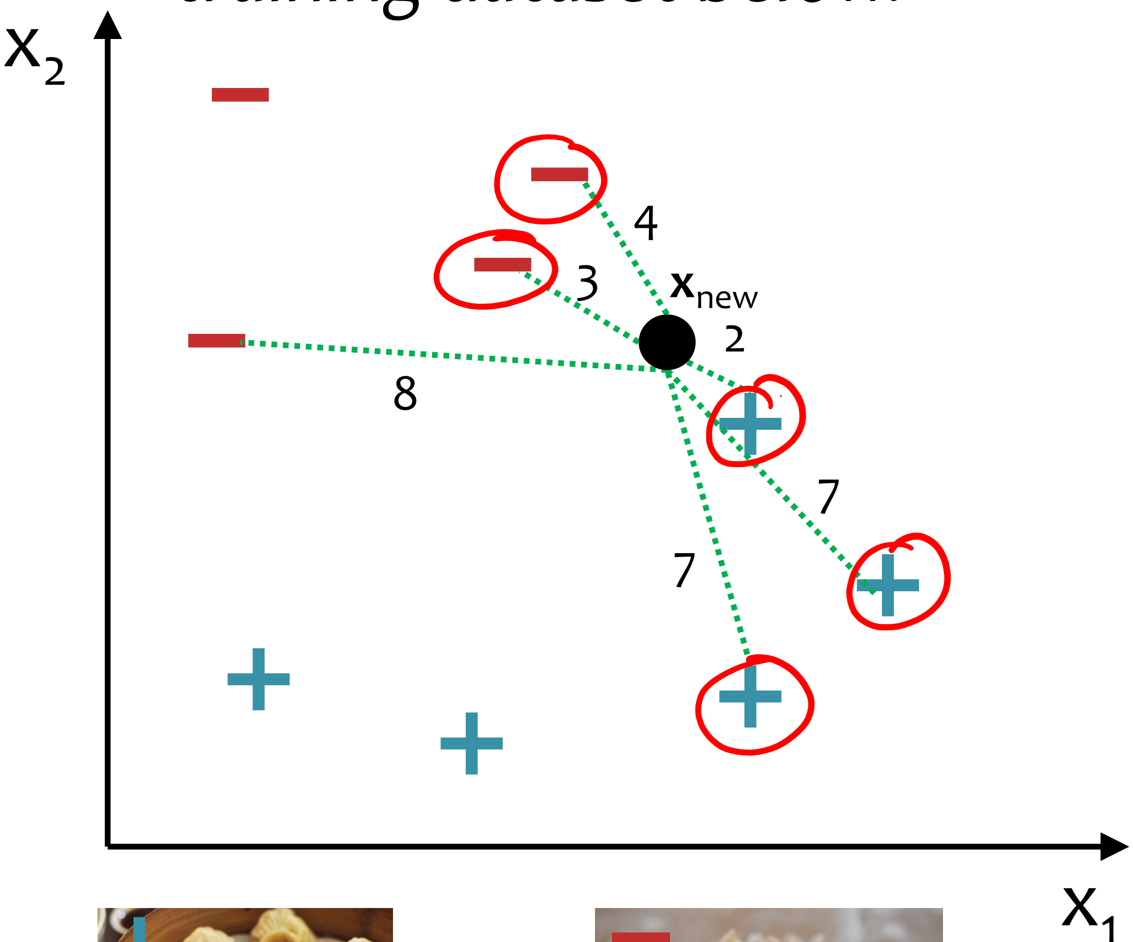
def train($\mathcal{D}$)**:**
    Store $\mathcal{D}$

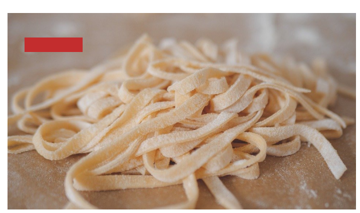
def h($\boldsymbol{x}'$)**:**
    Let S = the set of k points in $\mathcal{D}$ nearest to $\boldsymbol{x}'$
        according to distance function
        d(**u**, **v**)
    Let v = majority_vote(S)
    return v


新年
快樂
HAPPY NEW YEAR

k-Nearest Neighbors

Suppose we have the training dataset below.





How should we label the new point?

It depends on k:

if k=1, $h(\mathbf{x}_{new})$ = +1

if k=3, $h(\mathbf{x}_{new})$ = -1

if k=5, $h(\mathbf{x}_{new})$ = +1

KNN: Remarks

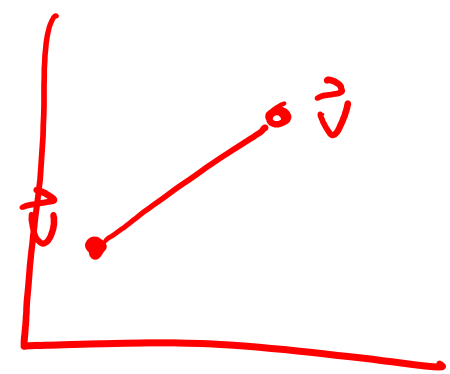
Distance Functions:

- KNN requires a **distance function**

$$d : \mathbb{R}^M \times \mathbb{R}^M \rightarrow \mathbb{R}$$

- The most common choice is **Euclidean distance**

$$d(\boldsymbol{u}, \boldsymbol{v}) = \sqrt{\sum_{m=1}^{M} (u_m - v_m)^2}$$



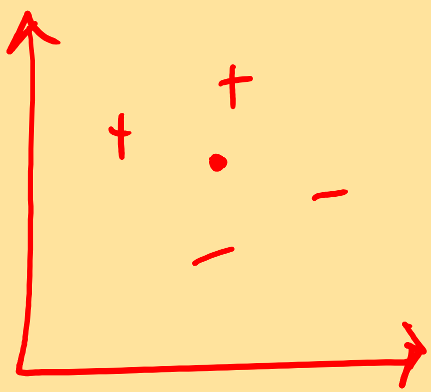
- But there are other choices (e.g. **Manhattan distance**)

$$d(\boldsymbol{u}, \boldsymbol{v}) = \sum_{m=1}^{M} |u_m - v_m|$$

KNN: Remarks

In-Class Exercises

How can we handle ties for even values of k?



$k=4$

Answer(s) Here:

- look at avg. distances to pluses/minuses respectively (distance-weighted KNN)
- increment/decrement k by 1
- randomly

KNN: Remarks

In-Class Exercises

How can we handle ties for even values of k?

Answer(s) Here:

- Consider another point
- Remove farthest of k points
- Weight votes by distance
- Consider another distance metric

KNN: Inductive Bias

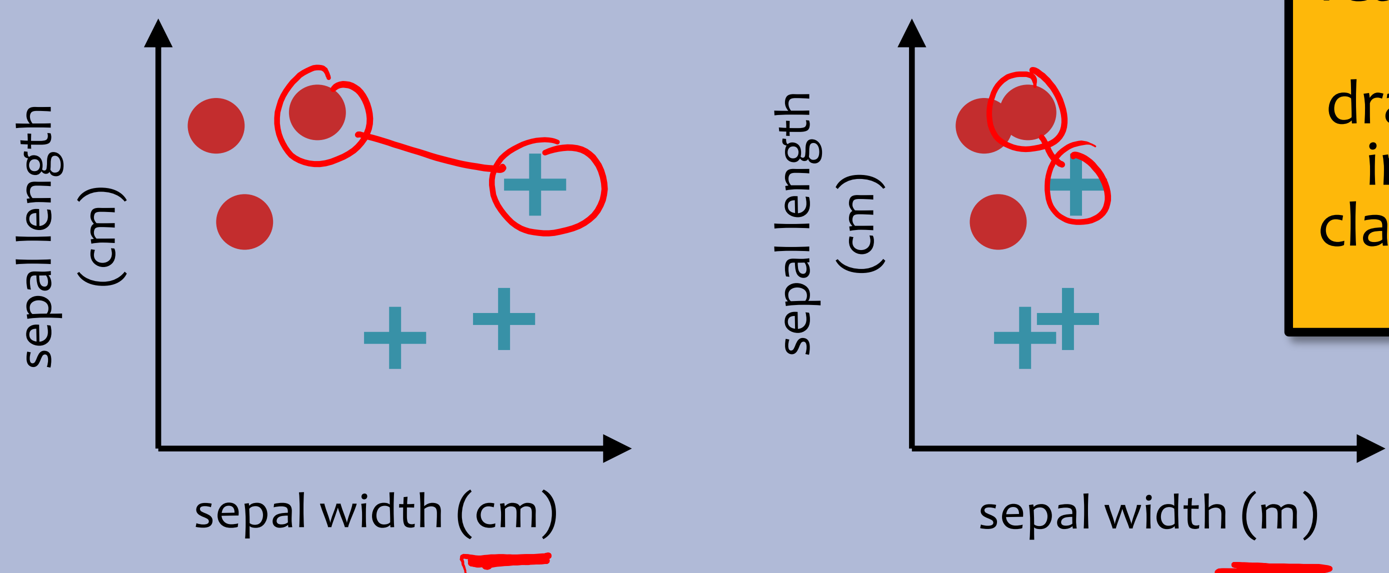
In-Class Exercise What is the inductive bias of KNN?

KNN: Inductive Bias

In-Class Exercise What is the inductive bias of KNN?

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

Example: two features for KNN



big problem: feature scale can dramatically influence classification results!

KNN: Computational Efficiency

- Suppose we have N training examples and each one has M features
- Computational complexity when 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)

for $i = 1, \ldots, N$:
for $m = 1, \ldots, M$:

$d(x', x^{(i)})$

KNN: Theoretical Guarantees

Cover & Hart (1967)

Let h(x) be a Nearest Neighbor (k=1) binary classifier. As the number of training examples N goes to infinity…

$$\text{error}_{\text{true}}(h) < 2 \times \text{Bayes Error Rate}$$

"In this sense, it may be said that half the classification information in an infinite sample set is contained in the nearest neighbor."

very informally, Bayes Error Rate can be thought of as: '*the best you could possibly do*'

Decision Boundary Example

Dataset: Outputs {+,-}; Features x_1 and x_2

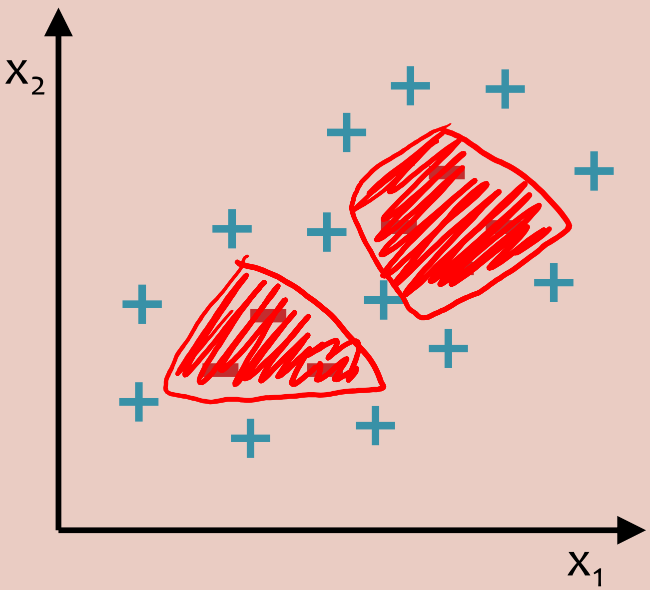
A = Yes B = No C = toxic

In-Class Exercise

Question: Q1

A. Can a **k-Nearest Neighbor classifier with k=1** achieve **zero training error** on this dataset?

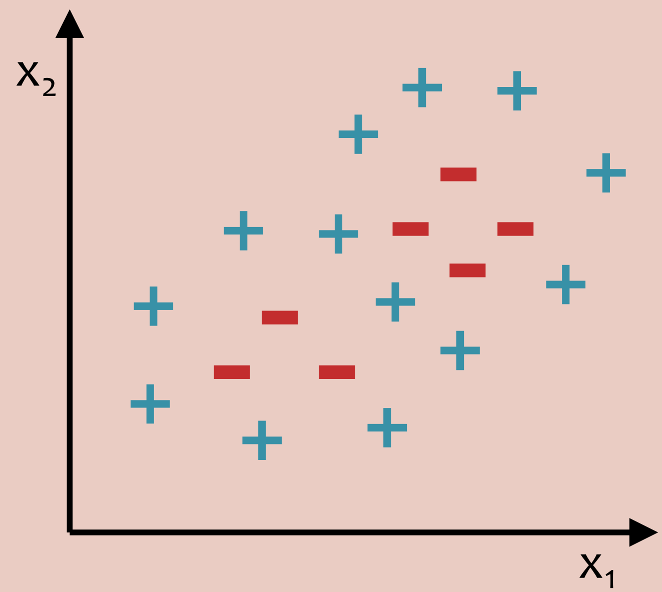
B. **If 'Yes'**, draw the learned decision boundary. **If 'No'**, why not?



Question: Q2

A. Can a **Decision Tree classifier** achieve **zero training error** on this dataset?

B. **If 'Yes'**, draw the learned decision boundary. **If 'No'**, why not?



Decision Boundary Example

Whiteboard:

- Decision Tree boundary with continuous features (saving this for a short video)

KNN ON FISHER IRIS DATA


sepal
petal

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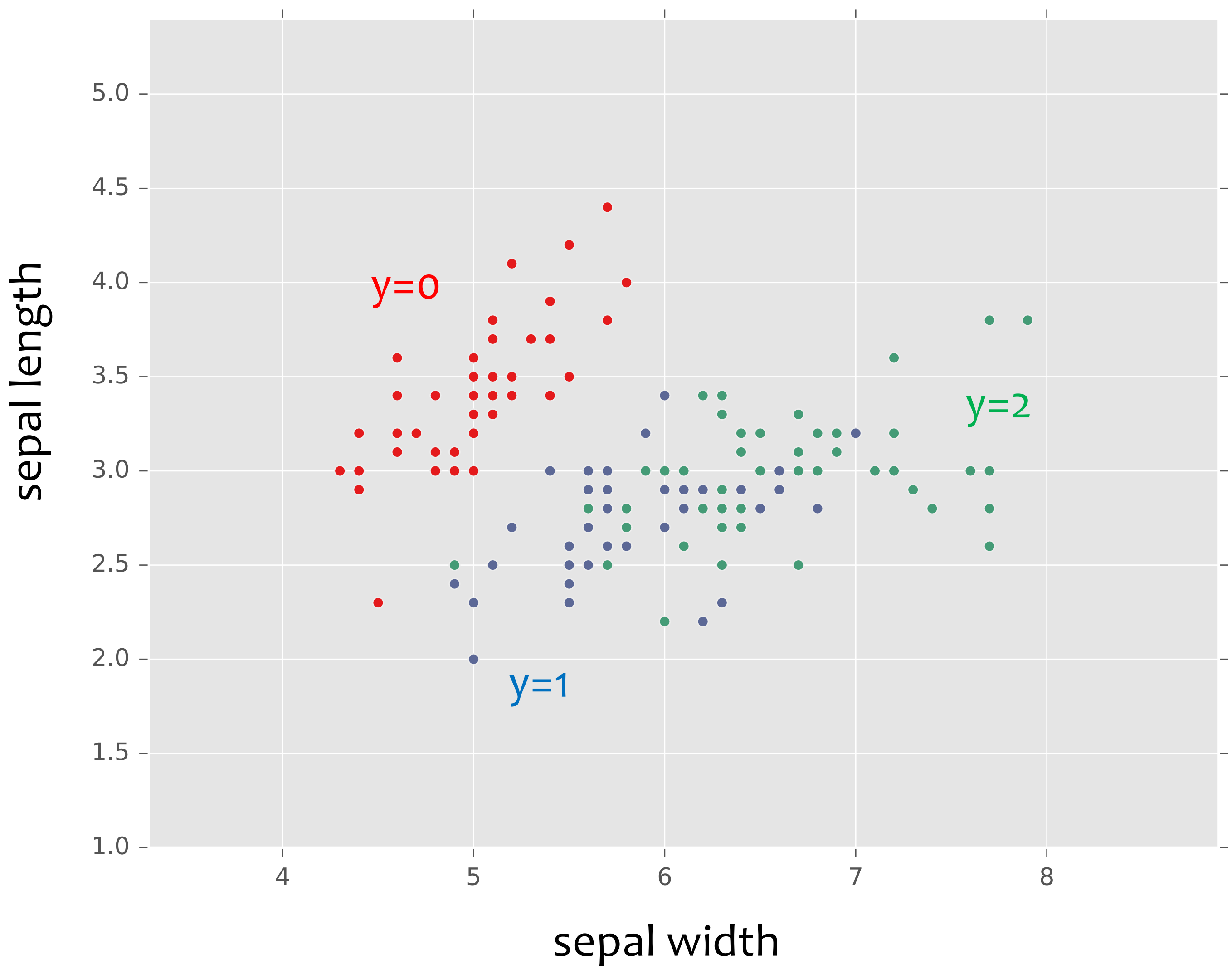
0	5.3	3.7
1	4.9	2.4
1	5.7	2.8
1	6.3	3.3
1	6.7	3.0

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

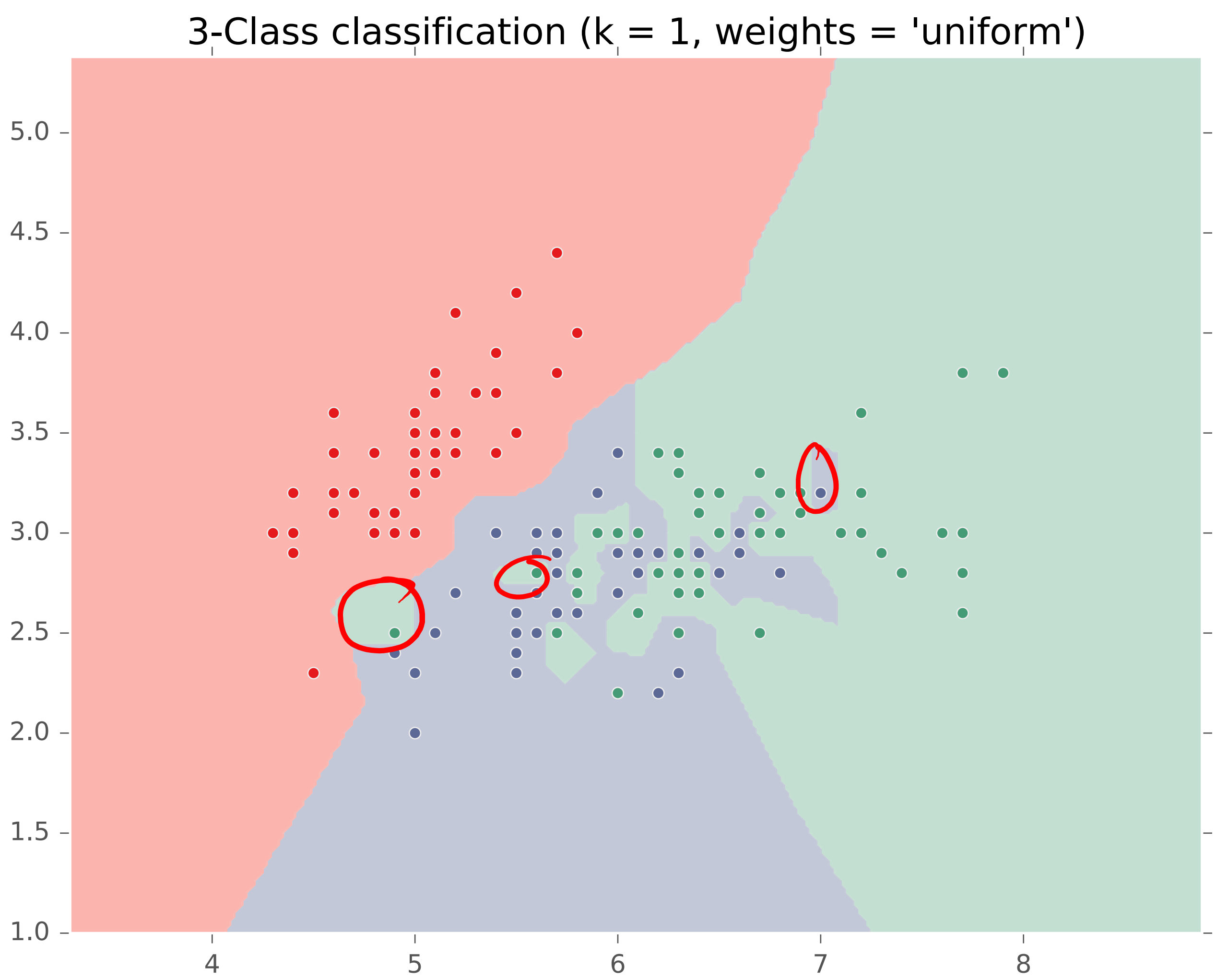
Full dataset: https://en.wikipedia.org/wiki/Iris_flower_data_set

KNN on Fisher Iris Data

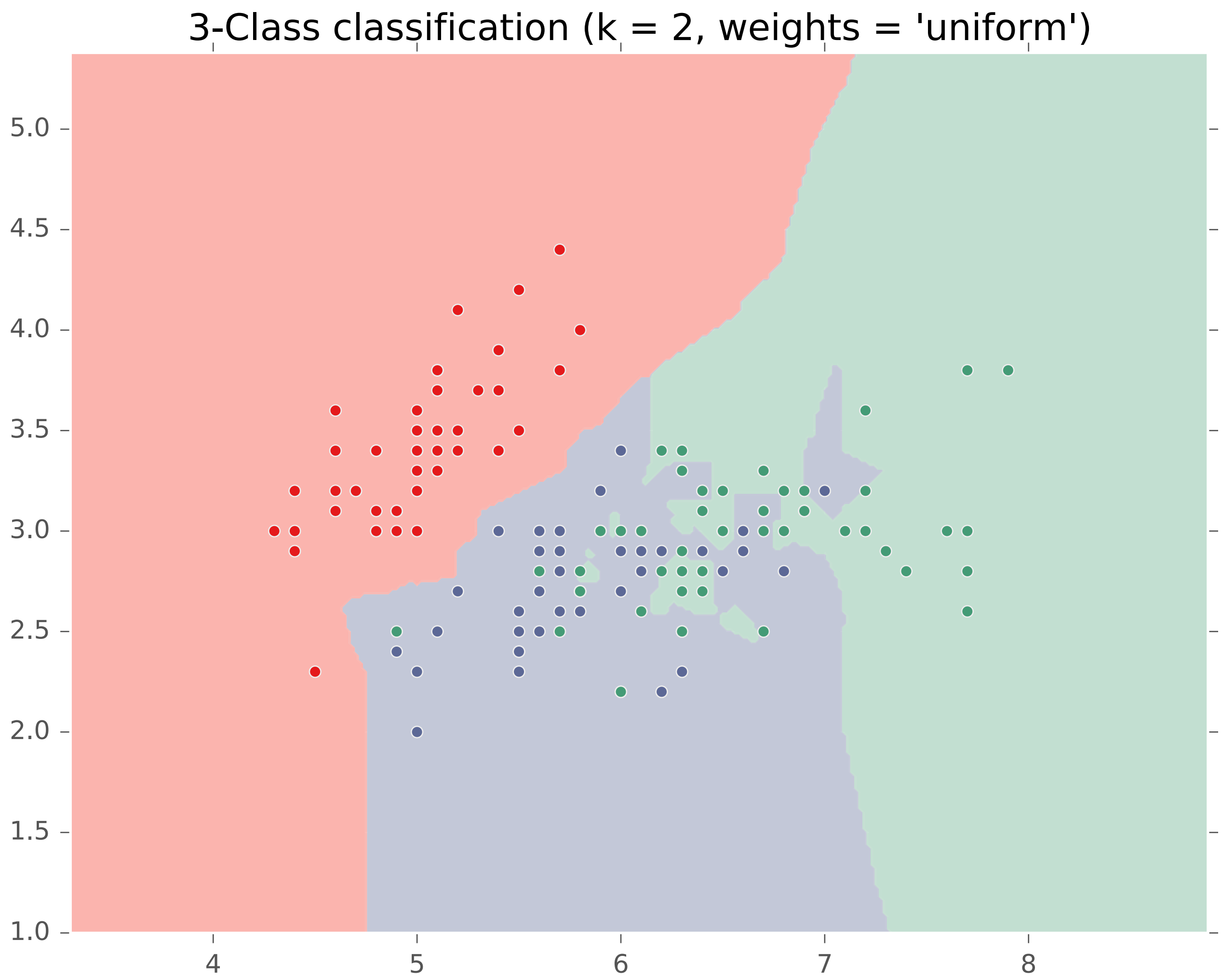


KNN on Fisher Iris Data

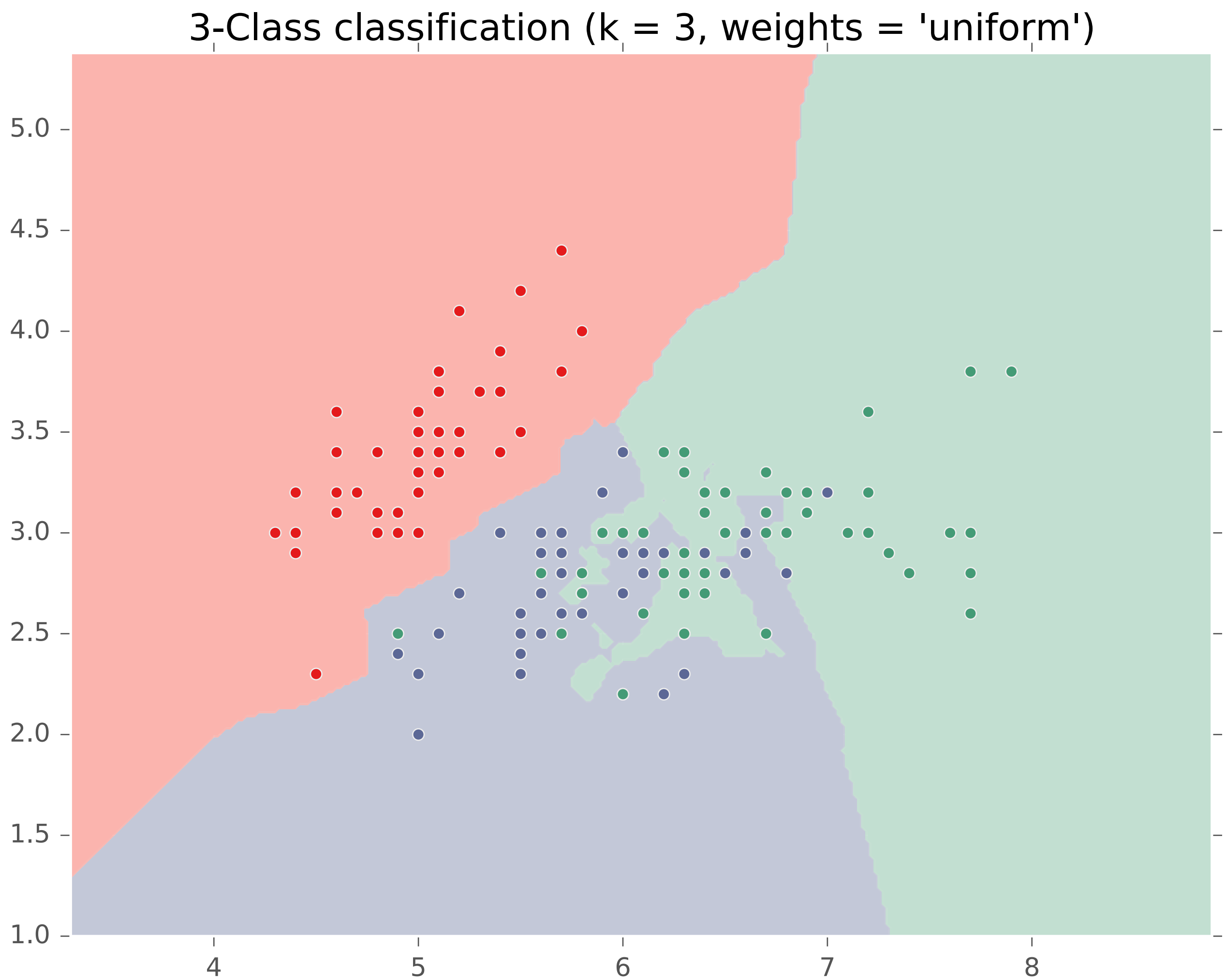
Special Case: Nearest Neighbor



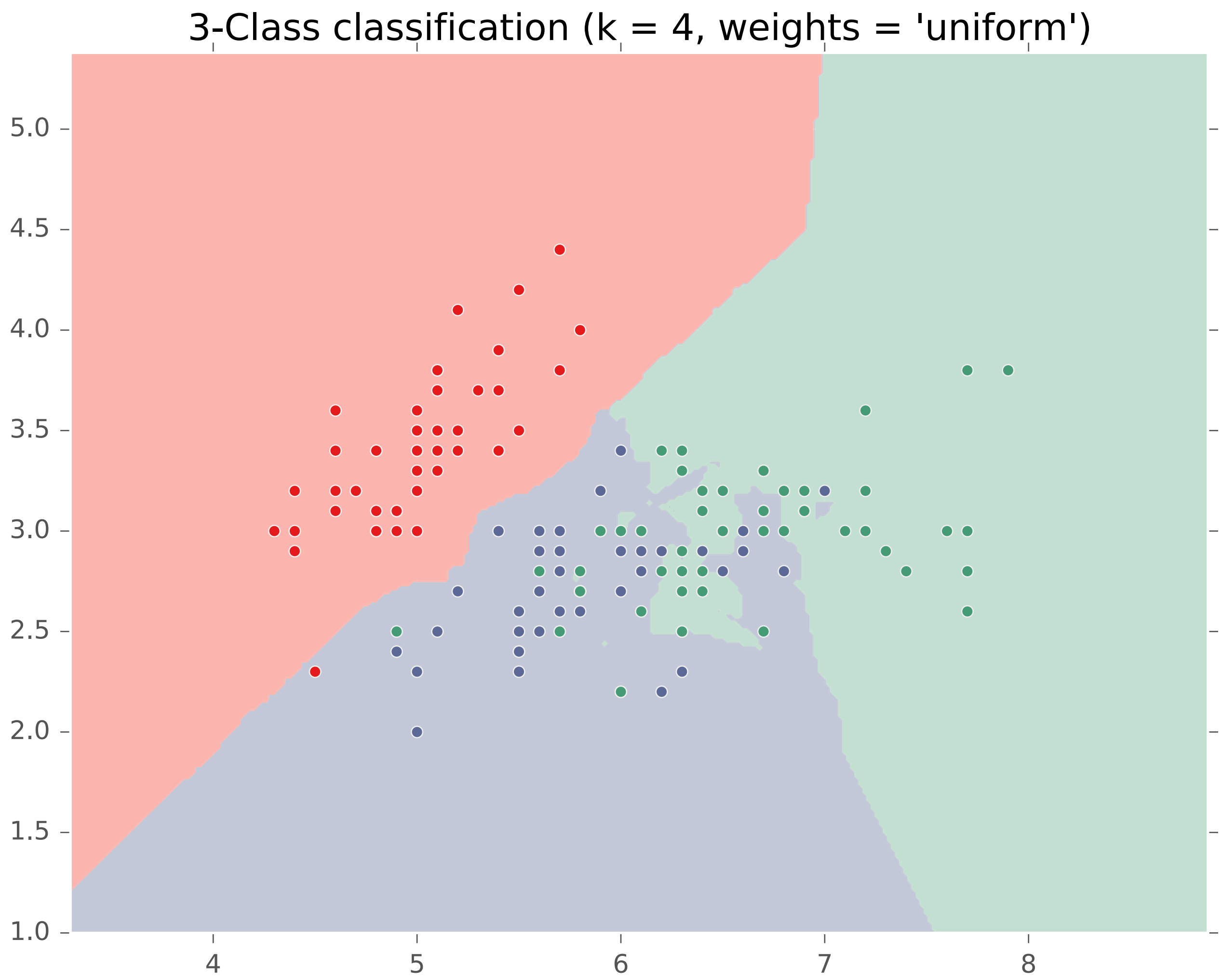
KNN on Fisher Iris Data



KNN on Fisher Iris Data



KNN on Fisher Iris Data



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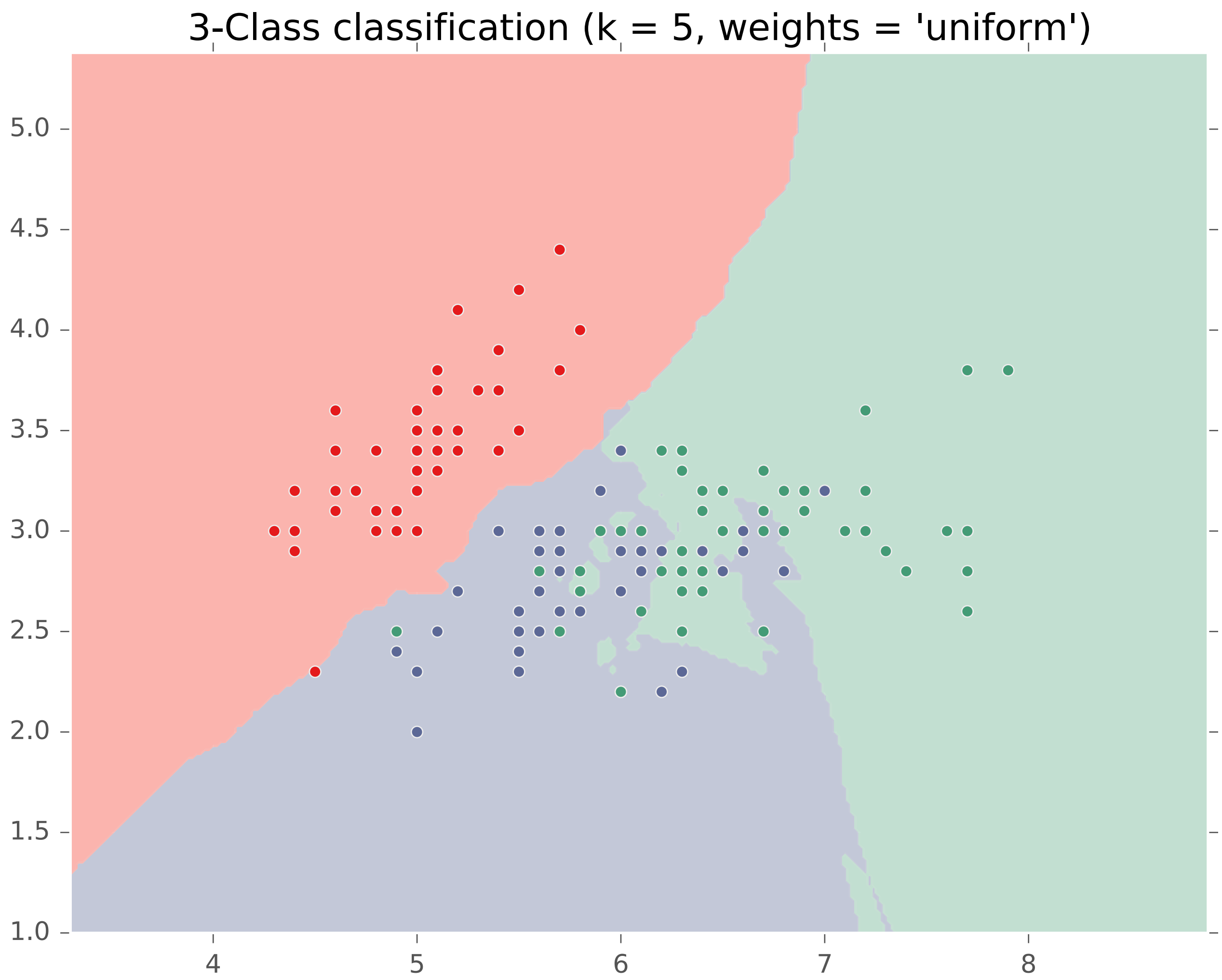

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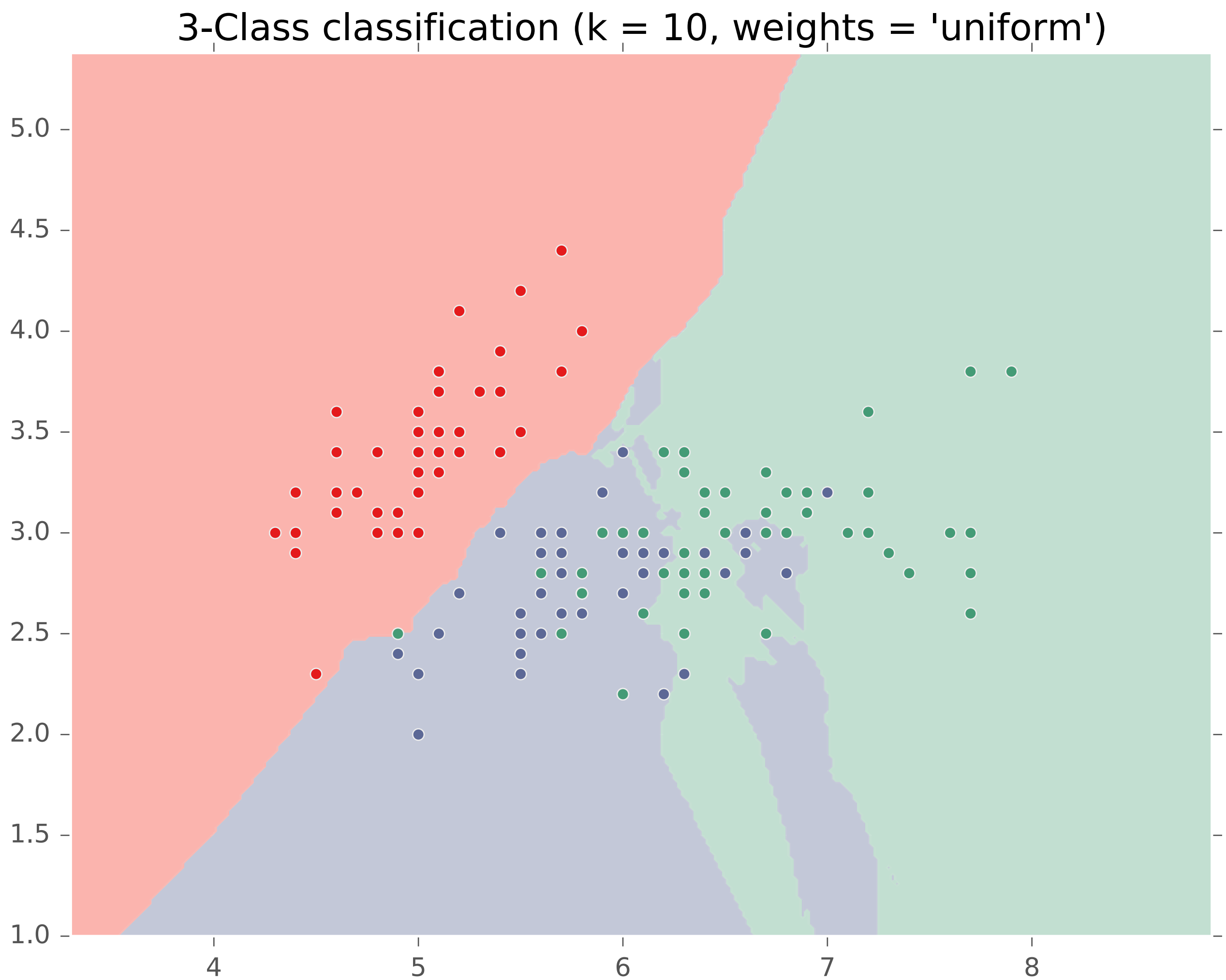

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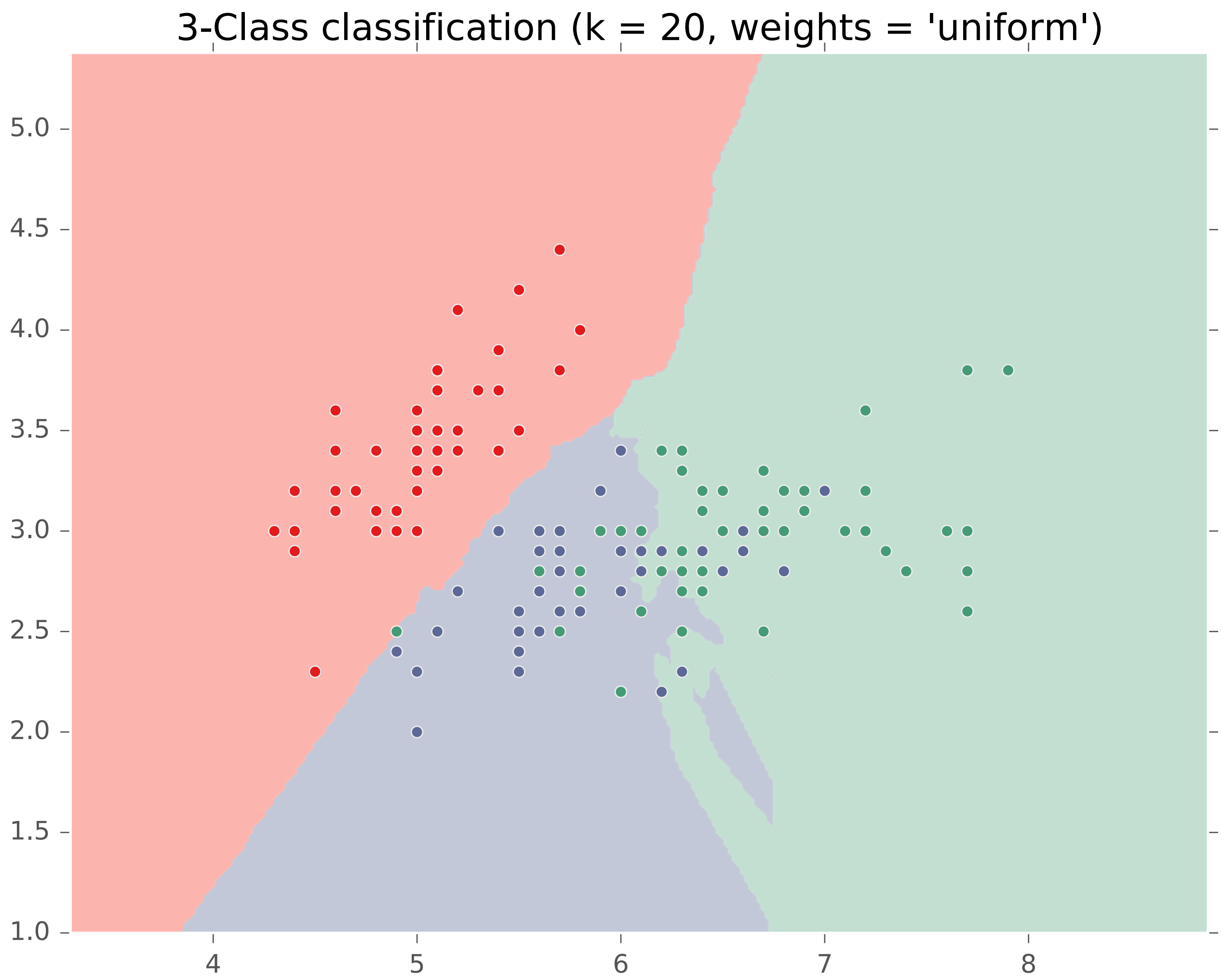

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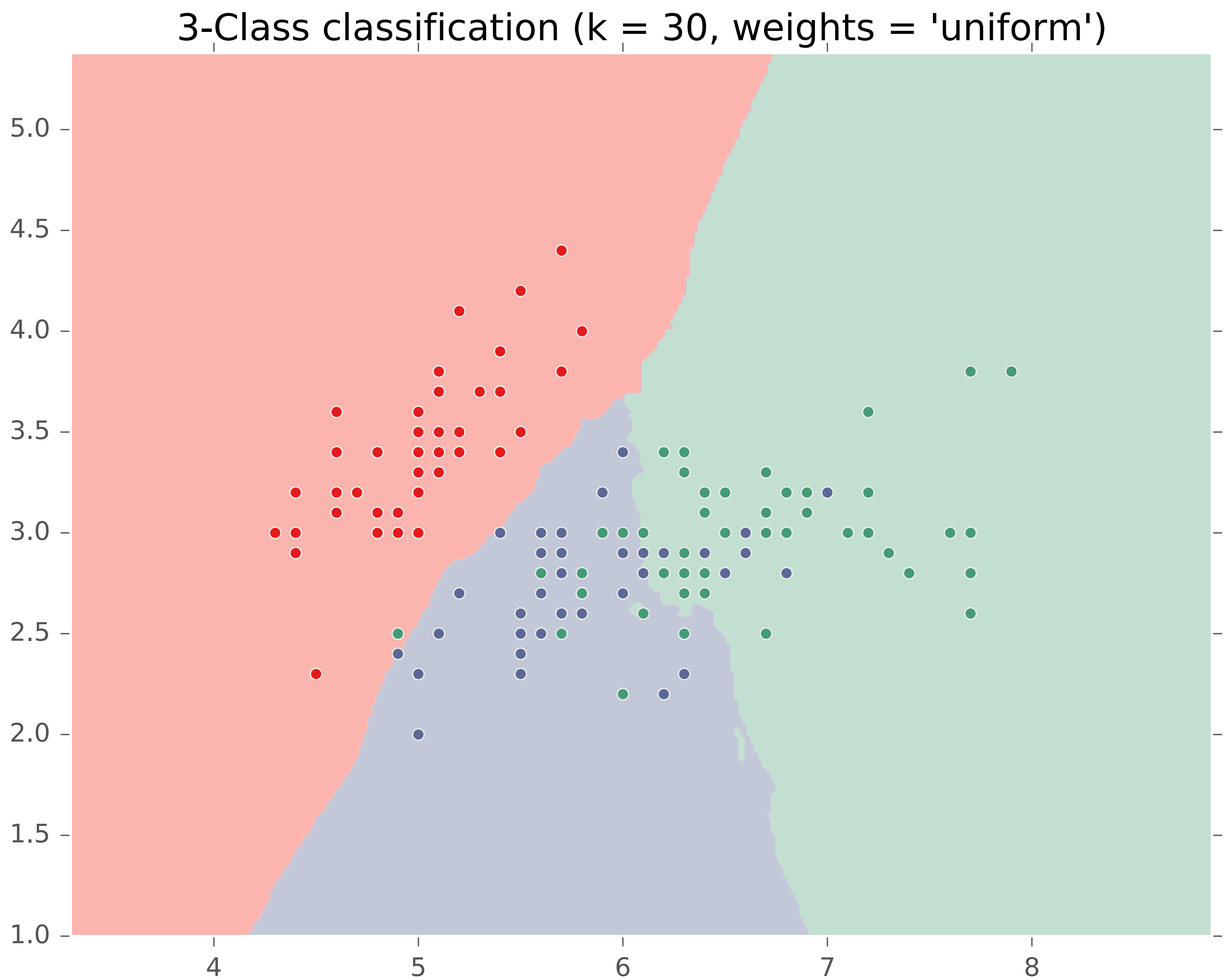

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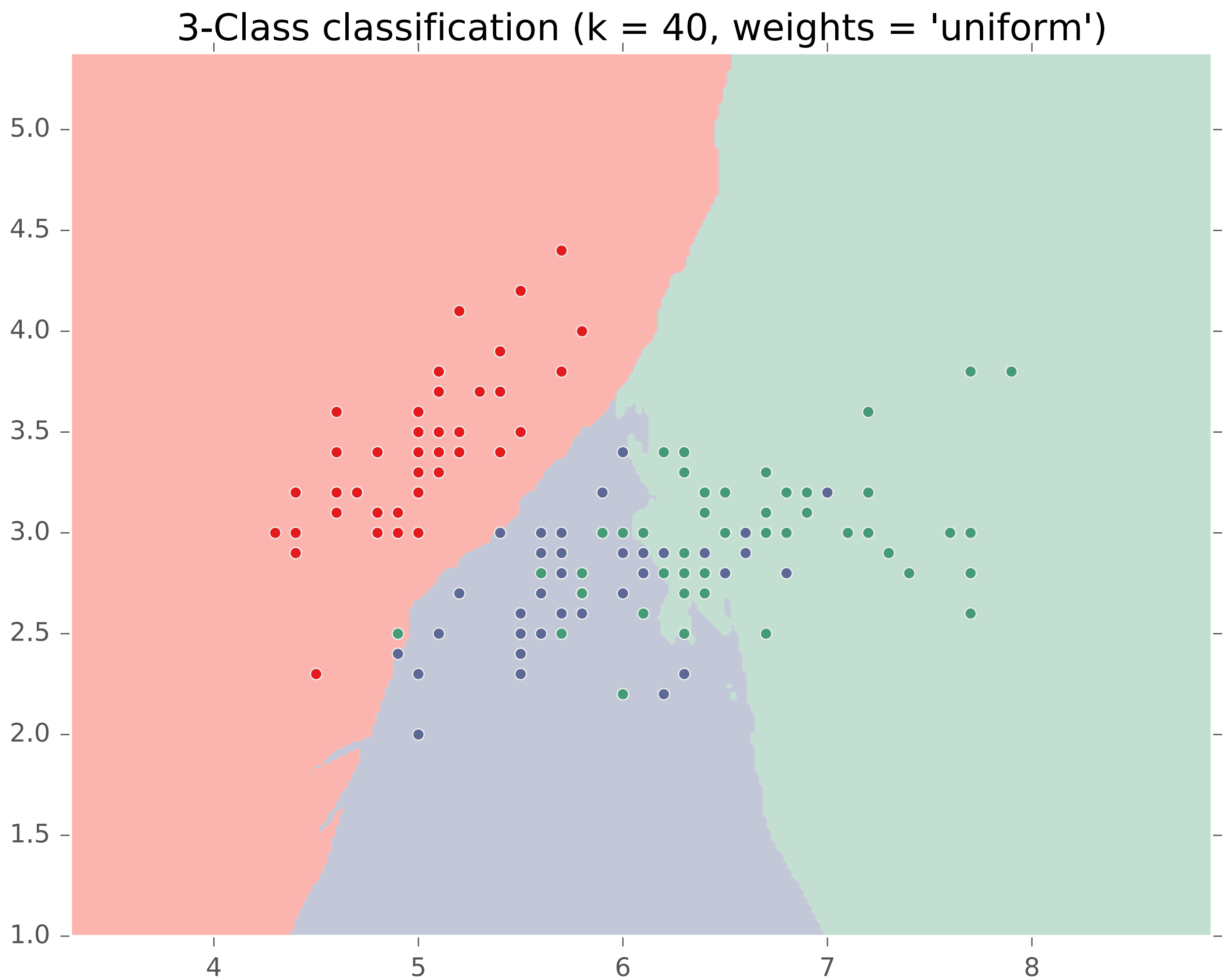

KNN on Fisher Iris Data

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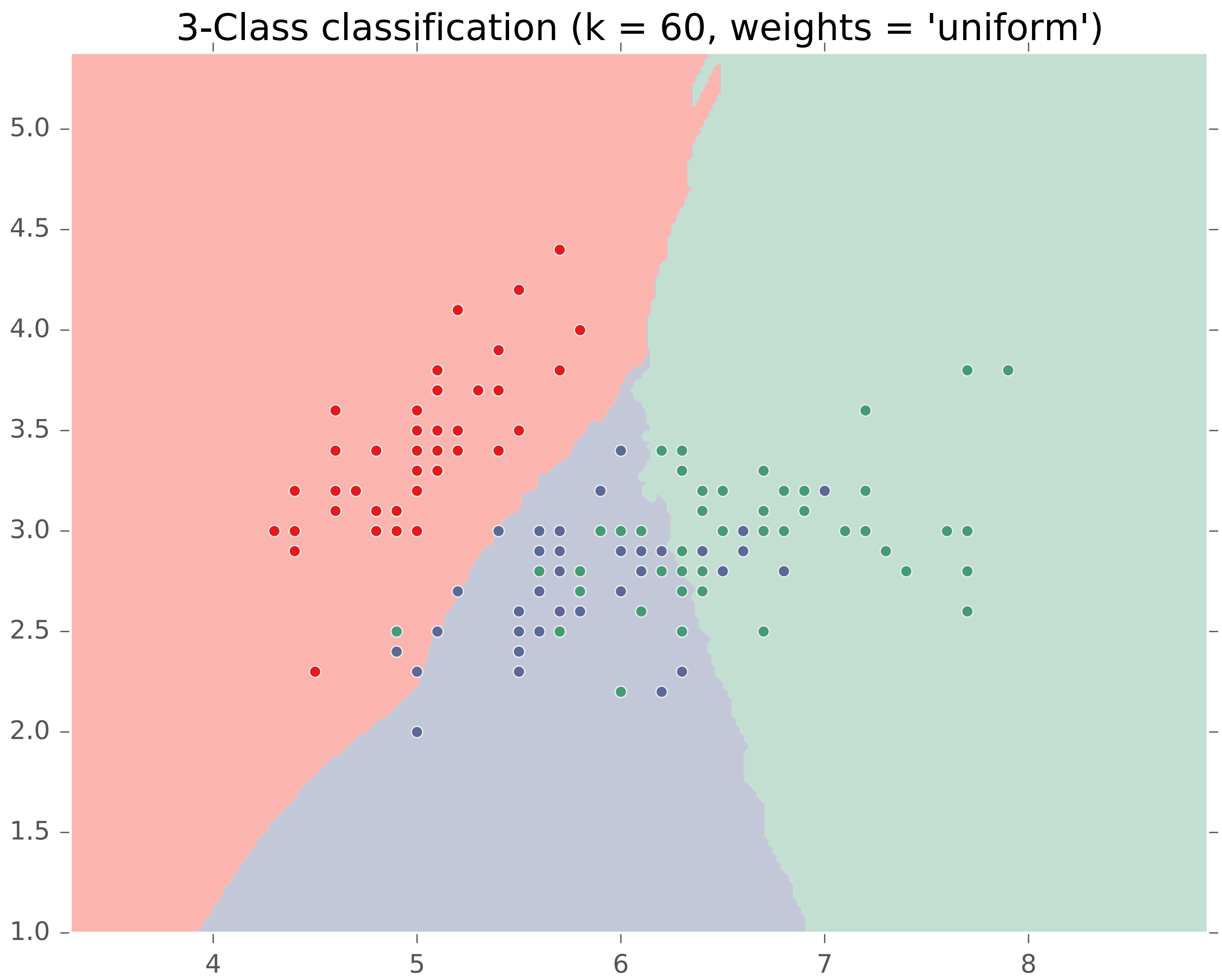
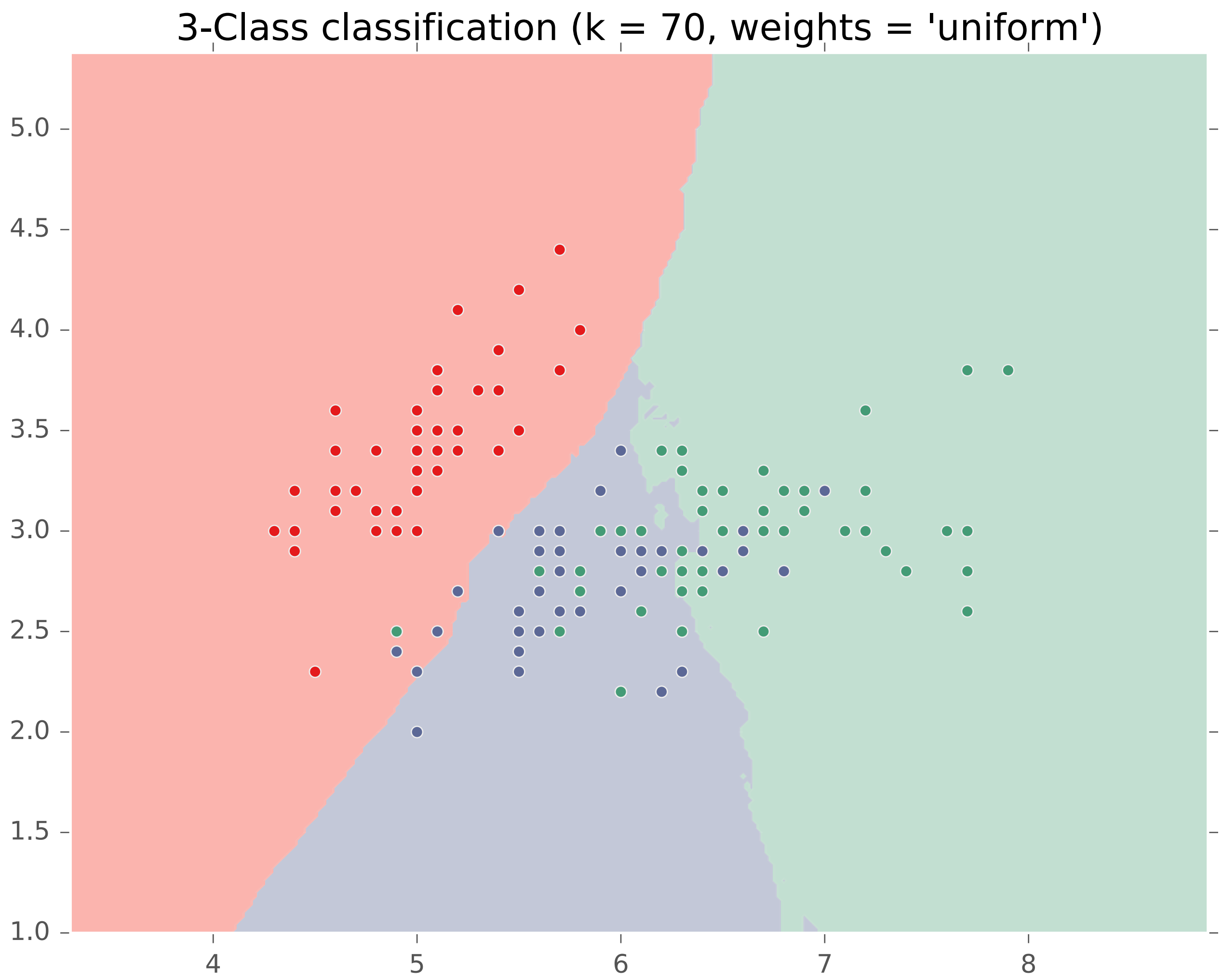


KNN on Fisher Iris Data



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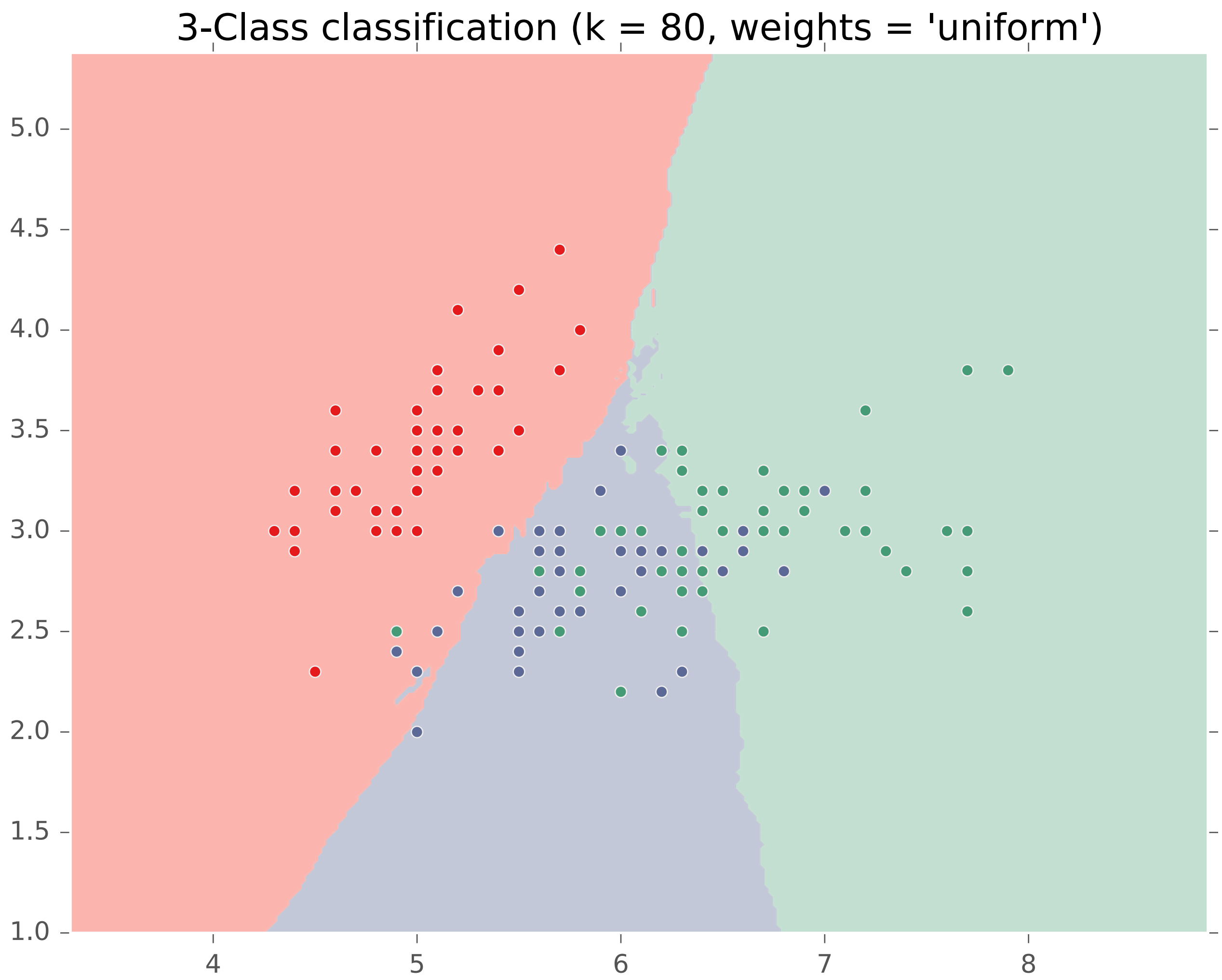

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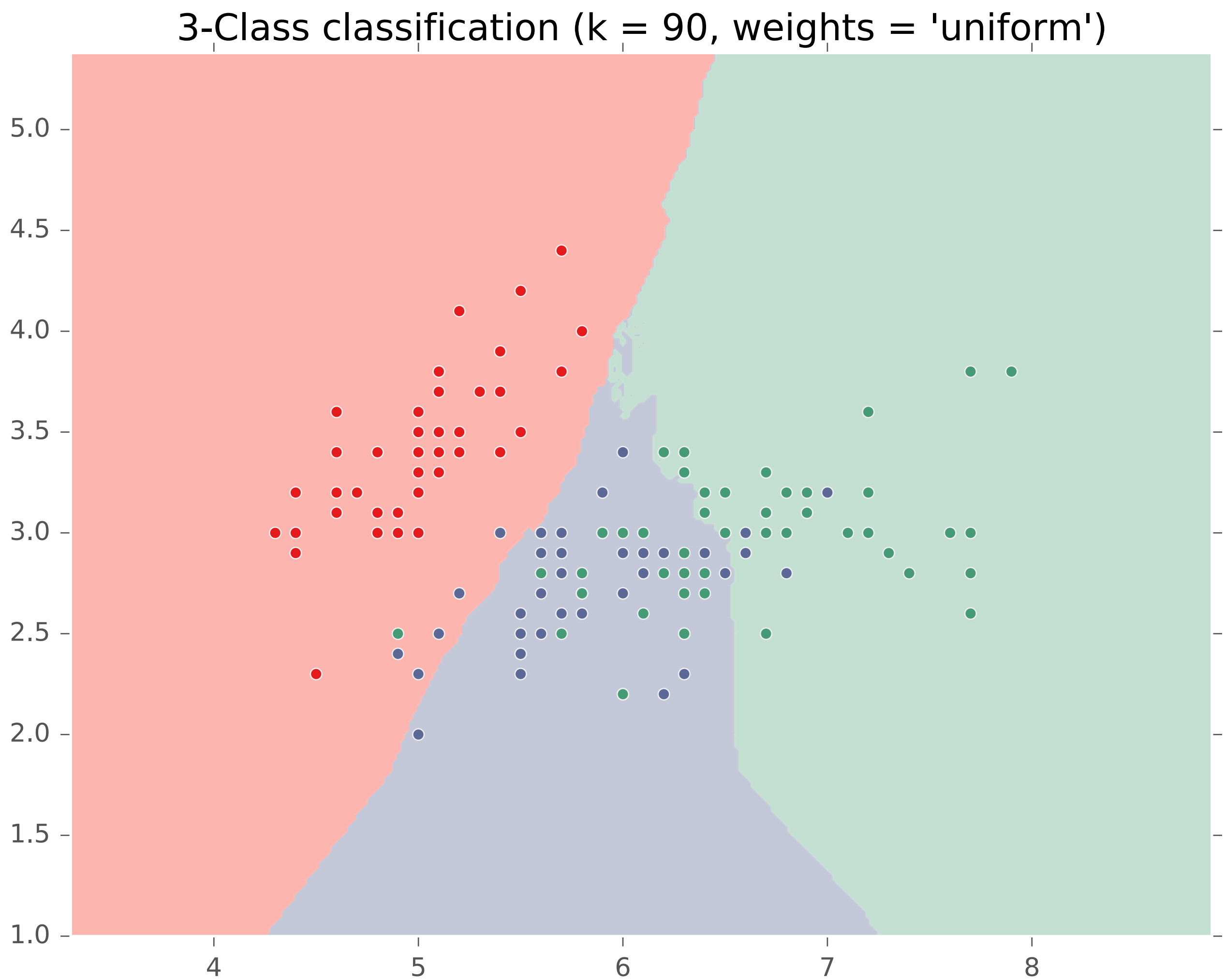

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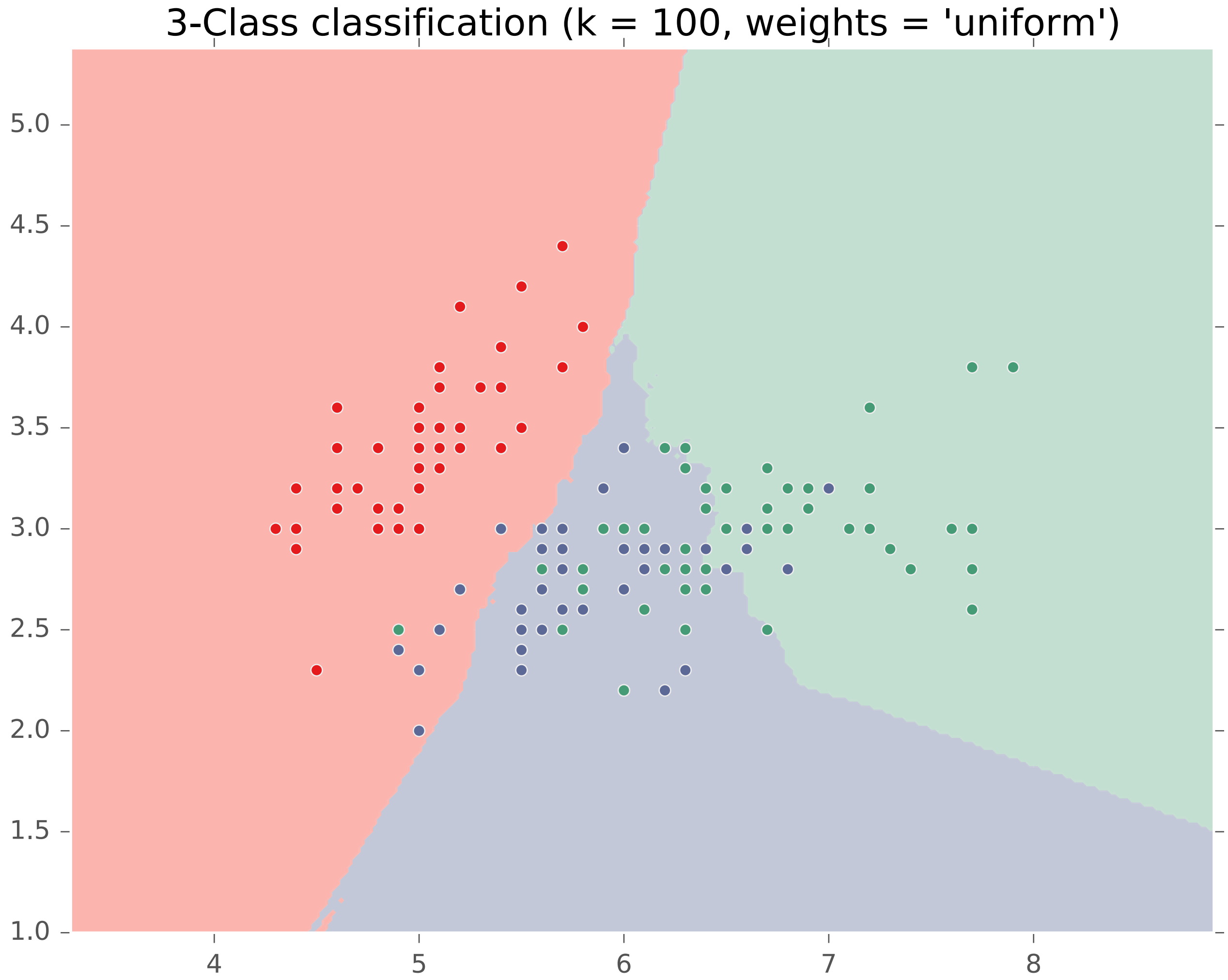

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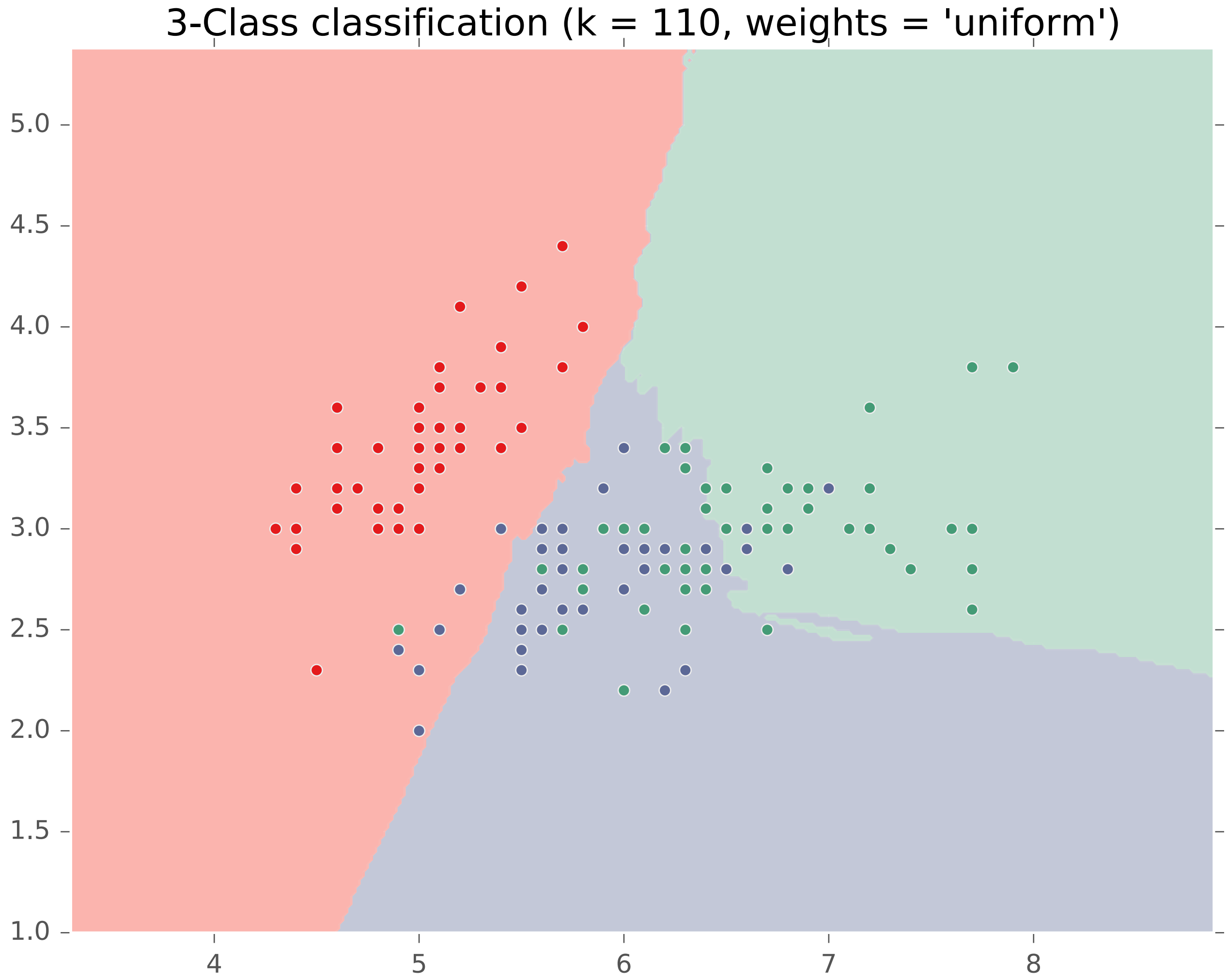
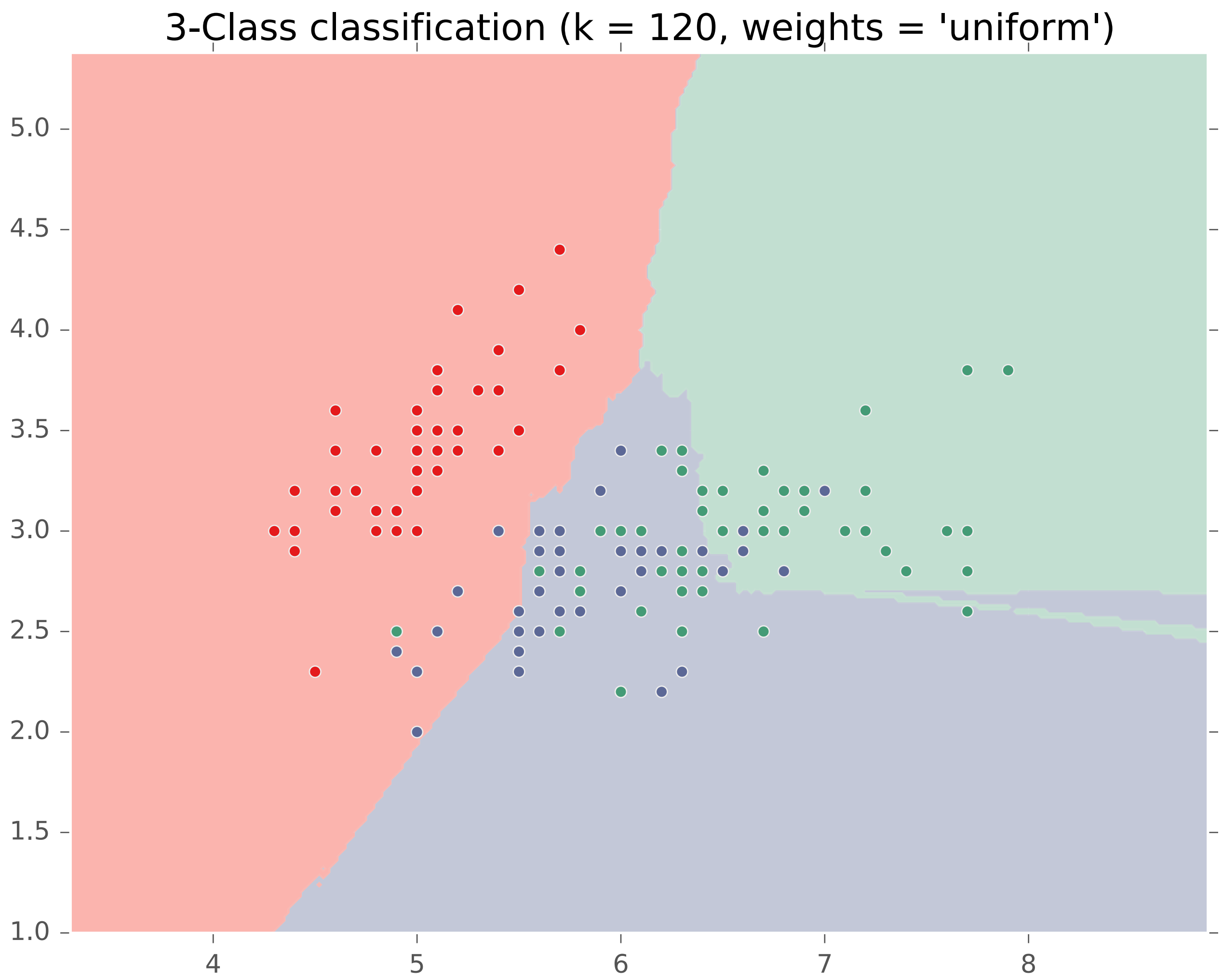
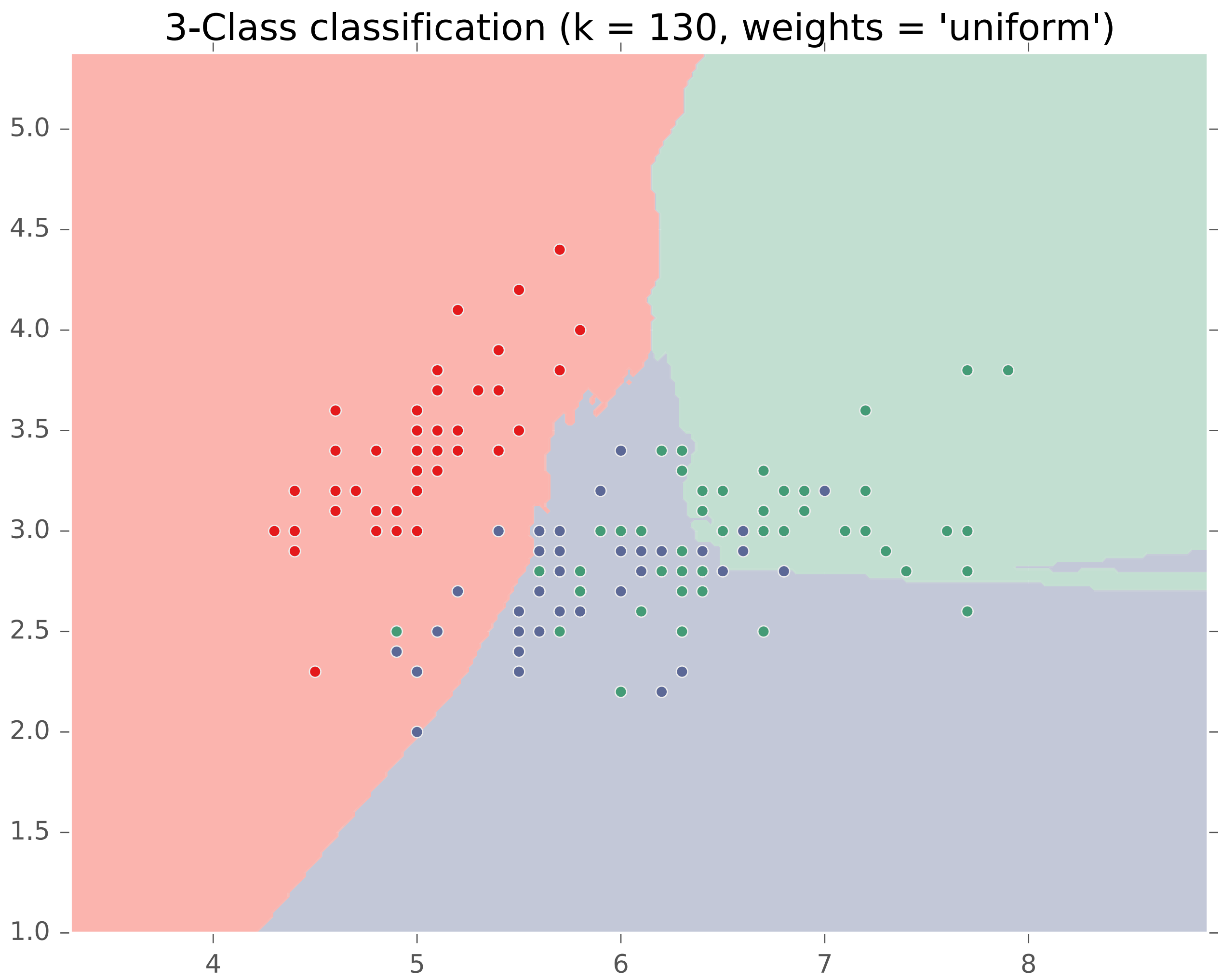


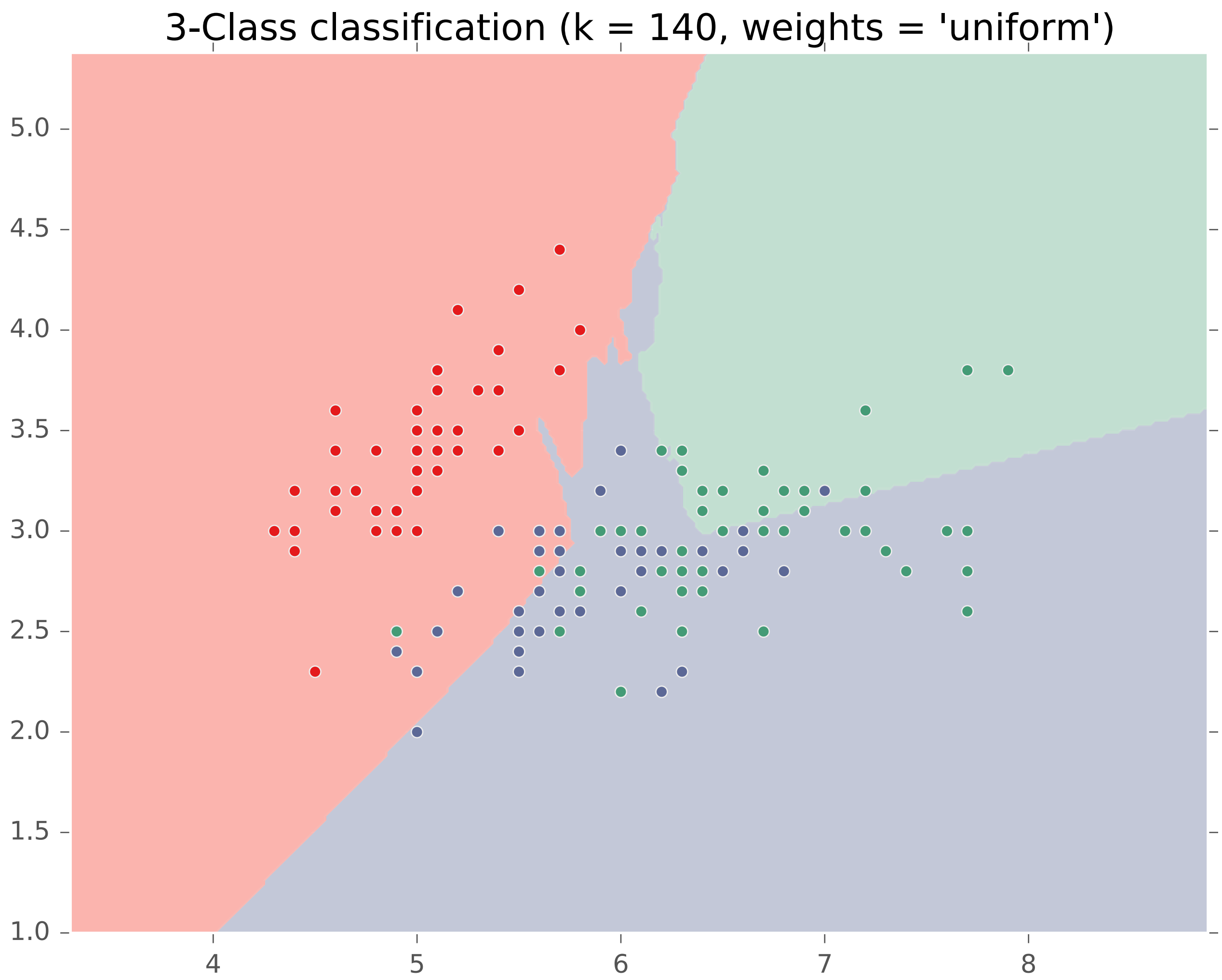
KNN on Fisher Iris Data



KNN on Fisher Iris Data

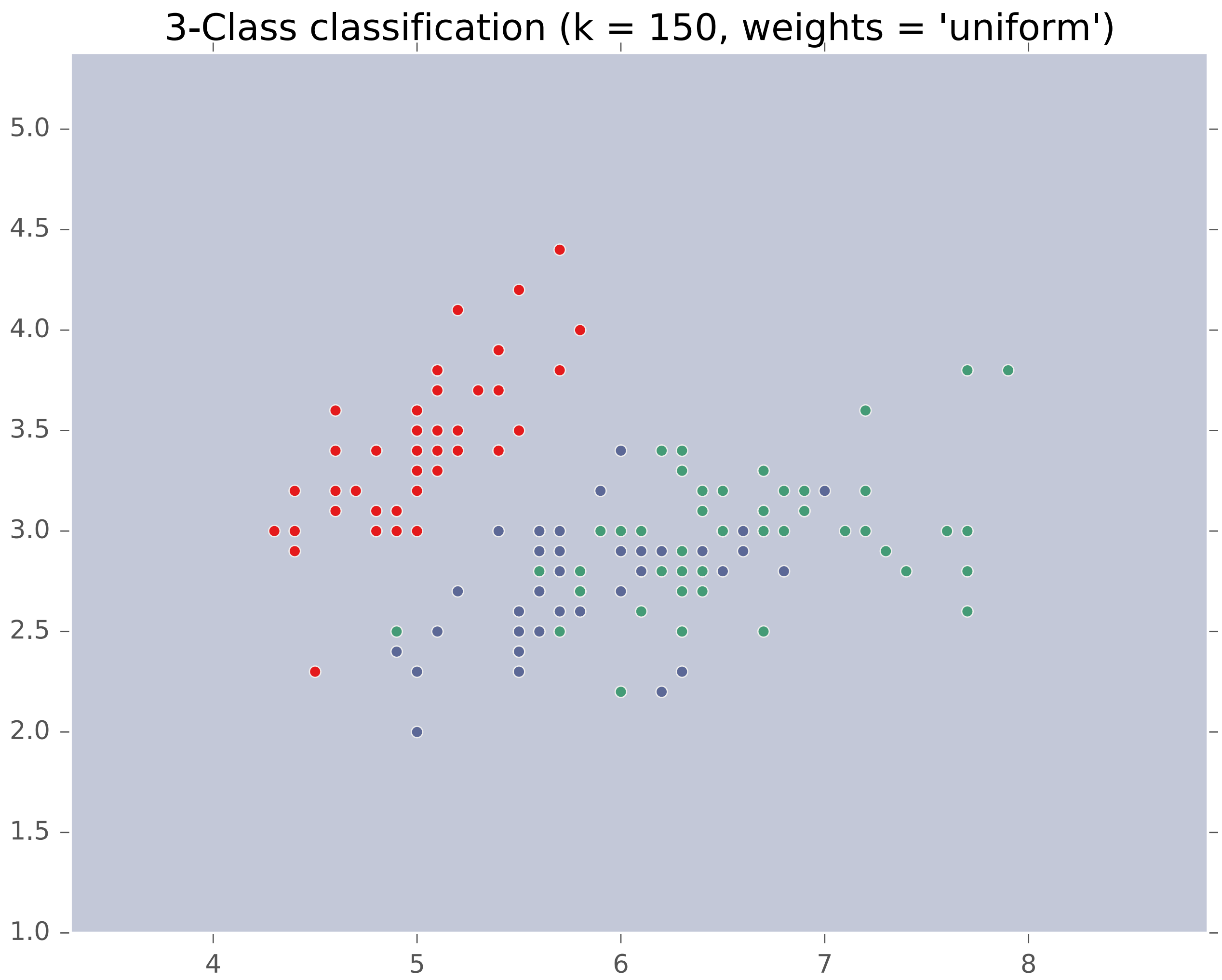


KNN on Fisher Iris Data



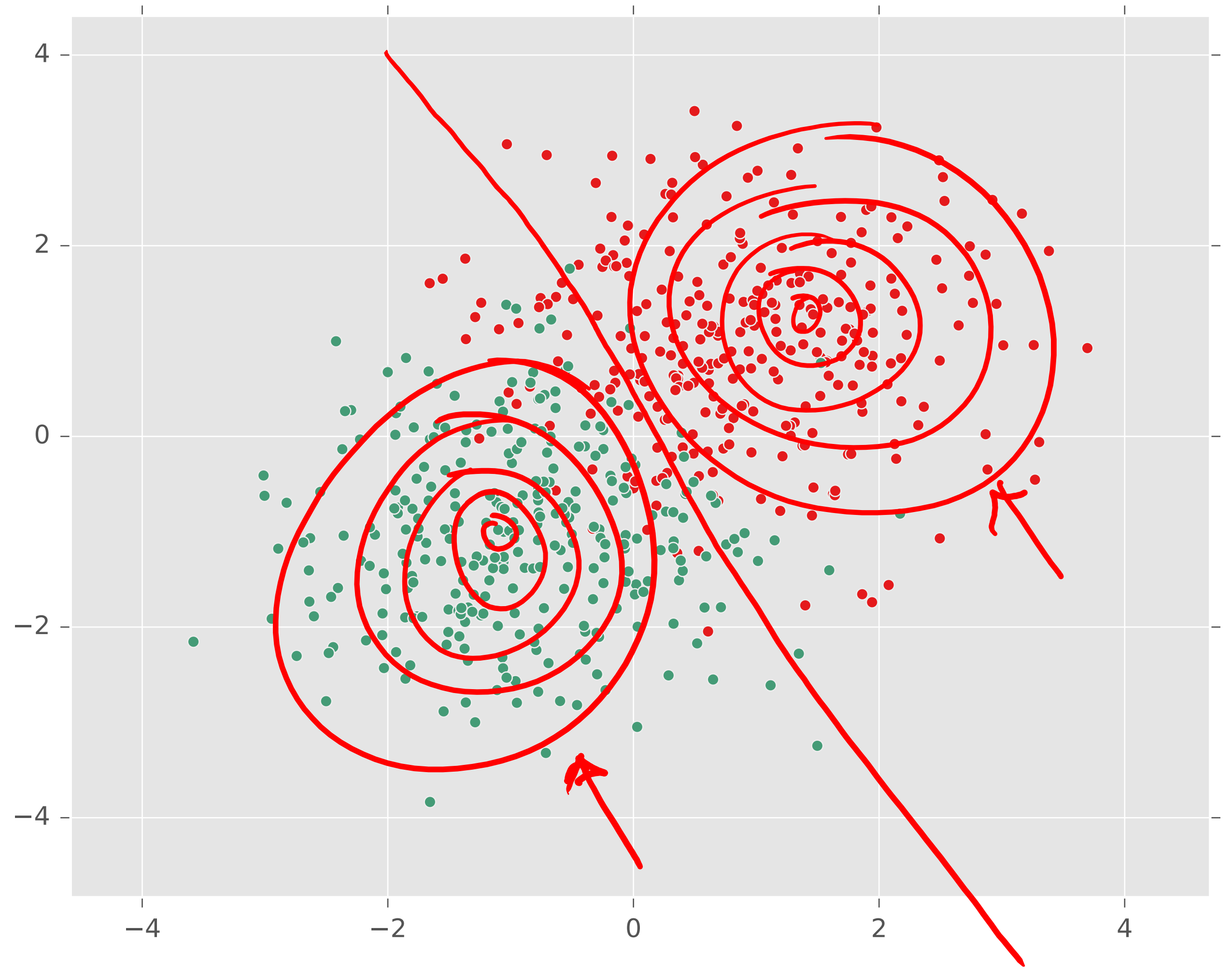
KNN on Fisher Iris Data

Special Case: Majority Vote

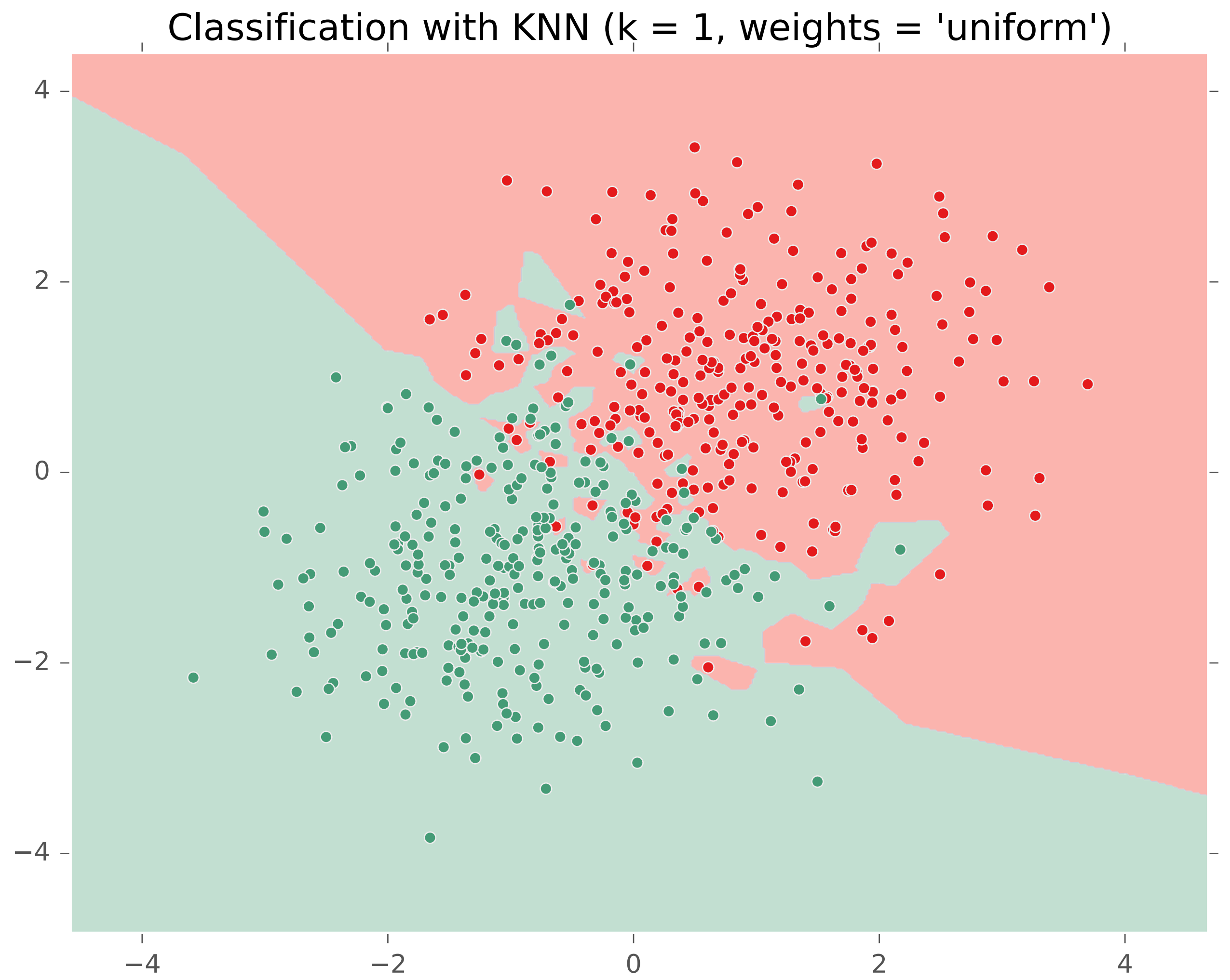


KNN ON GAUSSIAN DATA

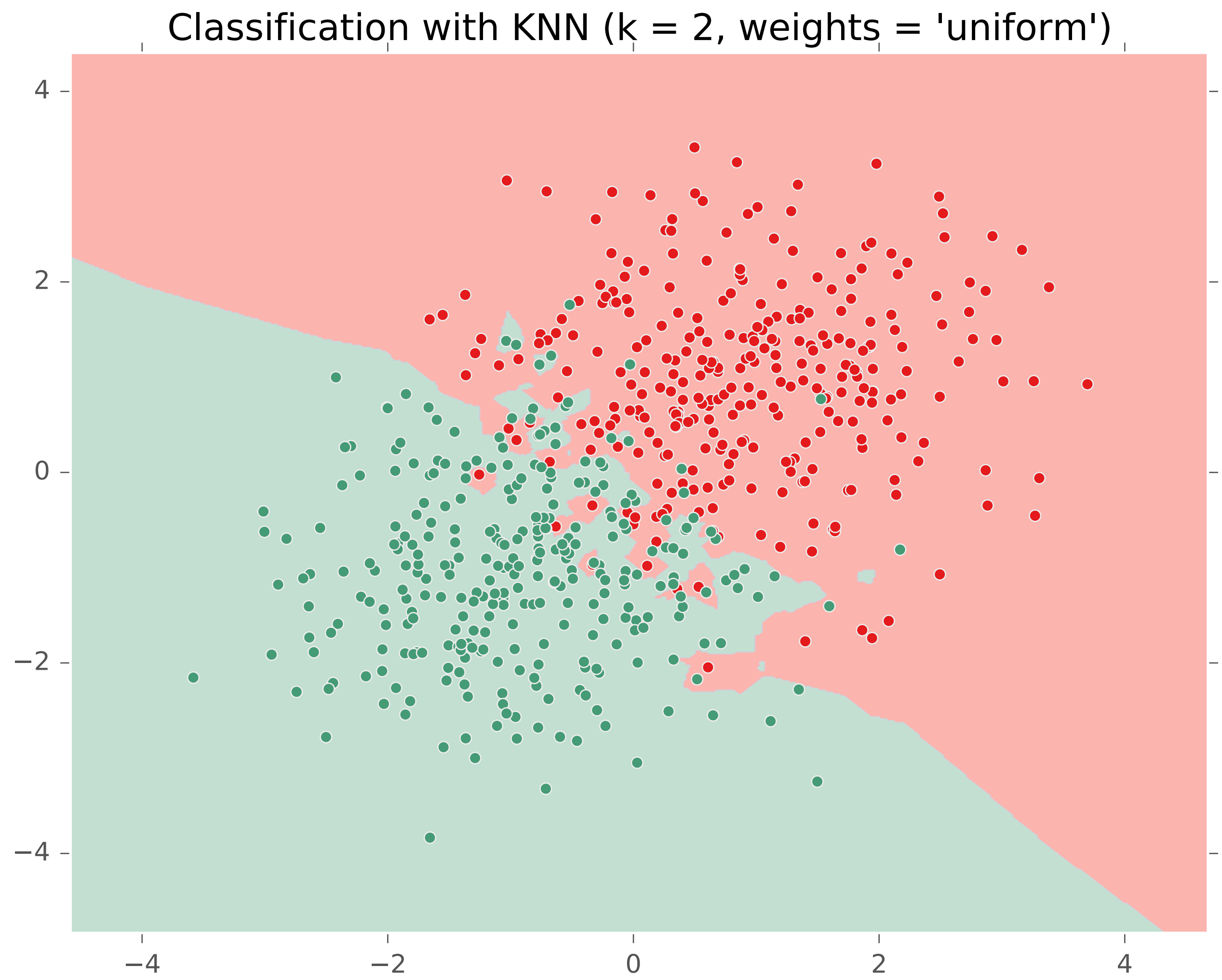
KNN on Gaussian Data



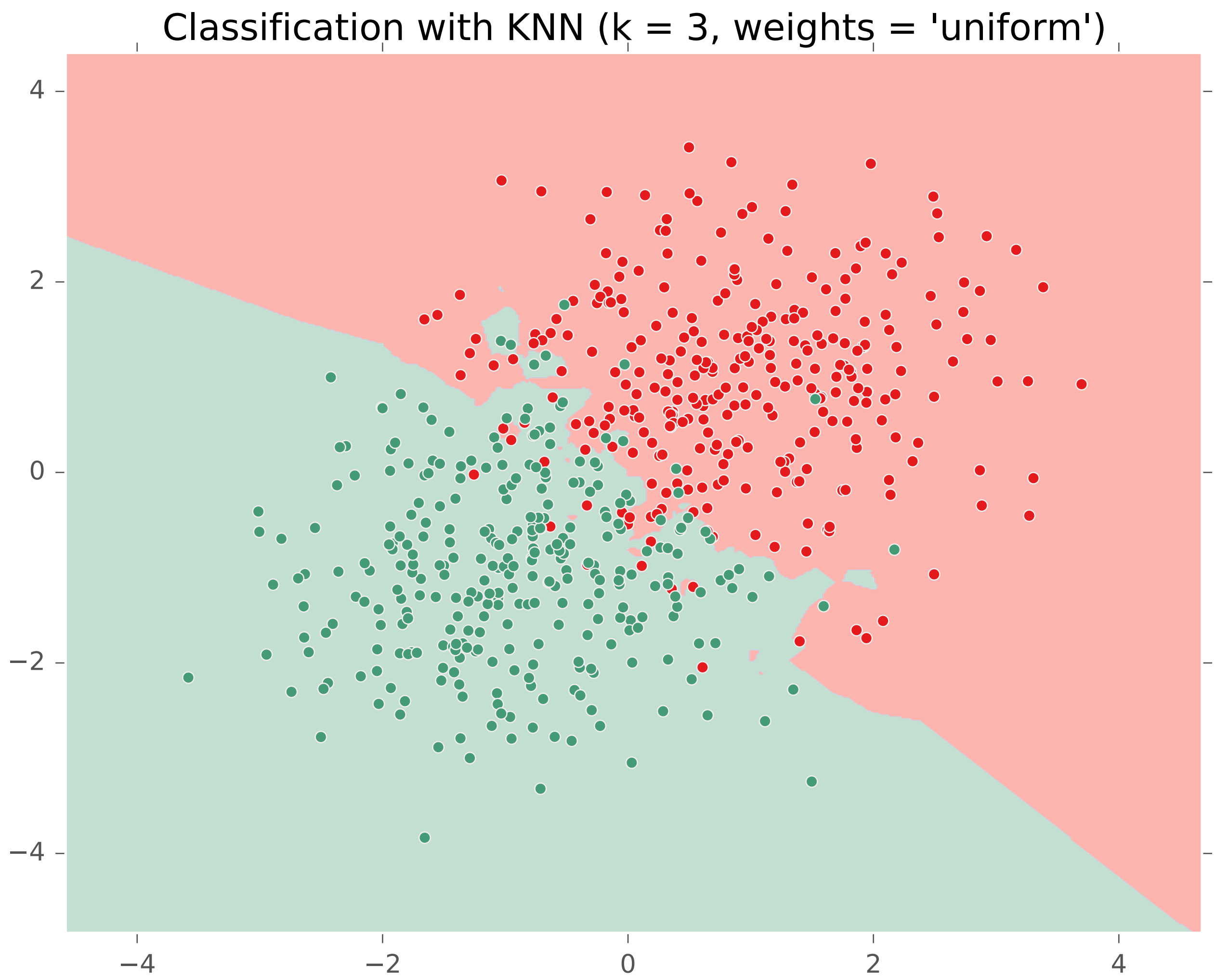
KNN on Gaussian Data



KNN on Gaussian Data



KNN on Gaussian Data



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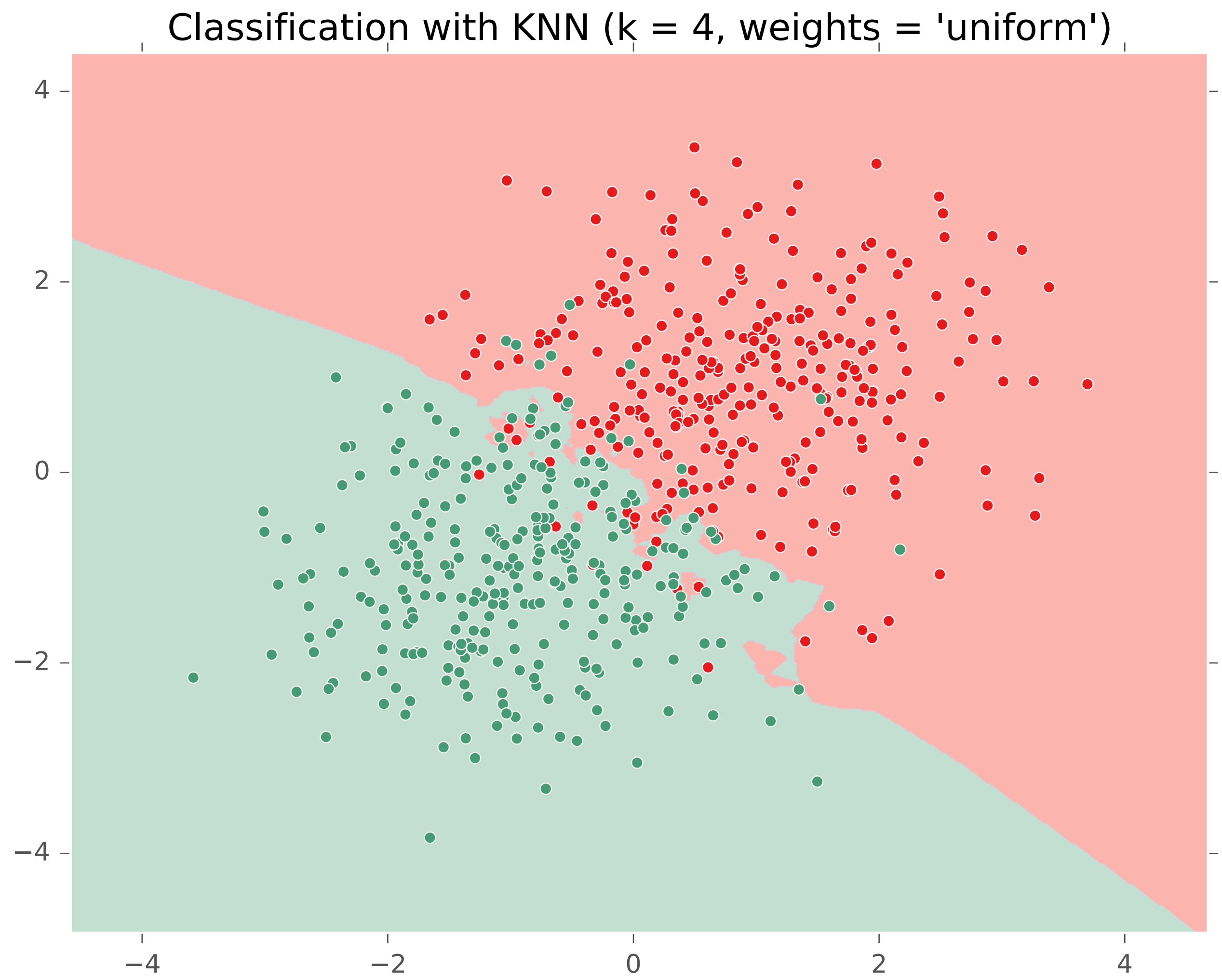
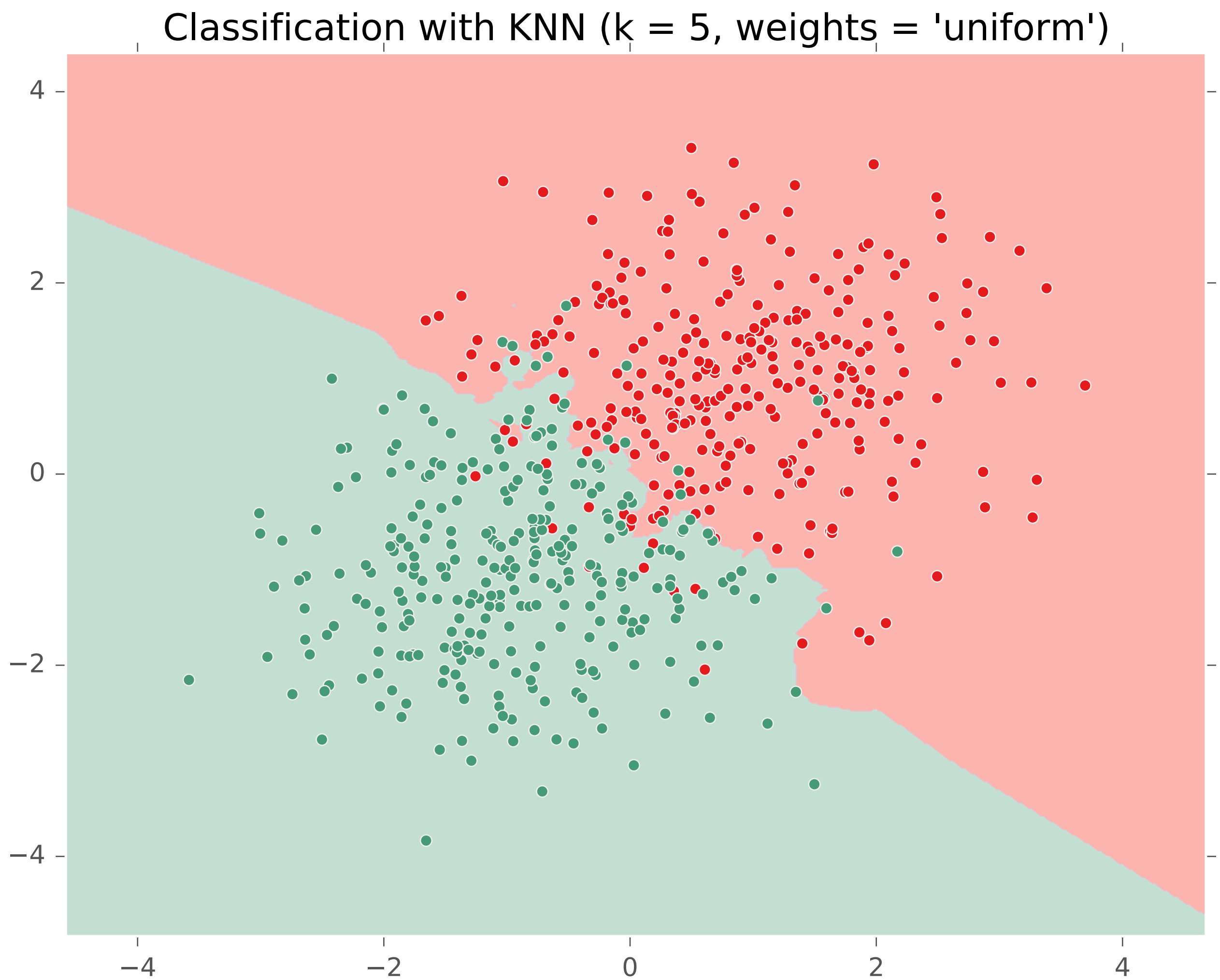


KNN on Gaussian Data



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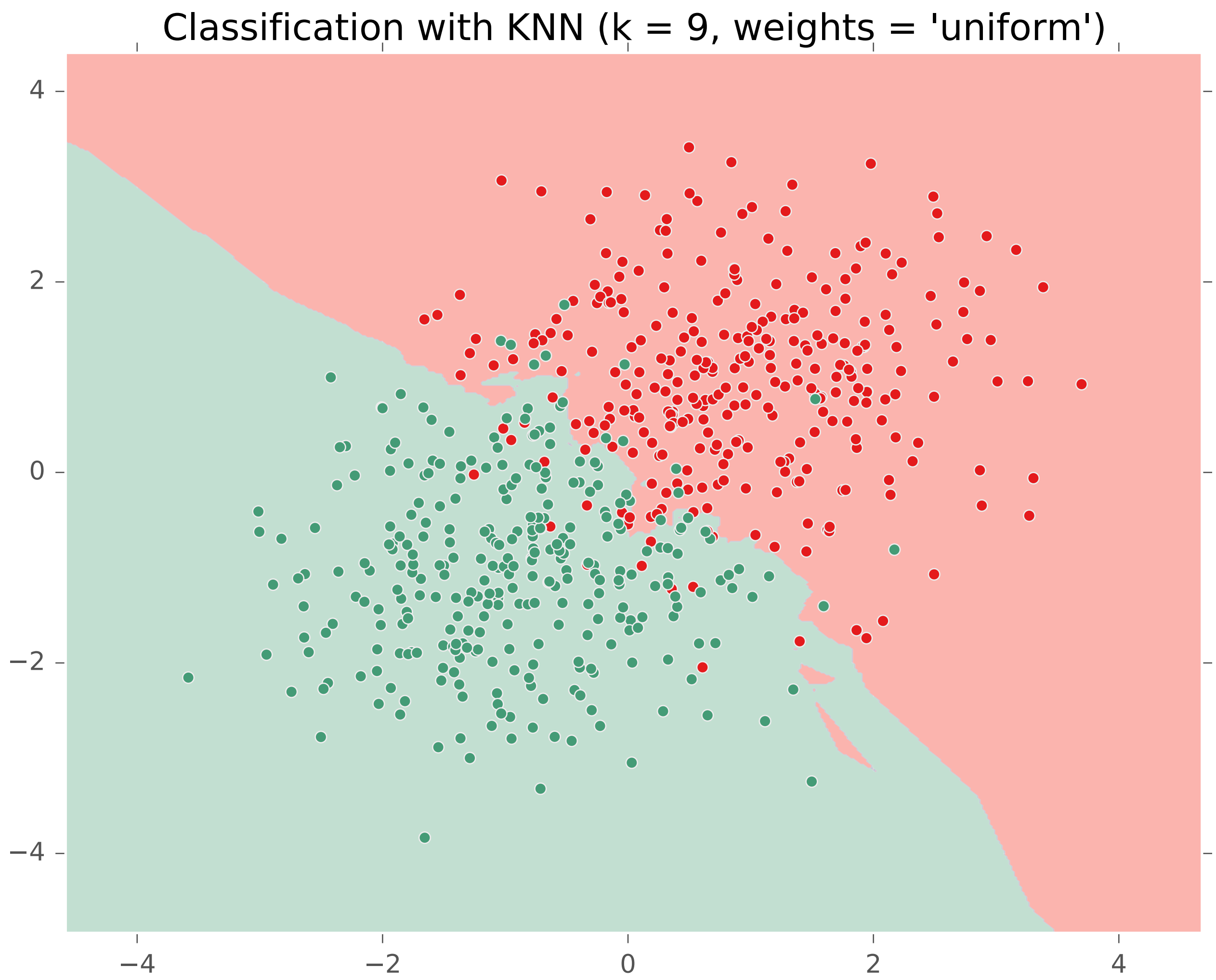

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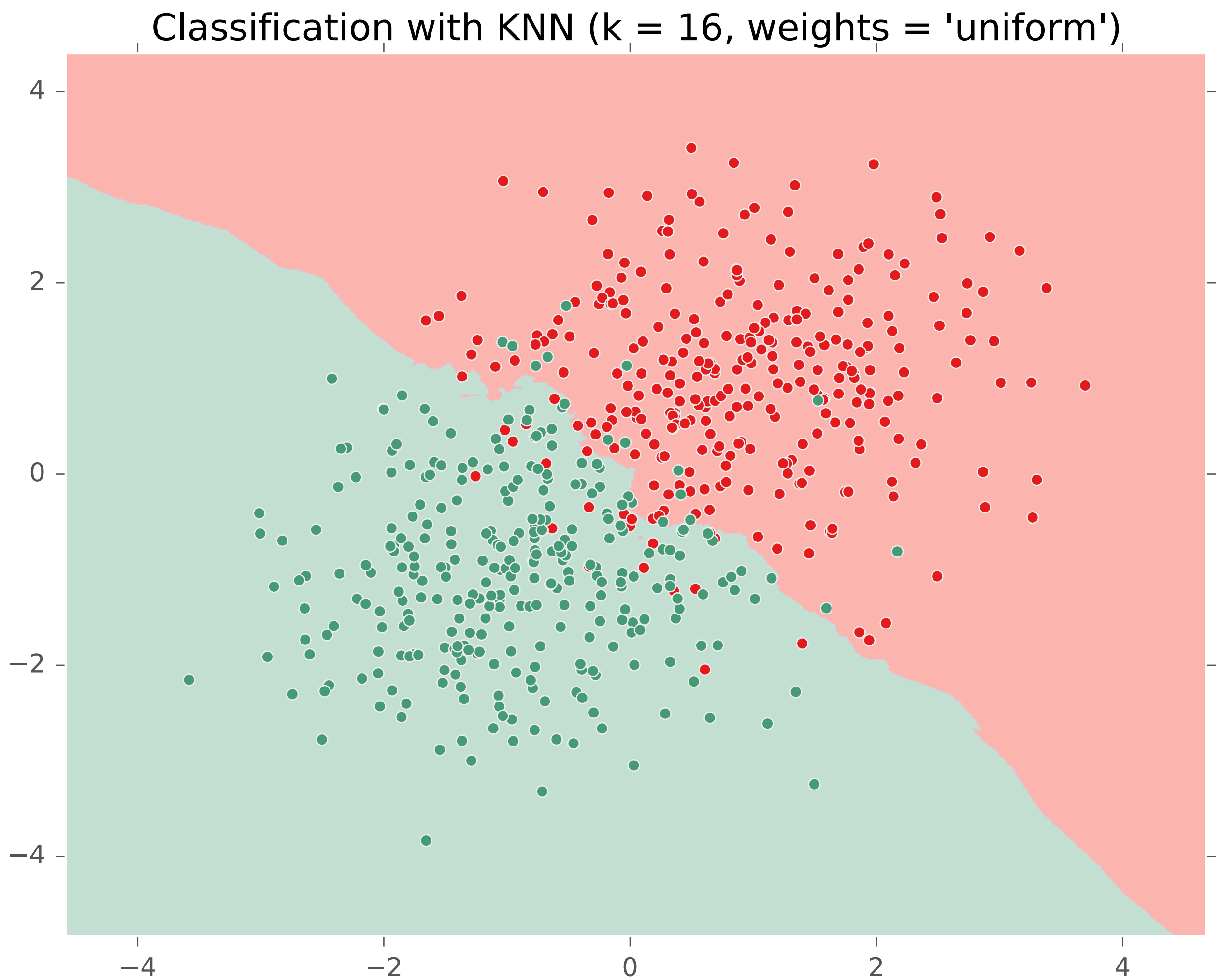

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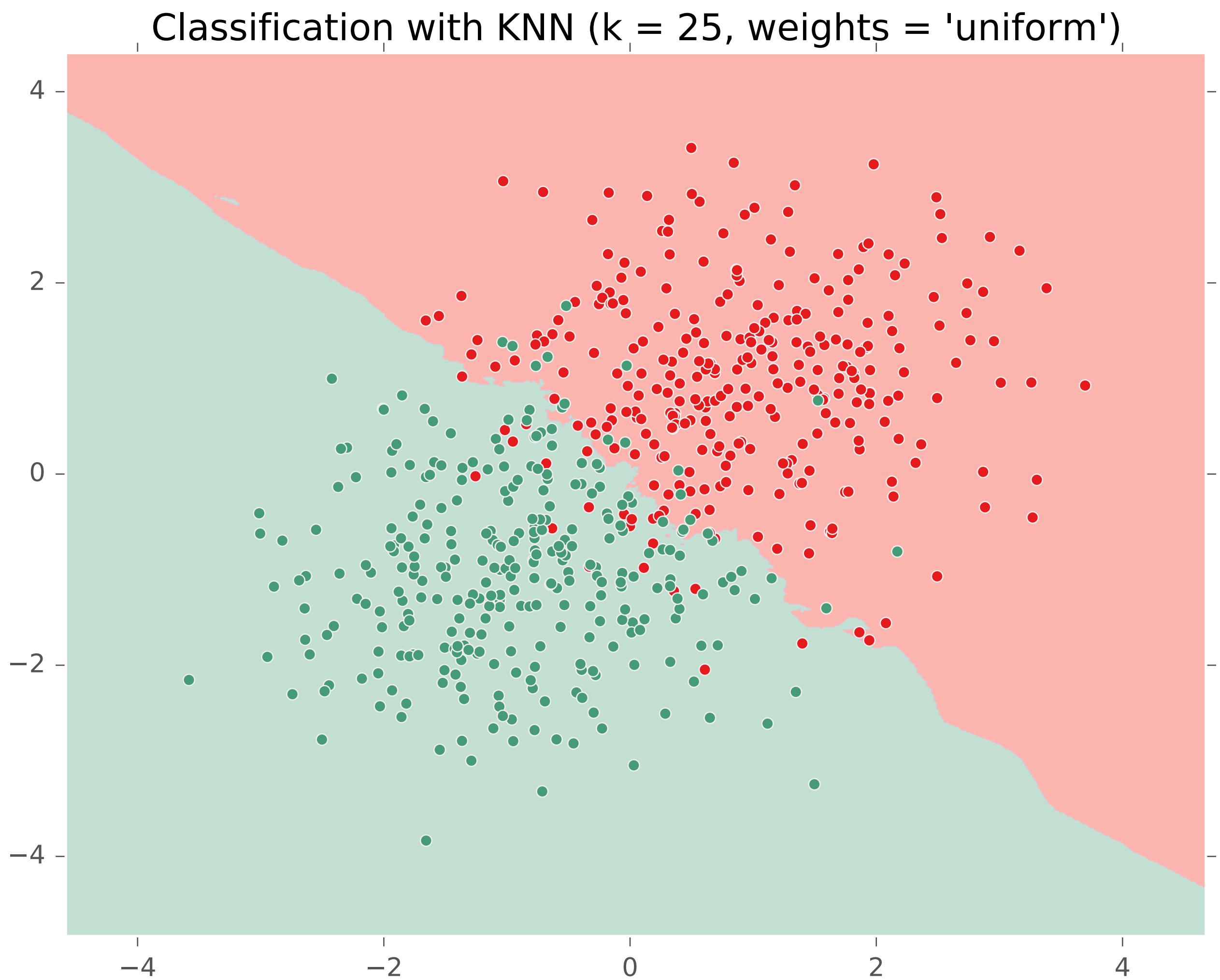
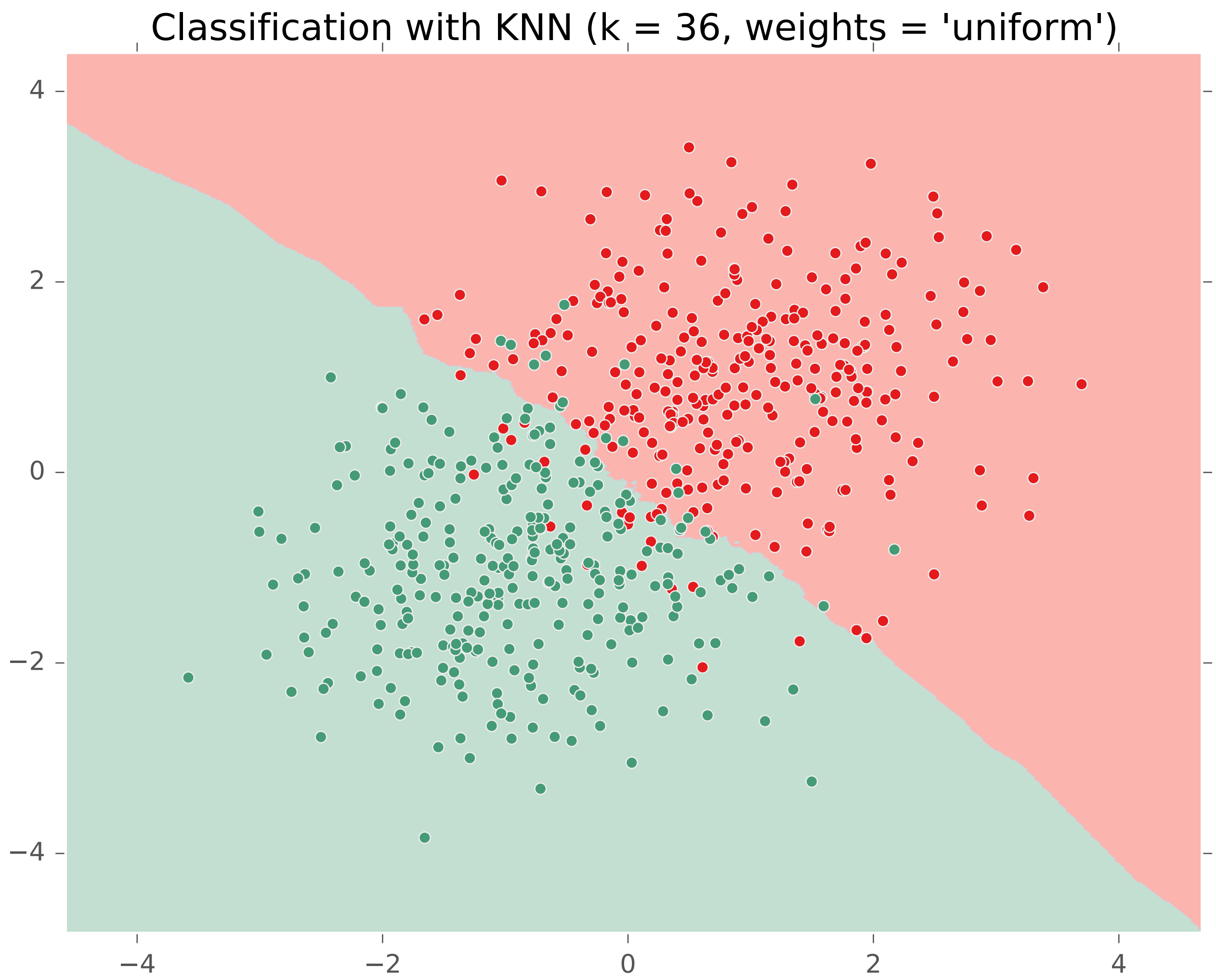
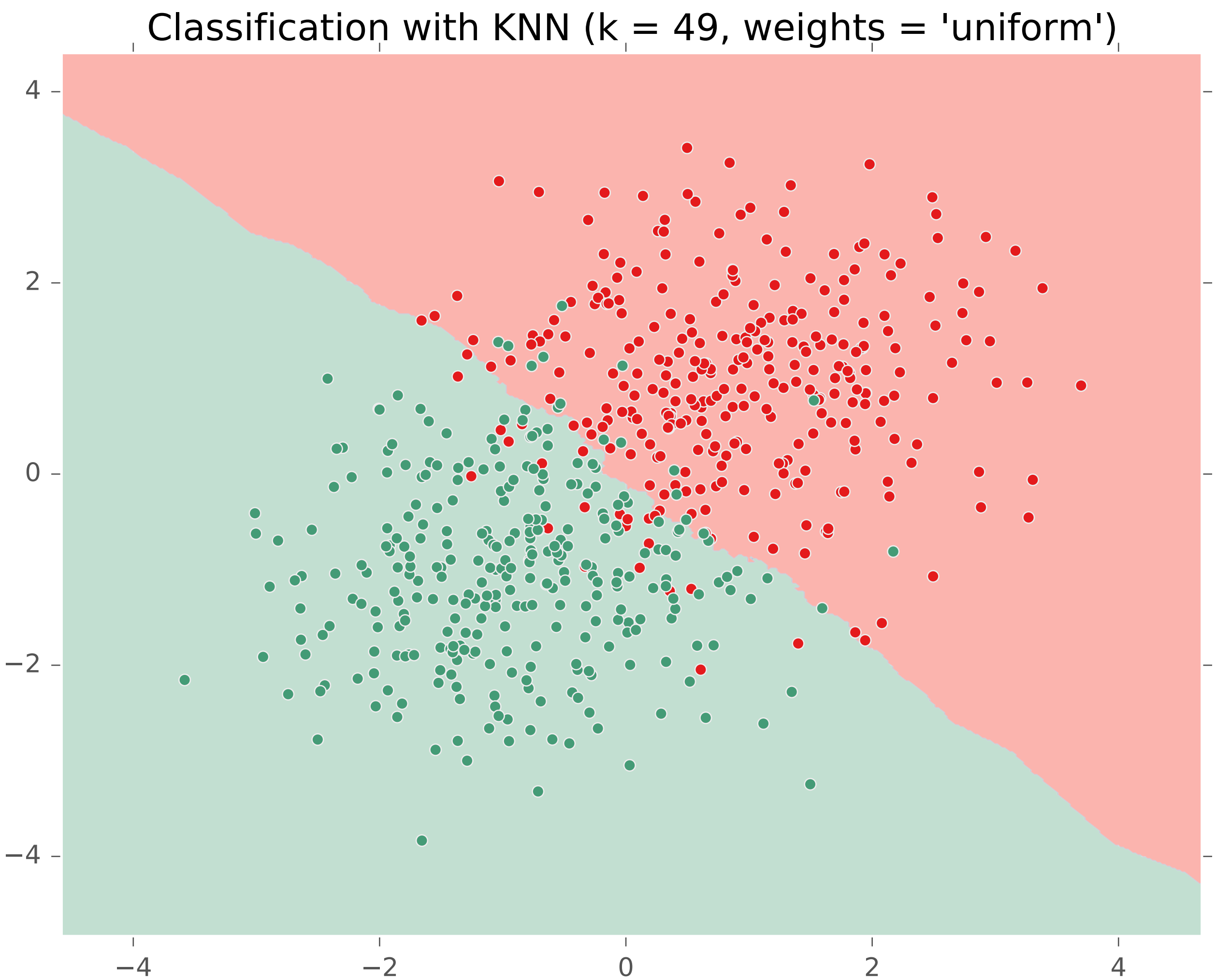


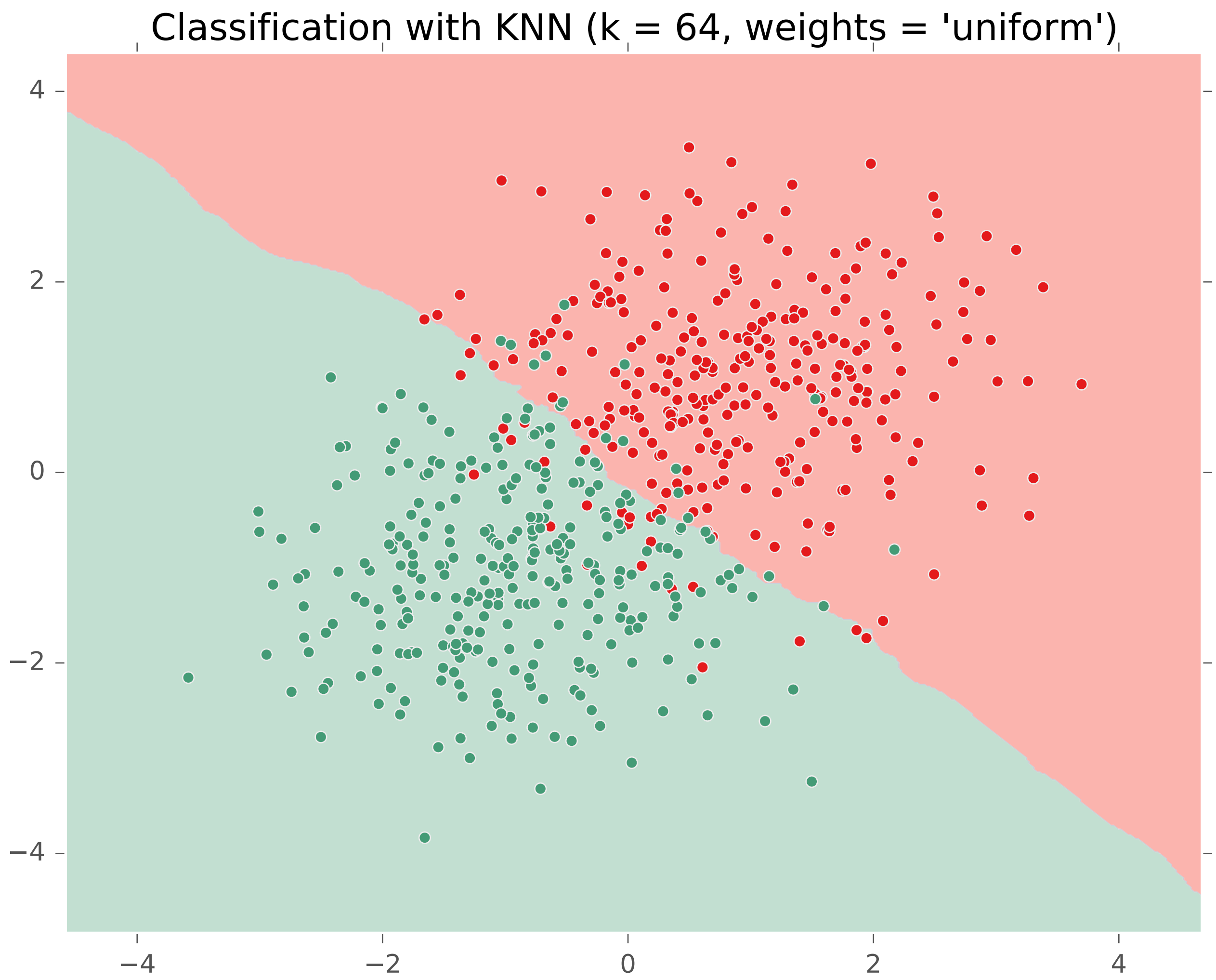
KNN on Gaussian Data



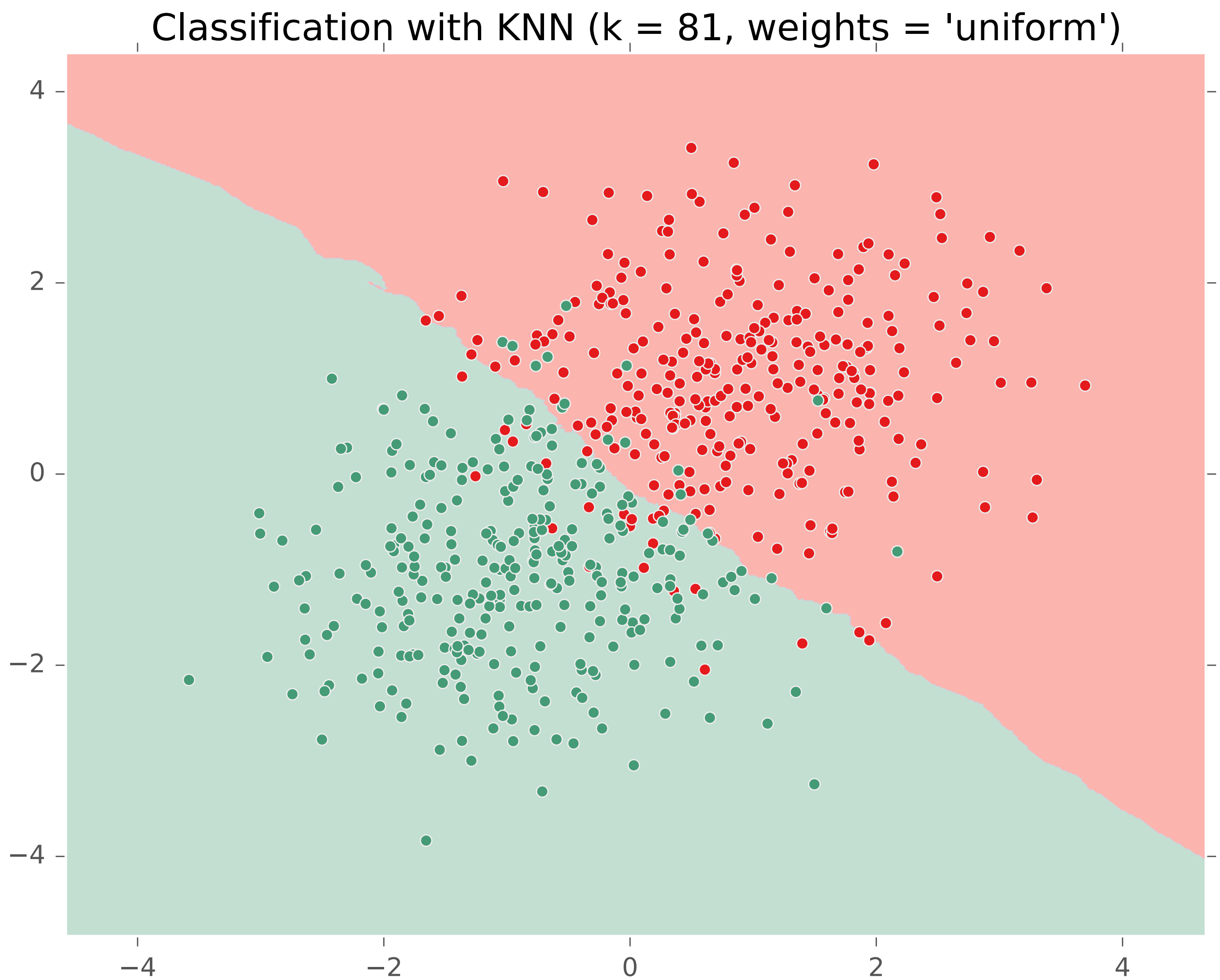
KNN on Gaussian Data



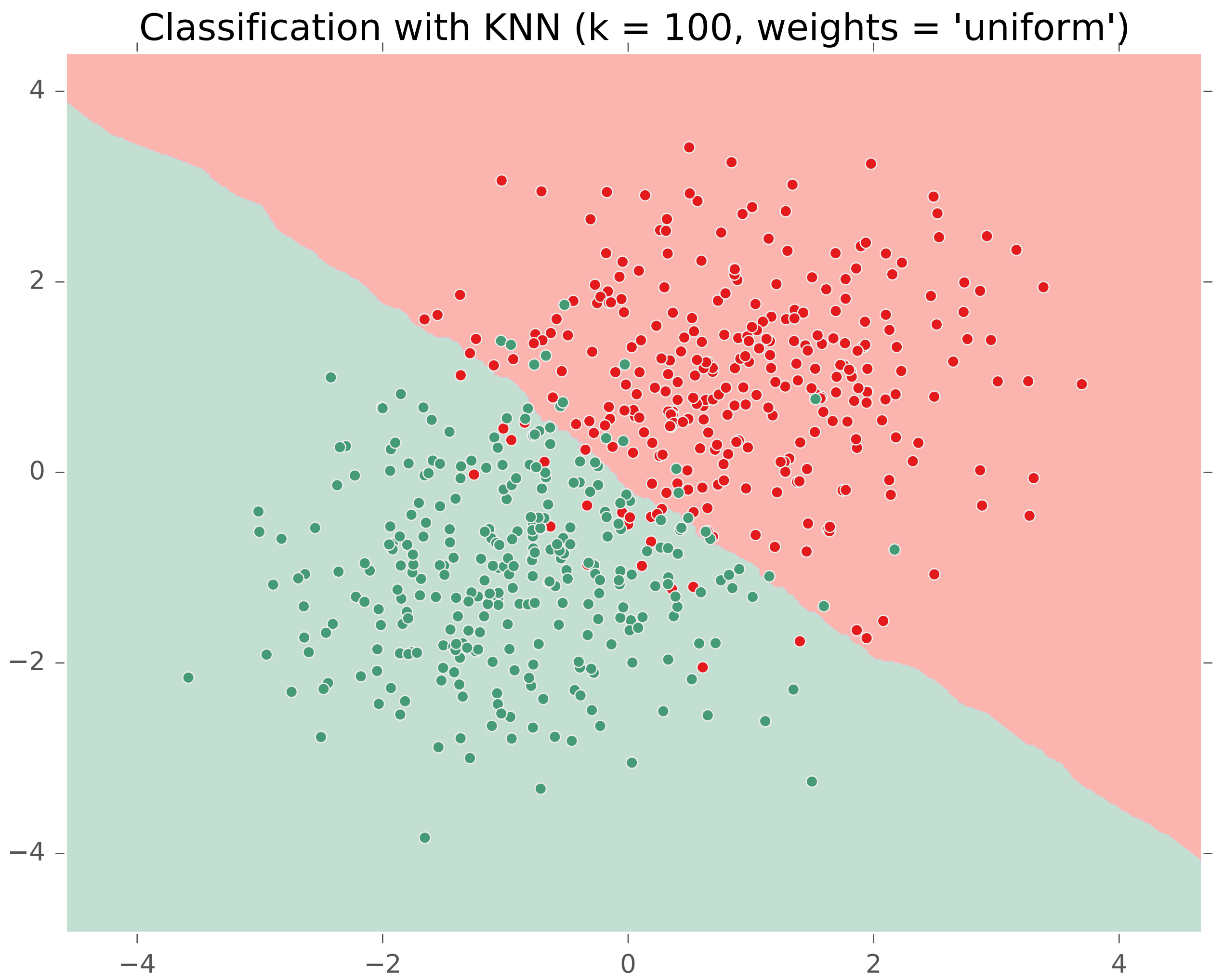
KNN on Gaussian Data



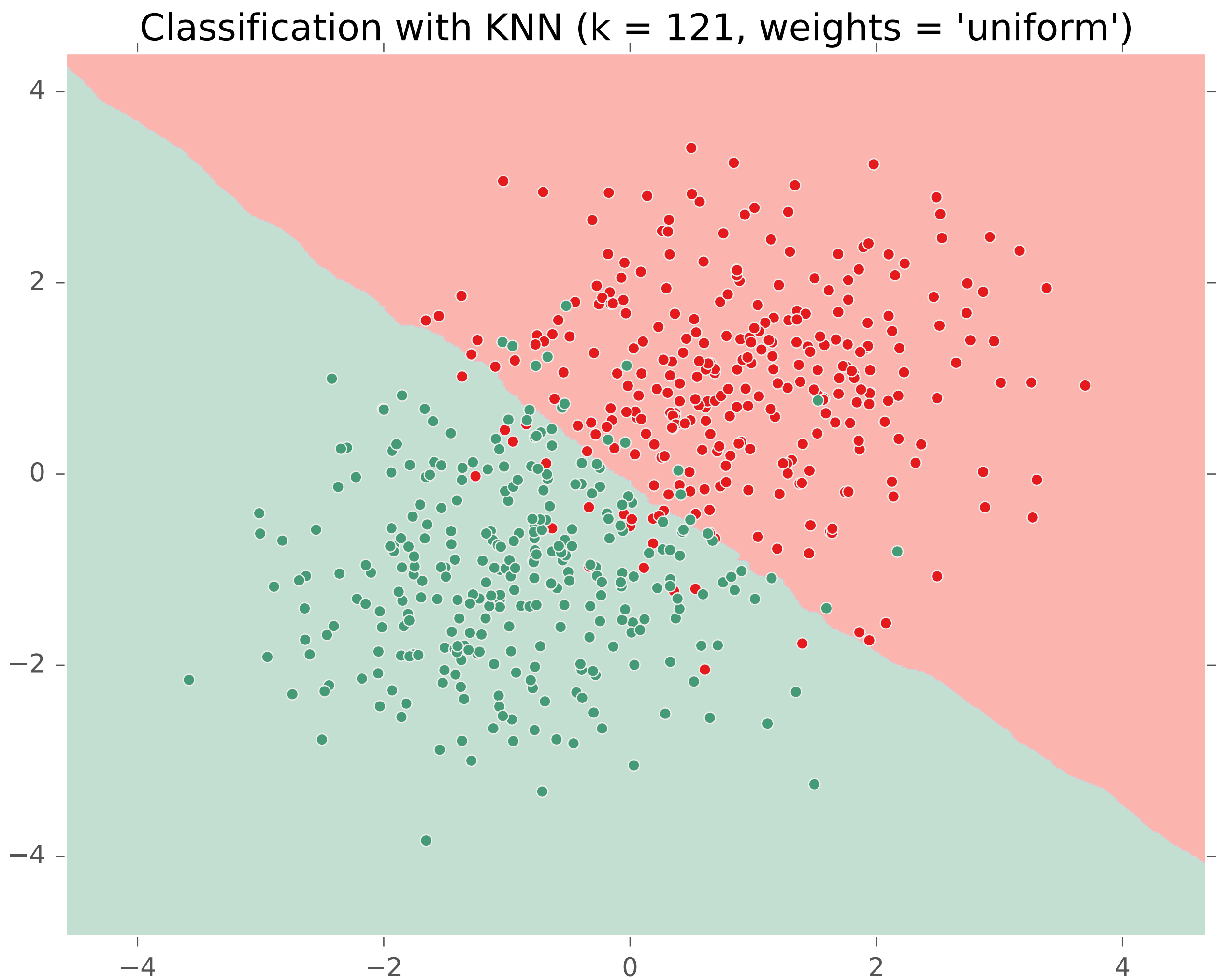
KNN on Gaussian Data



KNN on Gaussian Data



KNN on Gaussian Data



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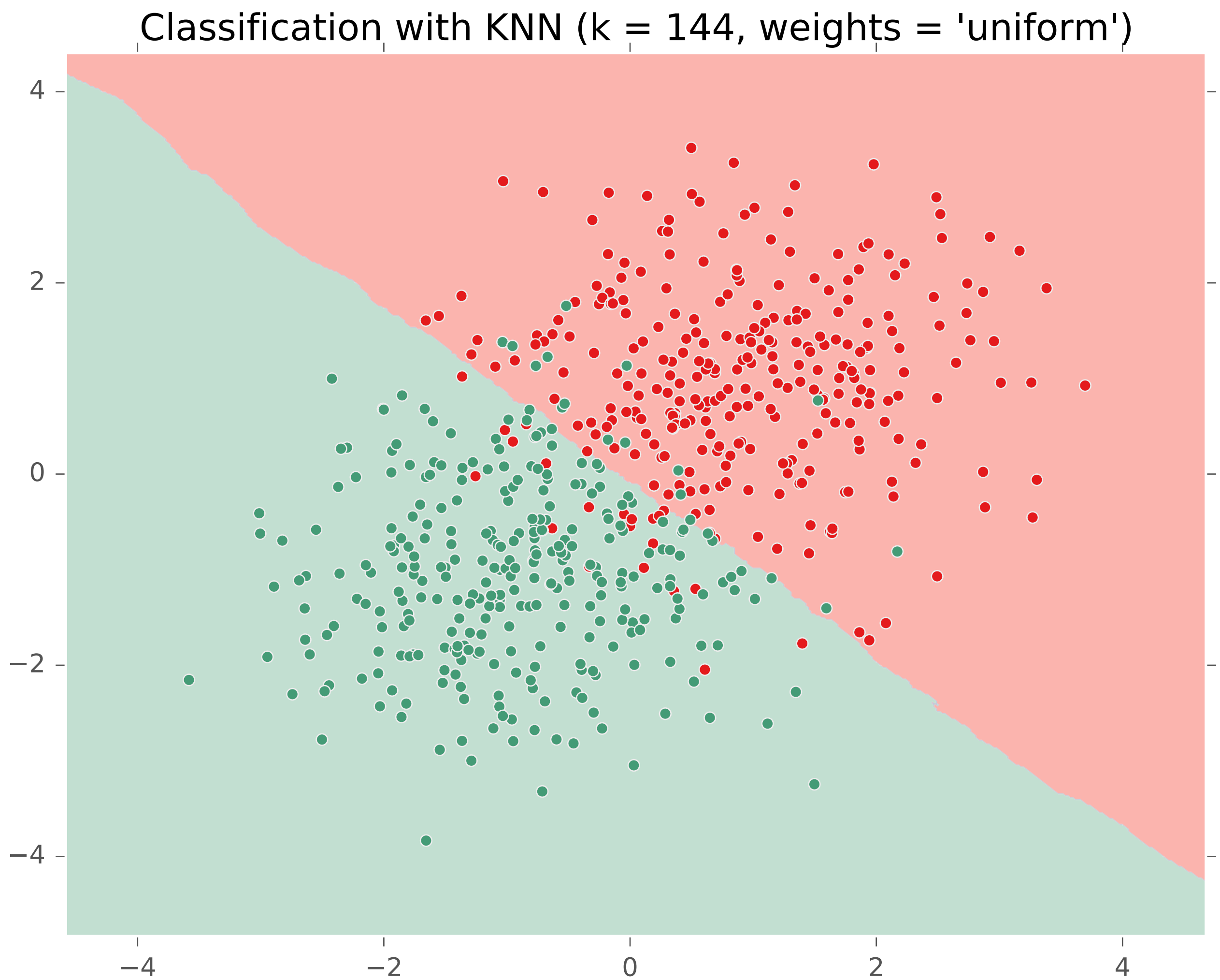
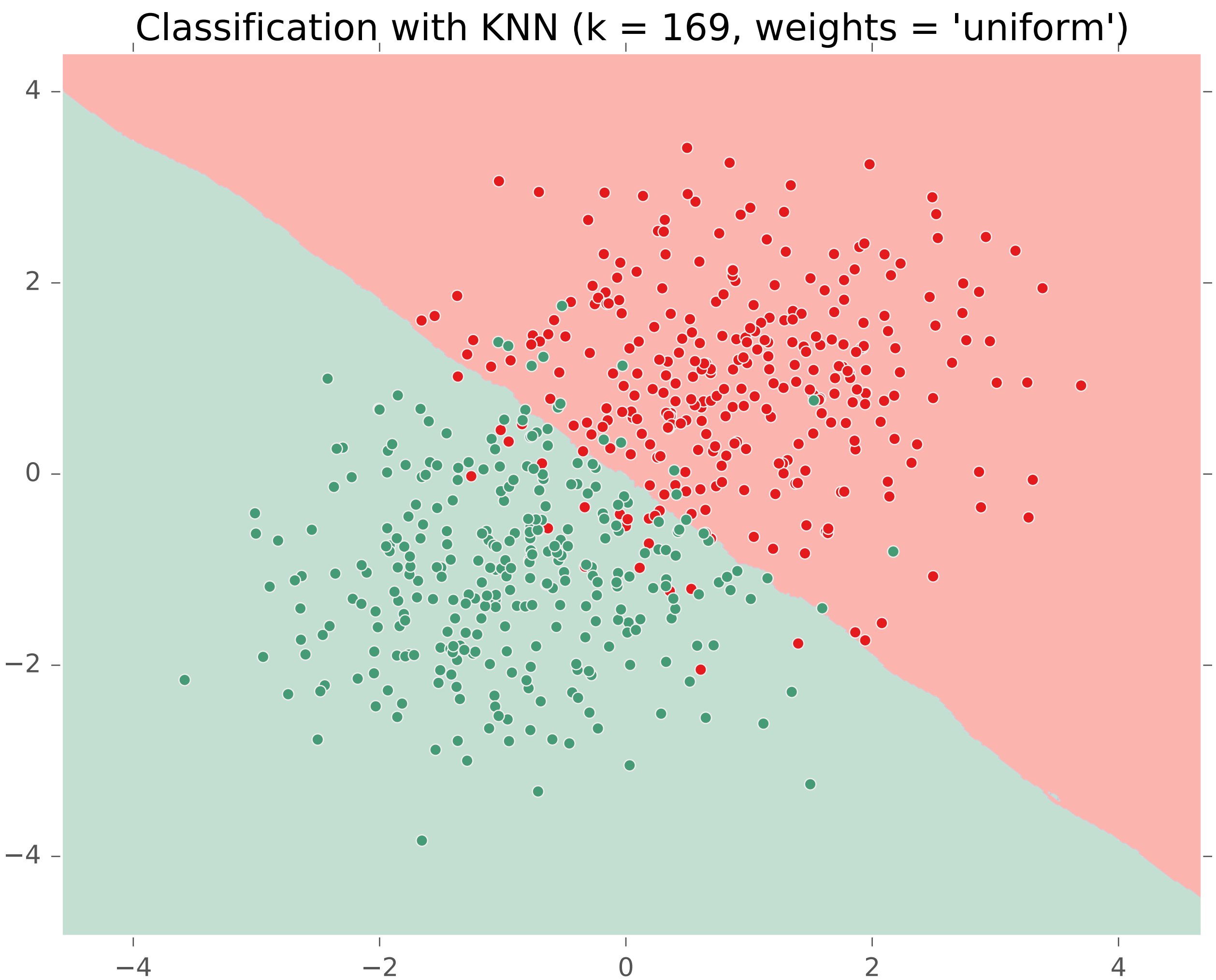


KNN on Gaussian Data



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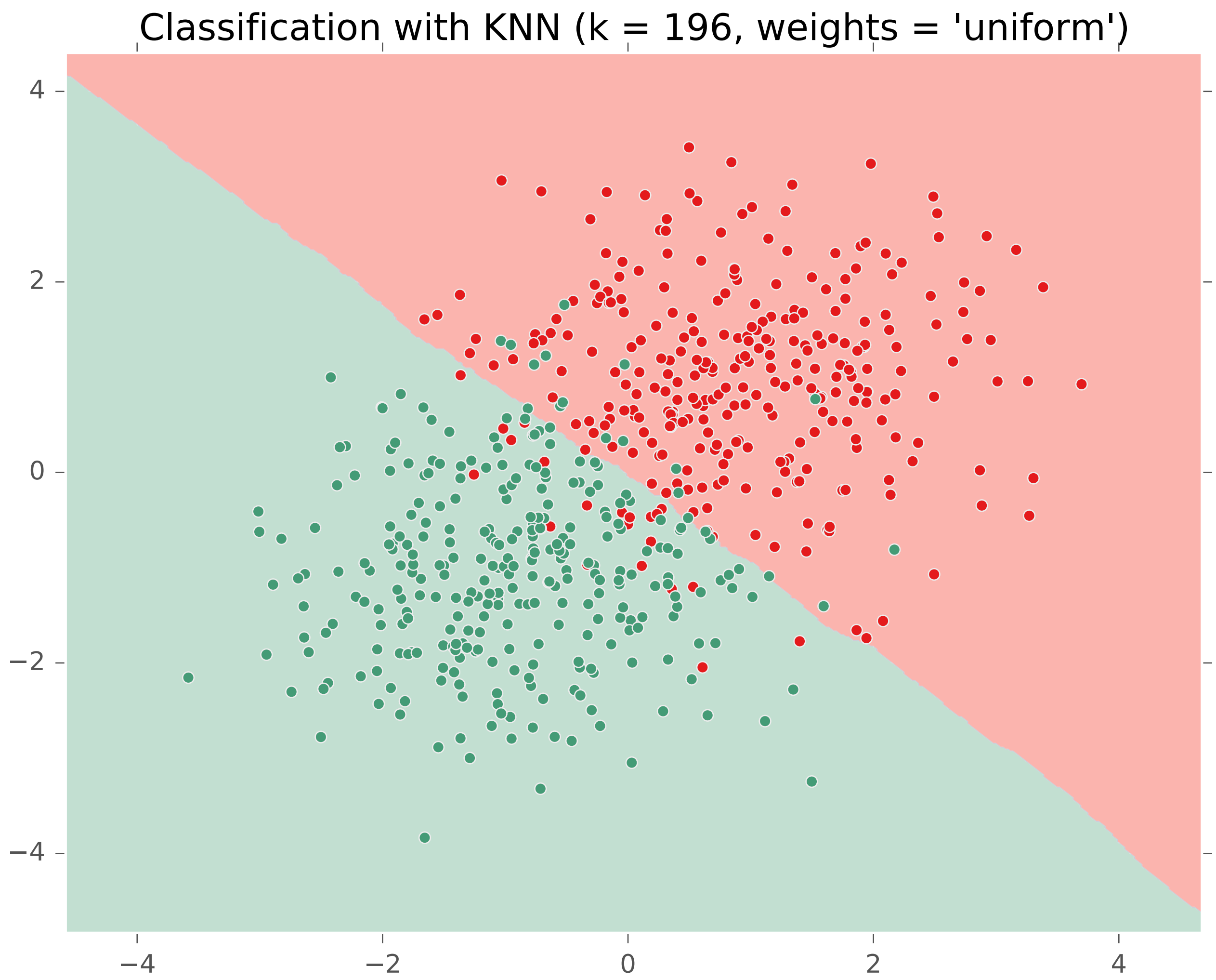
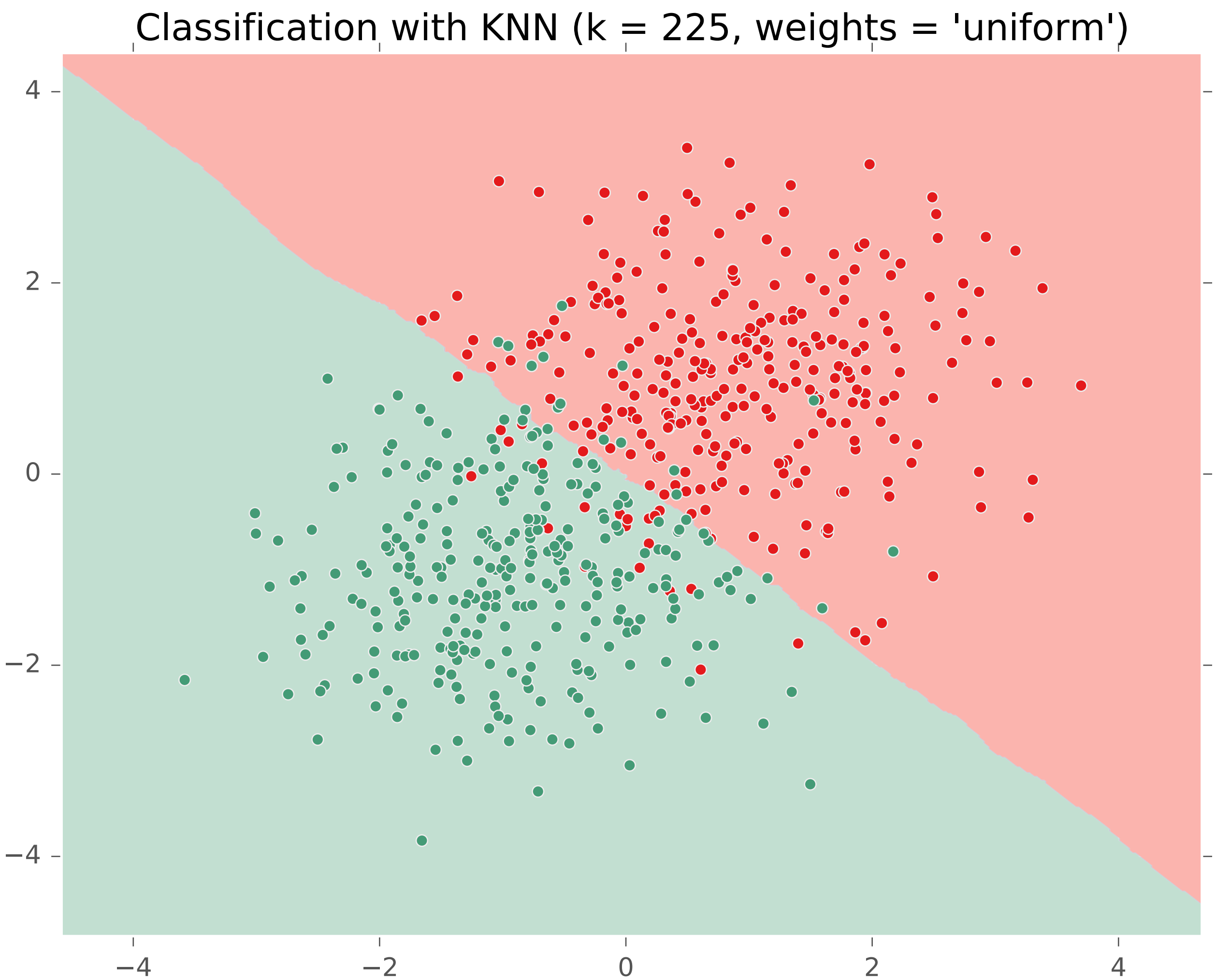
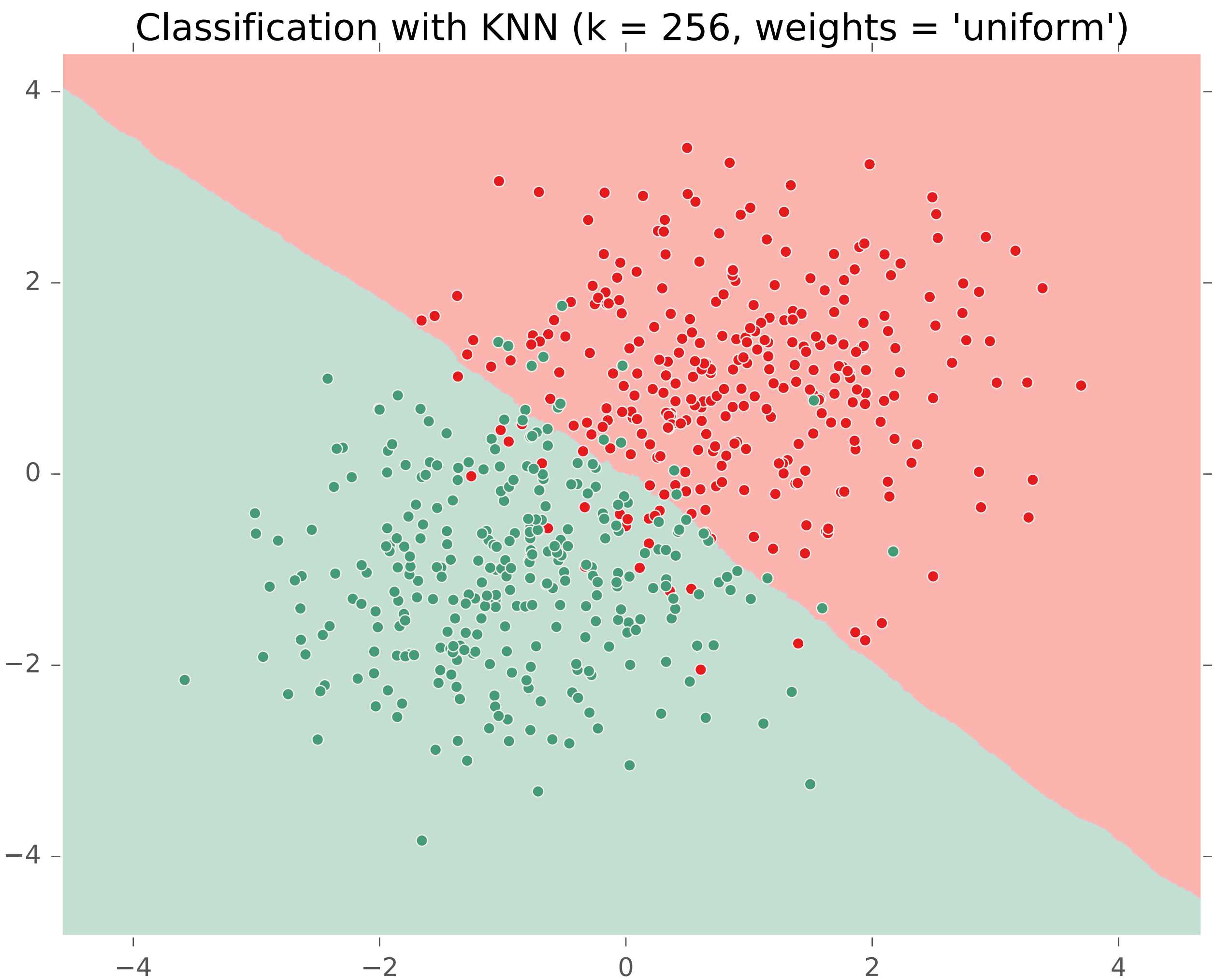


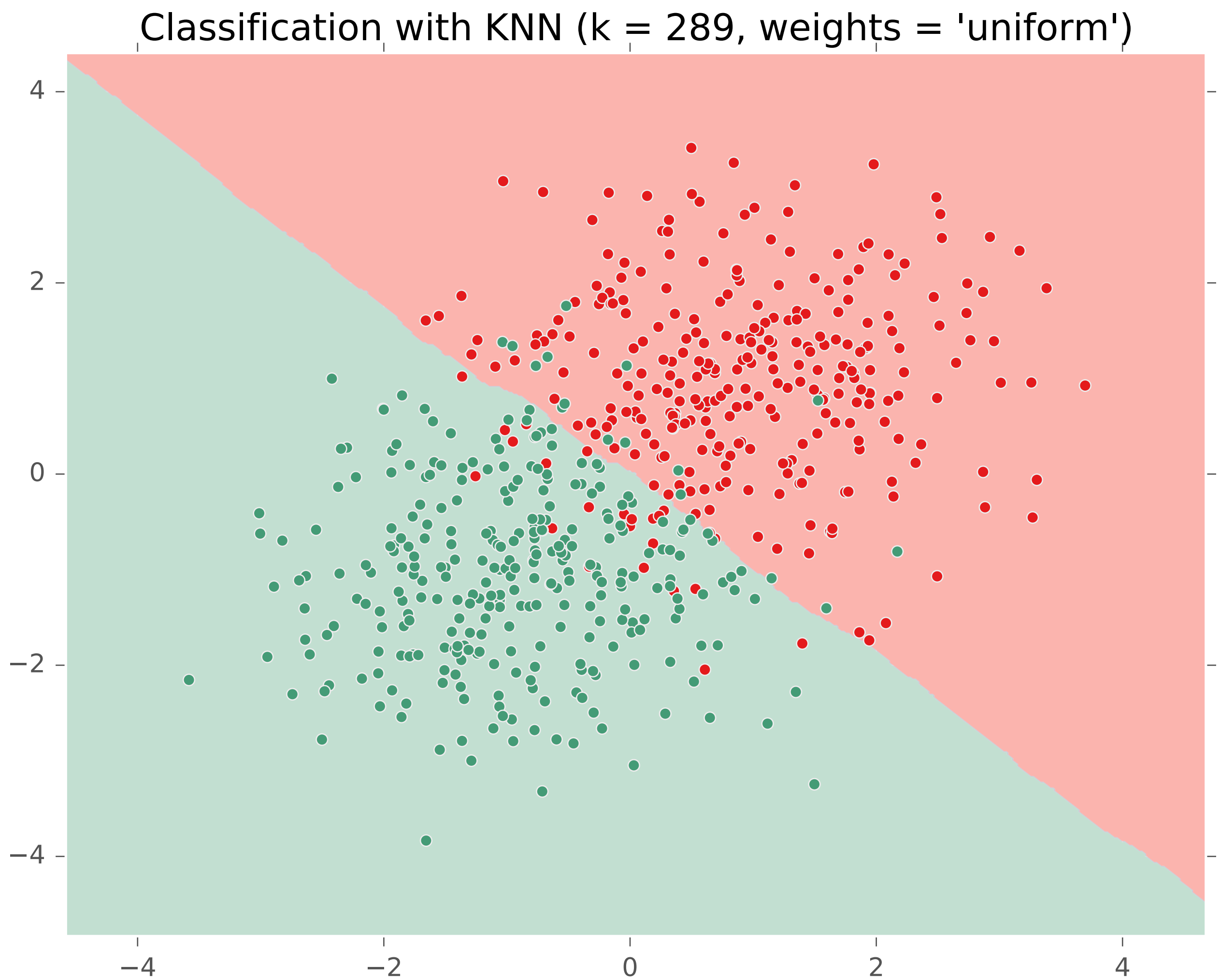
KNN on Gaussian Data



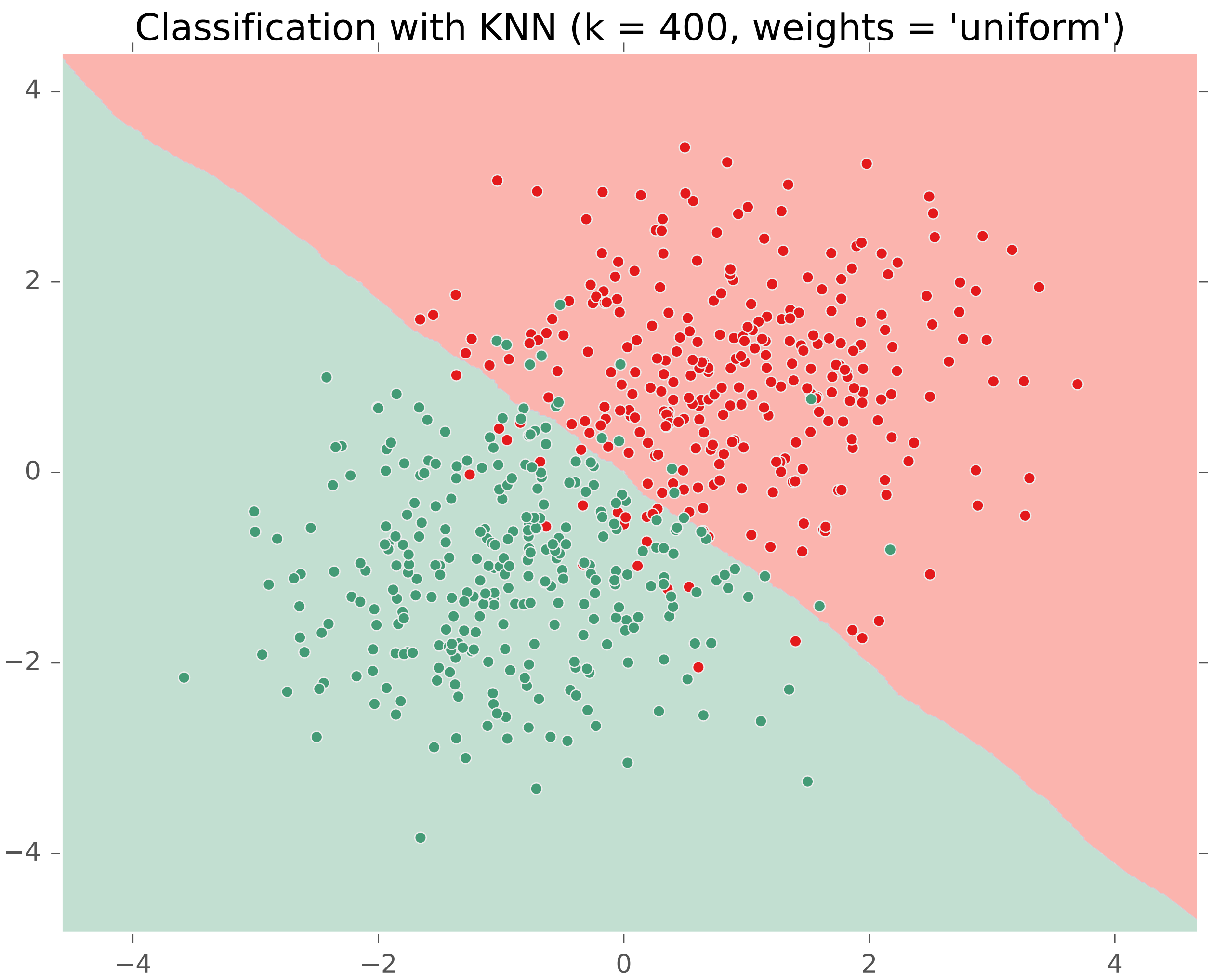
KNN on Gaussian Data



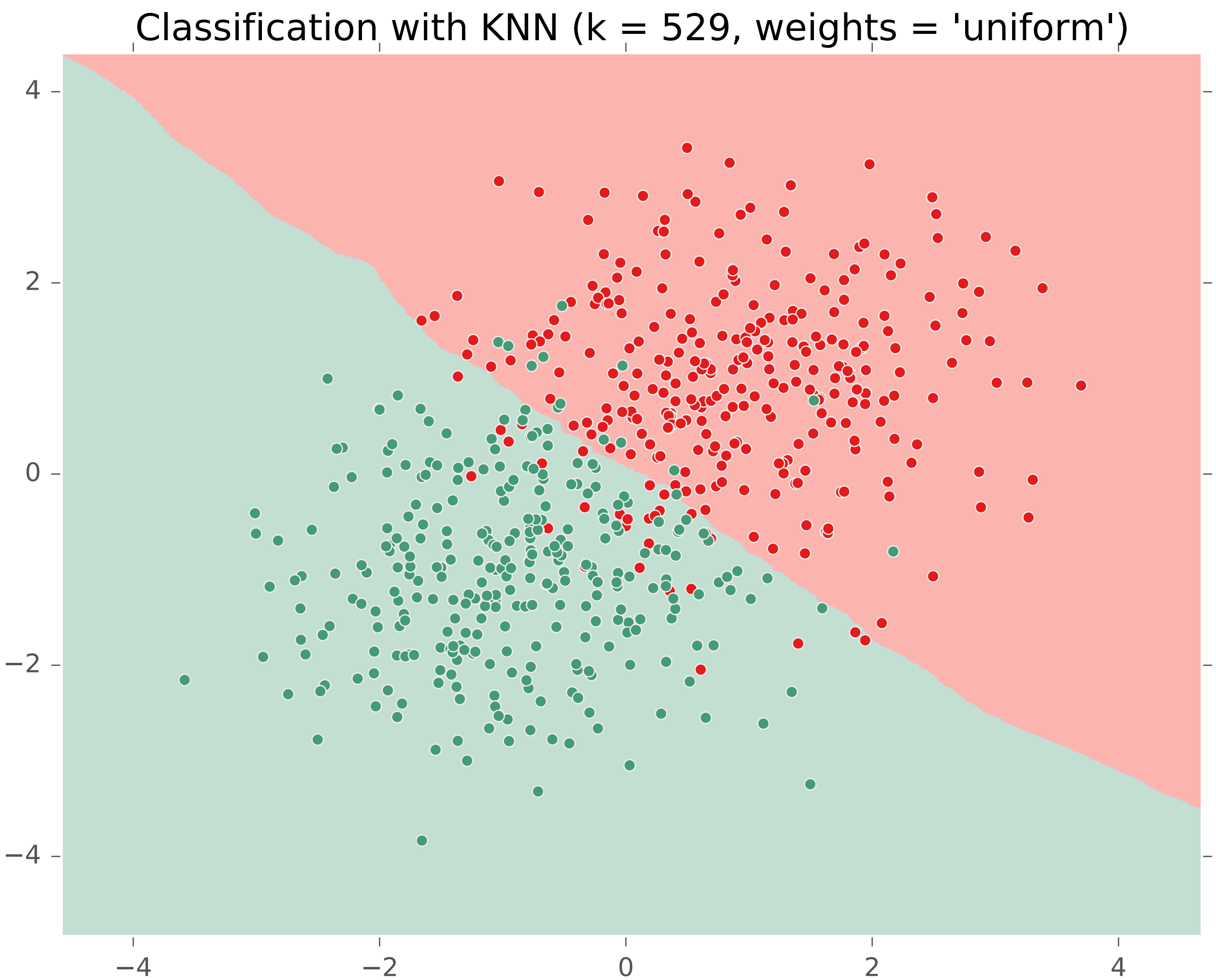
KNN on Gaussian Data



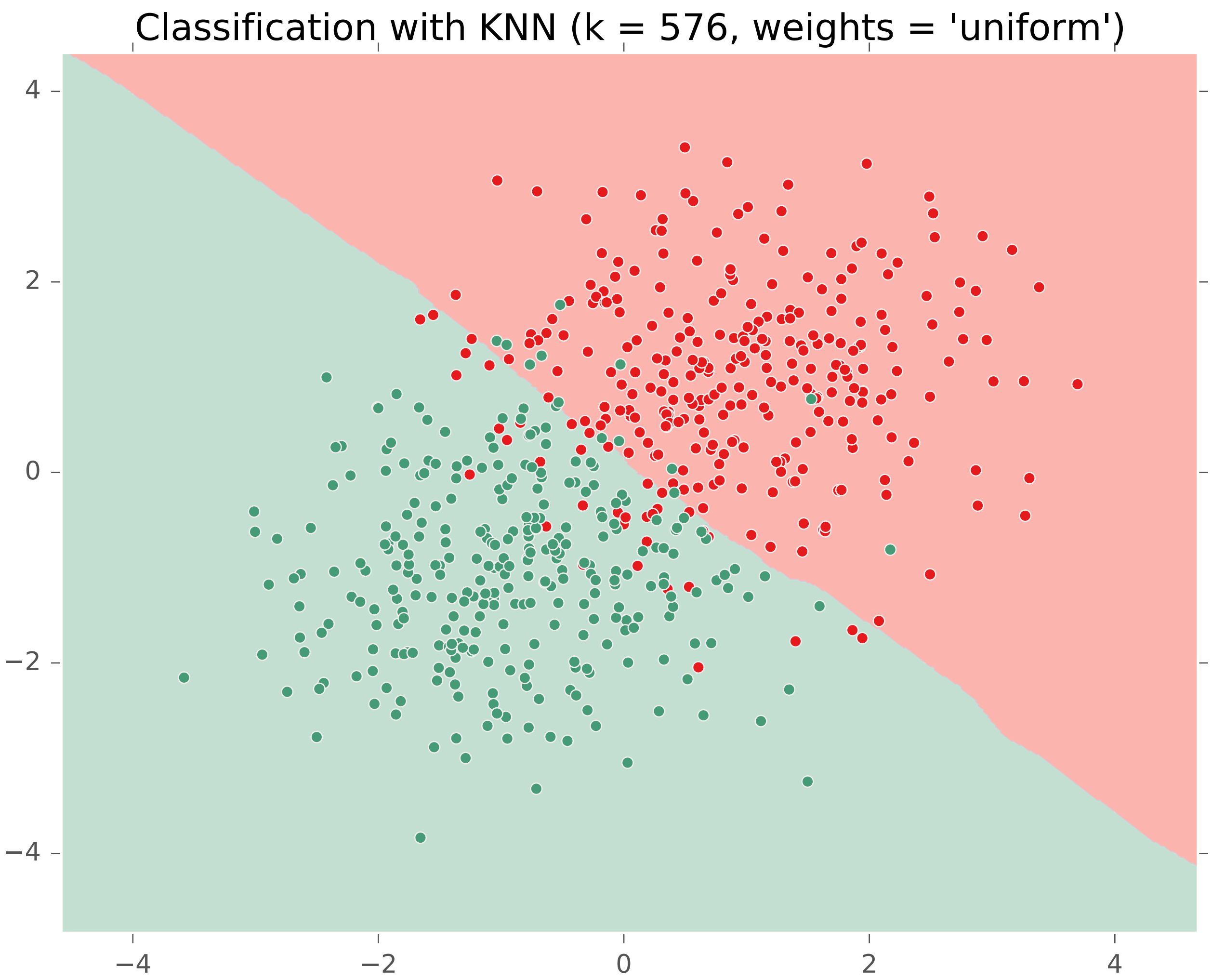
KNN on Gaussian Data



KNN on Gaussian Data



KNN on Gaussian Data



KNN Learning Objectives

You should be able to…

- Describe a dataset as points in a high dimensional space [CIML]
- Implement k-Nearest Neighbors with O(N) prediction
- Describe the inductive bias of a k-NN classifier and relate it to feature scale [a la. CIML]
- Sketch the decision boundary for a learning algorithm (compare k-NN and DT)
- State Cover & Hart (1967)'s large sample analysis of a nearest neighbor classifier
- Invent "new" k-NN learning algorithms capable of dealing with even k

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

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.

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

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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- *Def*: **model parameters** are the numeric values or structure selected by the learning algorithm that give rise to a hypothesis
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Model Selection

Example: Perceptron

- model = set of all linear separators
- parameters = vector of weights (one for each feature)
- learning algorithm = mistake based updates to the parameters
- hyperparameters = none (unless using some variant such as averaged perceptron)

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

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

Model Selection

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

Statistics

- *Def*: a **model** defines the data generation pro… family of para… distributions)
- *Def*: **model par…** values that giv… particular prob… distribution in…
- *Def*: **learnin…** (aka. estimation) is the proce… of finding the parame…s that best fit the data
- *Def*: **hyperparameters** are the parameters of a prior distribution over parameters

Machine Learning

- *Def*: (loosely) a **model** defines the … pace over which … forms its search
- … **parameters** are the … ues or structure … the learning algorithm … to a hypothesis
- … **ning algorithm** defines the d…a-driven search over the hypo…esis space (i.e. search for goo… …rameters)
- *Def*: **hyperparameters** are the tunable aspects of the model, that the learning algorithm does *not* select

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

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

Example of Hyperparameter Opt.

Whiteboard:

– Special cases of k-Nearest Neighbors
– Choosing k with validation data
– Choosing k with cross-validation

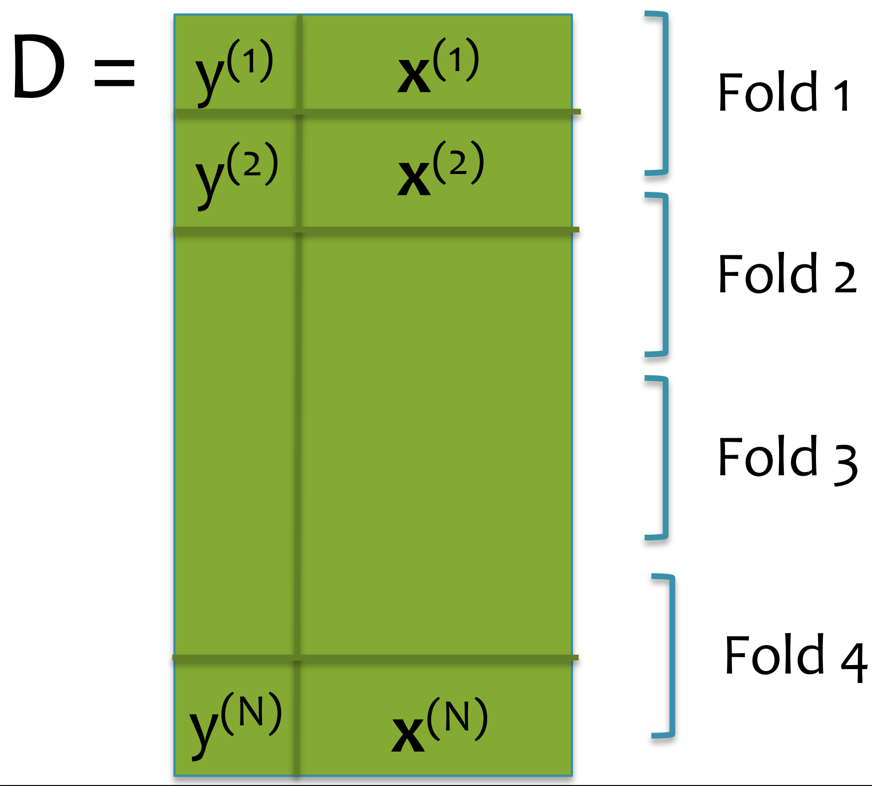
Cross-Validation

Cross validation is a method of estimating loss on held out data

Input: training data, learning algorithm, loss function (e.g. 0/1 error)

Output: an estimate of loss function on held-out data

Key idea: rather than just a single "validation" set, use many!
(Error is more stable. Slower computation.)



Algorithm:

Divide data into folds (e.g. 4)

1. Train on folds {1,2,3} and predict on {4}
2. Train on folds {1,2,4} and predict on {3}
3. Train on folds {1,3,4} and predict on {2}
4. Train on folds {2,3,4} and predict on {1}

Concatenate all the predictions and evaluate loss (*almost* equivalent to averaging loss over the folds)

Definition:
N-fold cross validation = cross validation with N folds

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
Cross-Validation	• training dataset • validation dataset	• cross-validation error	We estimate the error on held out data by repeatedly training on N-1 folds and predicting on the held-out fold
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

Experimental Design

Q: We pick the best hyperparameters by learning on the training data and evaluating error on the validation data. For our final model, should we also learn from just the training data?

A: No!

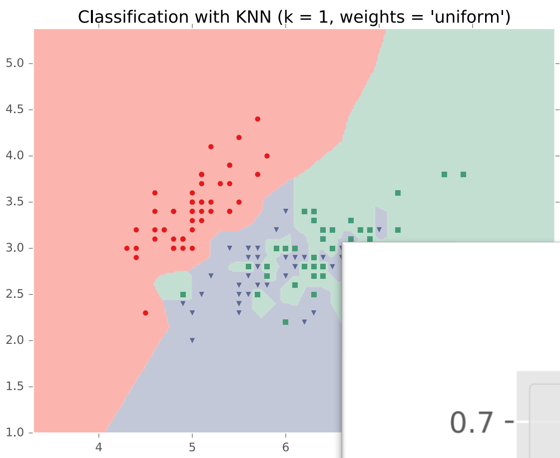
Let's assume that {train-original} is the original training data and {test} is the provided test dataset.

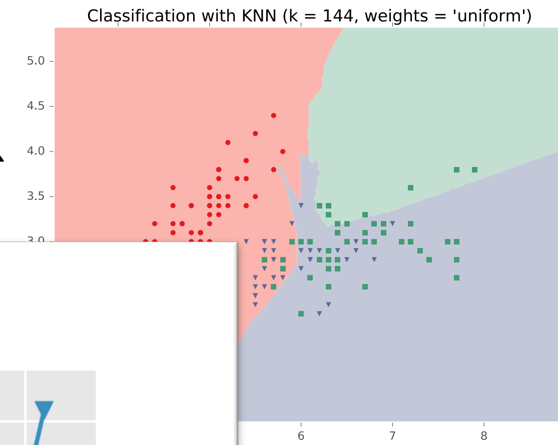
1. Split {train-original} into {train-subset} and {validation}.
2. Pick the hyperparameters that when training on {train-subset} give the lowest error on {validation}. Call these hyperparameters {best-hyper}.
3. Retrain a new model using {best-hyper} on {train-original} = {train-subset} ∪ {validation}.
4. Report test error by evaluating on {test}.

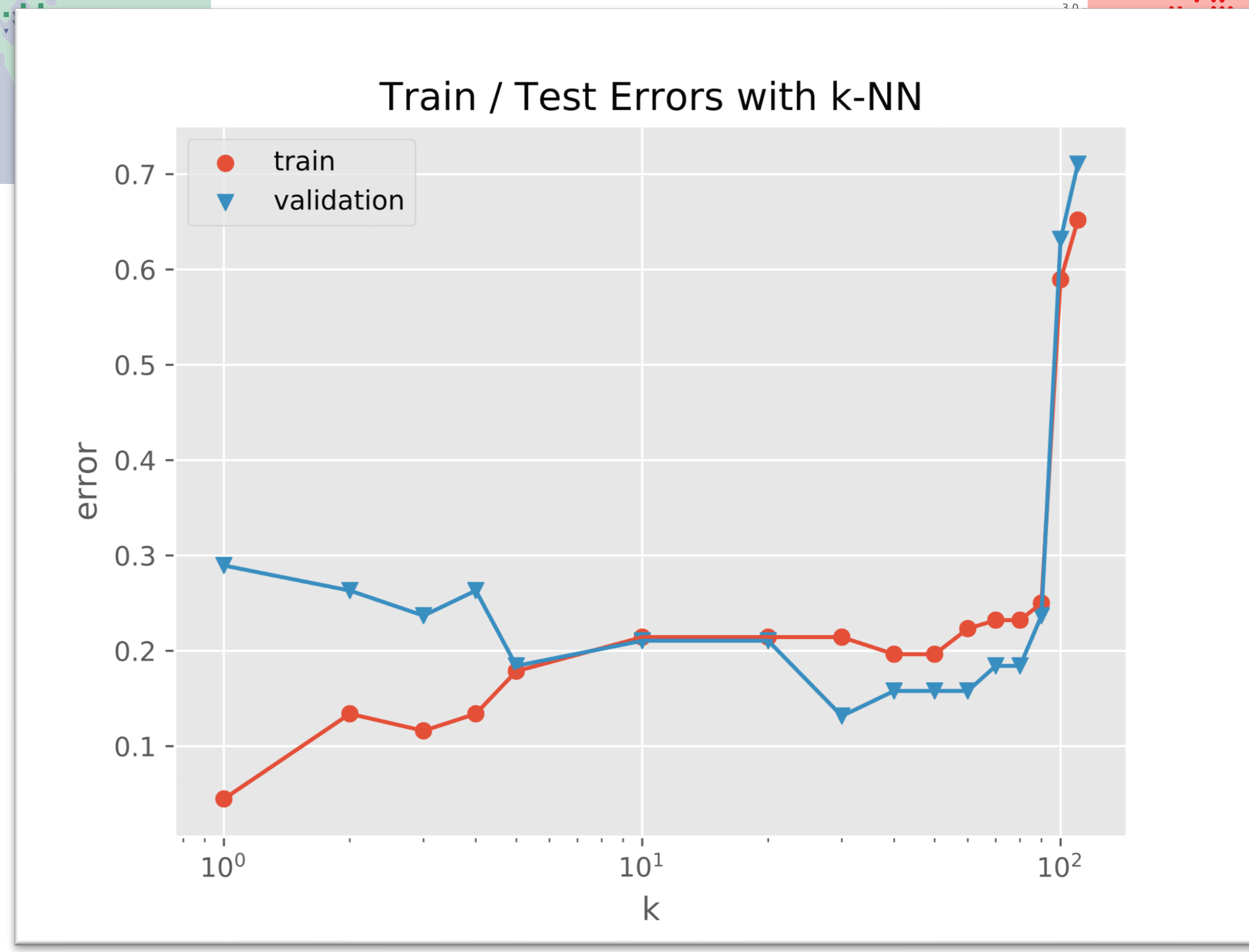
Alternatively, you could replace Steps 1-2 with the following:

1. Pick the hyperparameters that give the lowest cross-validation error on {train-original}. Call these hyperparameters {best-hyper}.

k-NN: Choosing k

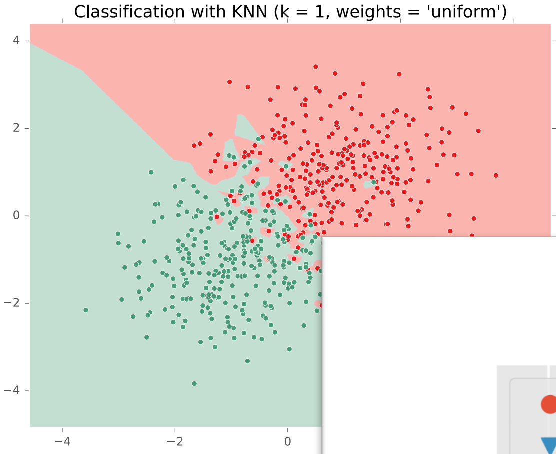


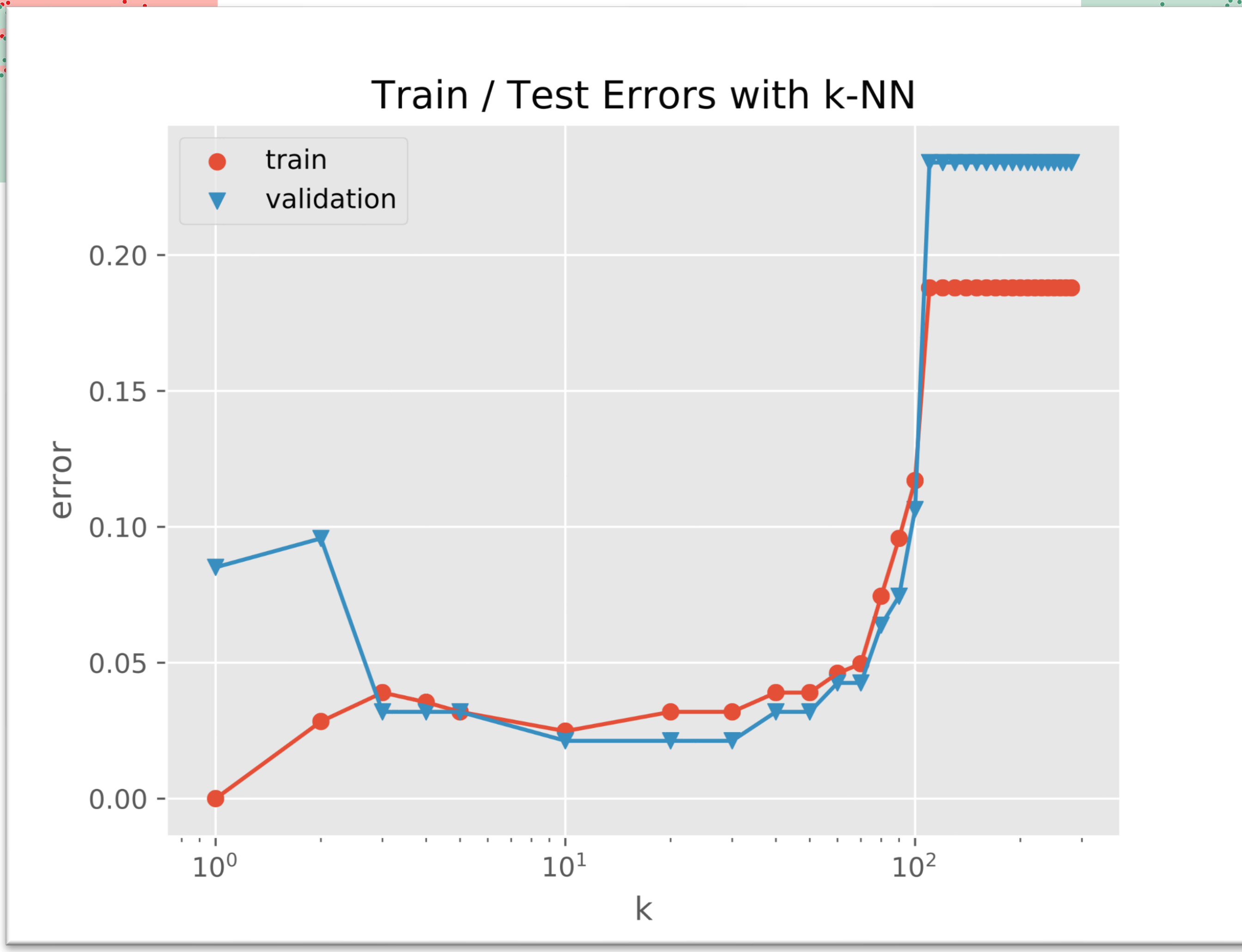


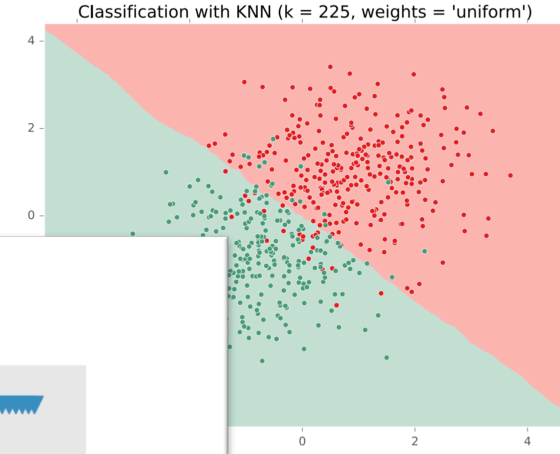


Fisher Iris Data: varying the value of k

k-NN: Choosing k







Gaussian Data: varying the value of k

HYPERPARAMETER OPTIMIZATION

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

Hyperparameter Optimization

Setting: suppose we have hyperparameters α, β, and χ and we wish to pick the "best" values for each one

Algorithm 1: Grid Search

- Pick a set of values for each hyperparameter
  $\alpha \in \{a_1, a_2, \ldots, a_n\}$, $\beta \in \{b_1, b_2, \ldots, b_n\}$, and $\chi \in \{c_1, c_2, \ldots, c_n\}$
- Run a grid search

```
for α ∈ {a_1, a_2, … , a_n}:
   for β ∈ {b_1, b_2, … , b_n}:
      for χ ∈ {c_1, c_2, … , c_n}:
         θ = train(D_train; α, β, χ)
          error = predict(D_validation; θ)
```

- return α, β, and χ with lowest validation error

Hyperparameter Optimization

Setting: suppose we have hyperparameters α, β, and χ and we wish to pick the "best" values for each one

Algorithm 2: Random Search

- Pick a range of values for each parameter
  $\alpha \in \{a_1, a_2, \ldots, a_n\}$, $\beta \in \{b_1, b_2, \ldots, b_n\}$, and $\chi \in \{c_1, c_2, \ldots, c_n\}$
- Run a random search

  for t = 1, 2, …, T:
     sample α uniformly from $\{a_1, a_2, \ldots, a_n\}$
     sample β uniformly from $\{b_1, b_2, \ldots, b_n\}$
     sample χ uniformly from $\{c_1, c_2, \ldots, c_n\}$
     $\theta = \text{train}(D_{train}; \alpha, \beta, \chi)$
     $\text{error} = \text{predict}(D_{validation}; \theta)$

- return α, β, and χ with lowest validation error

Hyperparameter Optimization

Question: Q3 A = toxic B = True C = False

True or False: given a finite amount of computation time, **grid search** is more likely to find good values for hyperparameters than **random search**.

Answer:

Hyperparameter Optimization

Question:

True or False: given a finite amount of computation time, grid search is more likely to find good values for hyperparameters than random search.

Answer:

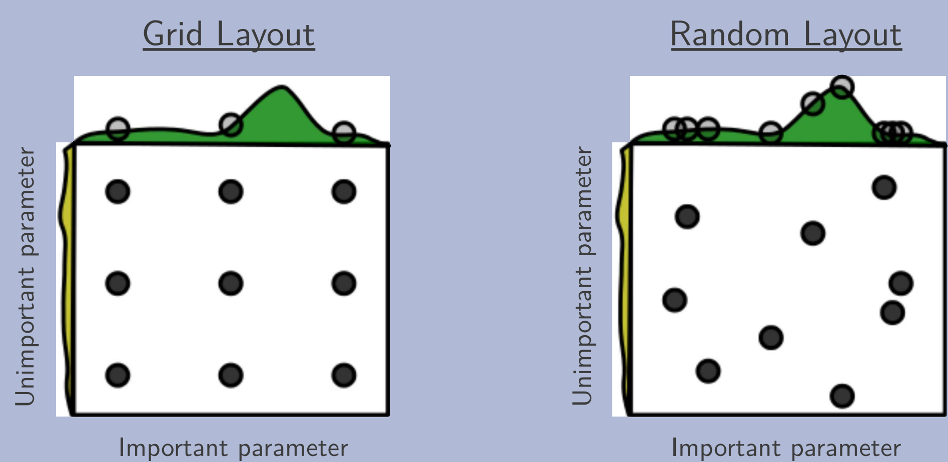


Figure 1: Grid and random search of nine trials for optimizing a function $f(x,y) = g(x) + h(y) \approx g(x)$ with low effective dimensionality. Above each square $g(x)$ is shown in green, and left of each square $h(y)$ is shown in yellow. With grid search, nine trials only test $g(x)$ in three distinct places. With random search, all nine trials explore distinct values of g. This failure of grid search is the rule rather than the exception in high dimensional hyper-parameter optimization.

Figure from Bergstra & Bengio (2012)

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
- Define "instance-based learning" or "nonparametric methods"
- Select an appropriate algorithm for optimizing (aka. learning) hyperparameters