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

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9/13/23

Front Matter

- Announcements:
  - HW2 released 9/6, due 9/15 (Friday!) at 11:59 PM
  - HW3 will be released on 9/15, due 9/23 at 11:59 PM
    - HW3 is a written-only homework
    - **You may only use at most 2 late days on HW3**
  - **Important scheduling note:** we will have lecture on 9/15 (Friday!) in lieu of recitation
    - This is to ensure that we cover enough material for you all to make a meaningful start on HW3
    - The HW3 recitation has been moved to 9/20 (next Wednesday)

Recall: Nearest Neighbor Pseudocode

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

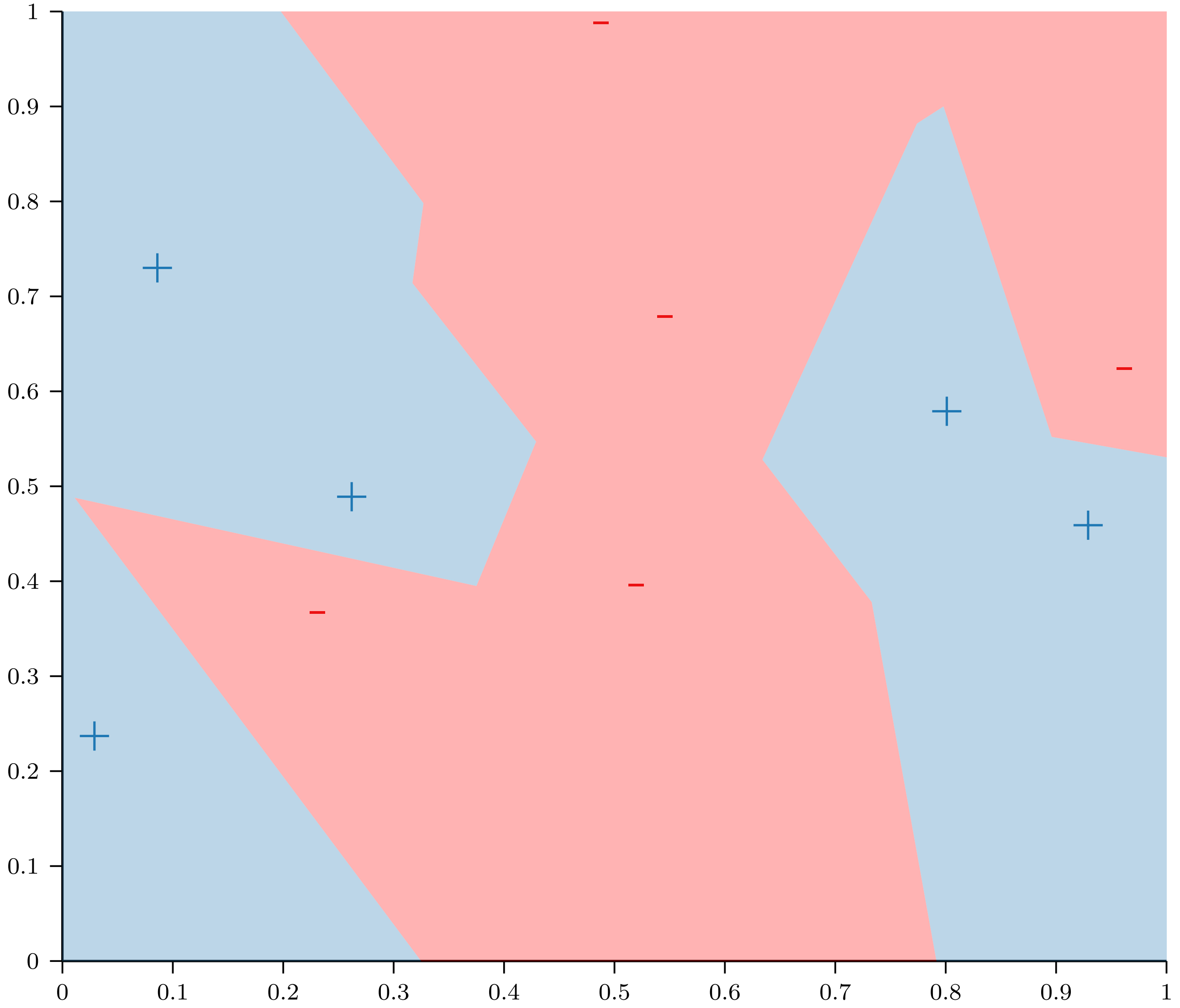
    store $\mathcal{D}$

def predict($\boldsymbol{x}'$):

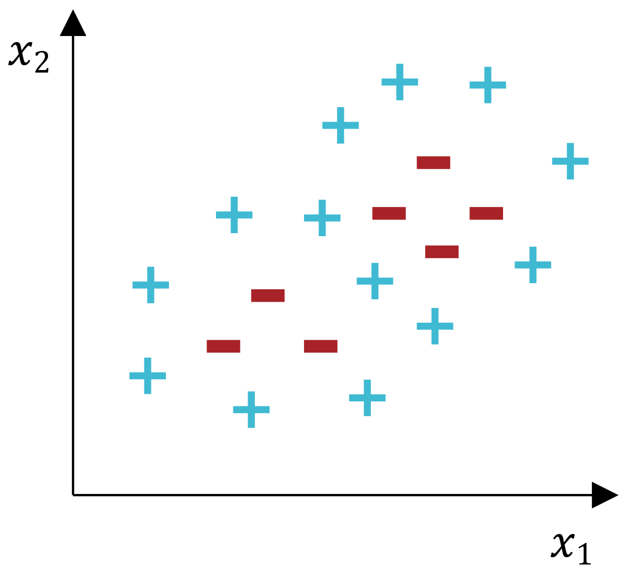
    find the nearest neighbor to $\boldsymbol{x}'$ in $\mathcal{D}$, $\boldsymbol{x}^{(i)}$

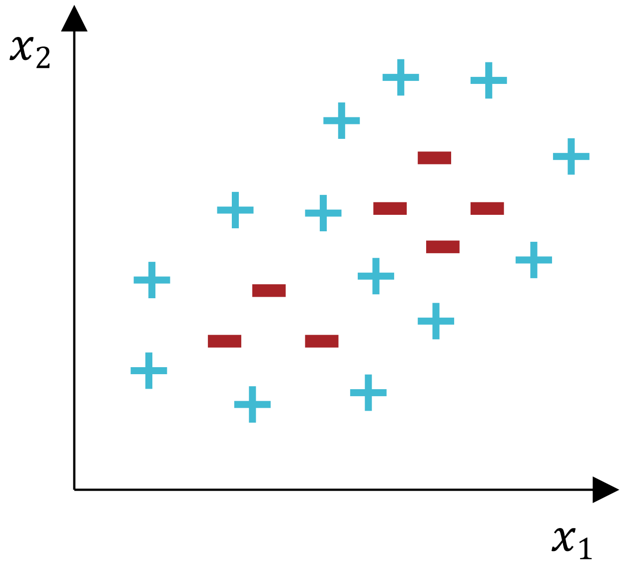
    return $y^{(i)}$

Recall: Nearest Neighbor Decision Boundary



Decision Boundary Exercise





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

Recall: 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)
```

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)

kNN on Fisher Iris Data

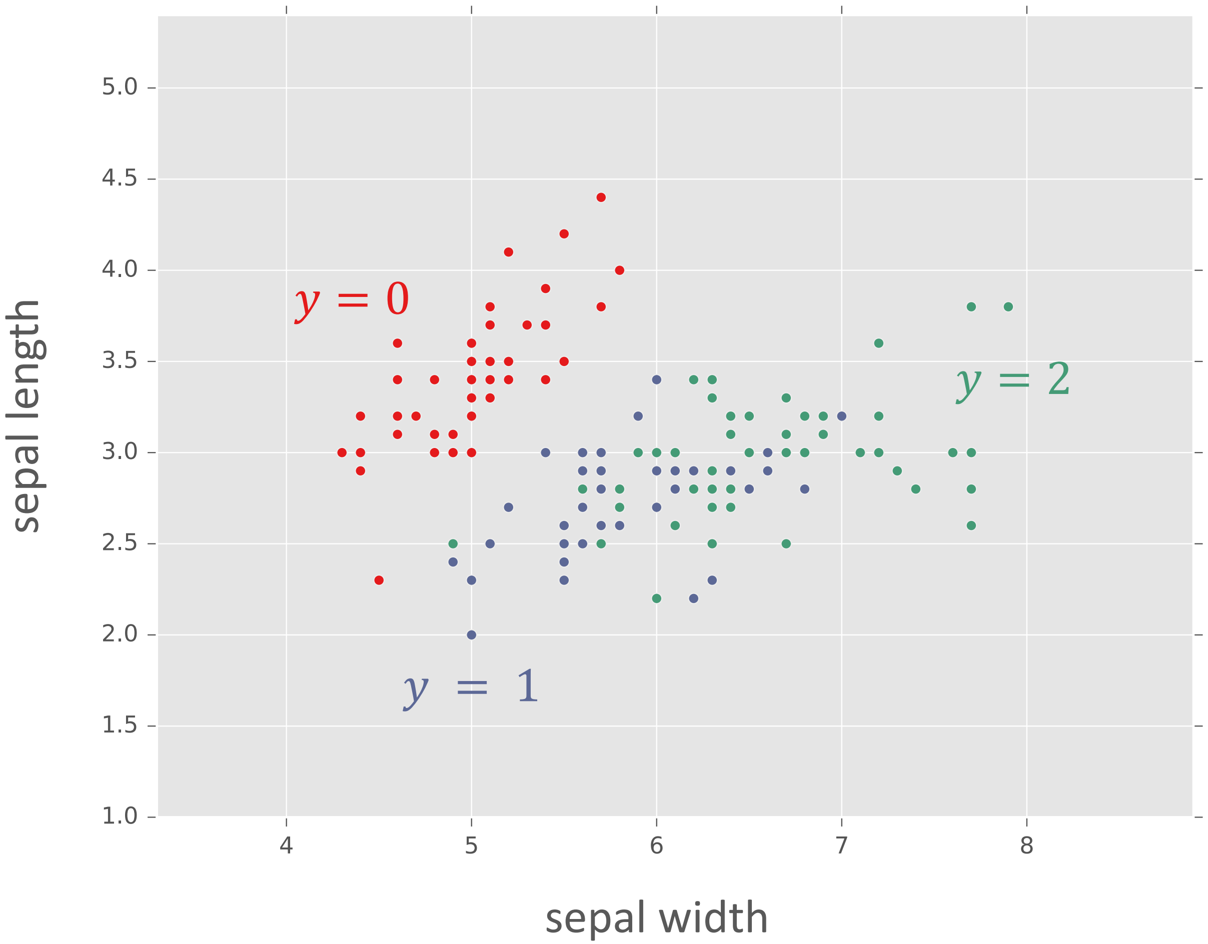


Figure courtesy of Matt Gormley

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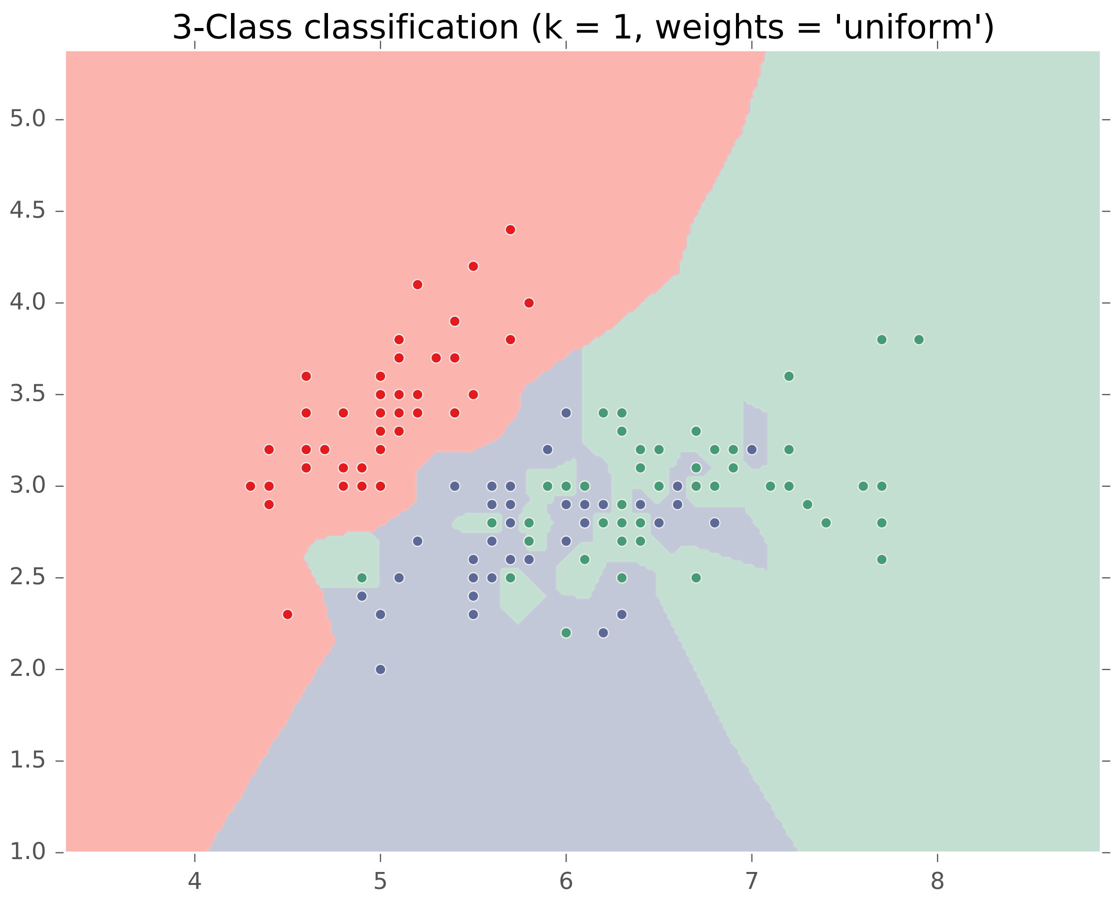

Figure courtesy of Matt Gormley

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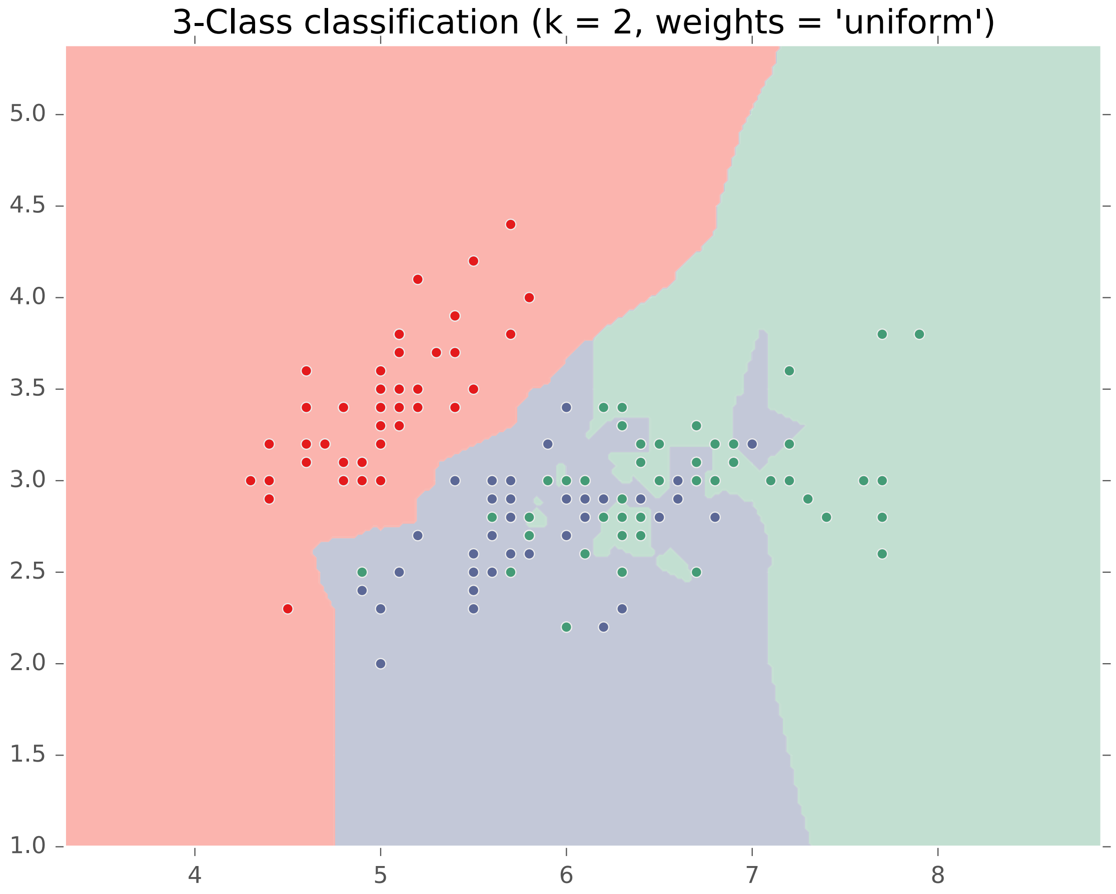

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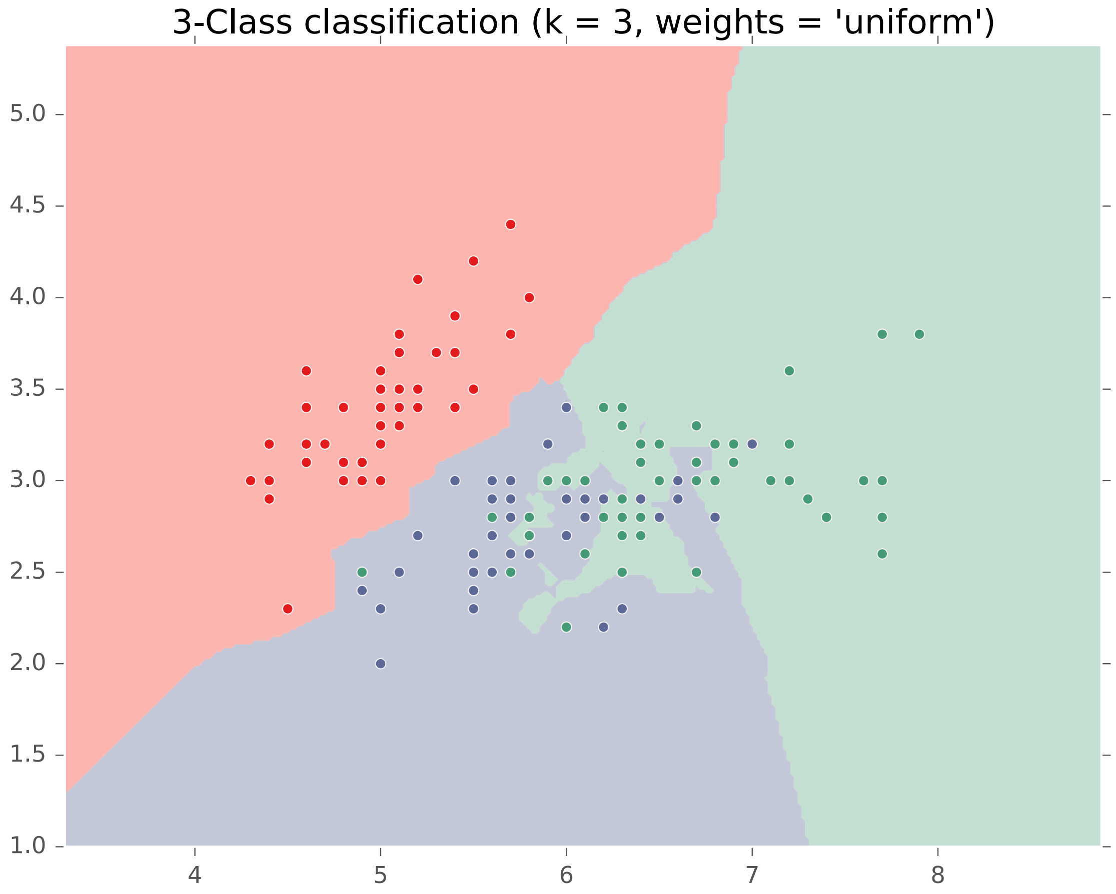

Figure courtesy of Matt Gormley

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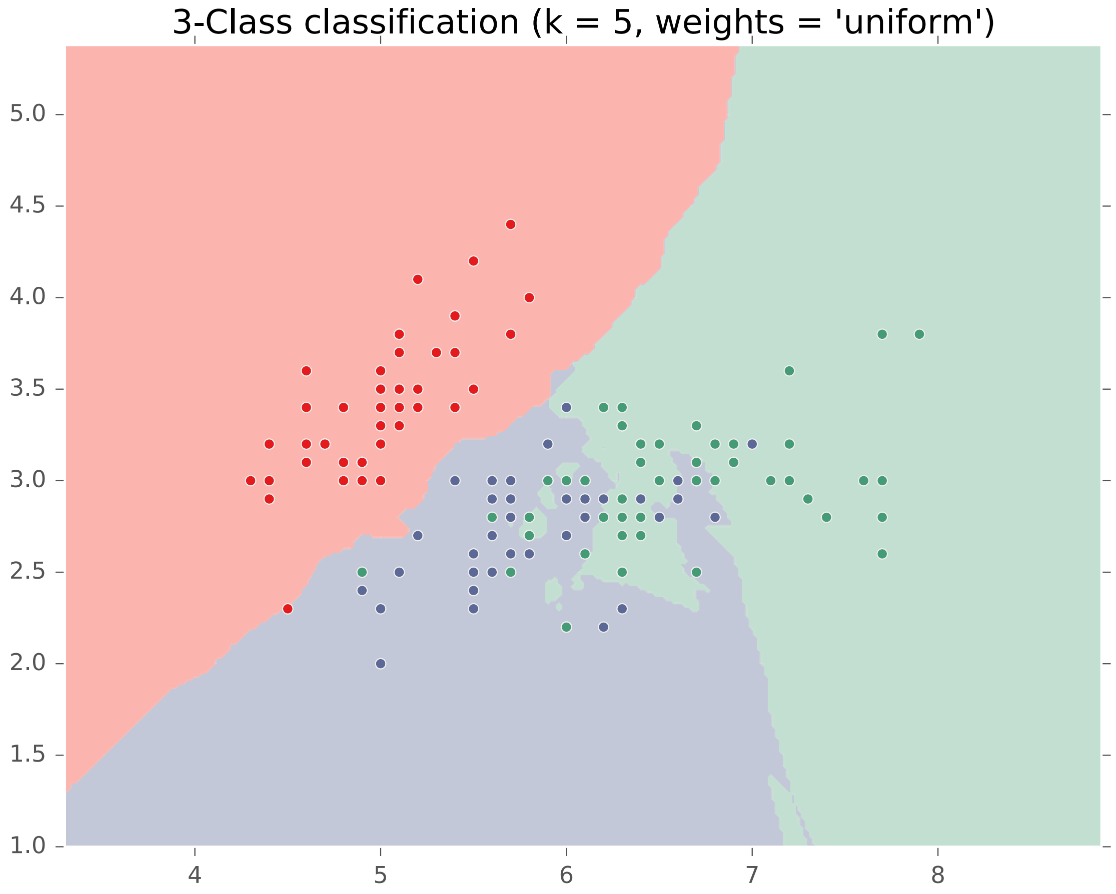

Figure courtesy of Matt Gormley

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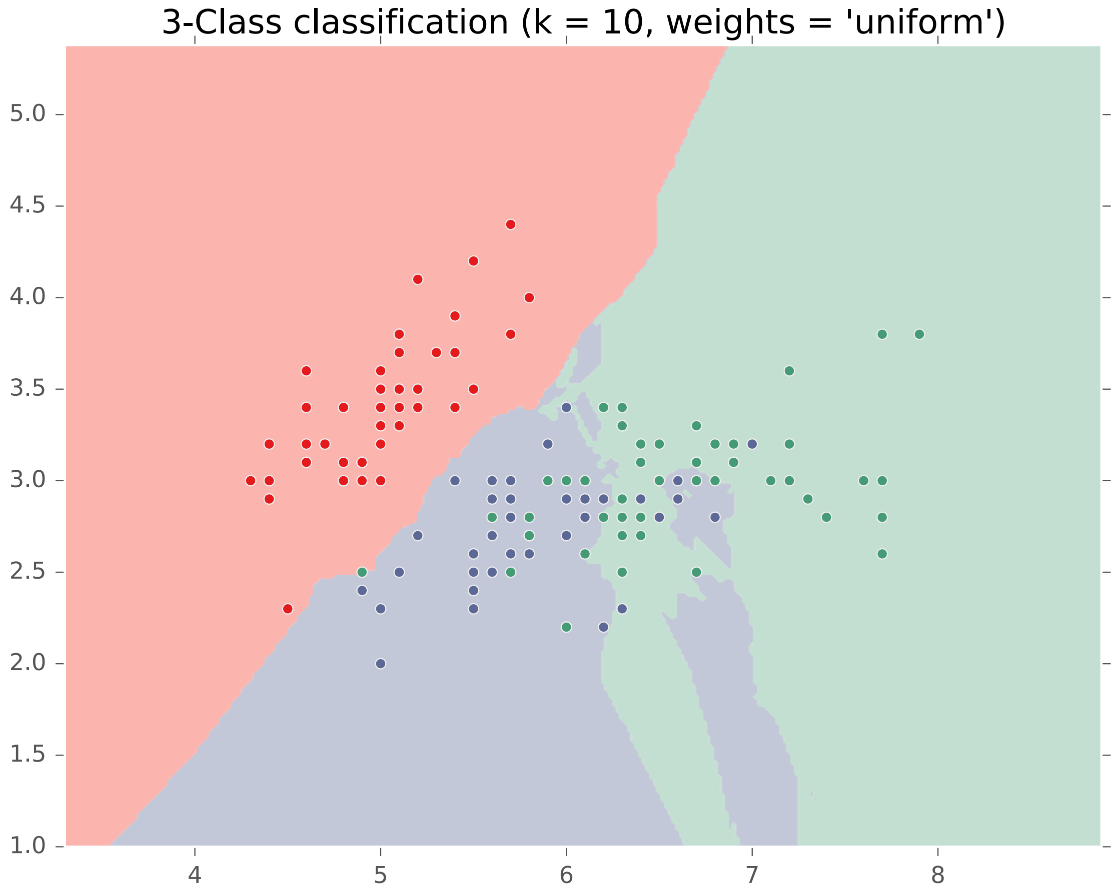

Figure courtesy of Matt Gormley

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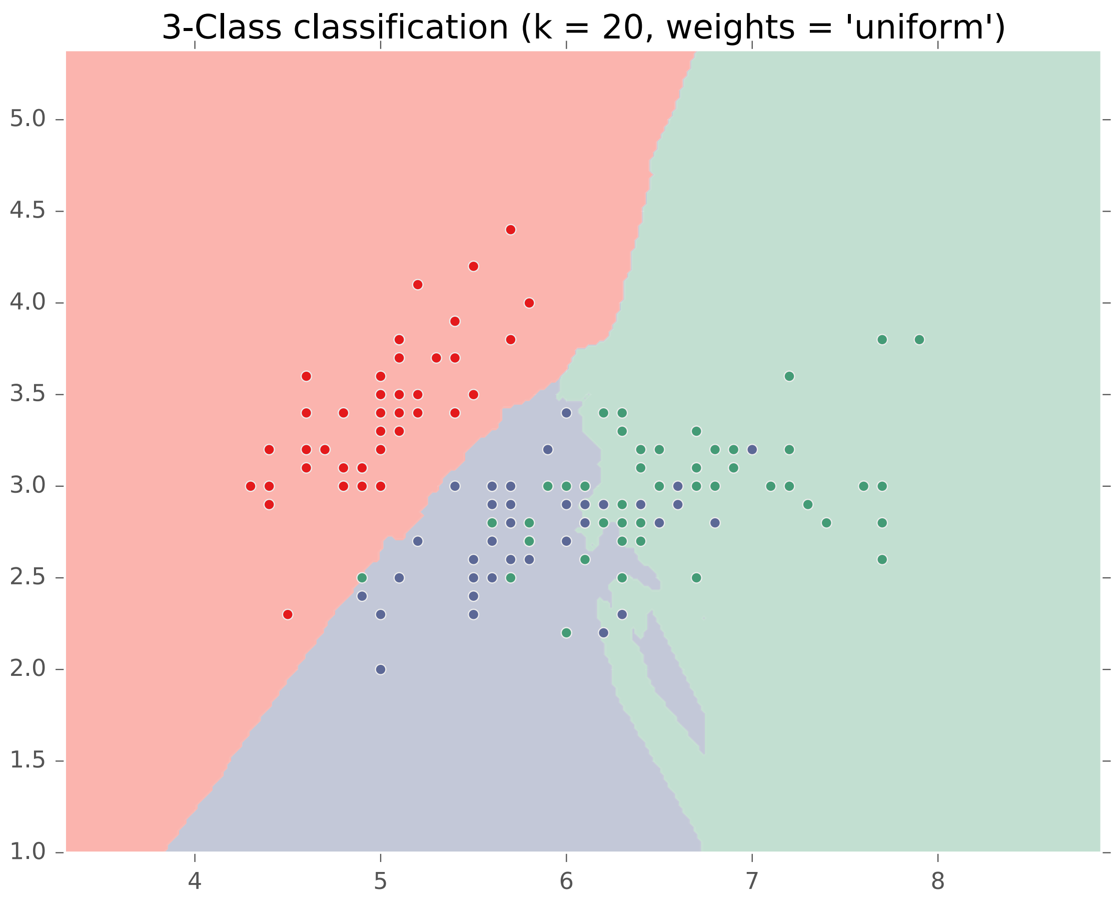
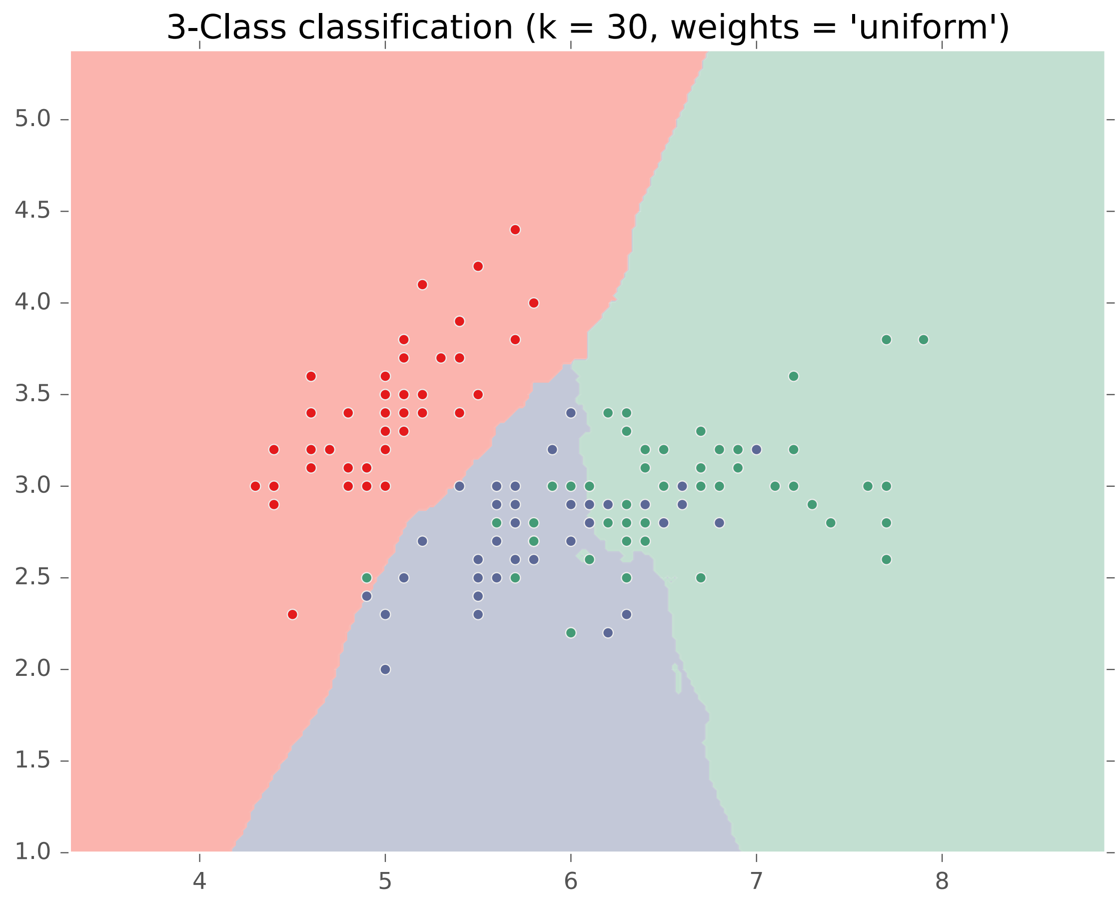


Figure courtesy of Matt Gormley

kNN on Fisher Iris Data



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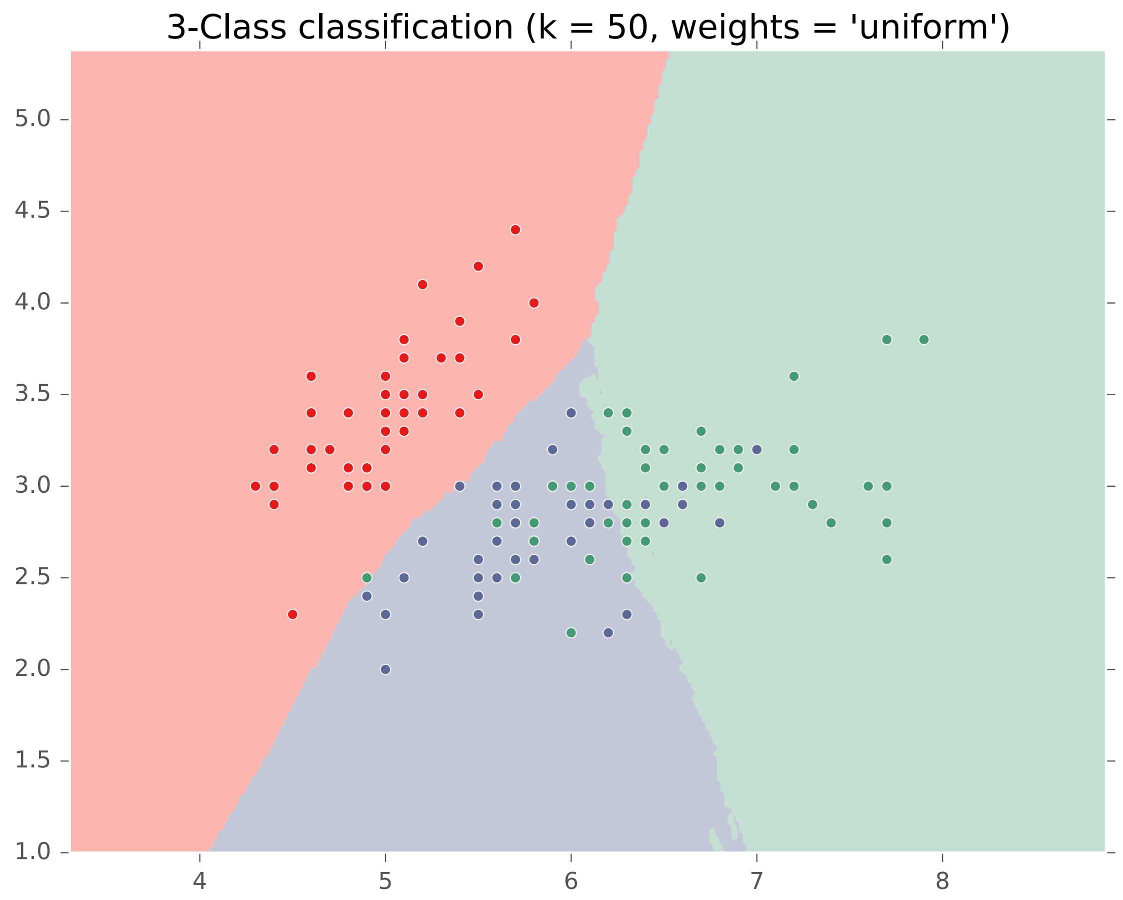

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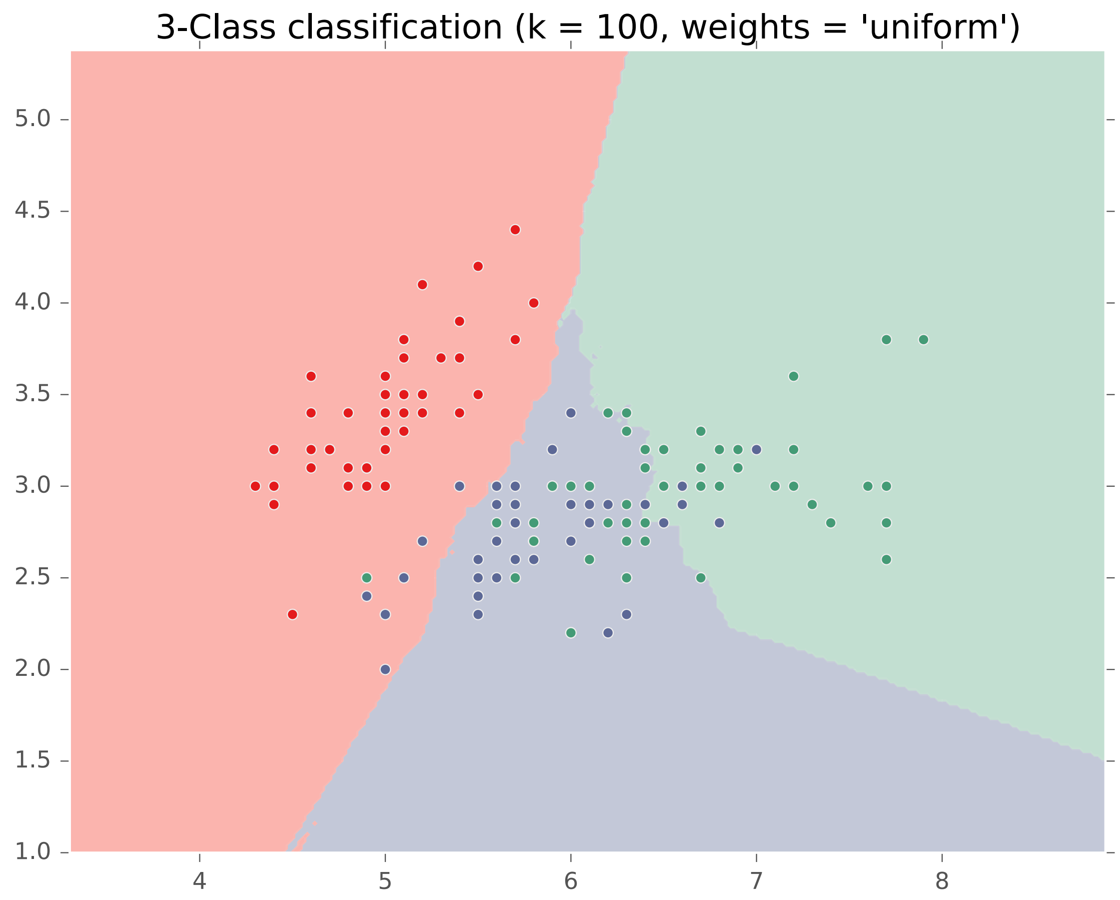

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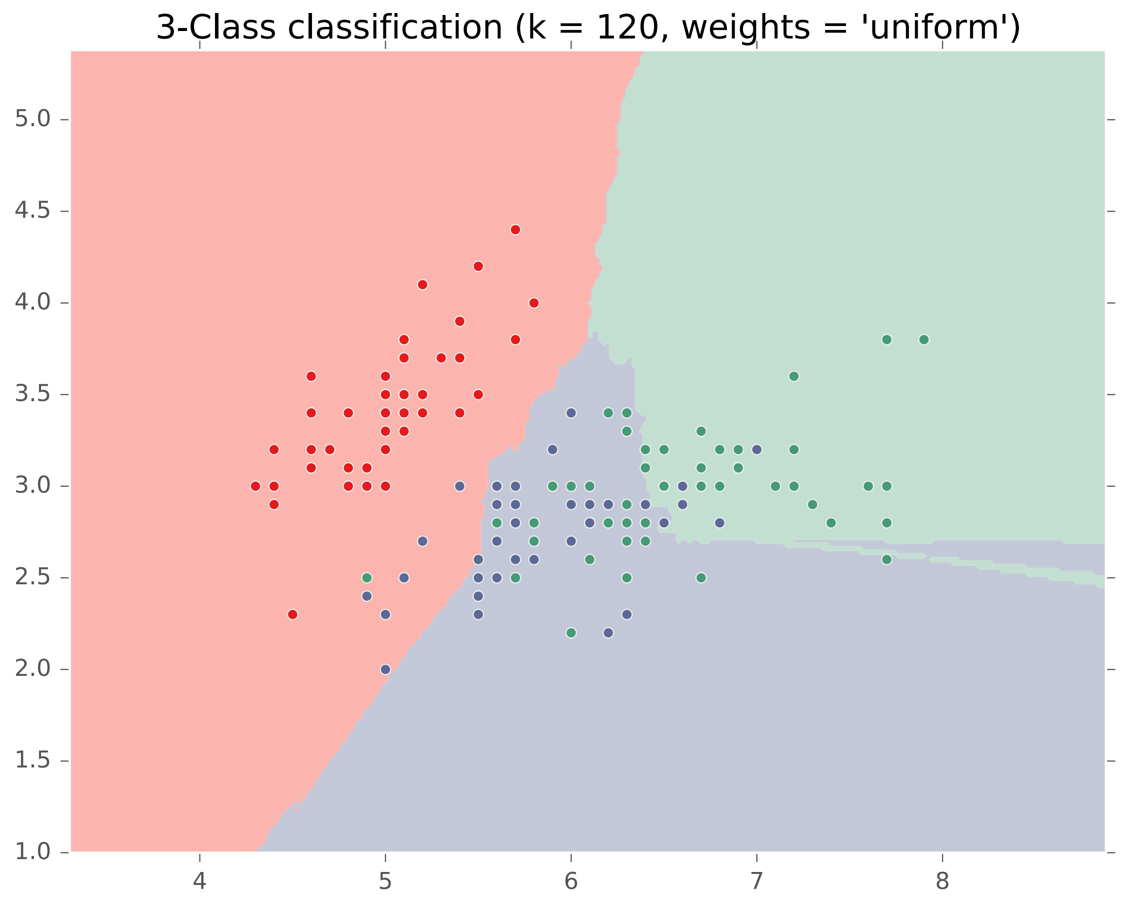

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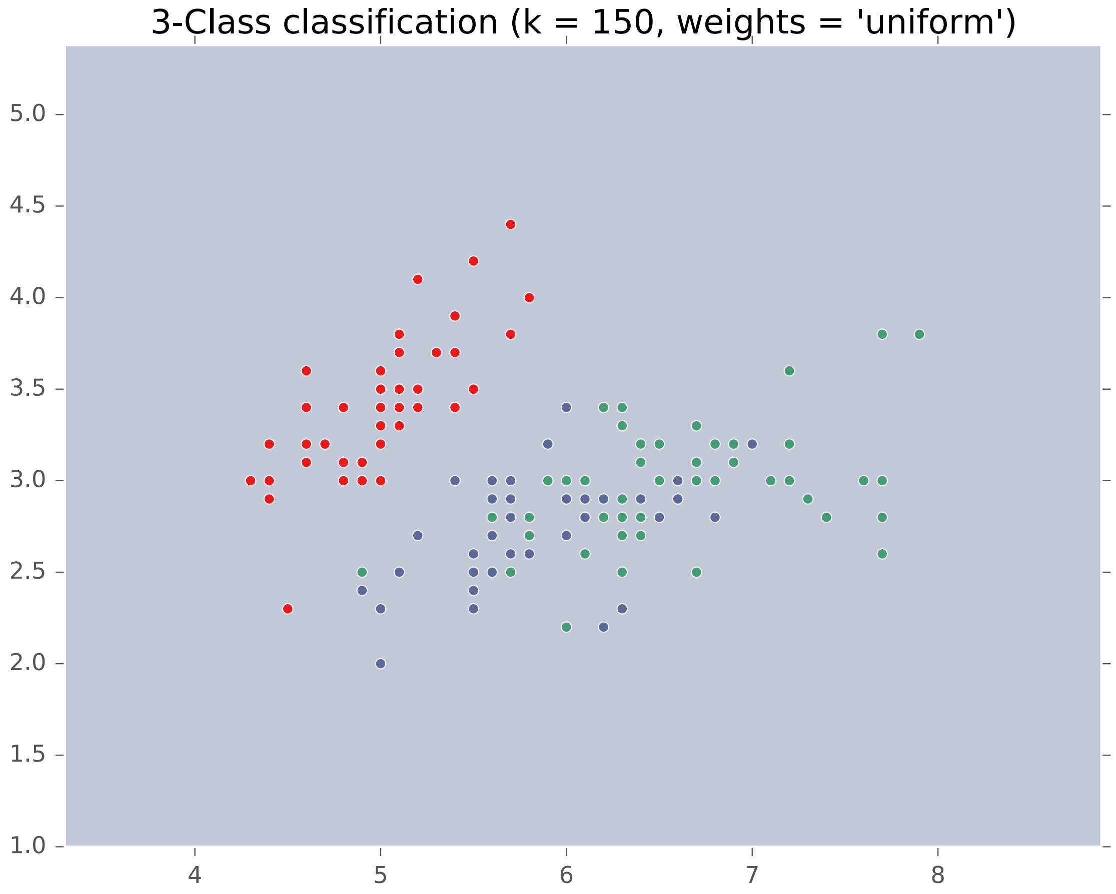

Figure courtesy of Matt Gormley

kNN with Euclidean Distance: Inductive Bias

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

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

How on earth do we go about setting k?

- This is effectively a question of model selection: every value of k corresponds to a different model.

- **WARNING**:
  - In some sense, our discussion of model selection is premature.
  - The models we have considered thus far are fairly simple.
  - In the real world, the models and the many decisions available to you will be much more complex than what we've seen so far.

Model Selection

- Terminology:
  - **Model** $\approx$ the hypothesis space in which the learning algorithm searches for a classifier to return
  - **Parameters** = numeric values or structure selected by the learning algorithm
  - **Hyperparameters** = tunable aspects of the model that need to be specified before learning can happen, set outside of the training procedure

- Example – Decision Trees:
  - Model = the set of all possible trees, potentially limited by some hyperparameter, e.g., max depth (see below)
  - Parameters = structure of a specific tree, i.e., the order in which features are split on
  - Hyperparameters = max depth, splitting criterion, etc…

Model Selection

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- Example – kNN:
  - Model = the set of all possible nearest neighbor classifiers
  - Parameters = none! kNN is a non-parametric model
  - Hyperparameters = k

Parametric vs. Nonparametric Models

- Parametric models (e.g., decision trees)
  - Have a parametrized form with parameters learned from training data
  - Can discard training data after parameters have been learned.
  - Cannot exactly model every target function
- Nonparametric models (e.g., kNN)
  - Have no parameters that are learned from training data; can still have *hyperparameters*
  - Training data generally needs to be stored in order to make predictions
  - Can recover any target function given enough data

Model Selection vs Hyperparameter Optimization

- Hyperparameter optimization can be considered a special case of model selection
  - Changing the hyperparameters changes the hypothesis space or the set of potential classifiers returned by the learning algorithm
- Deciding between a decision tree and kNN (model selection) vs. selecting a value of k for kNN (hyperparameter optimization)
- Both model selection and hyperparameter optimization happen outside the regular training procedure

Setting k

- When $k = 1$:
  - many, complicated decision boundaries
  - liable to overfit
- When $k = N$:
  - no decision boundaries; always predicts the most common label in the training data (majority vote)
  - liable to 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 $\to$ the Bayes error rate
- Practical heuristics:
  - $k = \lfloor \sqrt{N} \rfloor$
  - $k = 3$
- Perform model selection!

Model Selection with Test Sets?

- Given $\mathcal{D} = \mathcal{D}_{train} \cup \mathcal{D}_{test}$, suppose we have multiple candidate models:

$$\mathcal{H}_1, \mathcal{H}_2, \dots, \mathcal{H}_M$$

- Learn a classifier from each model using only $\mathcal{D}_{train}$:

$$h_1 \in \mathcal{H}_1, h_2 \in \mathcal{H}_2, \dots, h_M \in \mathcal{H}_M$$

- Evaluate each one using $\mathcal{D}_{test}$ and choose the one with lowest test error:

$$\hat{m} = \underset{m \in \{1,\dots,M\}}{\operatorname{argmin}} \; err(h_m, \mathcal{D}_{test})$$

- Is $err(h_{\hat{m}}, \mathcal{D}_{test})$ a good estimate of $err(h_{\hat{m}})$?

Model Selection with Validation Sets

- Given $\mathcal{D} = \mathcal{D}_{train} \cup \mathcal{D}_{val} \cup \mathcal{D}_{test}$, suppose we have multiple candidate models:

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- Evaluate each one using $\mathcal{D}_{val}$ and choose the one with lowest *validation* error:

$$\hat{m} = \underset{m \in \{1,\ldots,M\}}{\operatorname{argmin}} \; err(h_m, \mathcal{D}_{val})$$

Hyperparameter Optimization with Validation Sets

- Given $\mathcal{D} = \mathcal{D}_{train} \cup \mathcal{D}_{val} \cup \mathcal{D}_{test}$, suppose we have multiple candidate hyperparameter settings:

$$\theta_1, \theta_2, \dots, \theta_M$$

- Learn a classifier for each setting using only $\mathcal{D}_{train}$:

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Setting k for kNN with Validation Sets

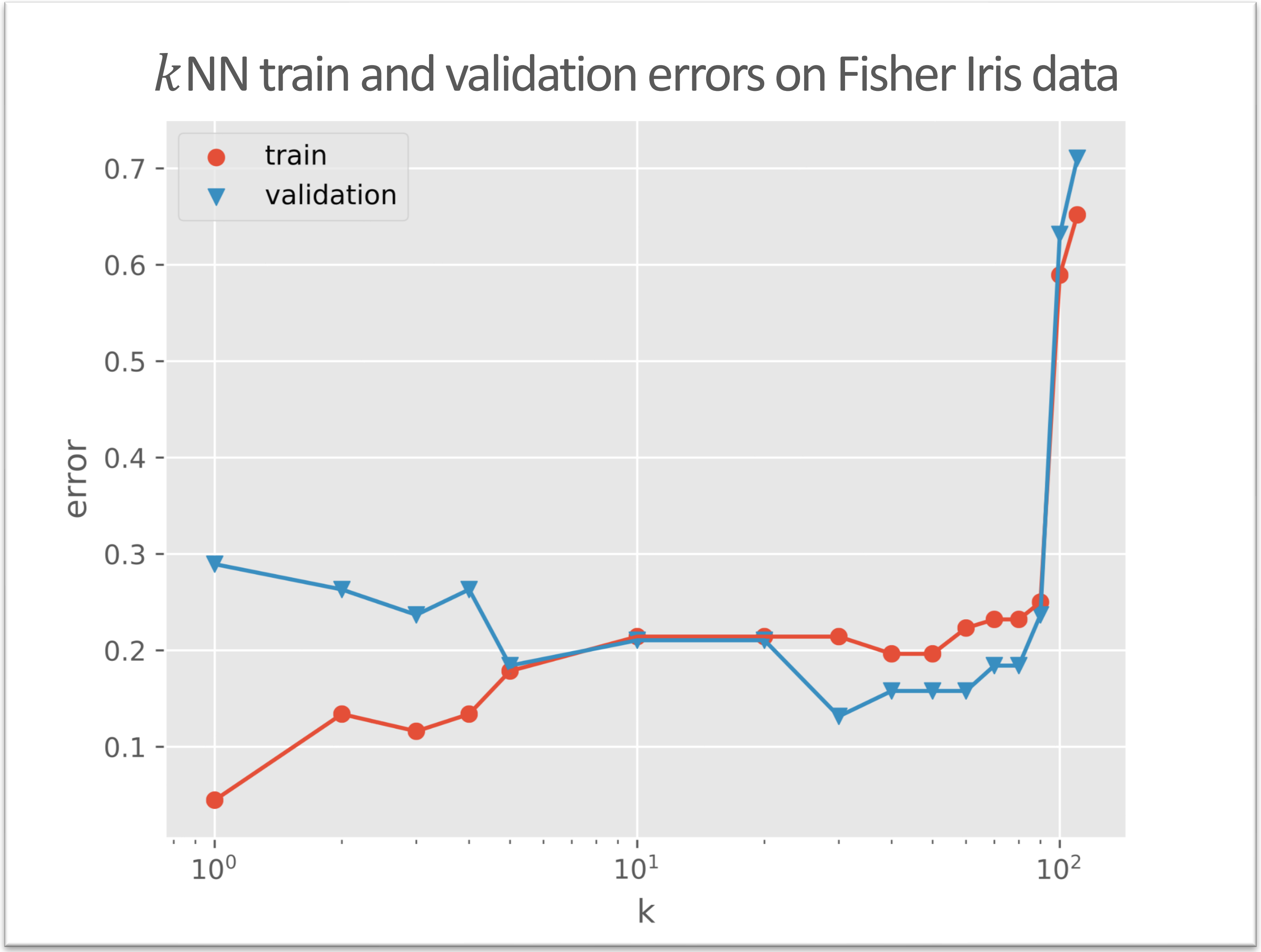


Figure courtesy of Matt Gormley

How should we partition our dataset?

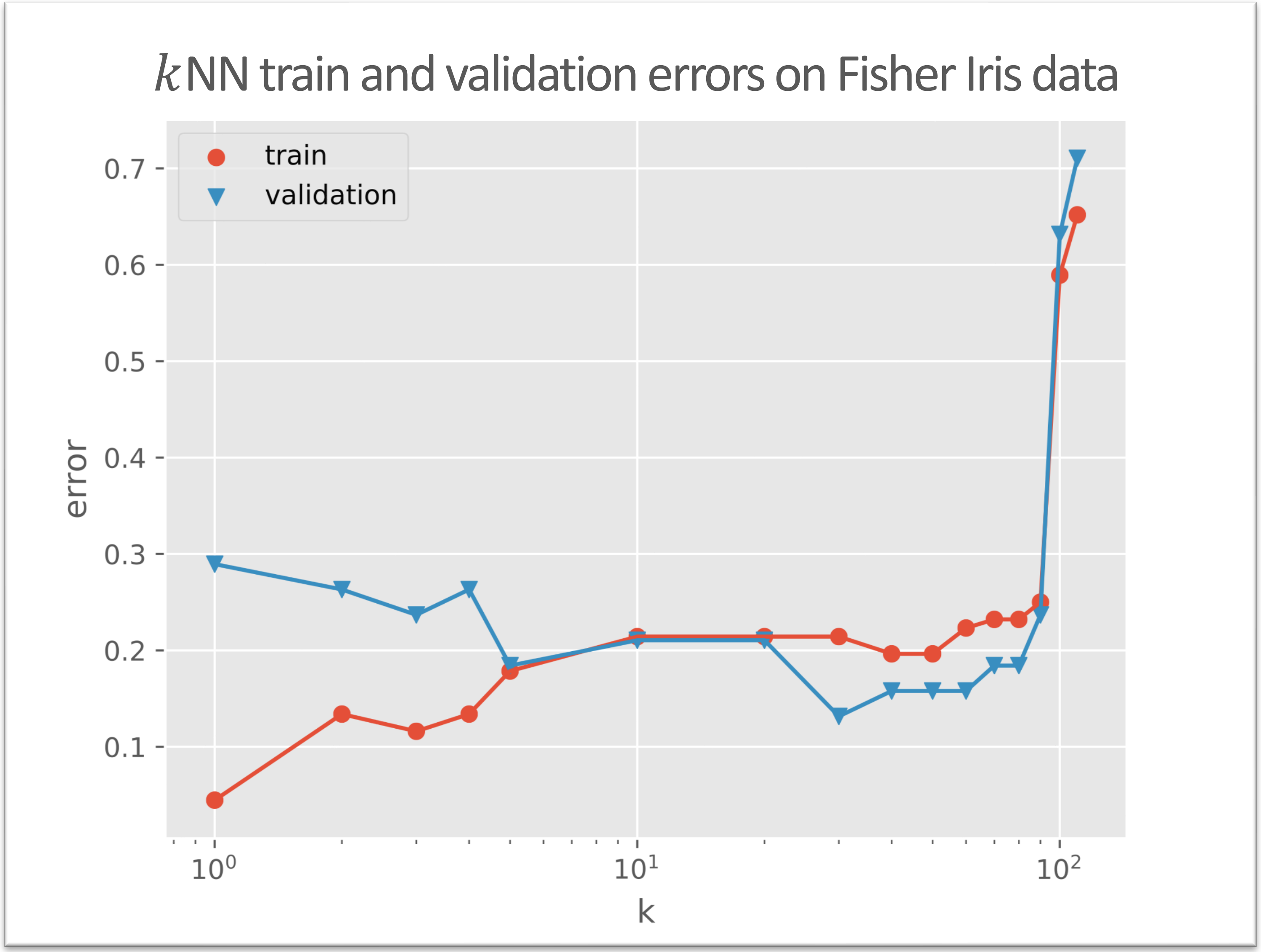
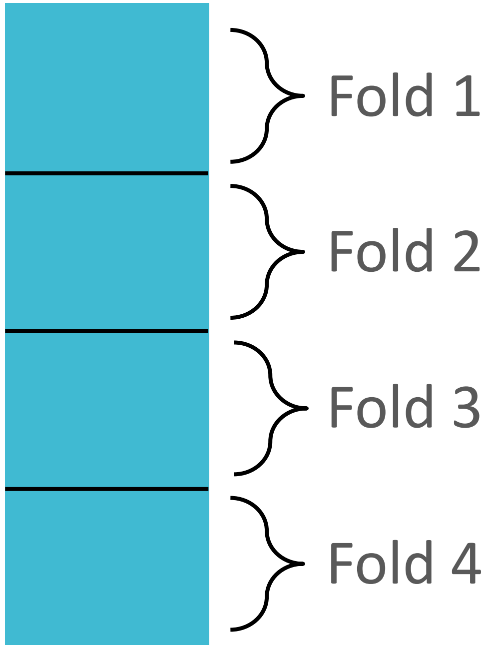


Figure courtesy of Matt Gormley

K-fold cross-validation

- Given $\mathcal{D}$, split $\mathcal{D}$ into K equally sized datasets or folds: $\mathcal{D}_1, \mathcal{D}_2, \ldots, \mathcal{D}_K$
- Use each one as a validation set once:



- Let h_{-i} be the classifier learned using $\mathcal{D}_{-i} = \mathcal{D} \backslash \mathcal{D}_i$ (all folds other than $\mathcal{D}_i$) and let $e_i = err(h_{-i}, \mathcal{D}_i)$
- The K-fold cross validation error is

$$err_{cv_K} = \frac{1}{K} \sum_{i=1}^{K} e_i$$

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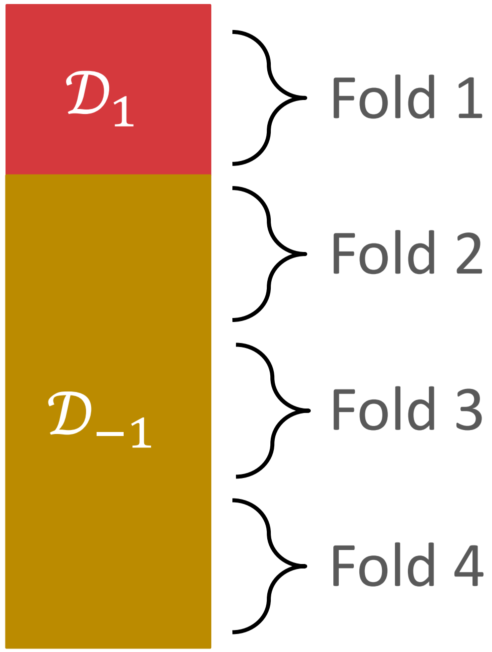

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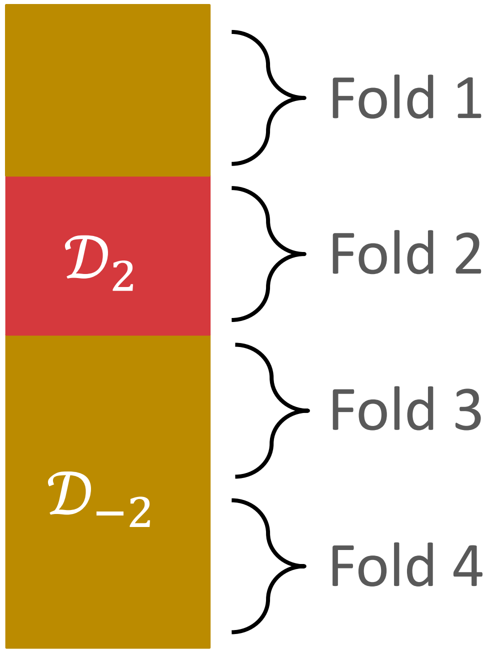

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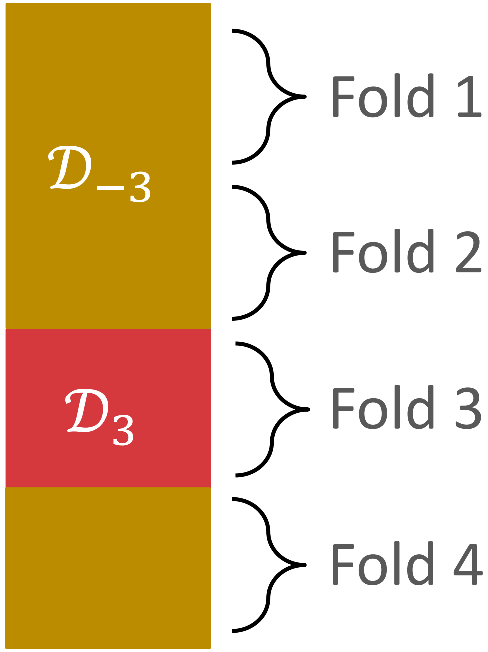

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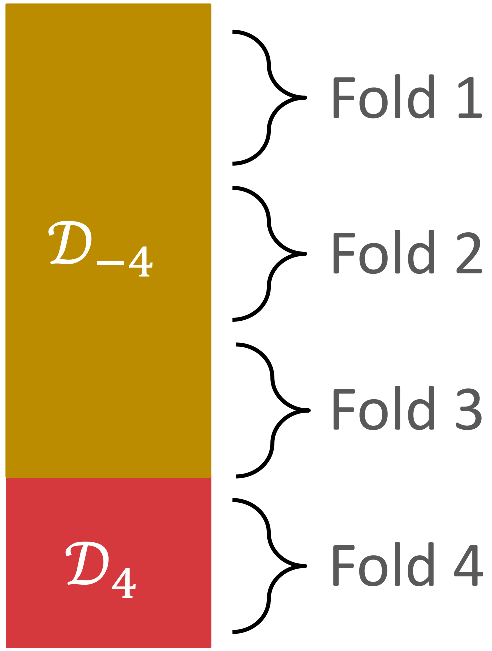

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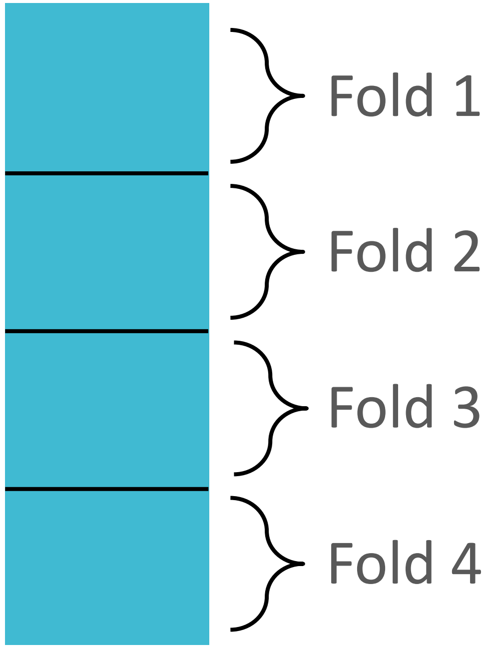

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- The K-fold cross validation error is

$$err_{cv_K} = \frac{1}{K} \sum_{i=1}^{K} e_i$$

- Special case when $K = N$: *Leave-one-out cross-validation*
- Choosing between m candidates requires training mK times

Summary

	Input	Output
Training	• training dataset • hyperparameters	• best model parameters
Hyperparameter Optimization	• training dataset • validation dataset	• best hyperparameters
Cross-Validation	• training dataset • validation dataset	• cross-validation error
Testing	• test dataset • classifier	• test error

Hyperparameter Optimization

- Given $\mathcal{D} = \mathcal{D}_{train} \cup \mathcal{D}_{val} \cup \mathcal{D}_{test}$, suppose we have multiple candidate hyperparameter settings:

$$\theta_1, \theta_2, \dots, \theta_M$$

- Learn a classifier for each setting using only $\mathcal{D}_{train}$:

$$h_1, h_2, \dots, h_M$$

- Evaluate each one using $\mathcal{D}_{val}$ and choose the one with lowest *validation* error:

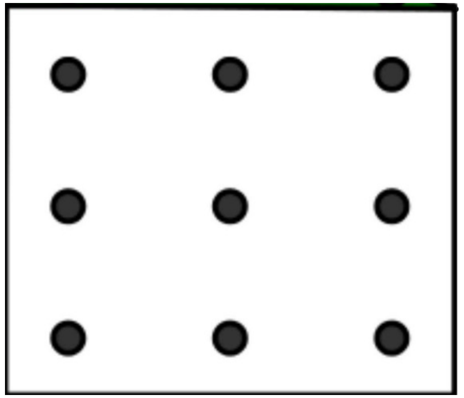
$$\hat{m} = \underset{m \in \{1,\dots,M\}}{\operatorname{argmin}} \; err(h_m, \mathcal{D}_{val})$$

General Methods for Hyperparameter Optimization

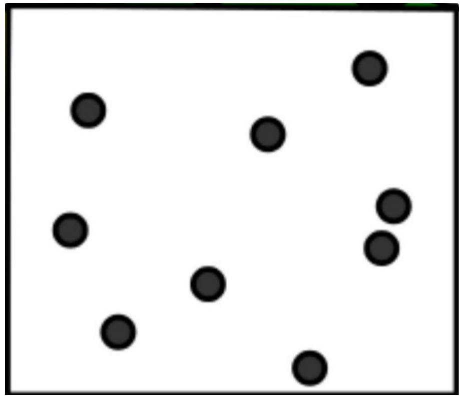
- Idea: set the hyperparameters to optimize some performance metric of the model
- Issue: if we have many hyperparameters that can all take on lots of different values, we might not be able to test all possible combinations
- Commonly used methods:
  - Grid search
  - Random search
  - Bayesian optimization (used by Google DeepMind to optimize the hyperparameters of AlphaGo: https://arxiv.org/pdf/1812.06855v1.pdf)
  - Evolutionary algorithms
  - Graduate-student descent

Grid Search vs. Random Search (Bergstra and Bengio, 2012)

Grid Layout



Random Layout



Source: https://jmlr.csail.mit.edu/papers/volume13/bergstra12a/bergstra12a.pdf

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
- Select an appropriate algorithm for optimizing (aka. learning) hyperparameters