10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
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Model Selection

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Lecture 4
January 29, 2018

Q&A

Q: How do we deal with ties in k-Nearest Neighbors (e.g. even k or equidistant points)?

A: I would ask you all for a good solution!

Q: How do we define a distance function when the features are categorical (e.g. weather takes values {sunny, rainy, overcast})?

A: Step 1: Convert from categorical attributes to numeric features (e.g. binary)

Step 2: Select an appropriate distance function (e.g. Hamming distance)

Reminders

- **Homework 2: Decision Trees**
  - Out: Wed, Jan 24
  - Due: Mon, Feb 5 at 11:59pm
- **10601 Notation Crib Sheet**

K-NEAREST NEIGHBORS

k-Nearest Neighbors

Chalkboard:

- KNN for binary classification
- Distance functions
- Efficiency of KNN
- Inductive bias of KNN
- KNN Properties

KNN ON FISHER IRIS DATA

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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Species	Sepal Length	Sepal Width
0	4.3	3.0
0	4.9	3.6
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

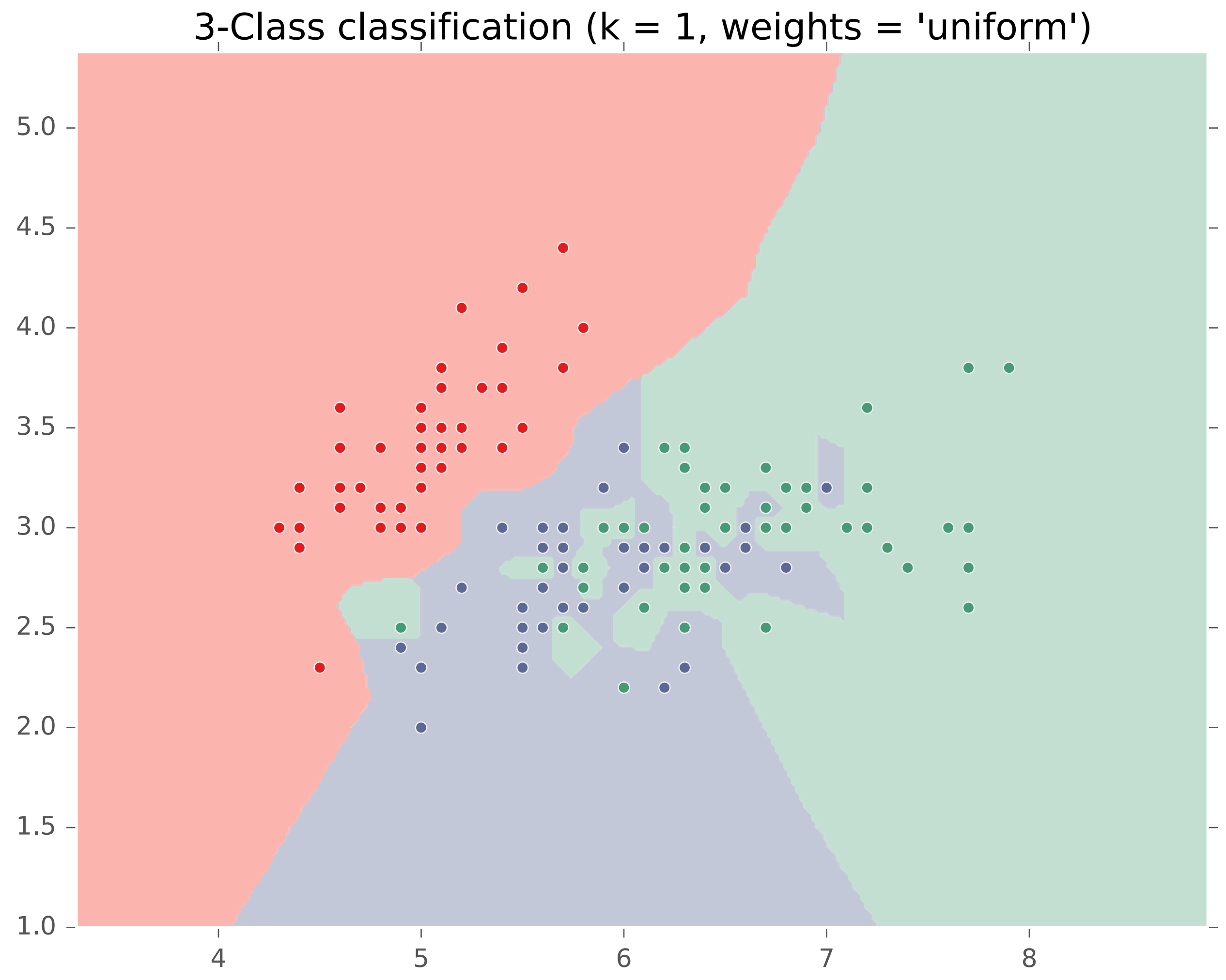
Deleted two of the four features, so that input space is 2D

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

KNN on Fisher Iris Data

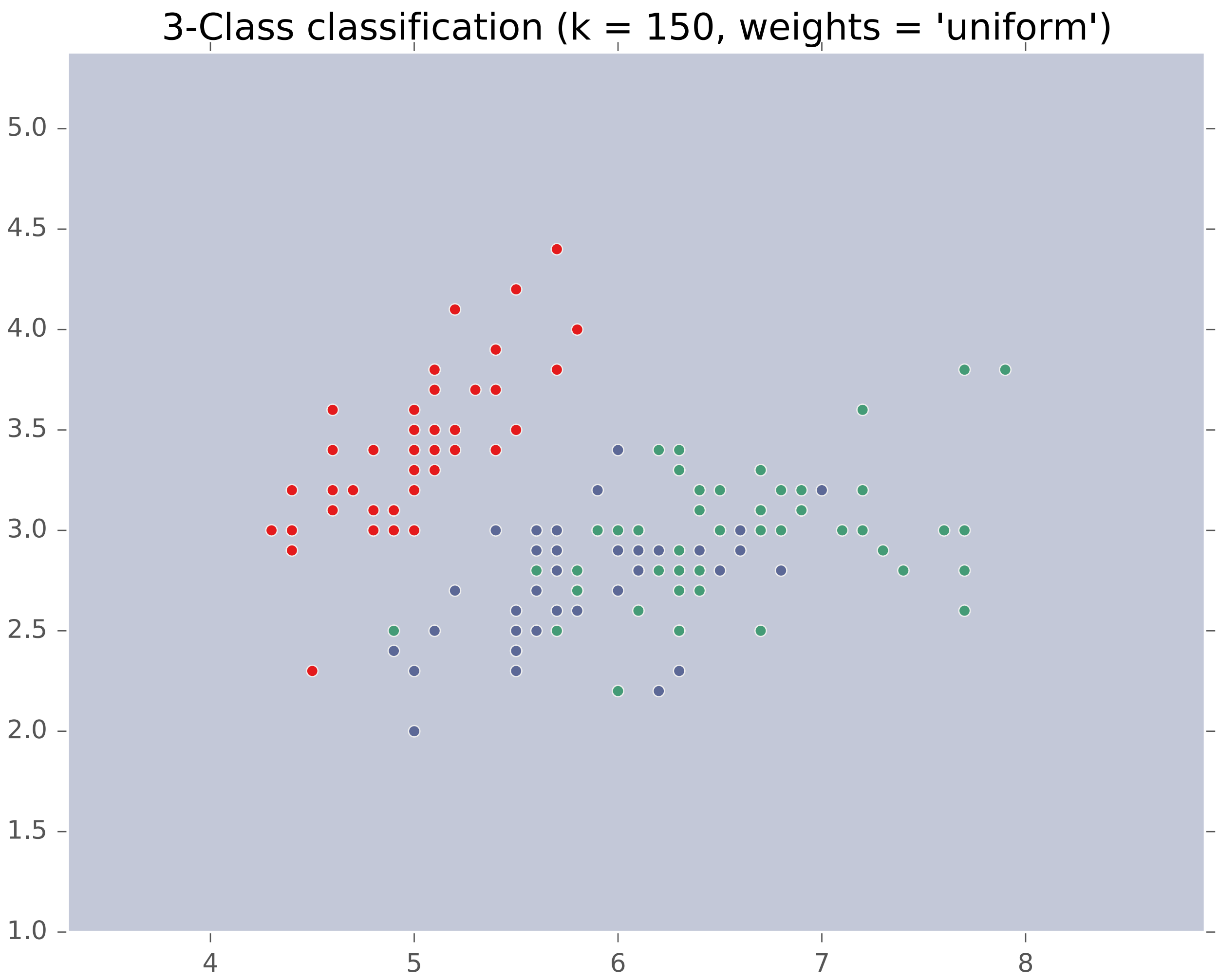
KNN on Fisher Iris Data

Special Case: Nearest Neighbor



KNN on Fisher Iris Data

Special Case: Majority Vote



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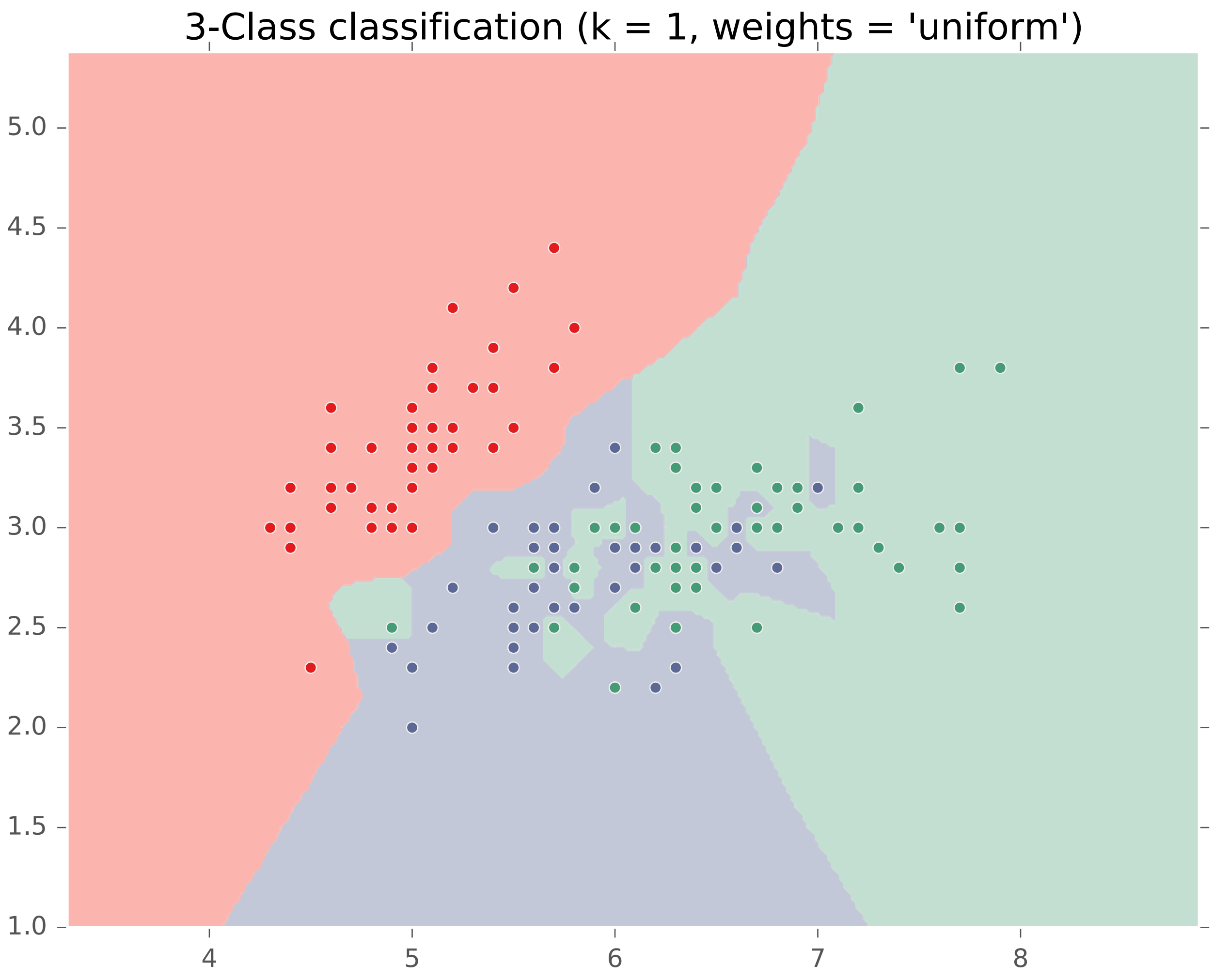

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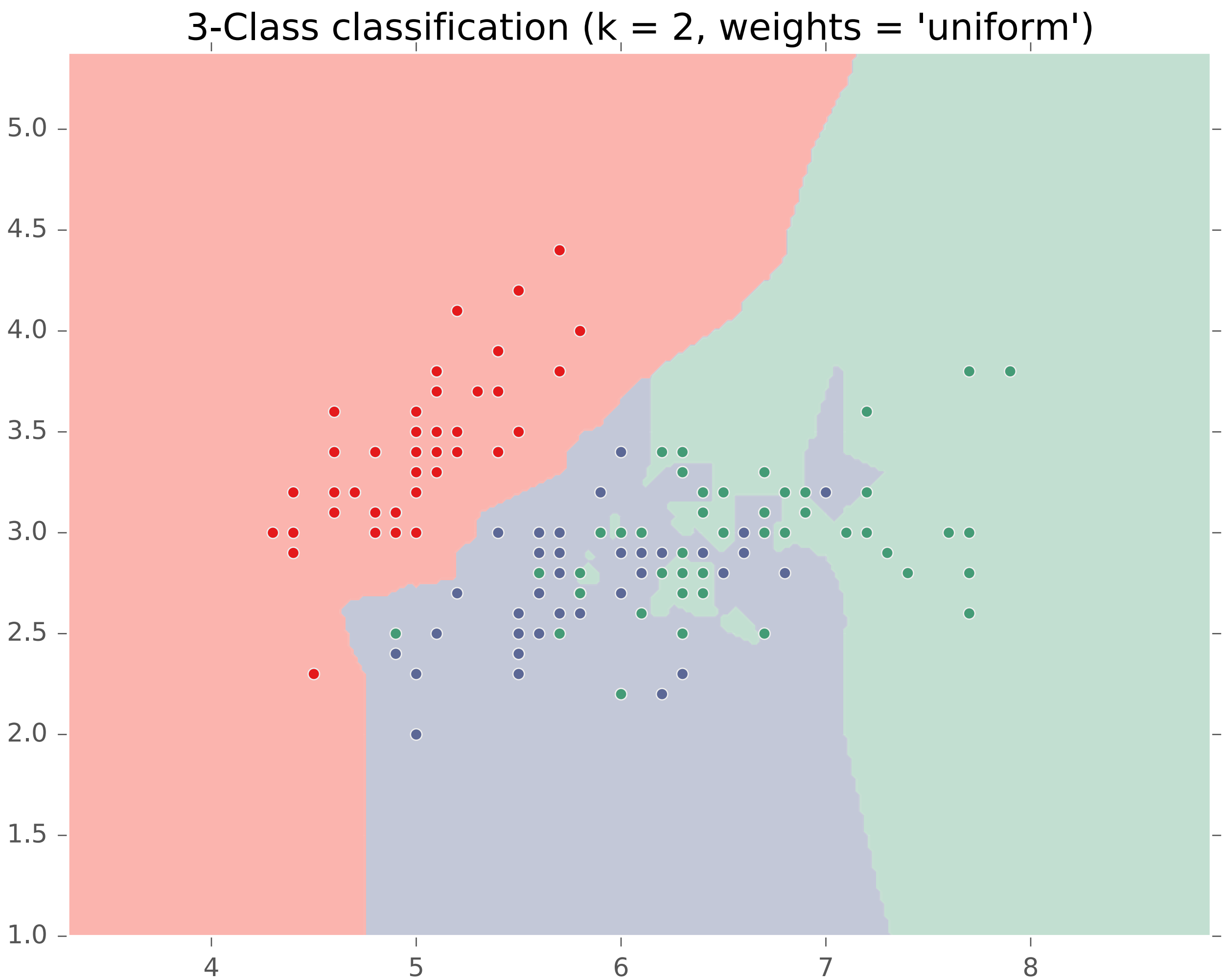

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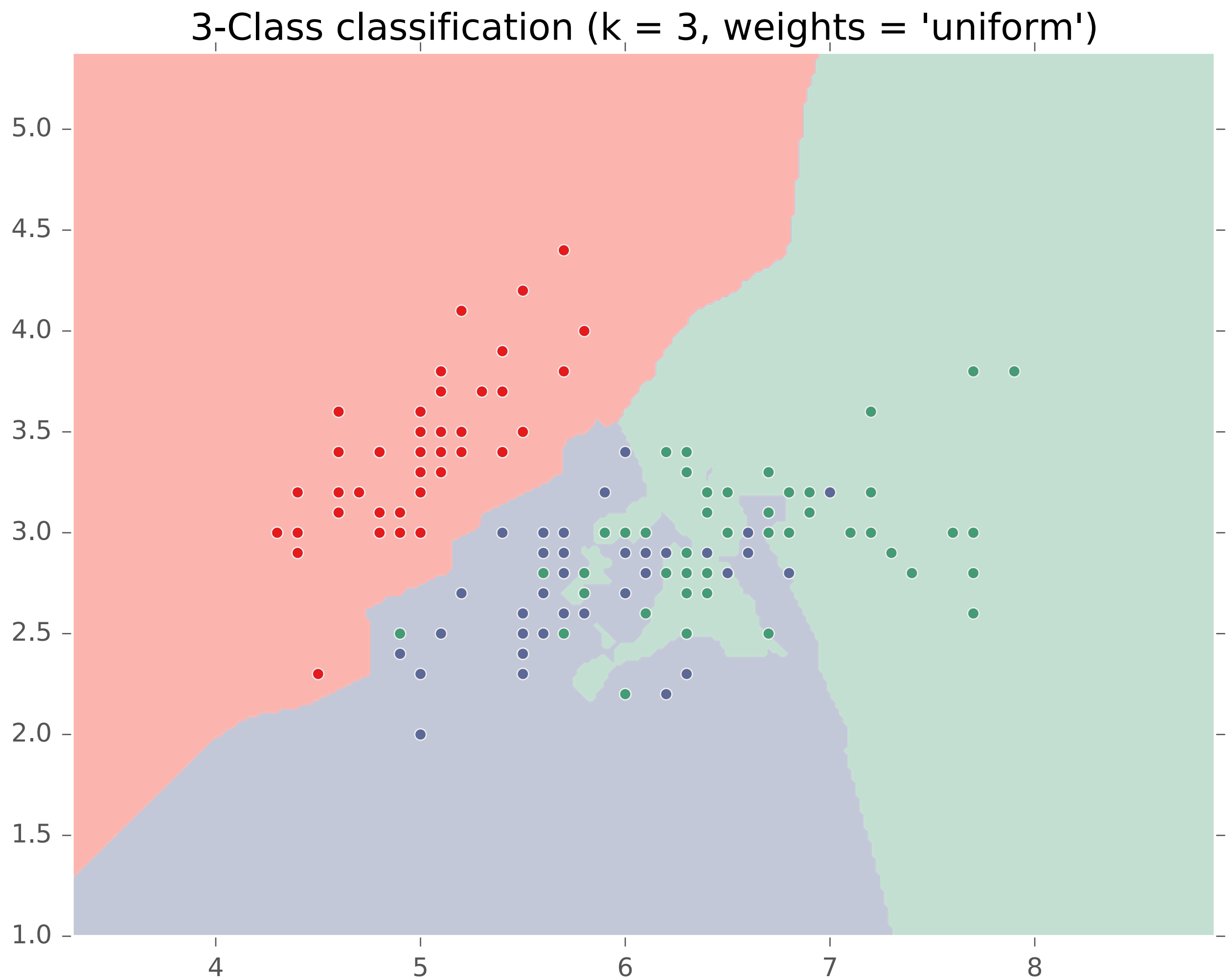

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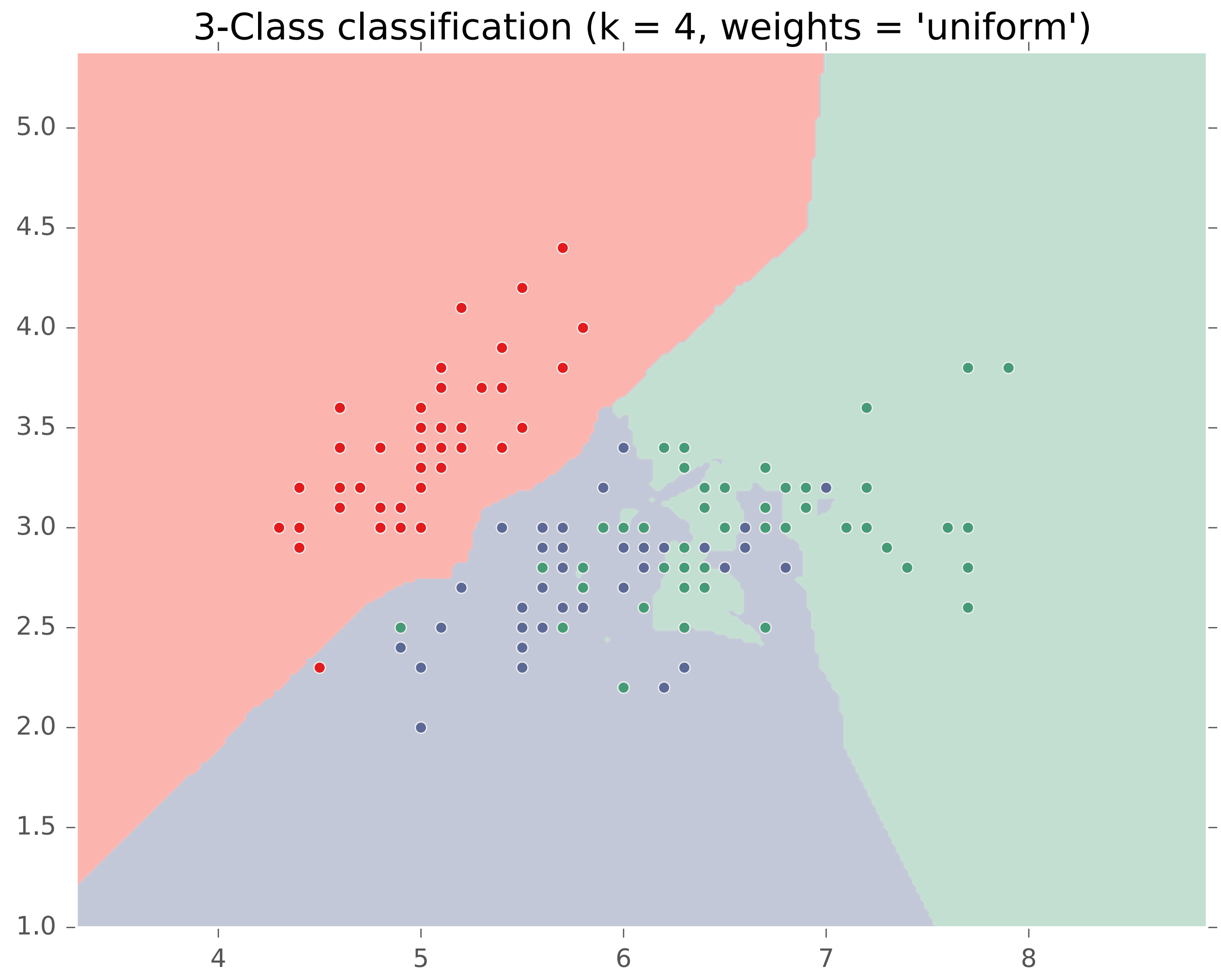

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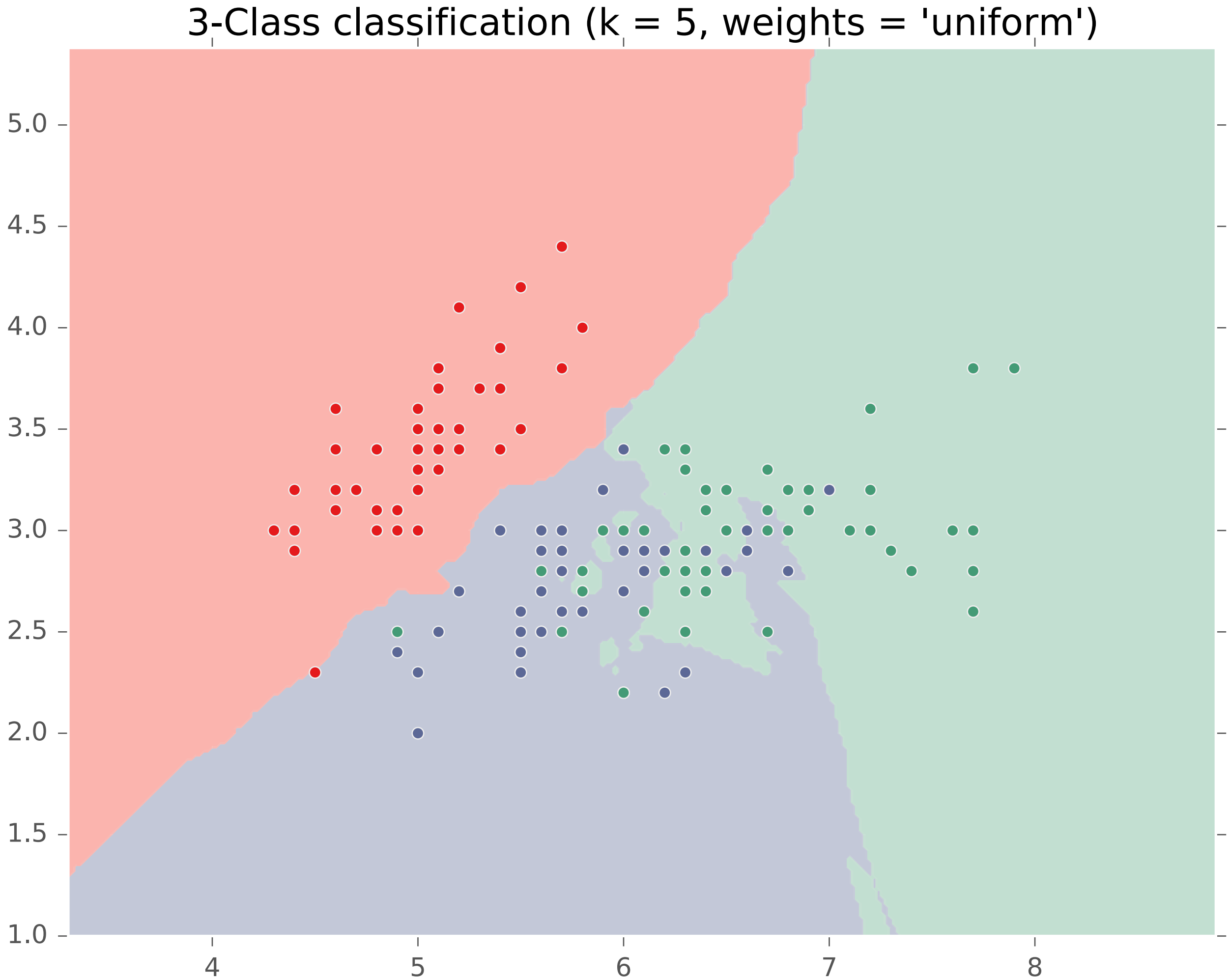

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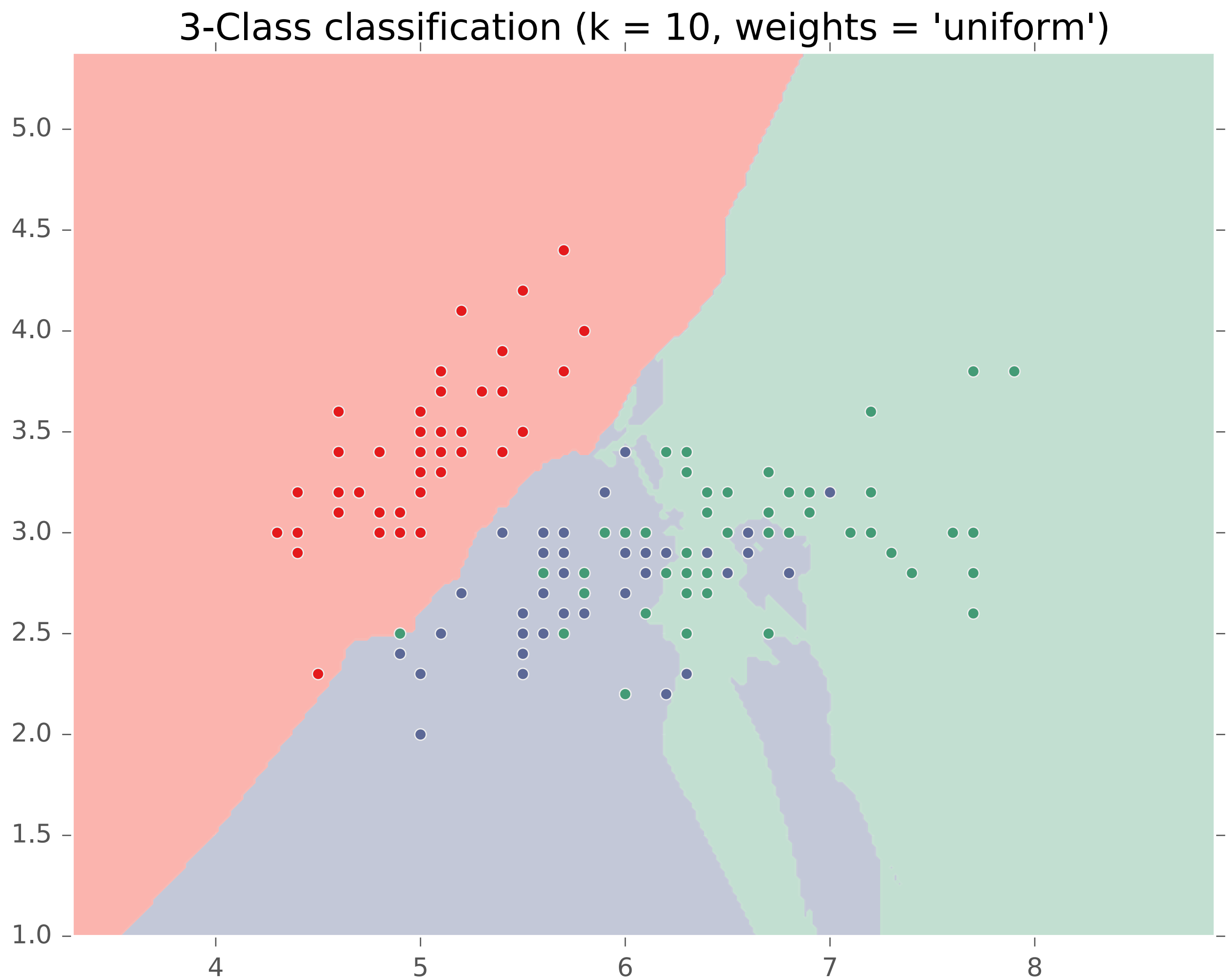

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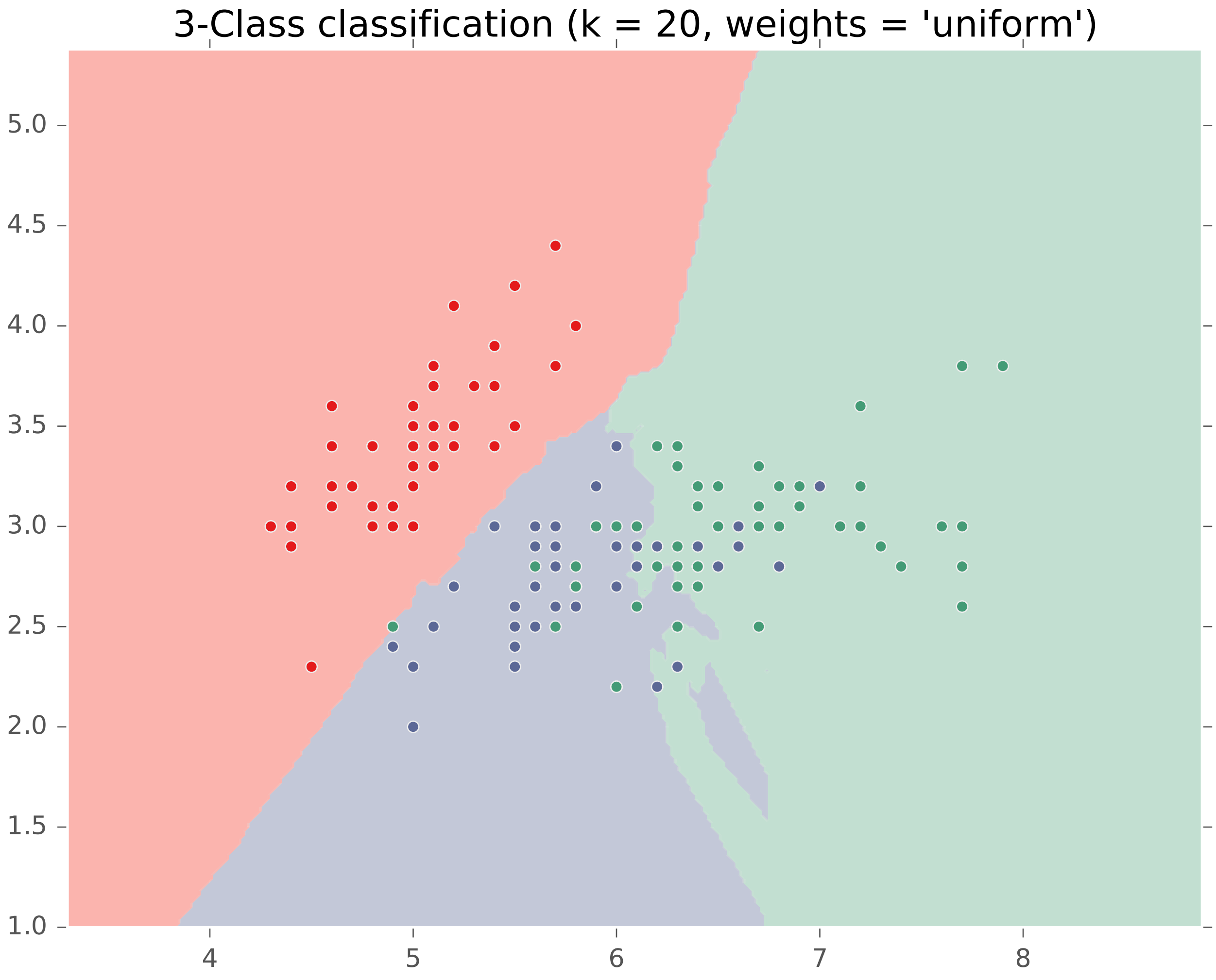

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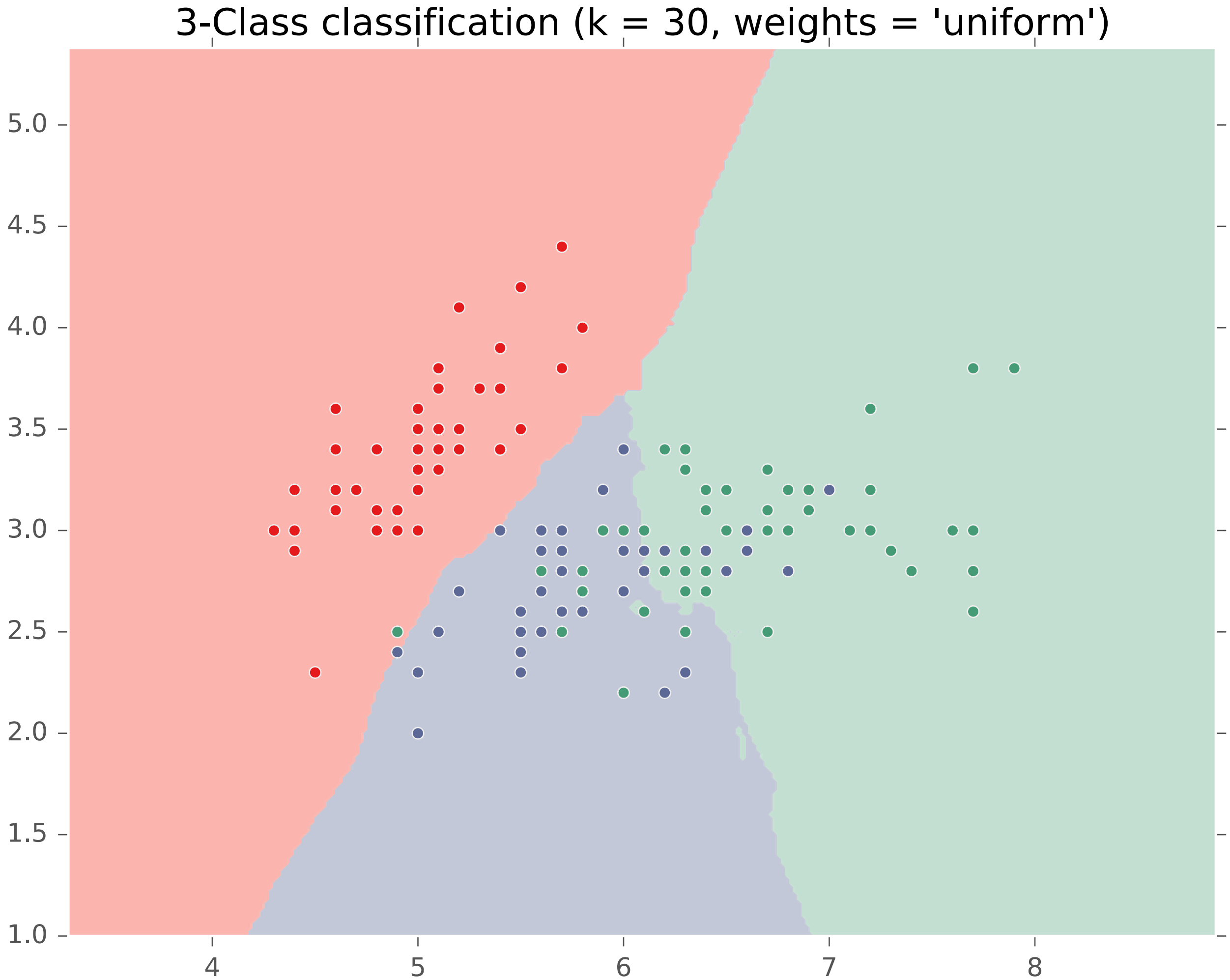

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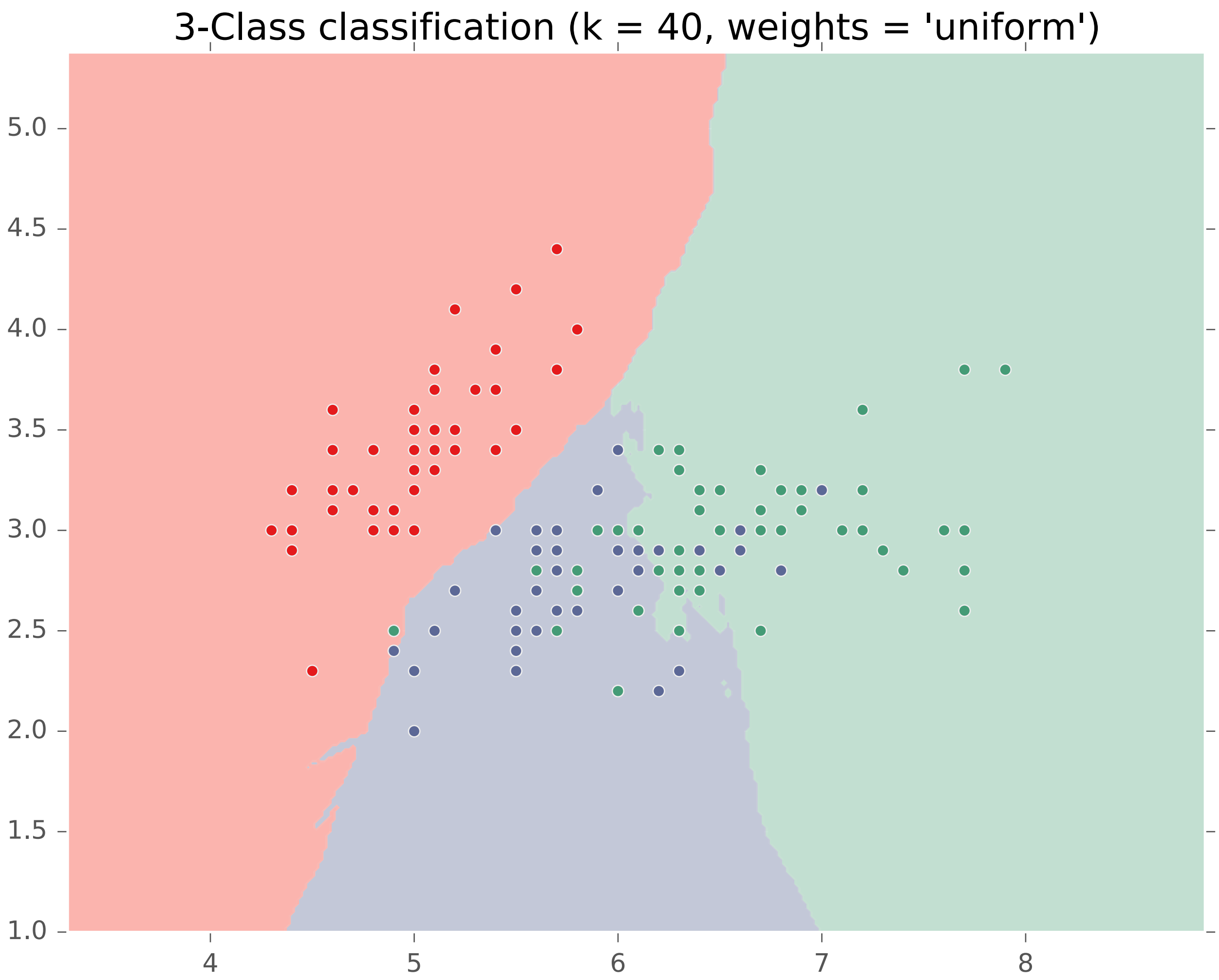

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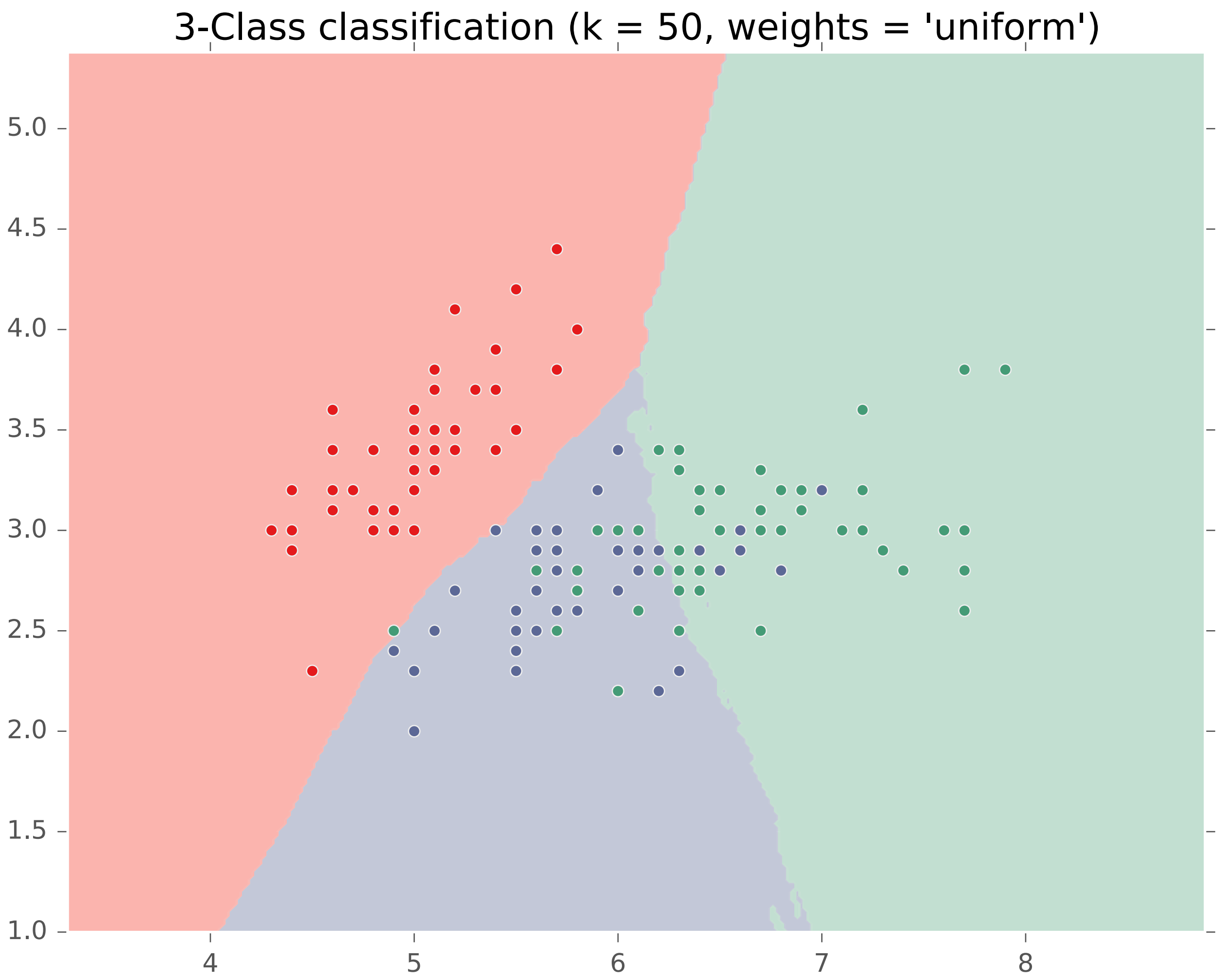

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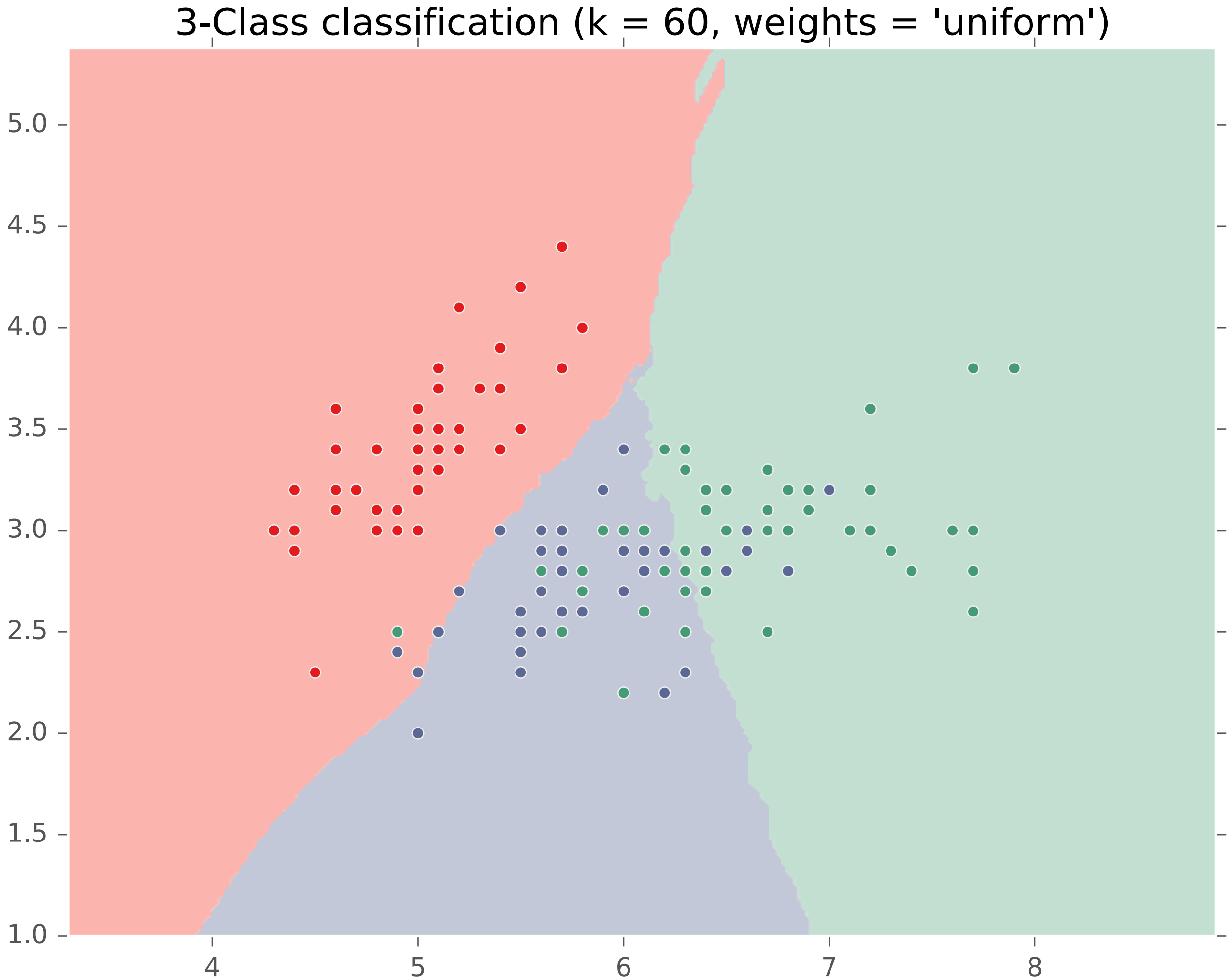

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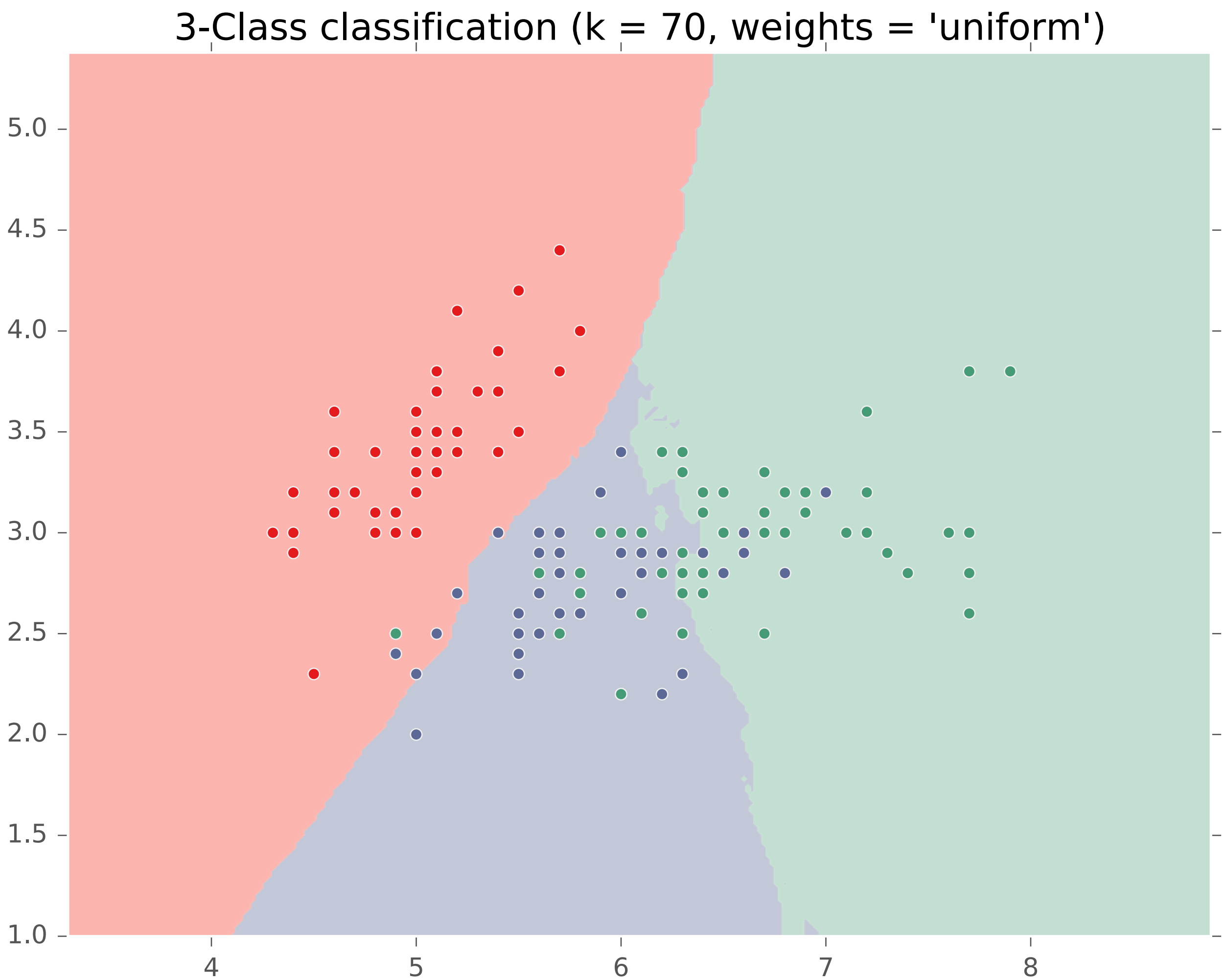

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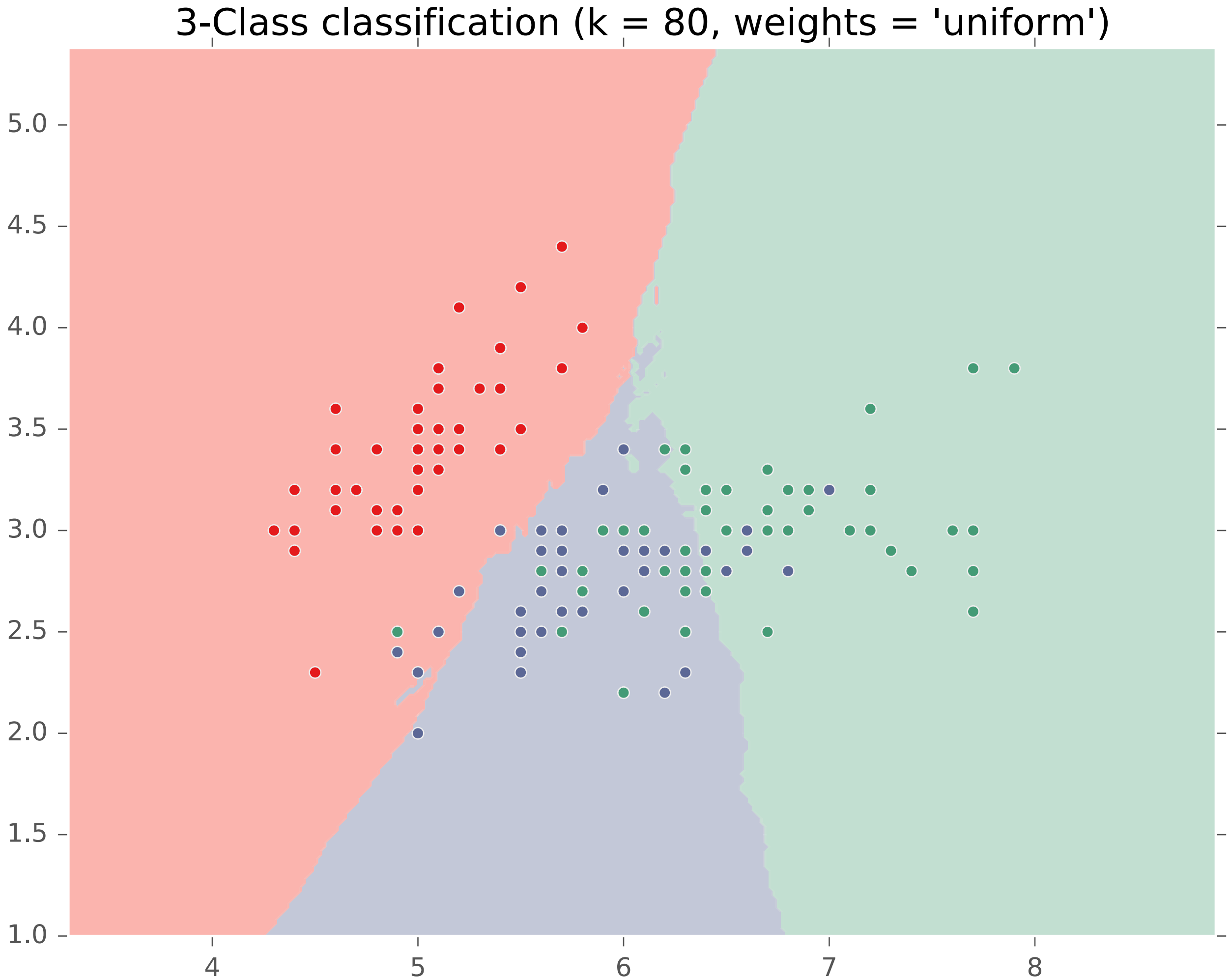

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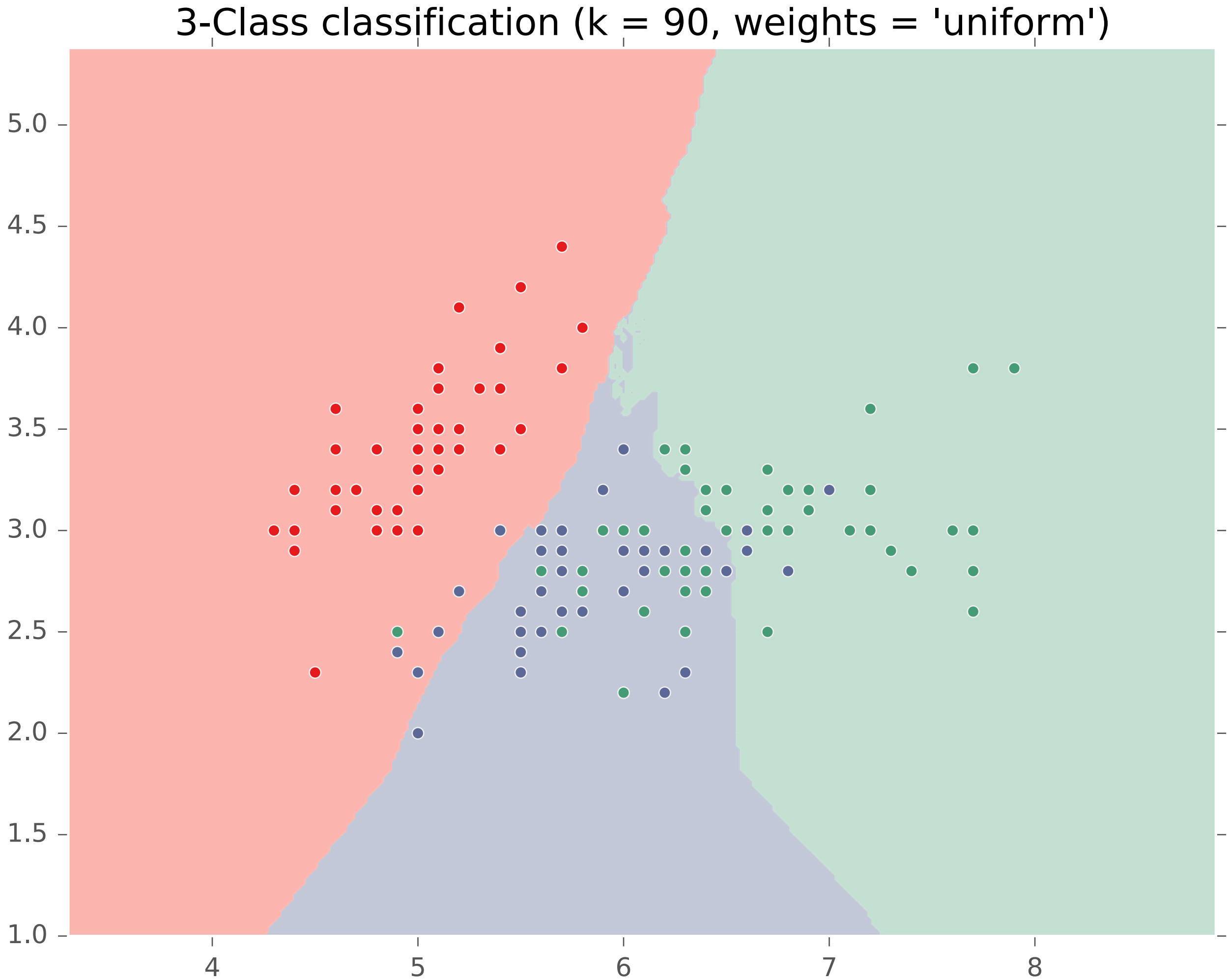

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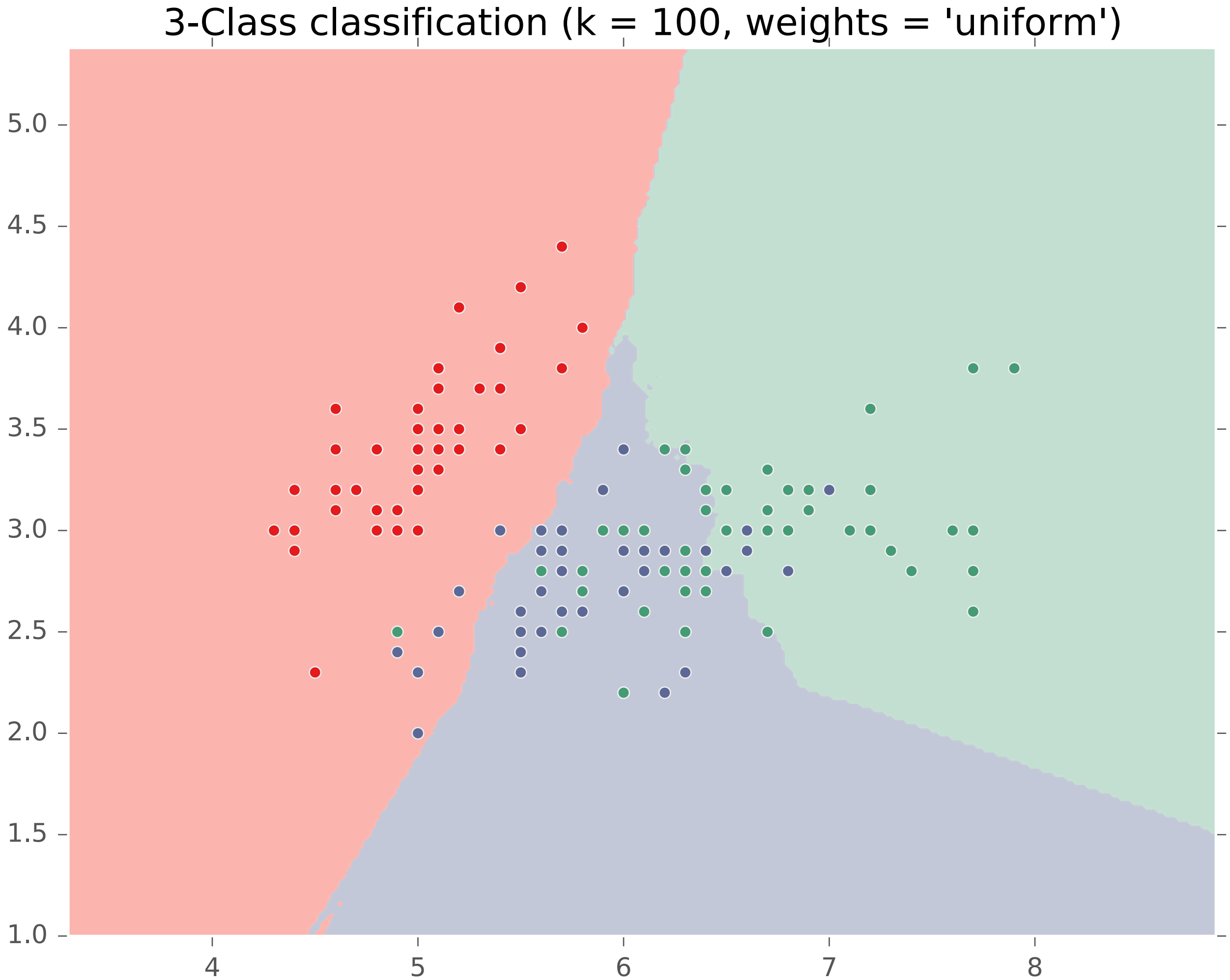

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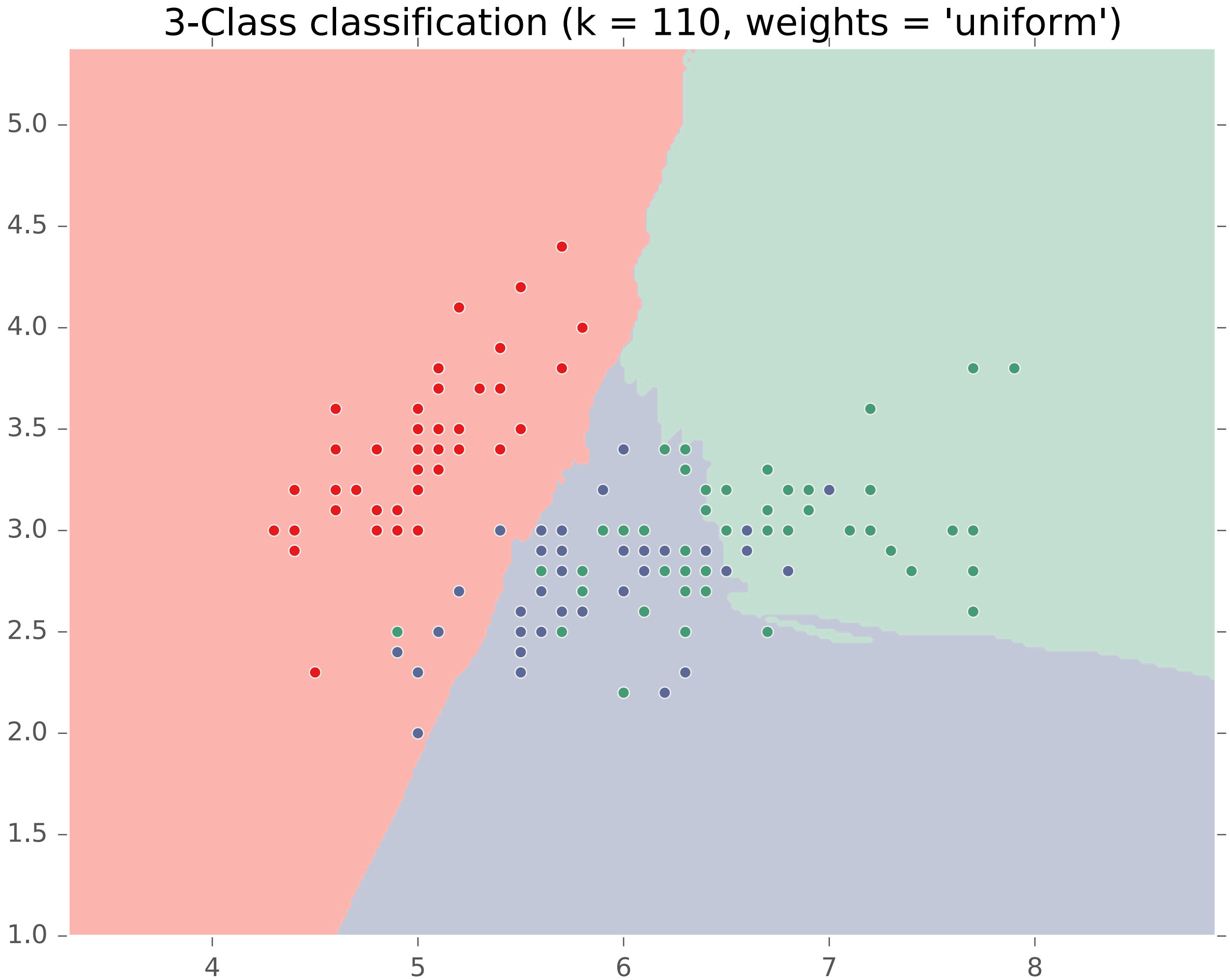

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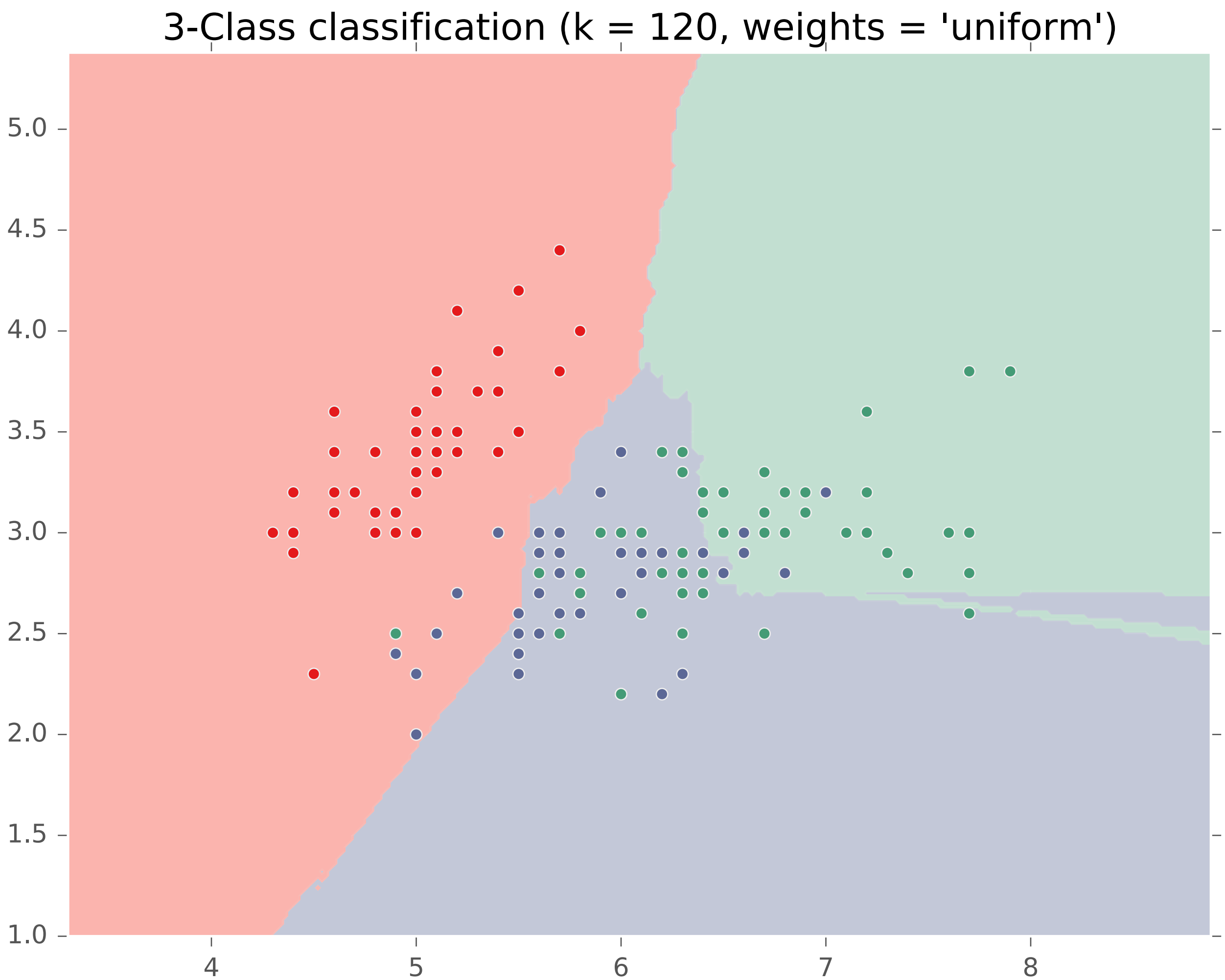

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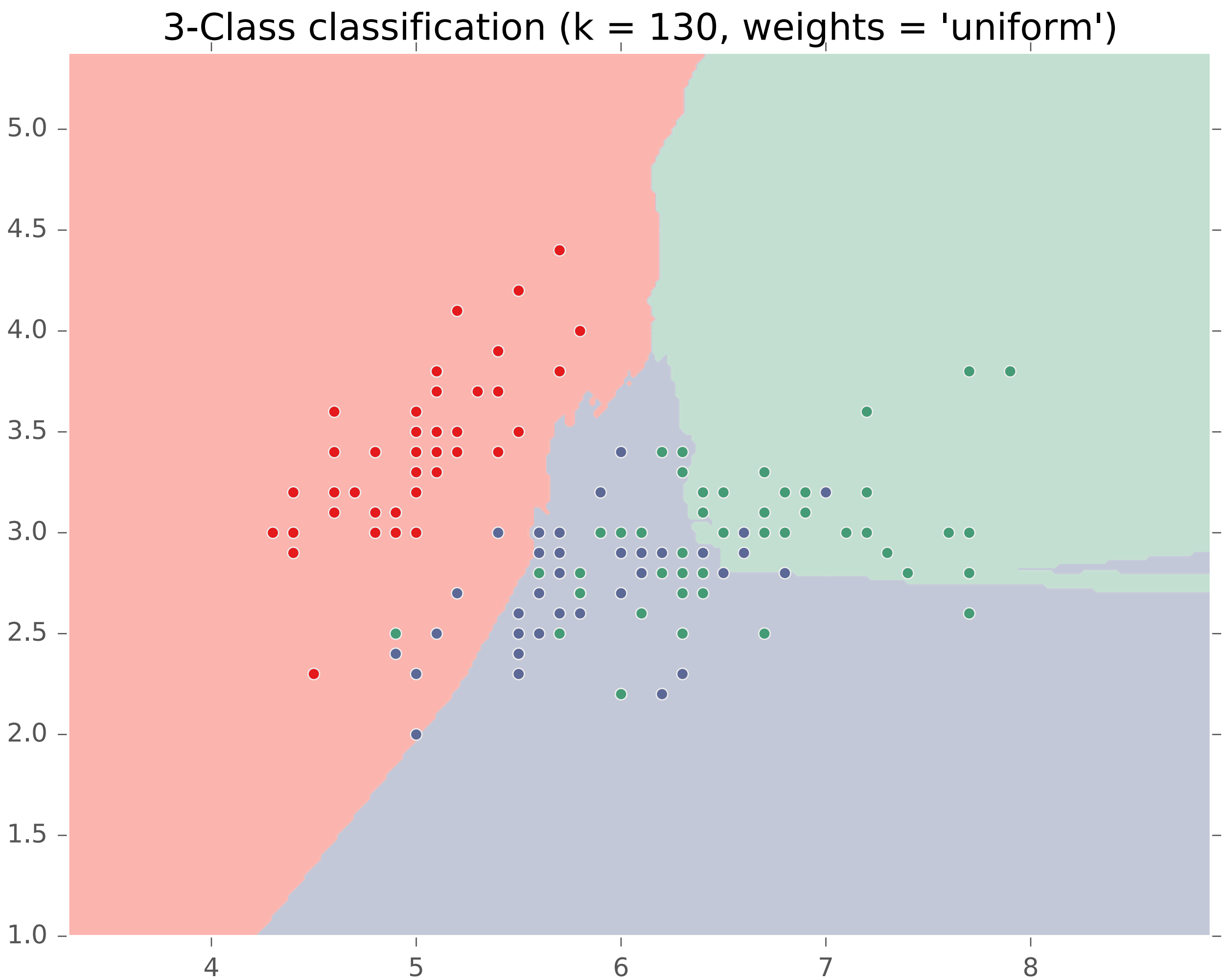

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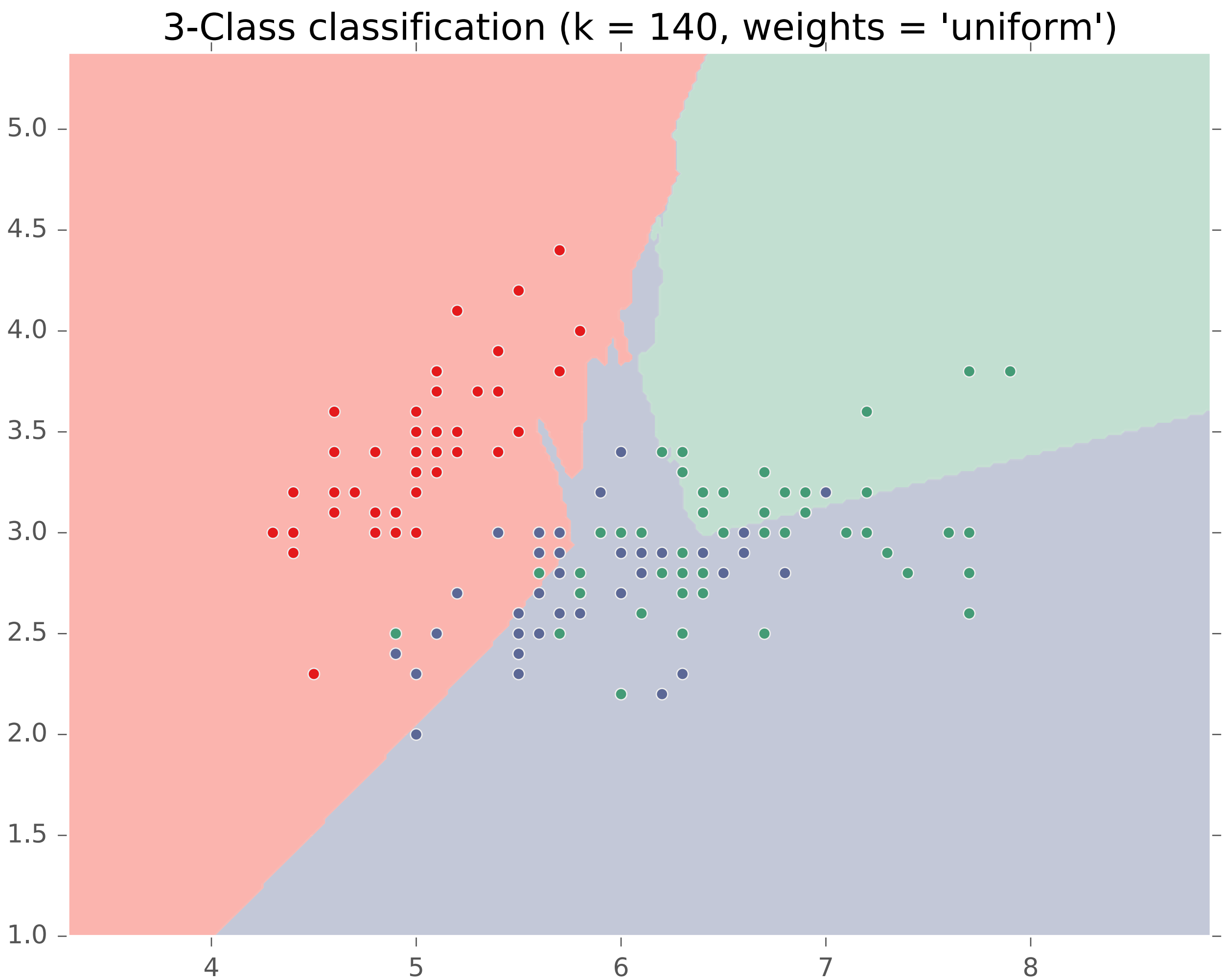

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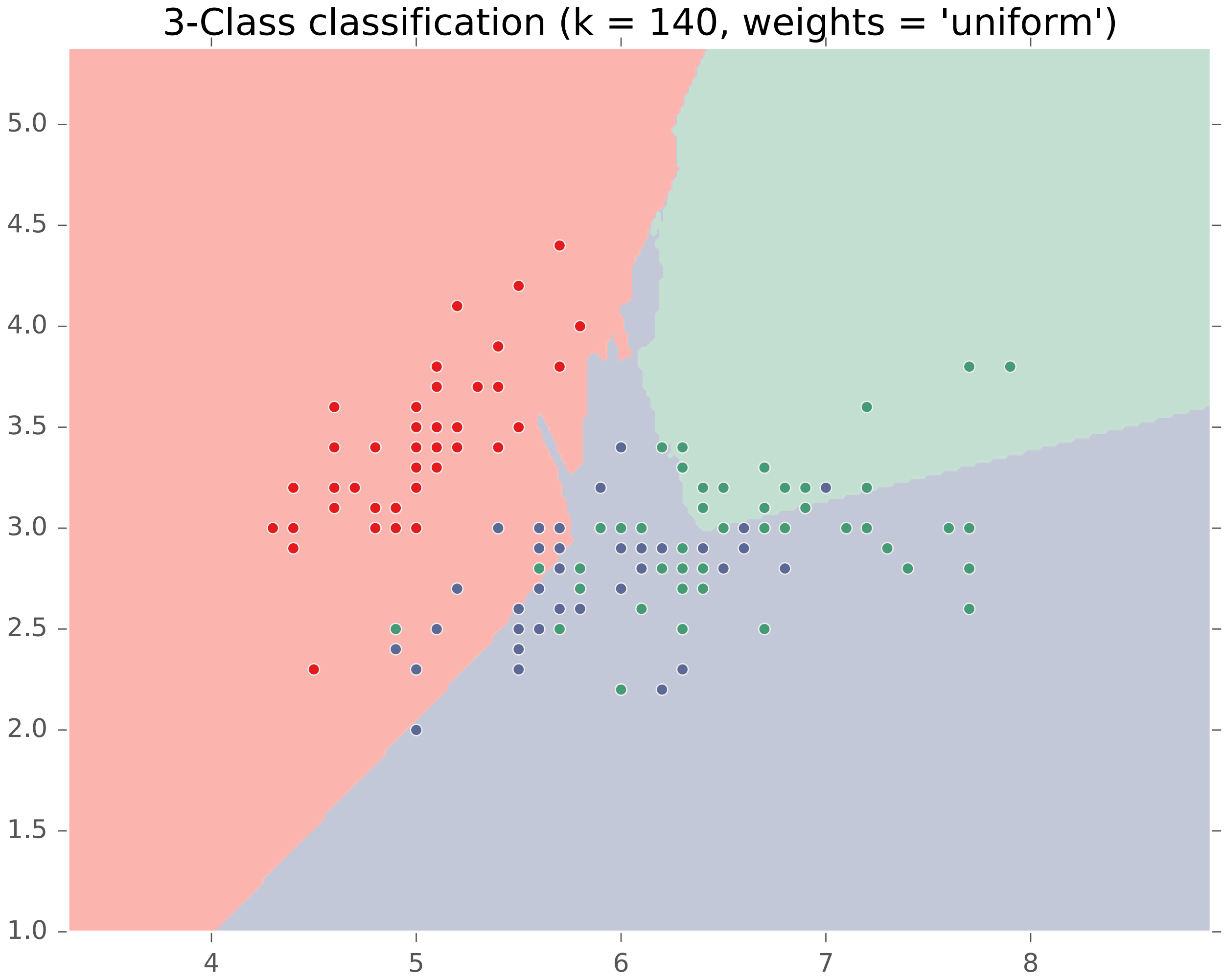
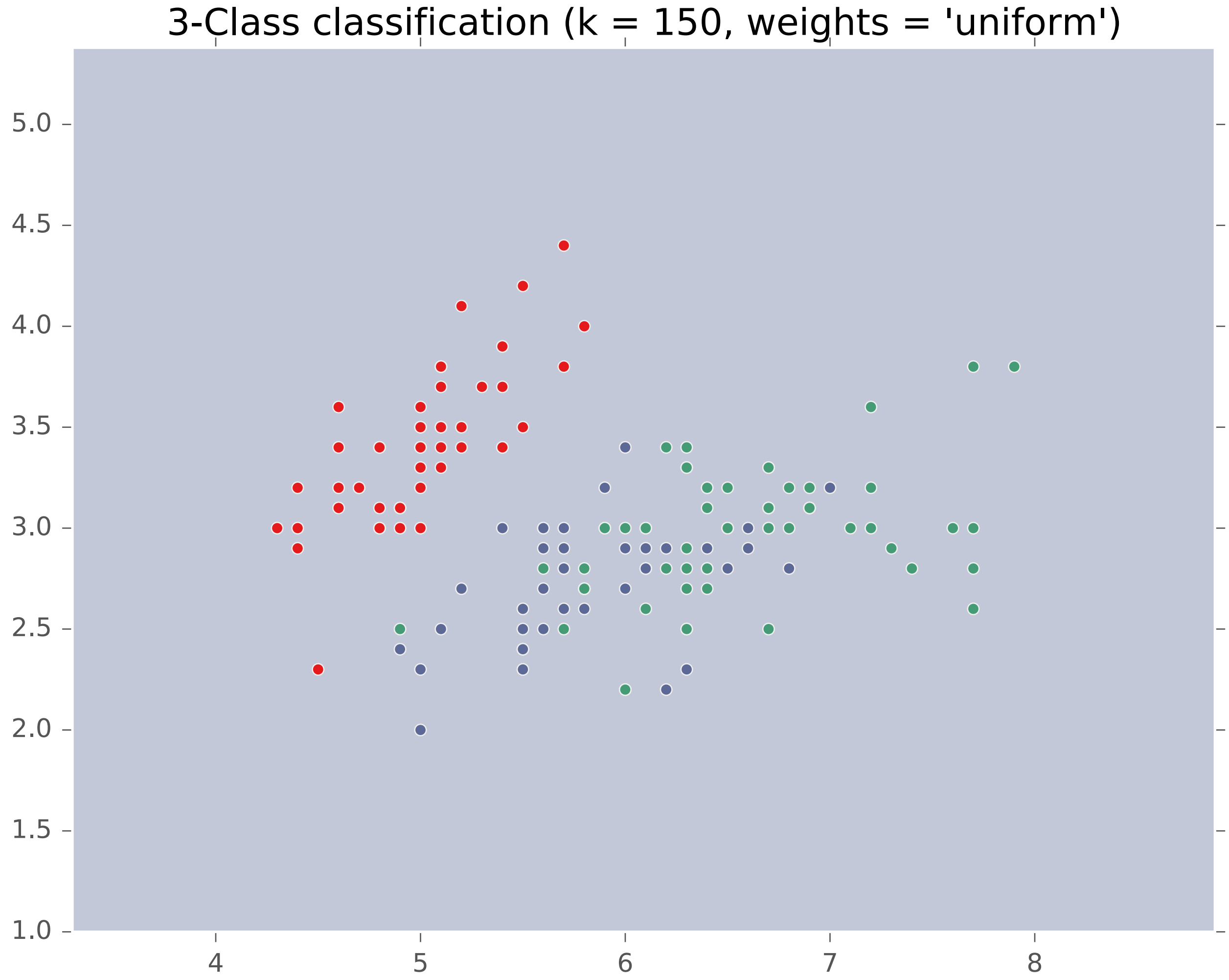


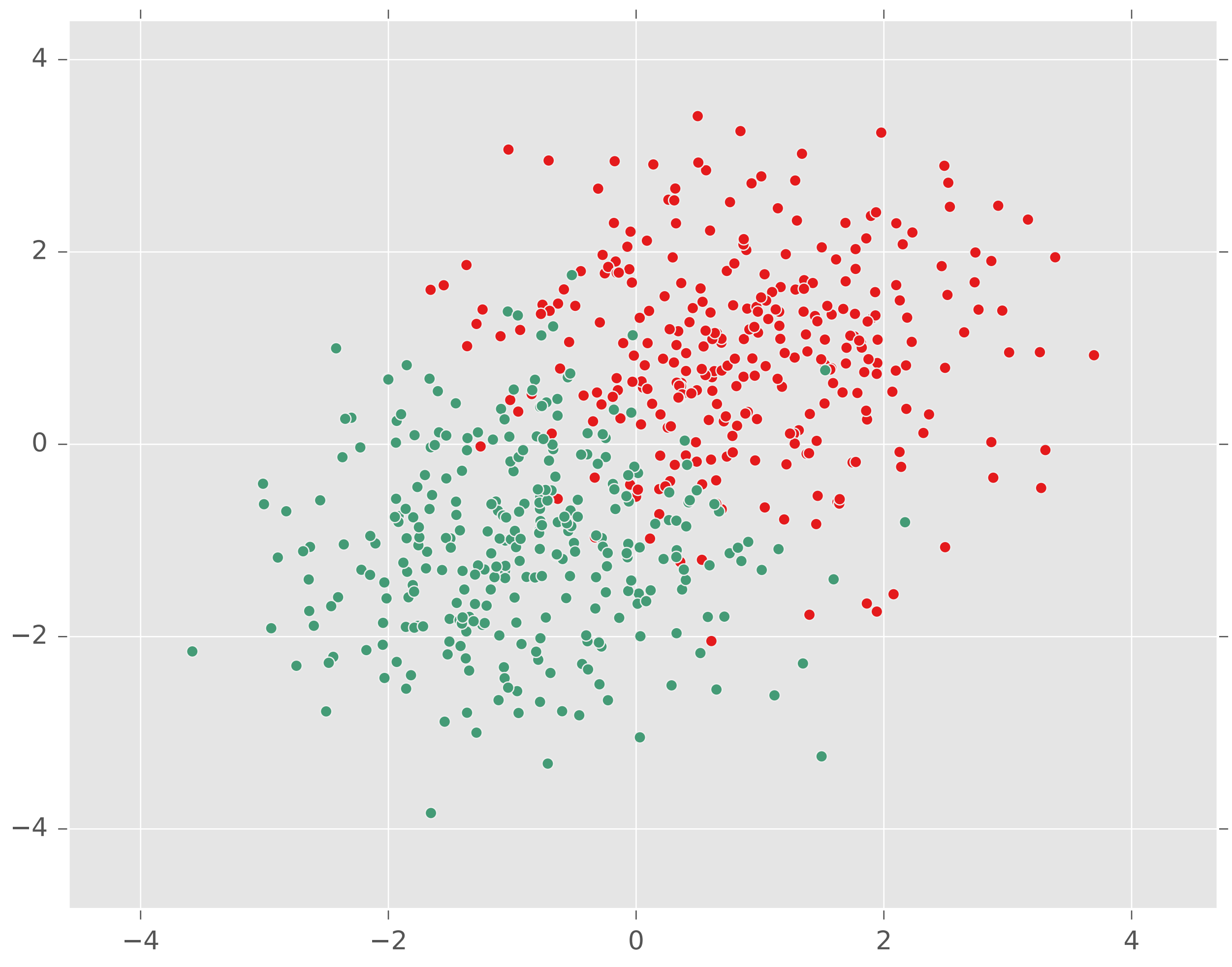
KNN on Fisher Iris Data

Special Case: Majority Vote



KNN ON GAUSSIAN DATA

KNN on Gaussian Data



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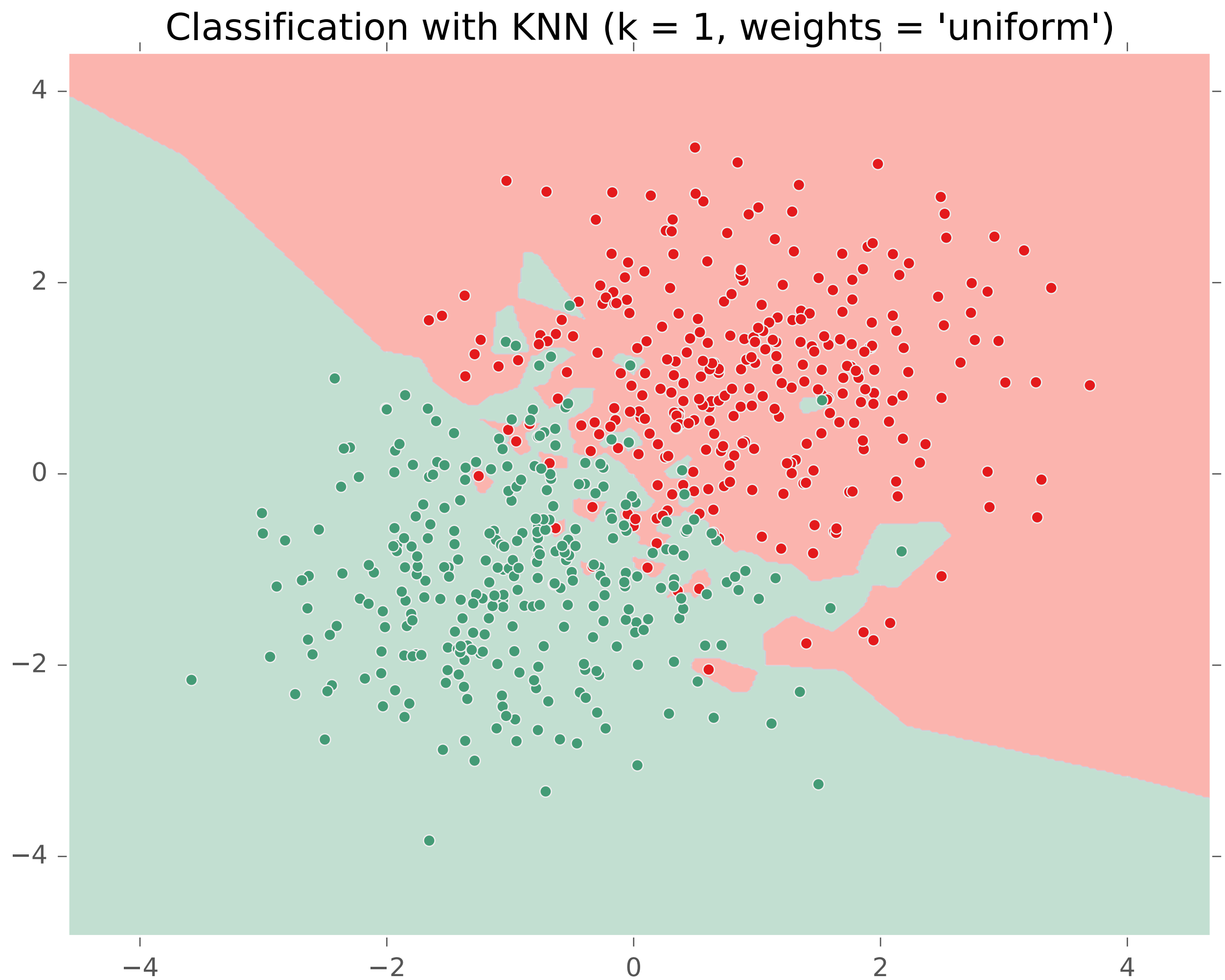

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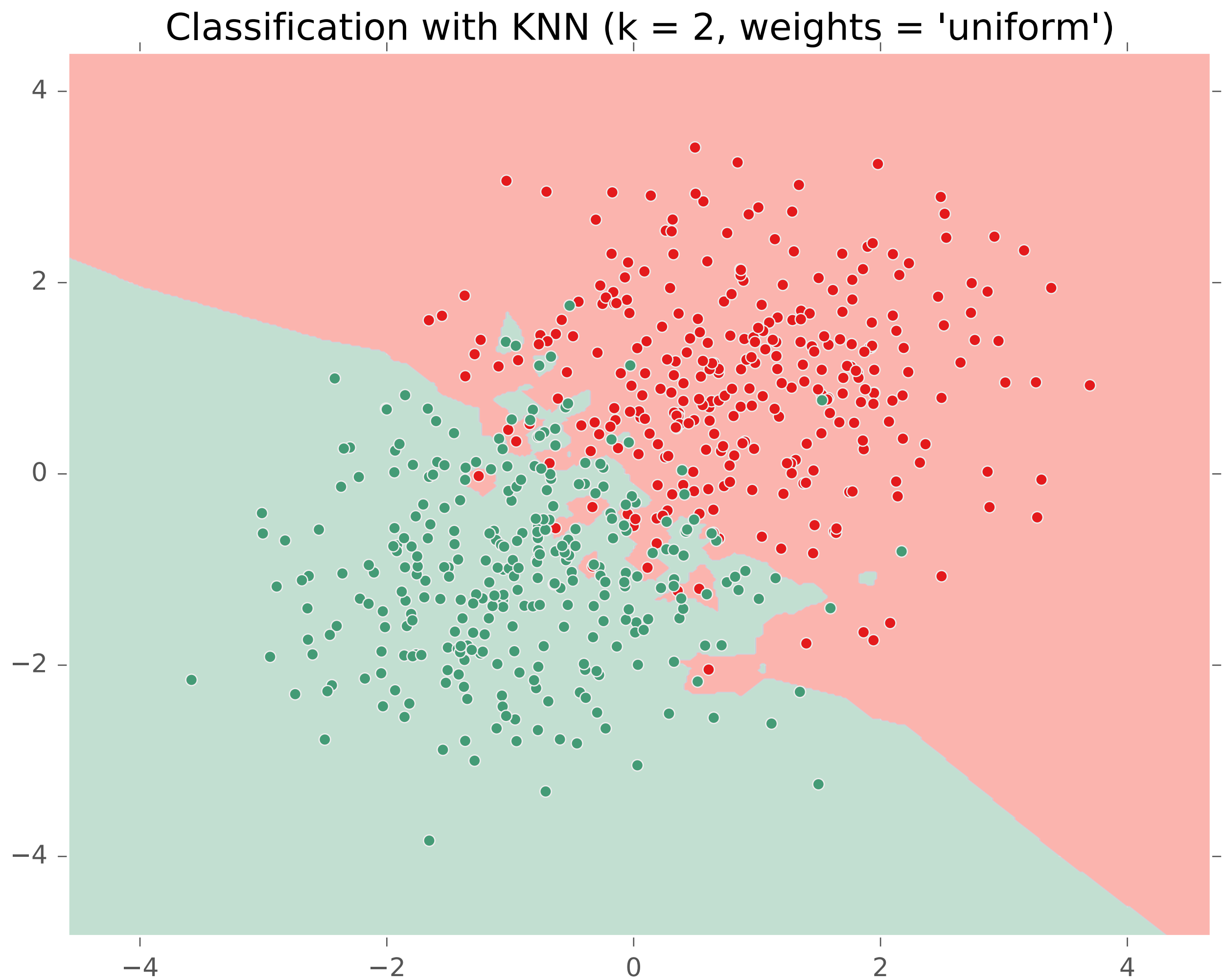

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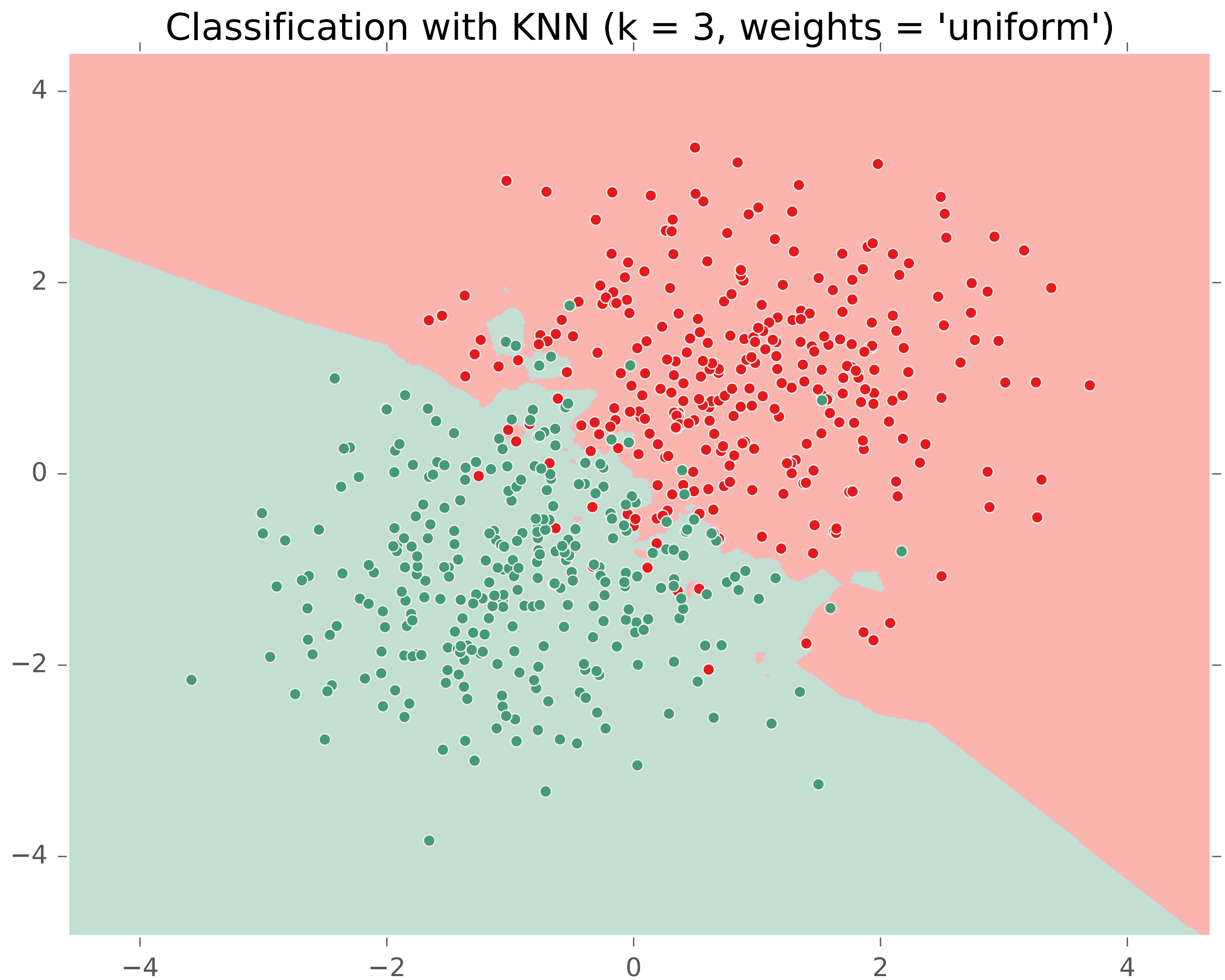

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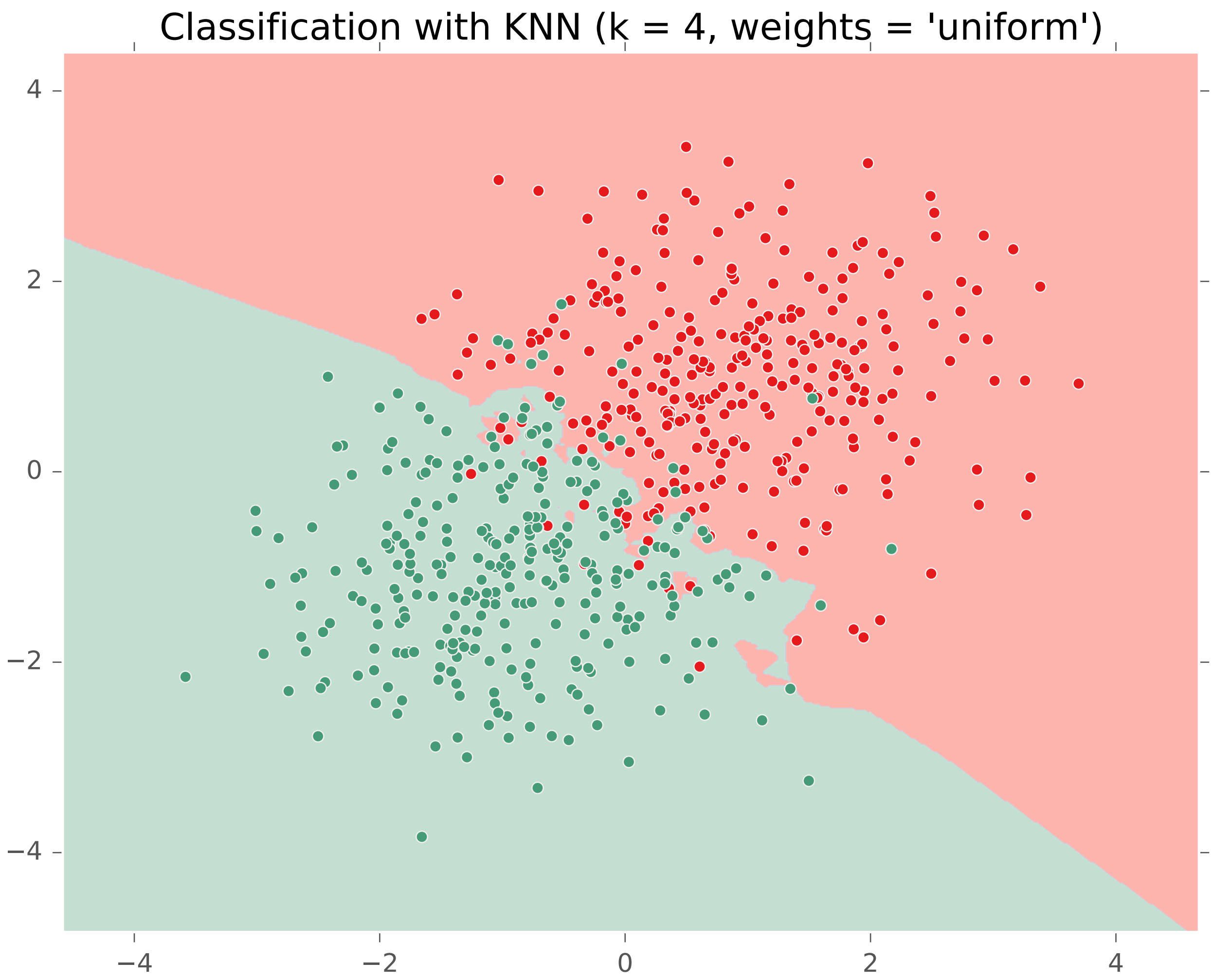

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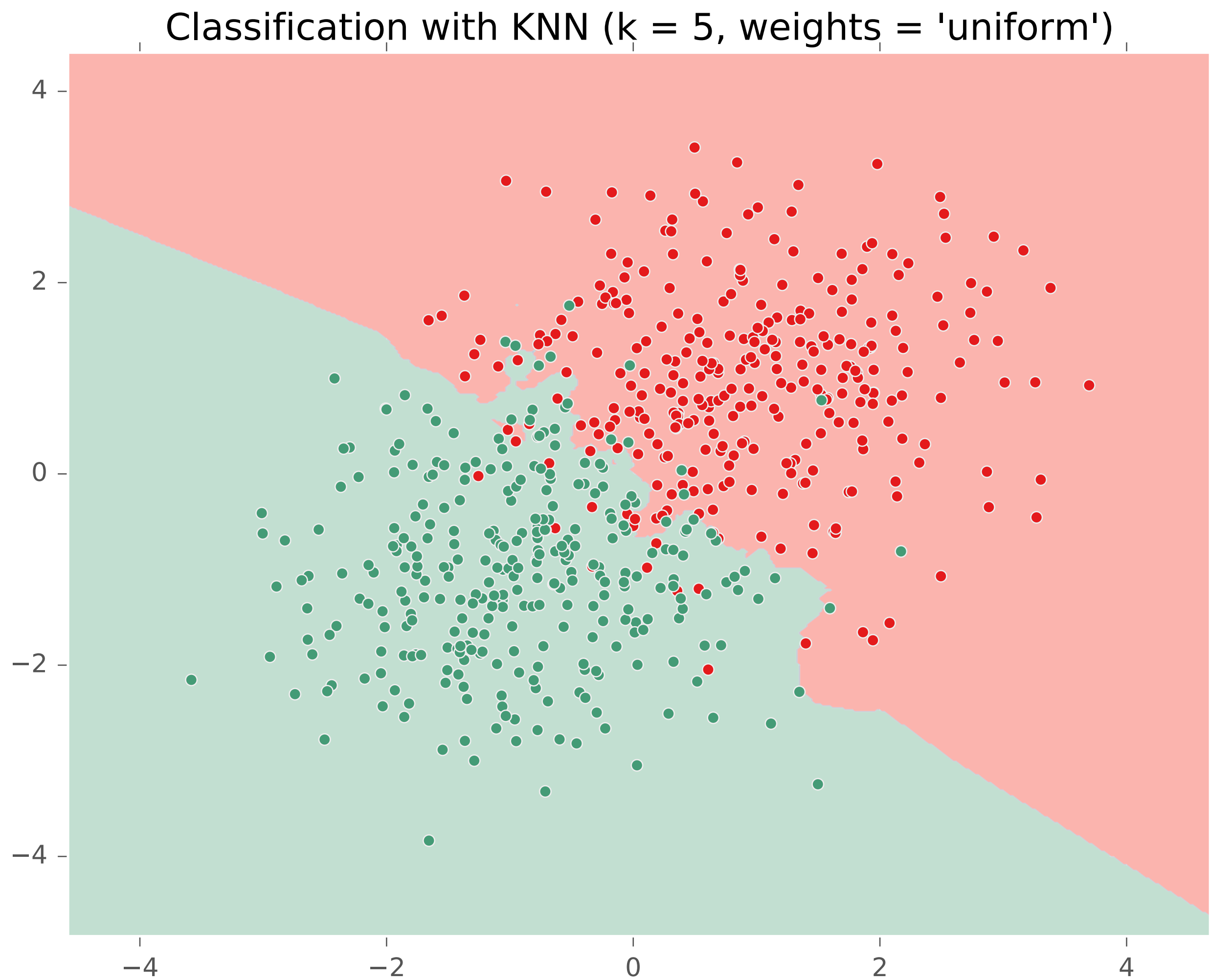

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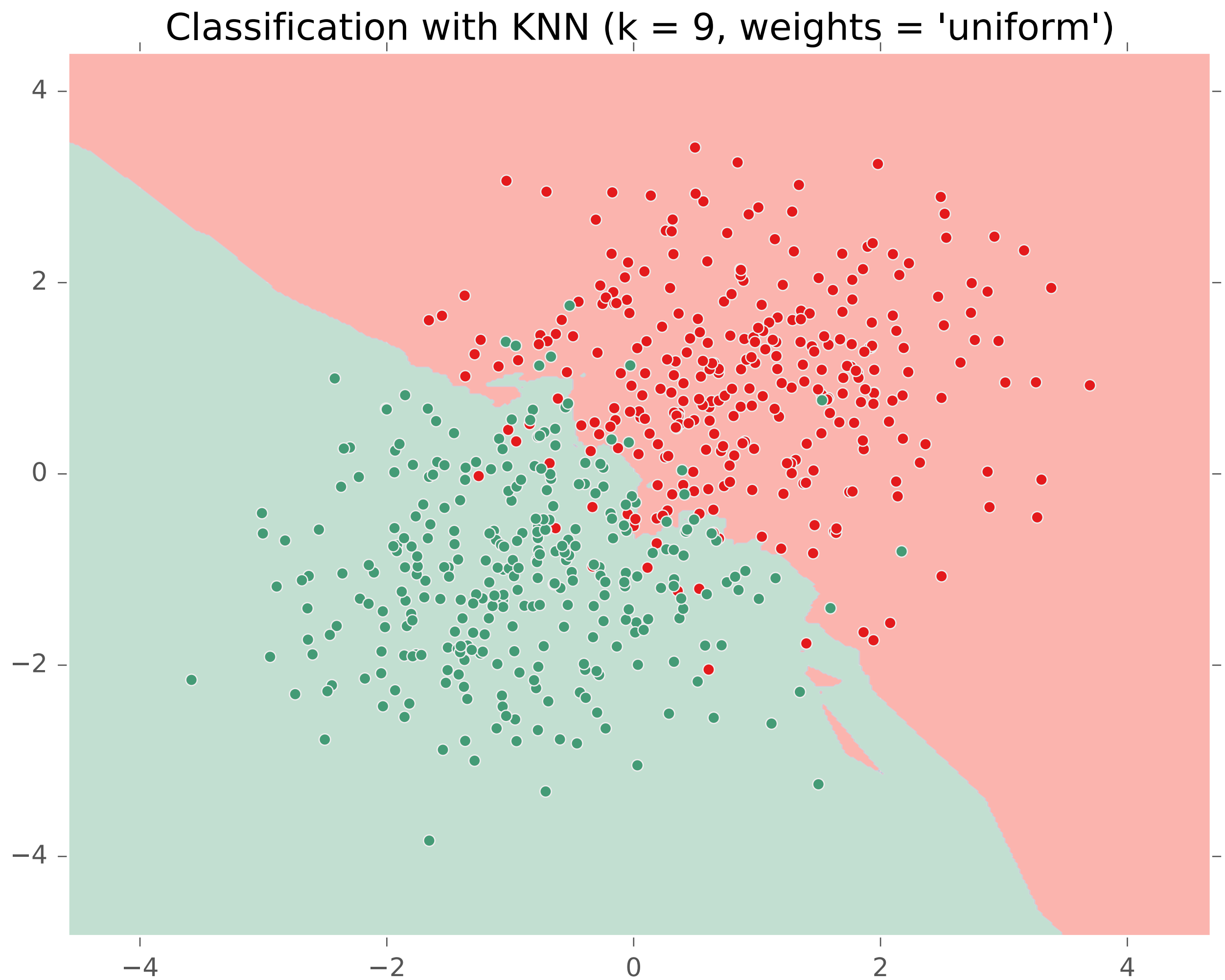

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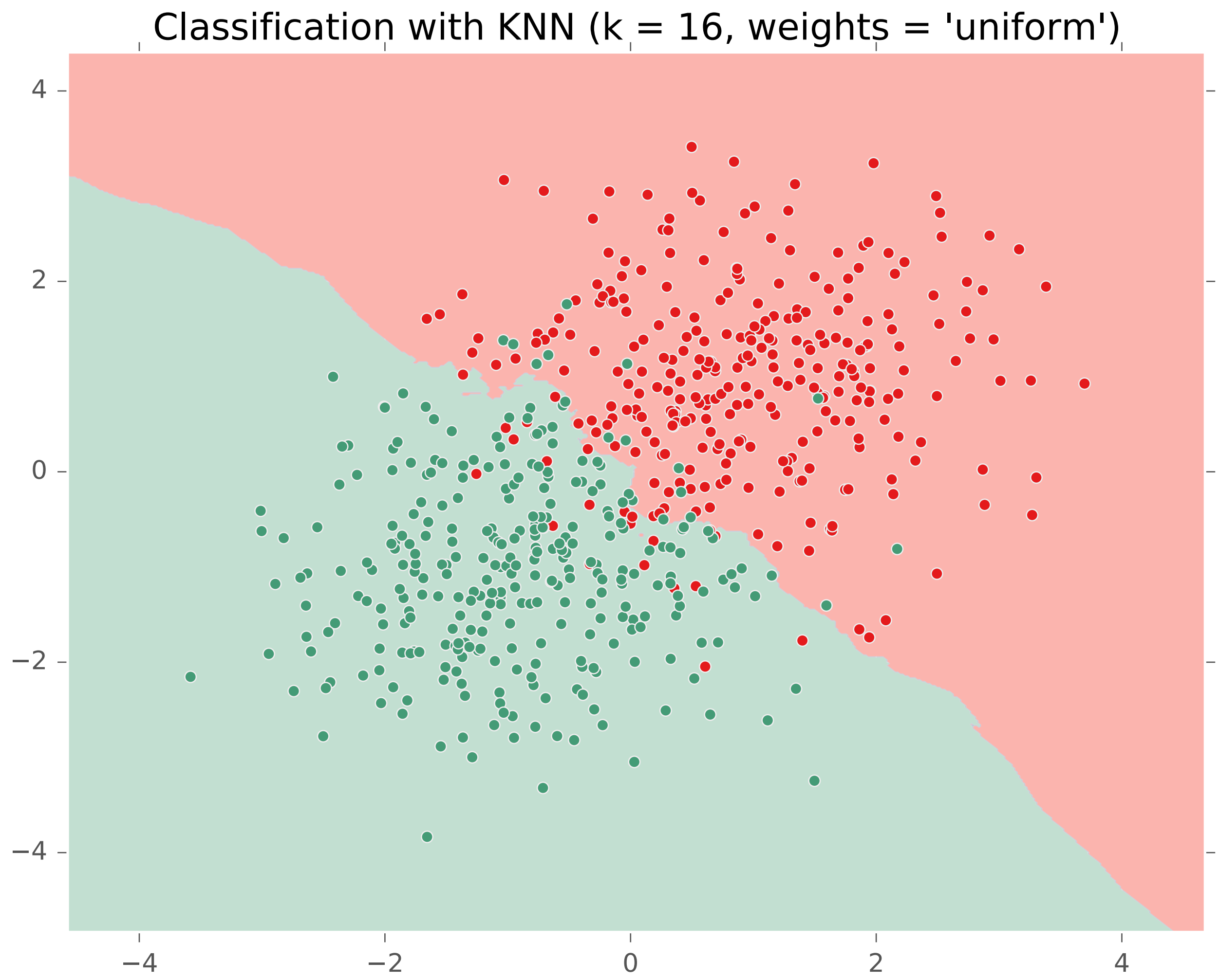

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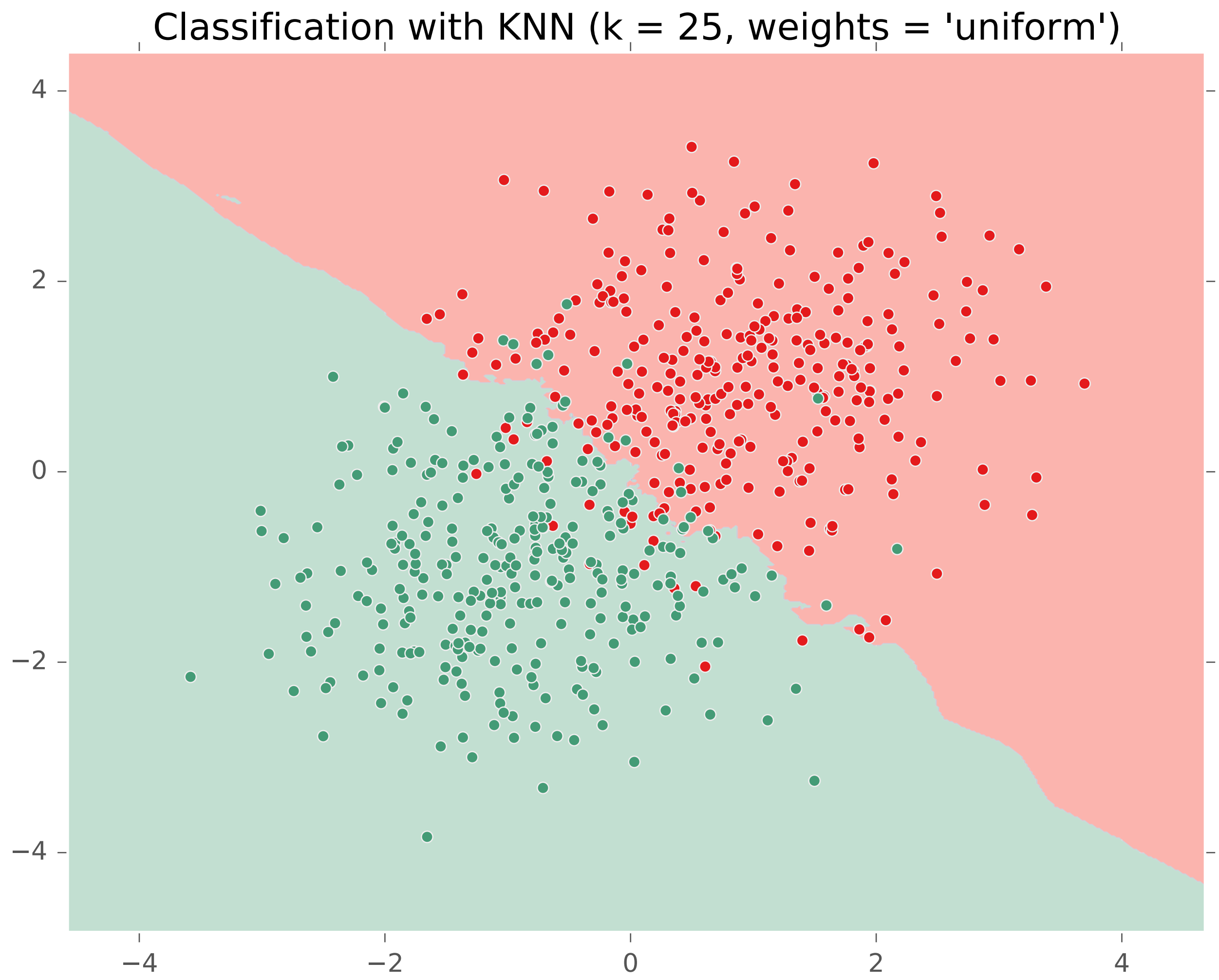

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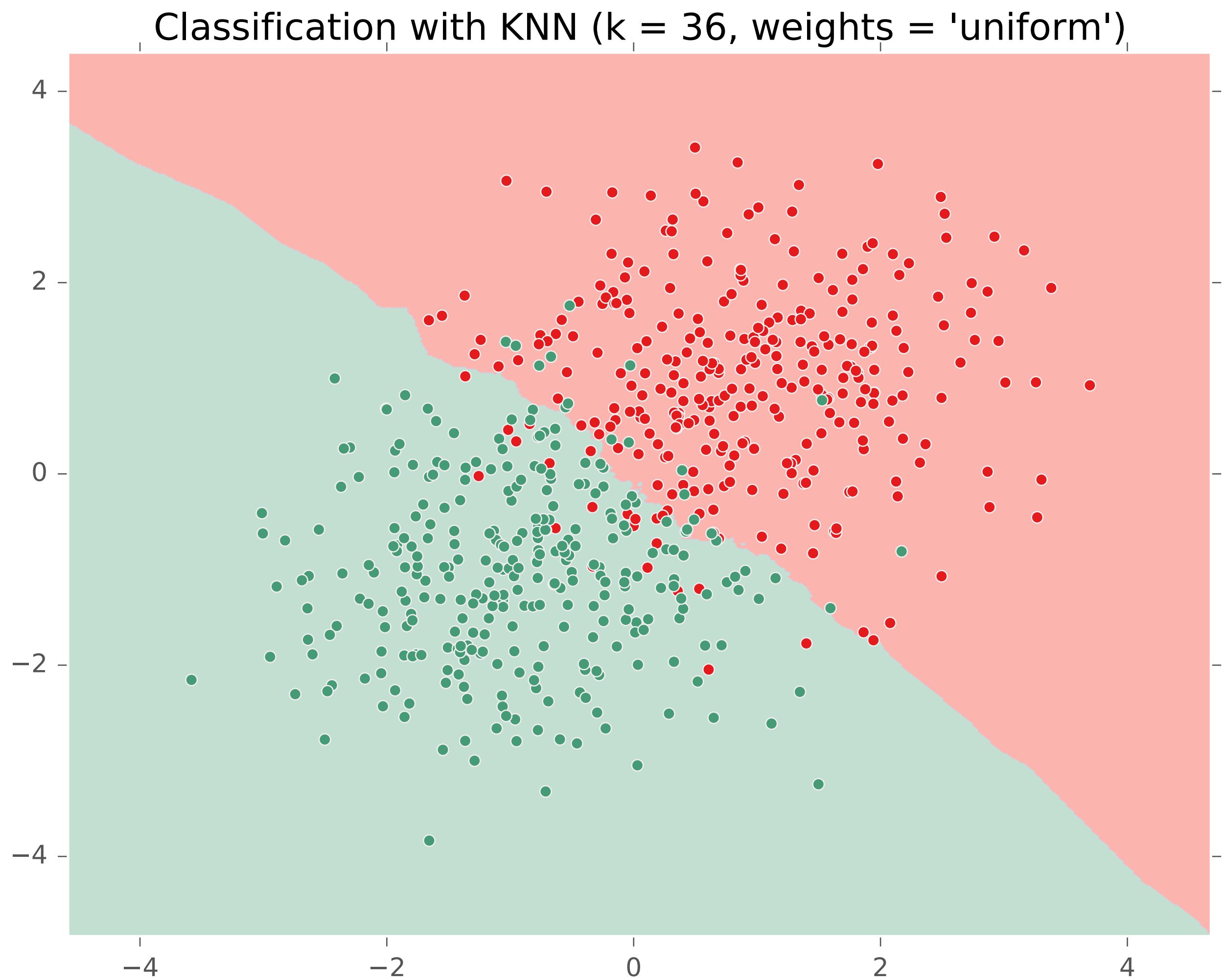

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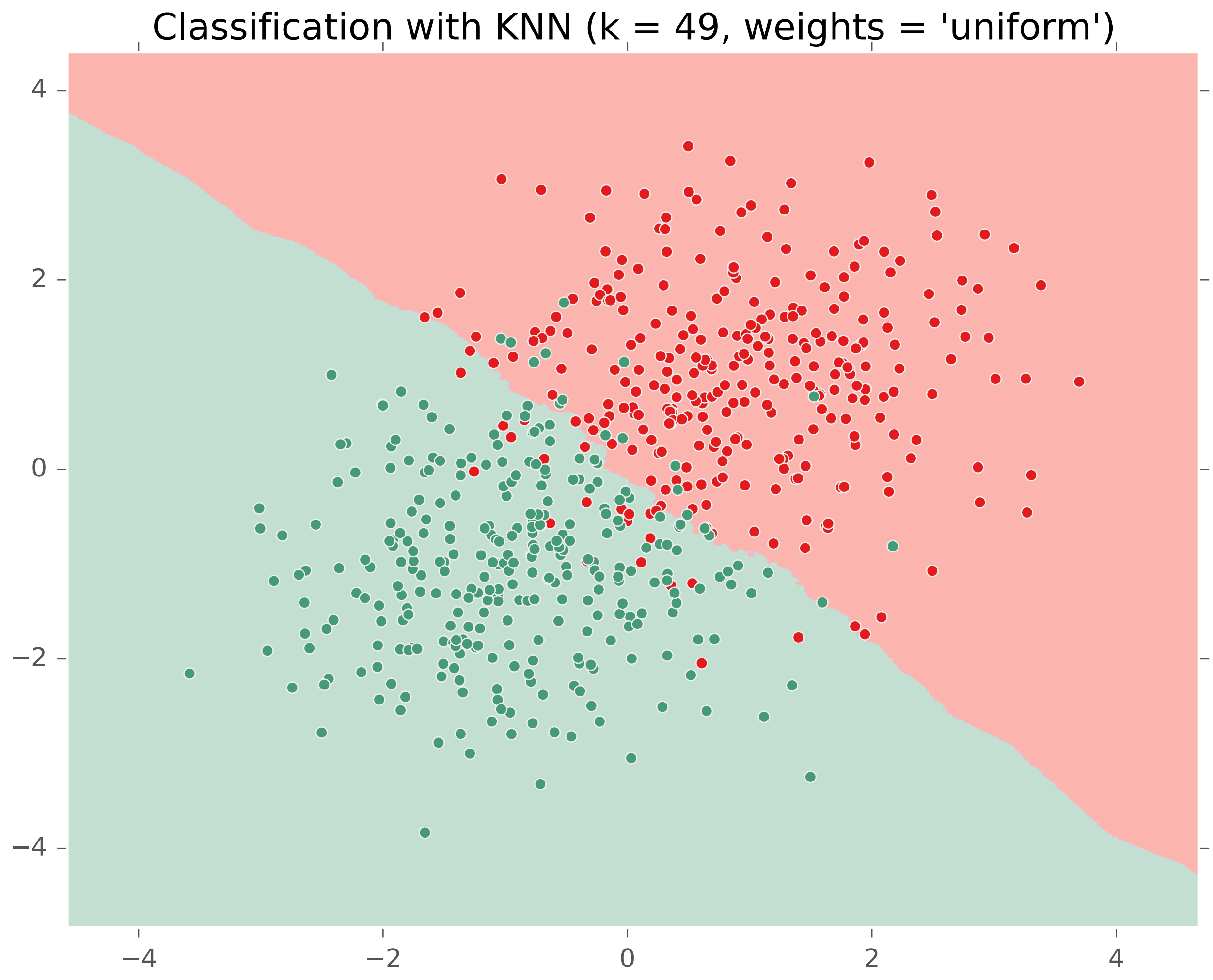

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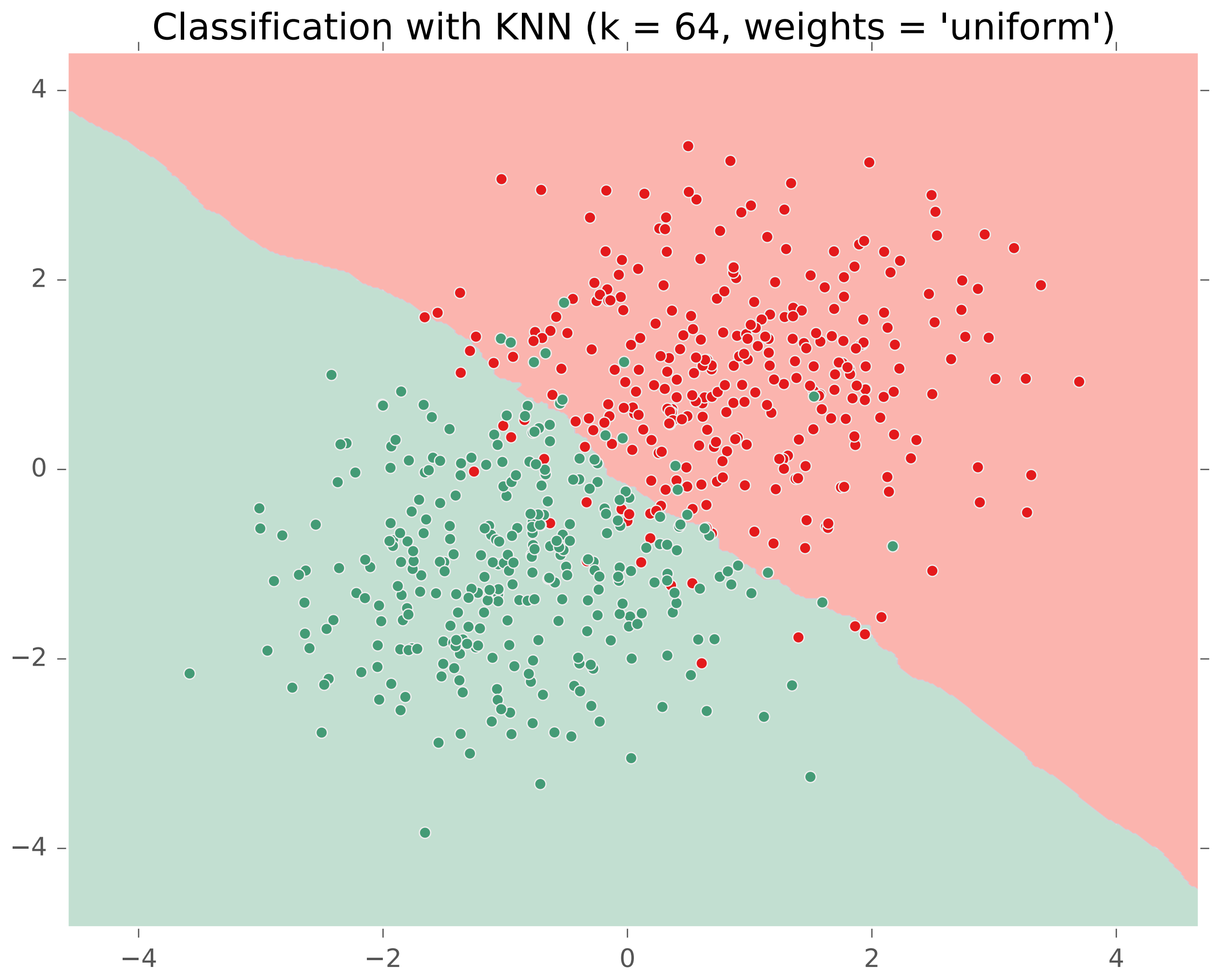

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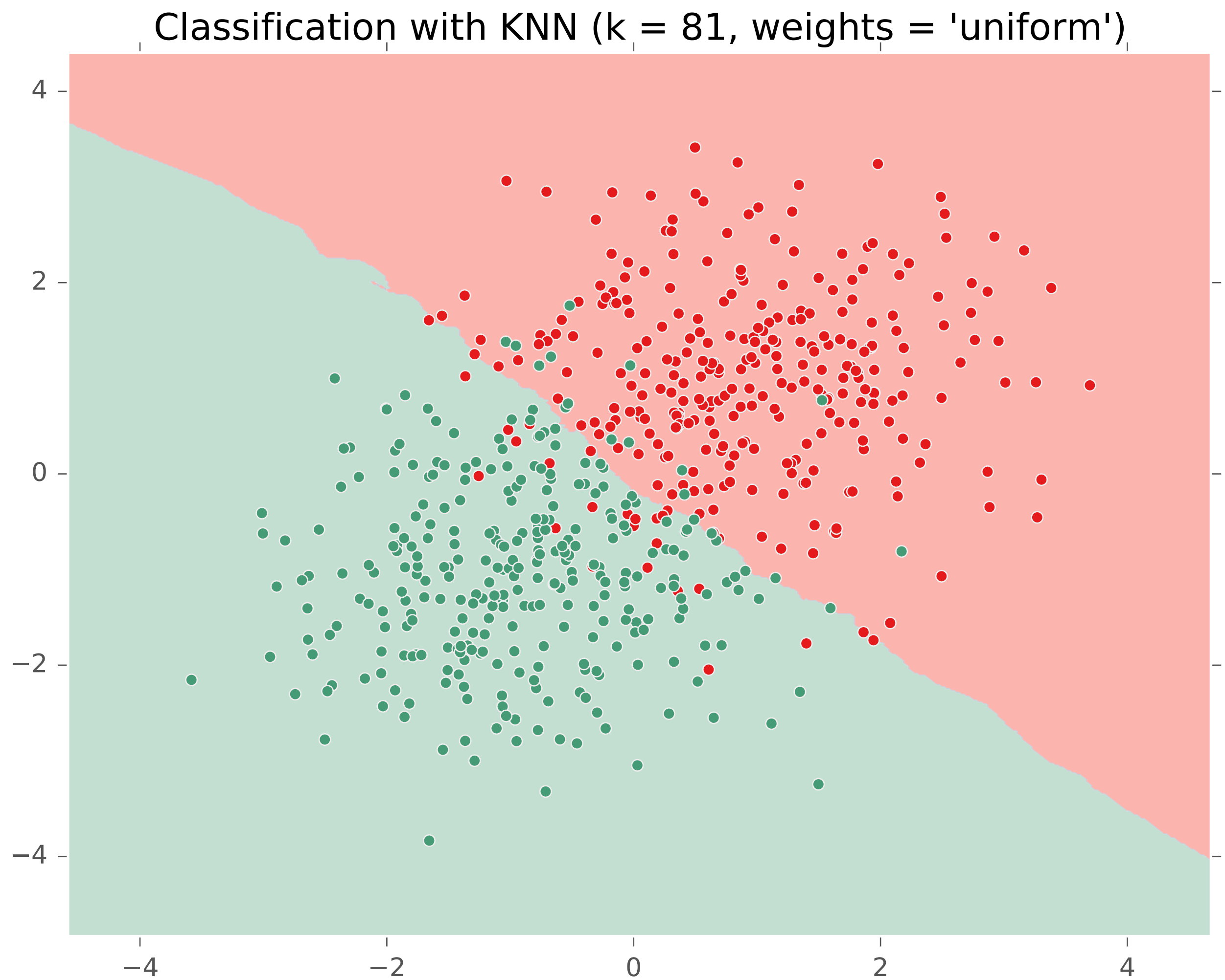

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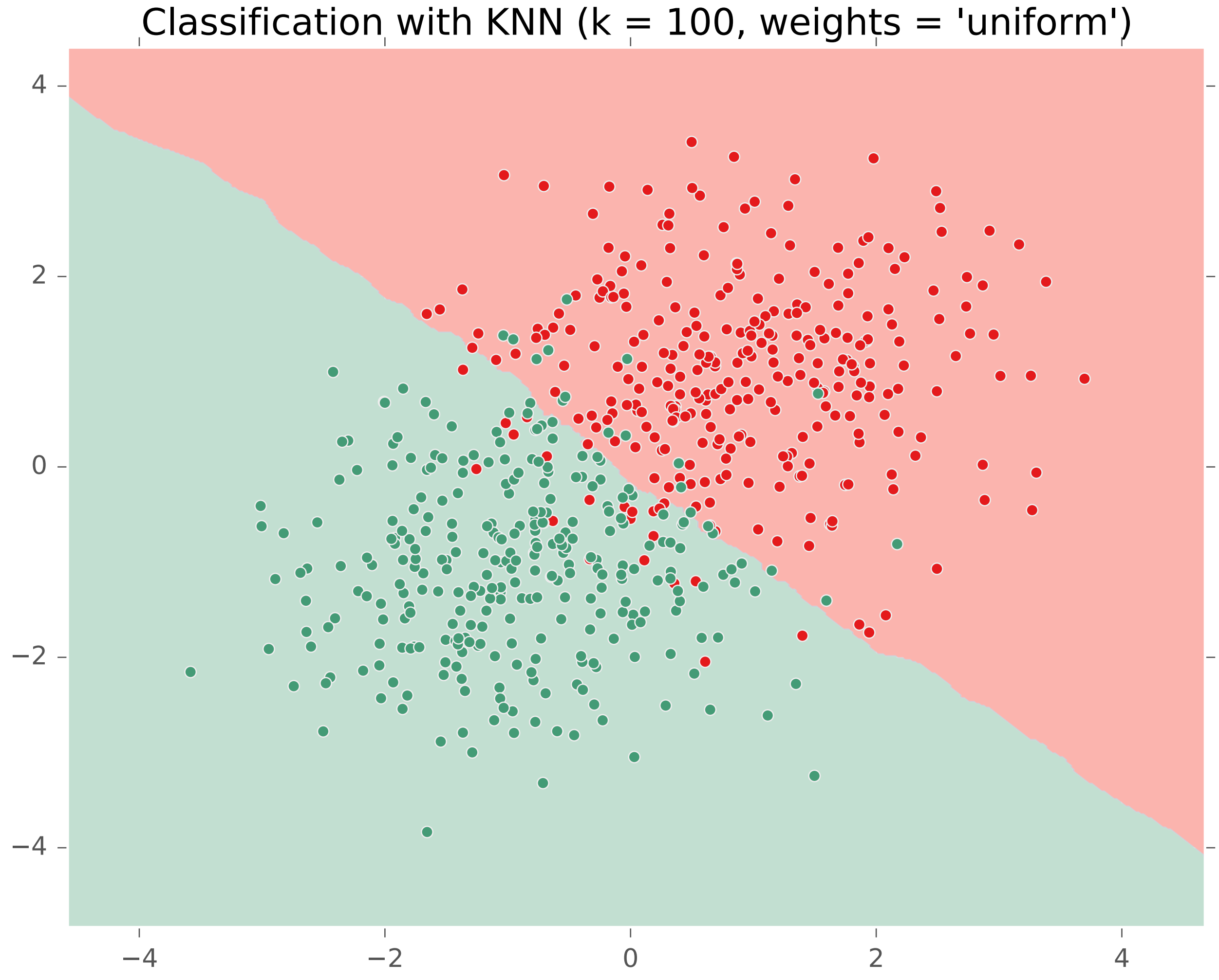

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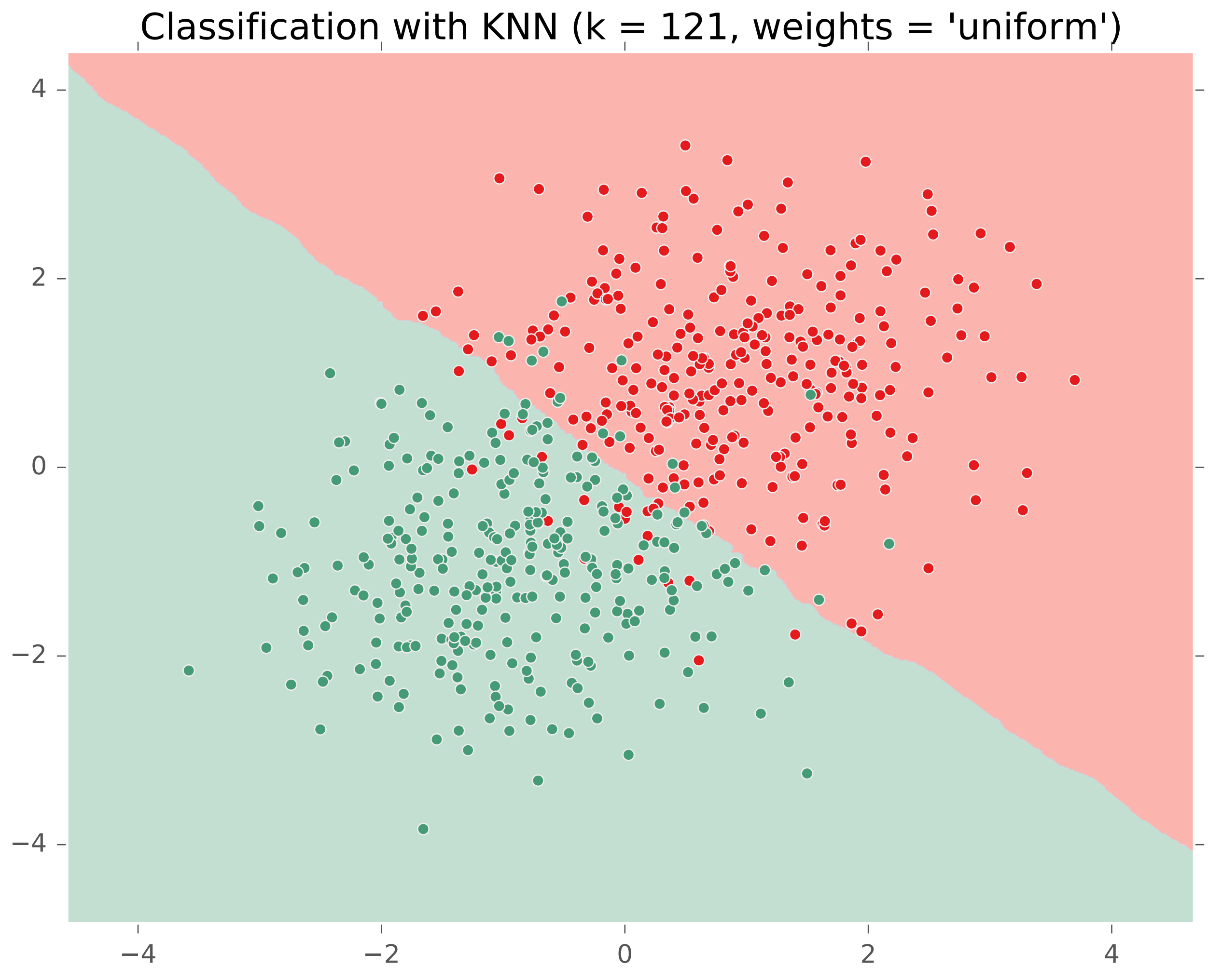

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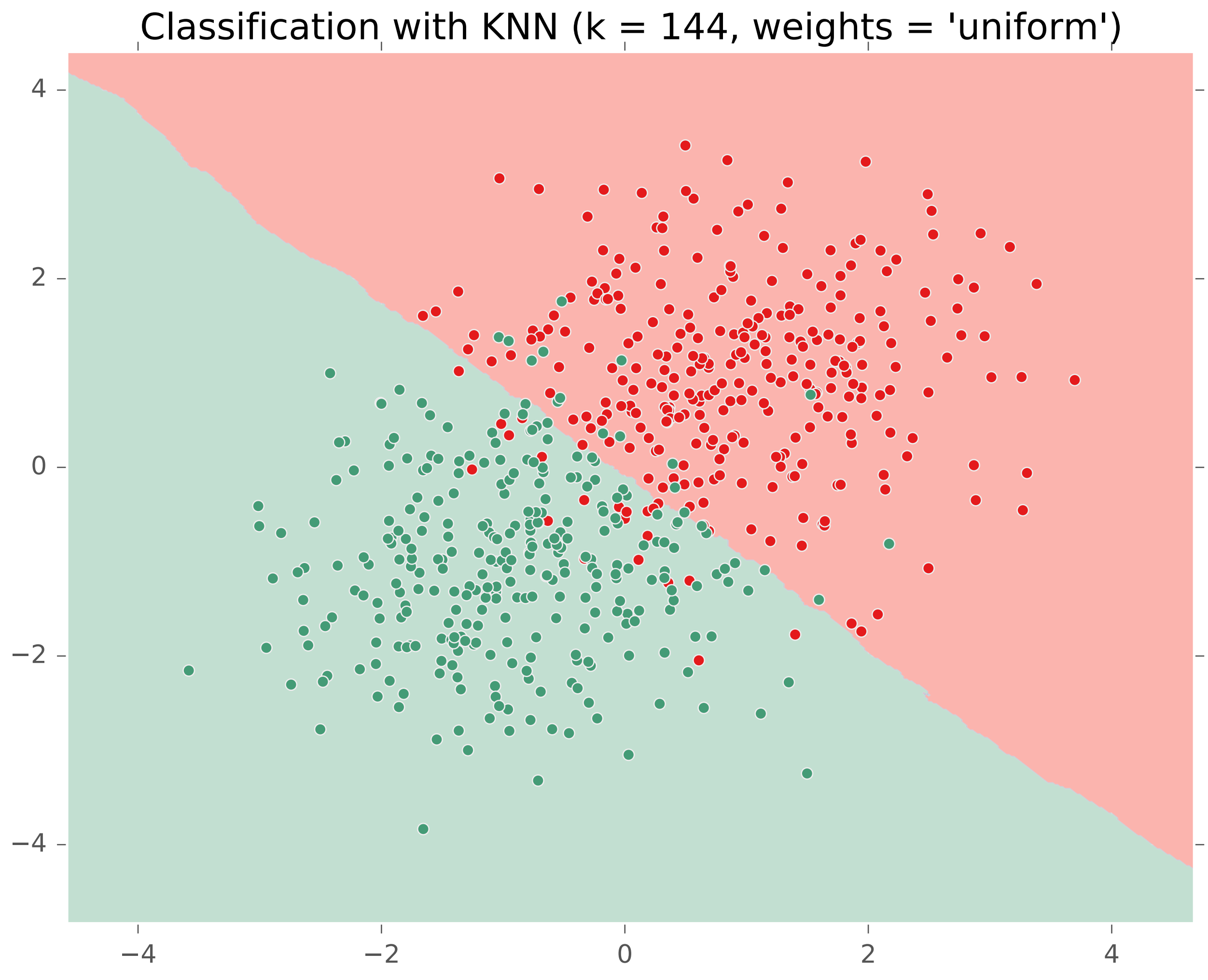

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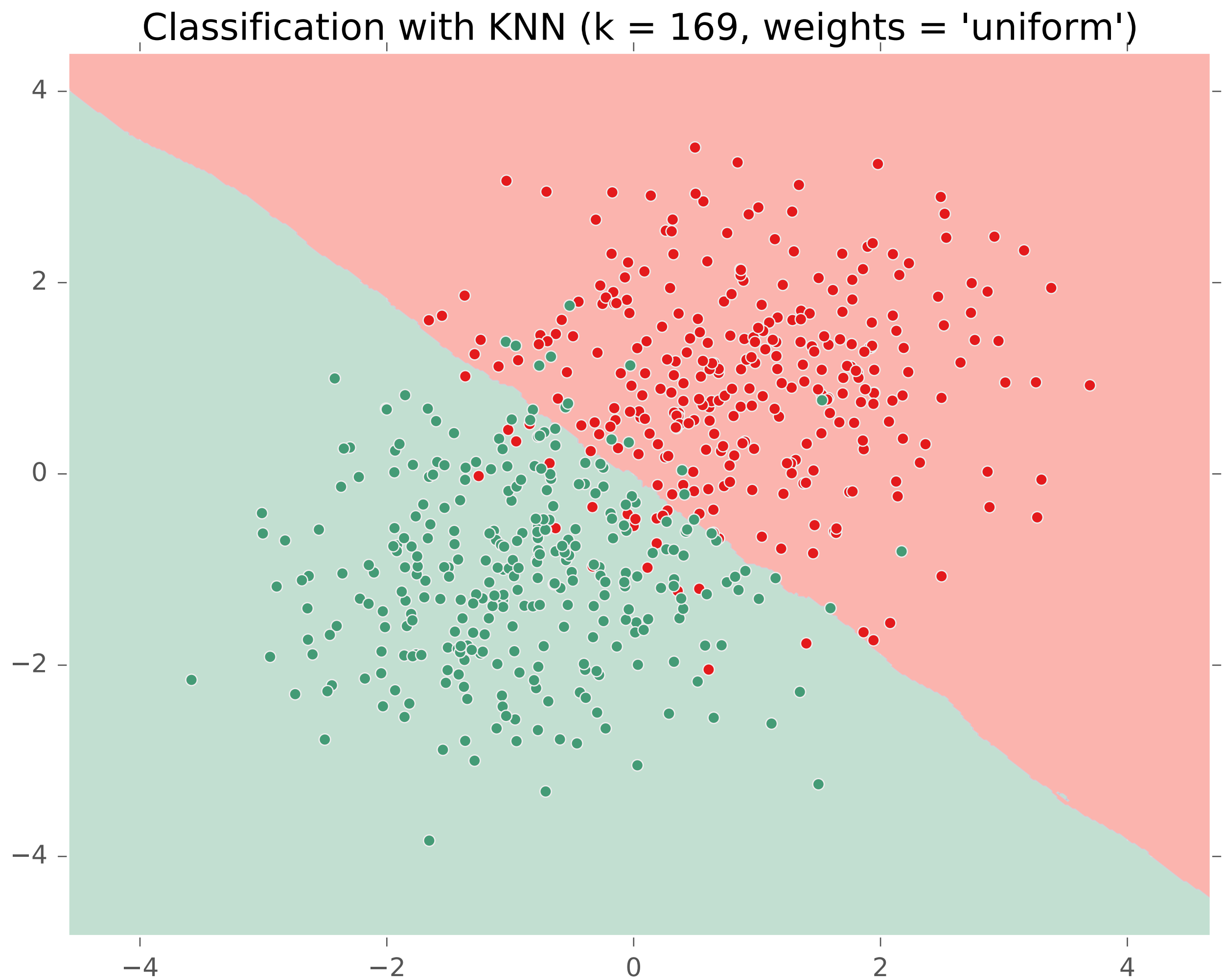

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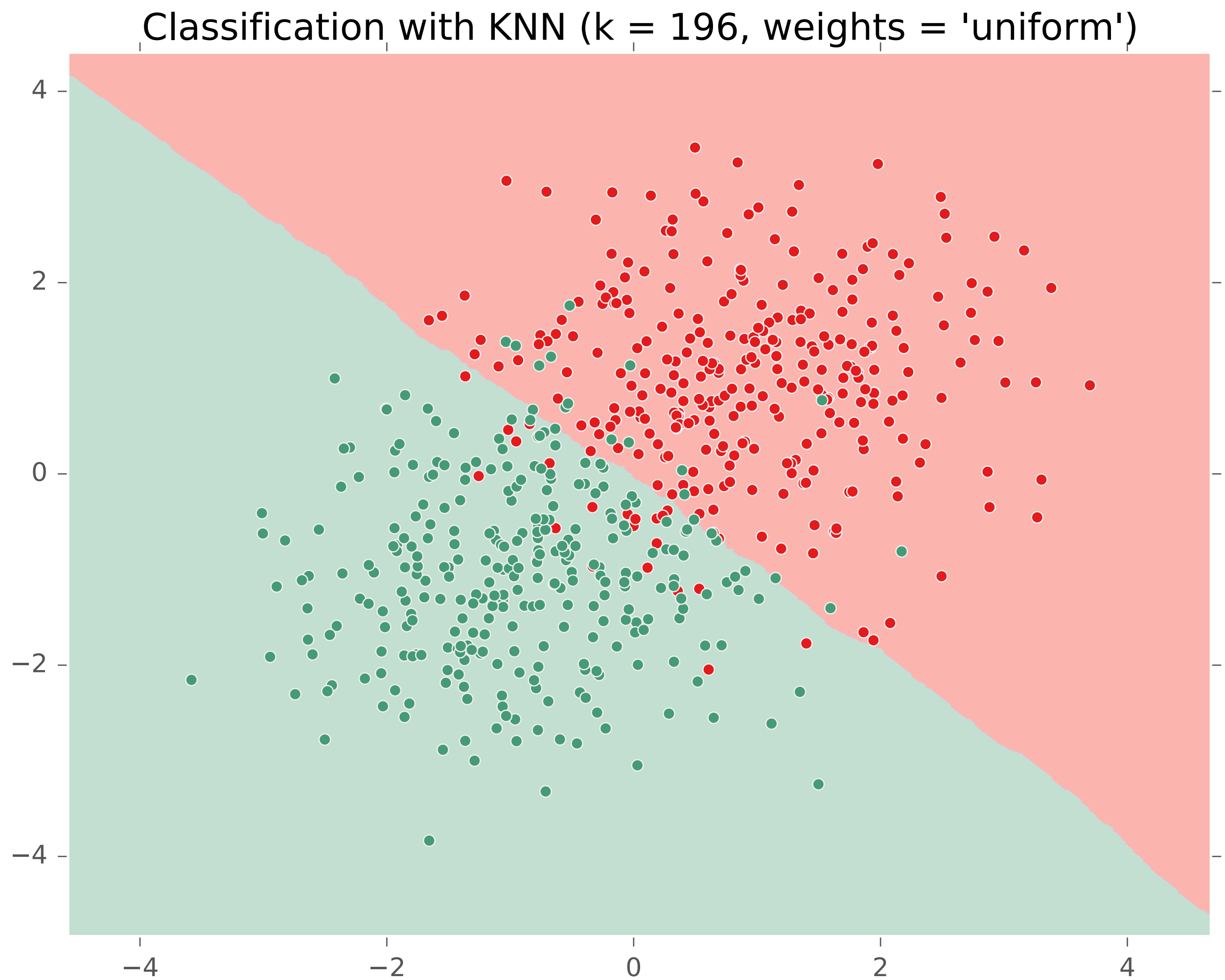

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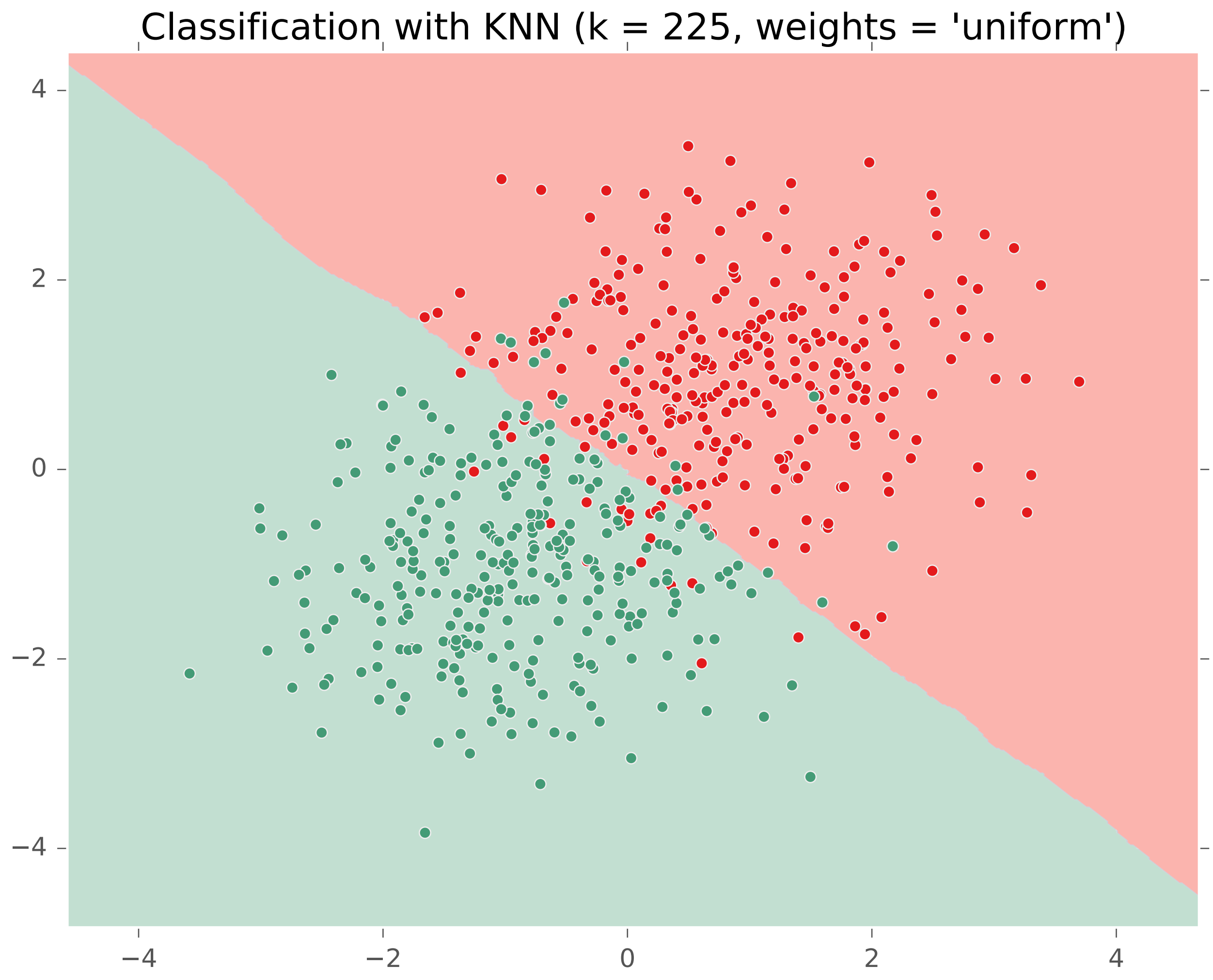

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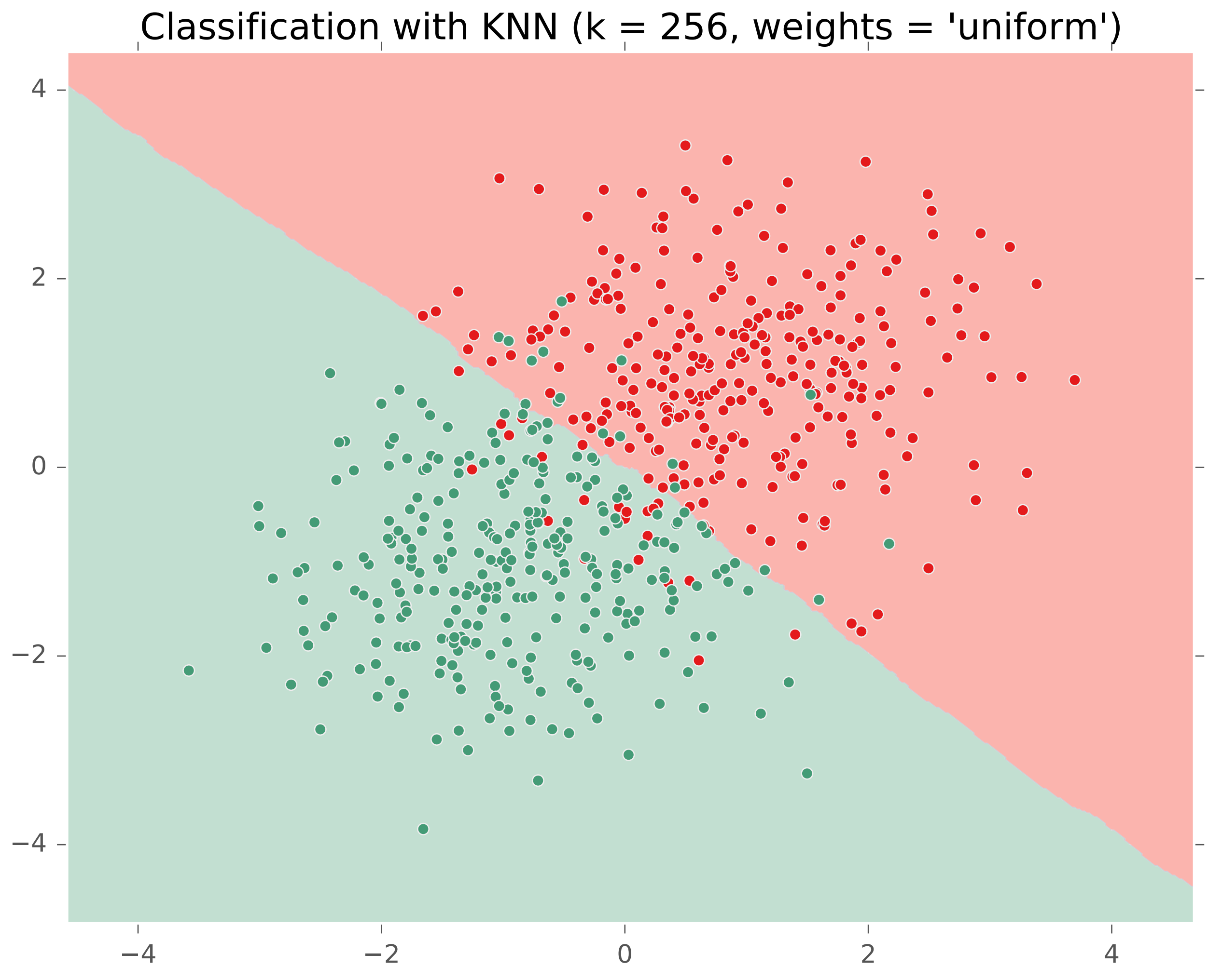

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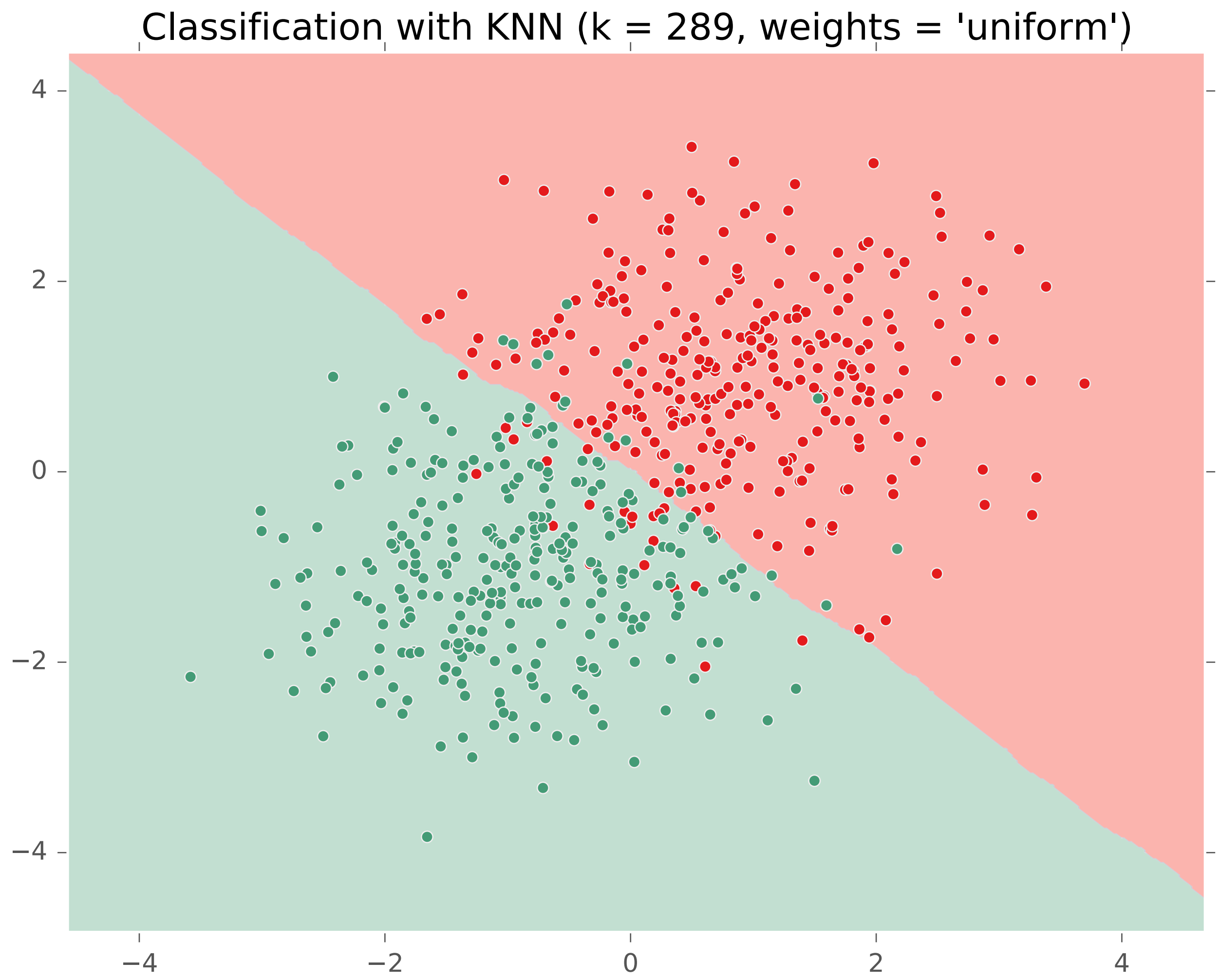

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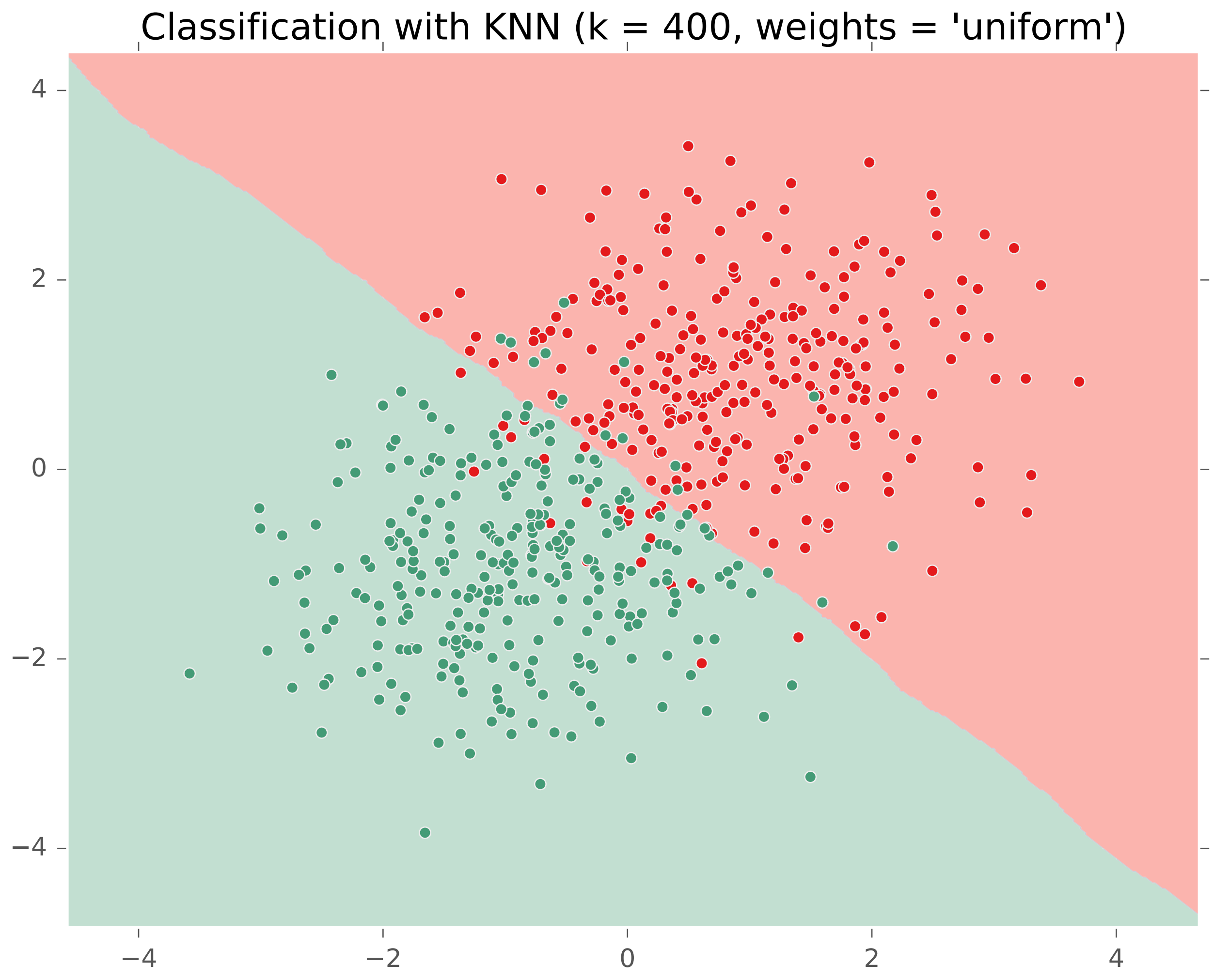

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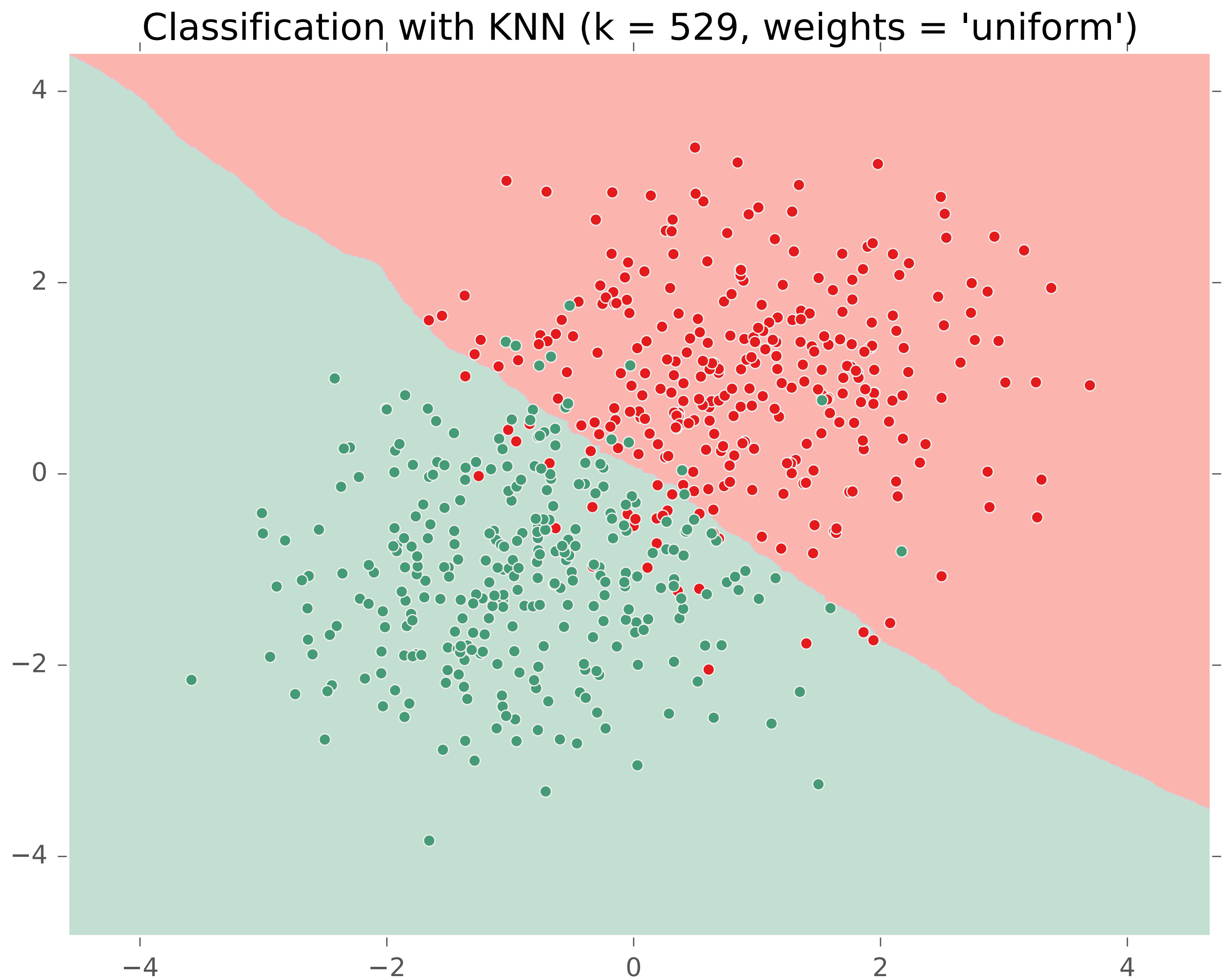

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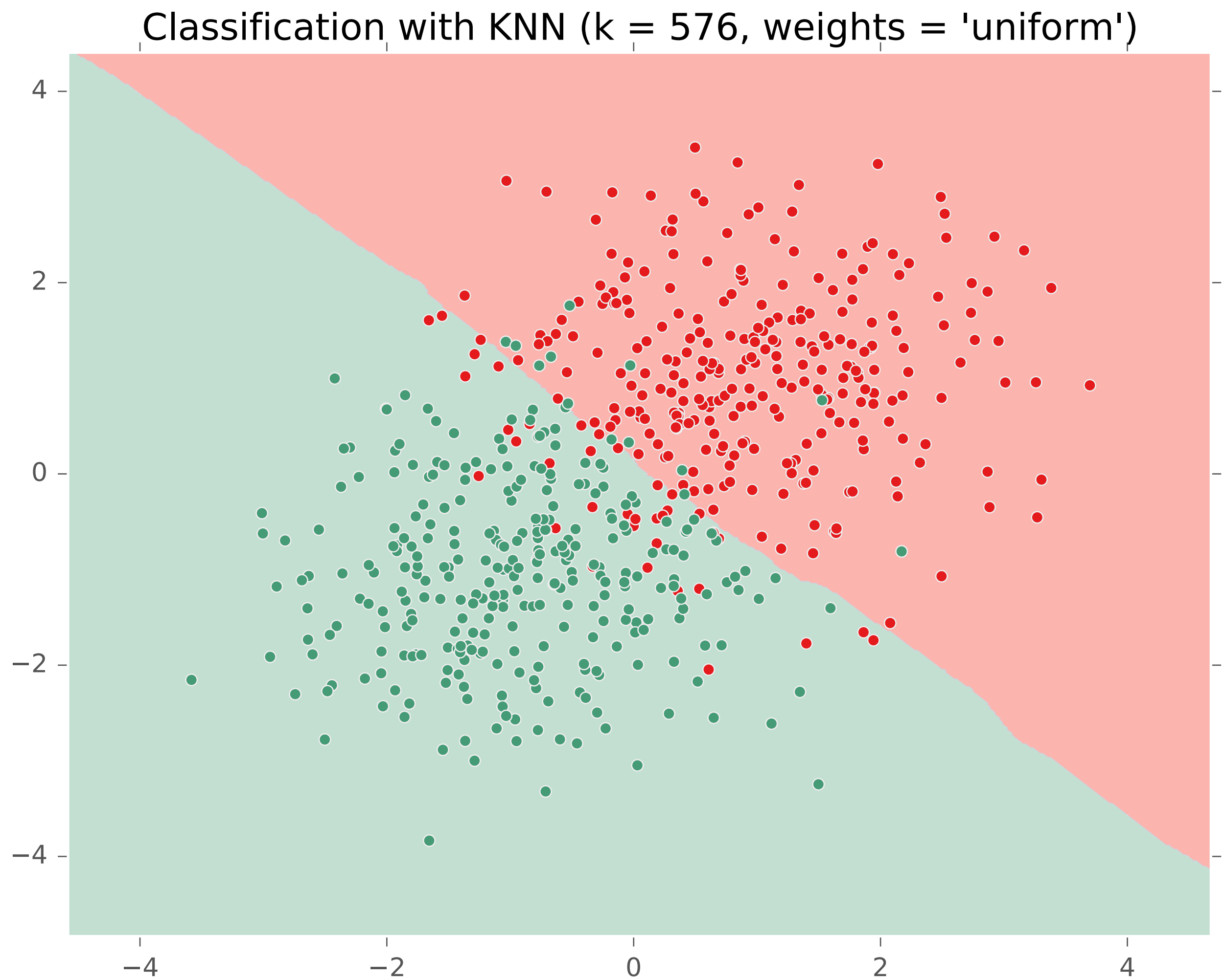

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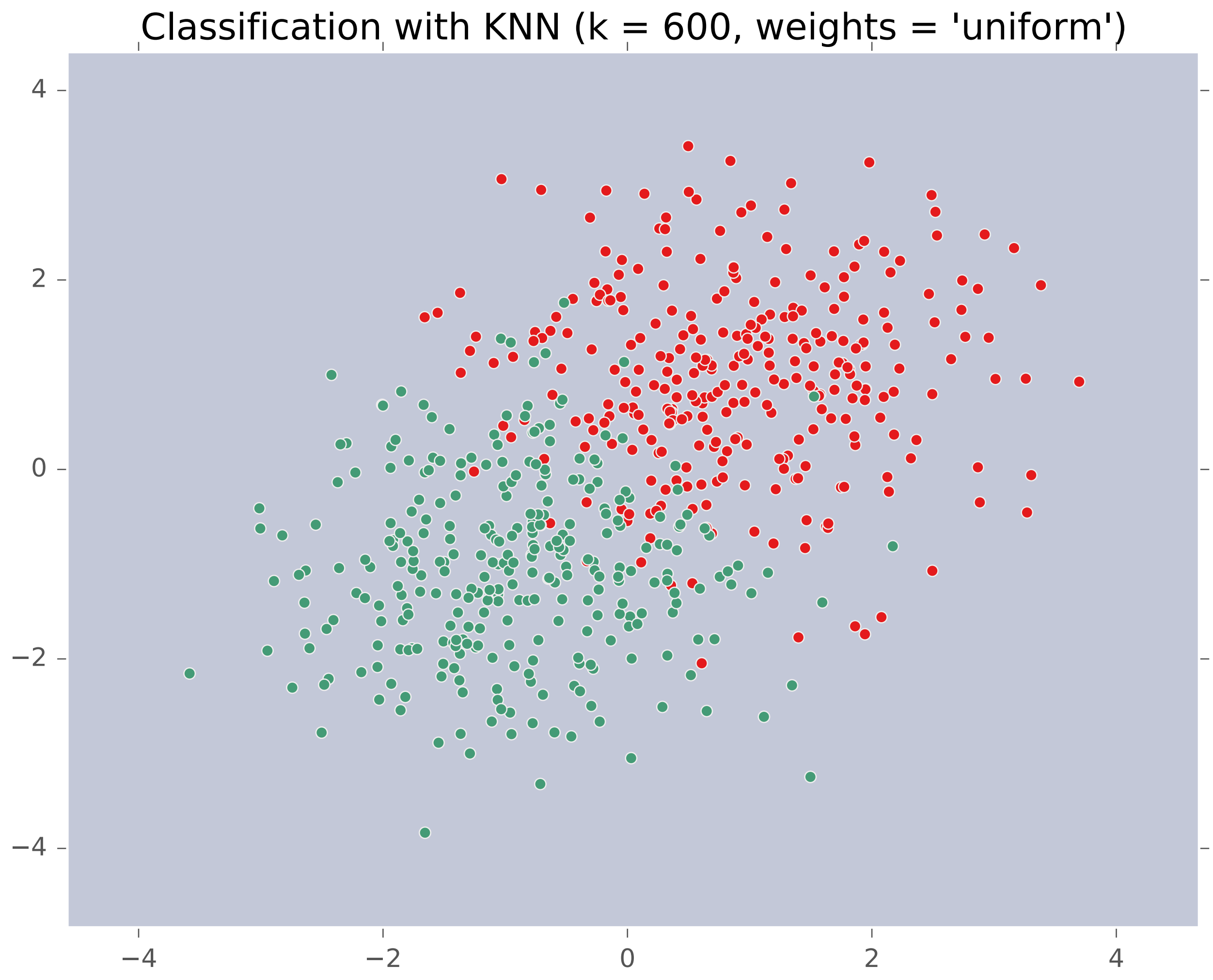

K-NEAREST NEIGHBORS

Questions

- How could k-Nearest Neighbors (KNN) be applied to **regression?**
- Can we do better than majority vote? (e.g. **distance-weighted** KNN)
- Where does the Cover & Hart (1967) **Bayes error rate bound** come from**?**

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
- Explain computational and geometric examples of the curse of dimensionality

k-Nearest Neighbors

But how do we choose 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

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

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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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

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Model Selection

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

Statistics

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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

Example of Hyperparameter Opt.

Chalkboard:

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

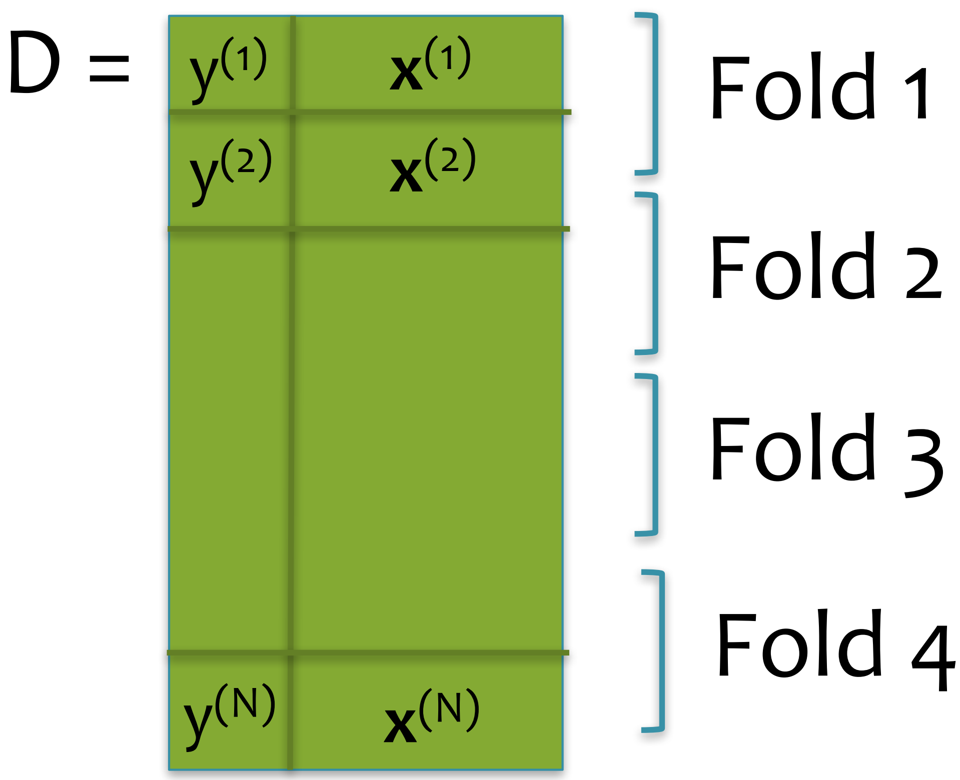
Cross-Validation

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)

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