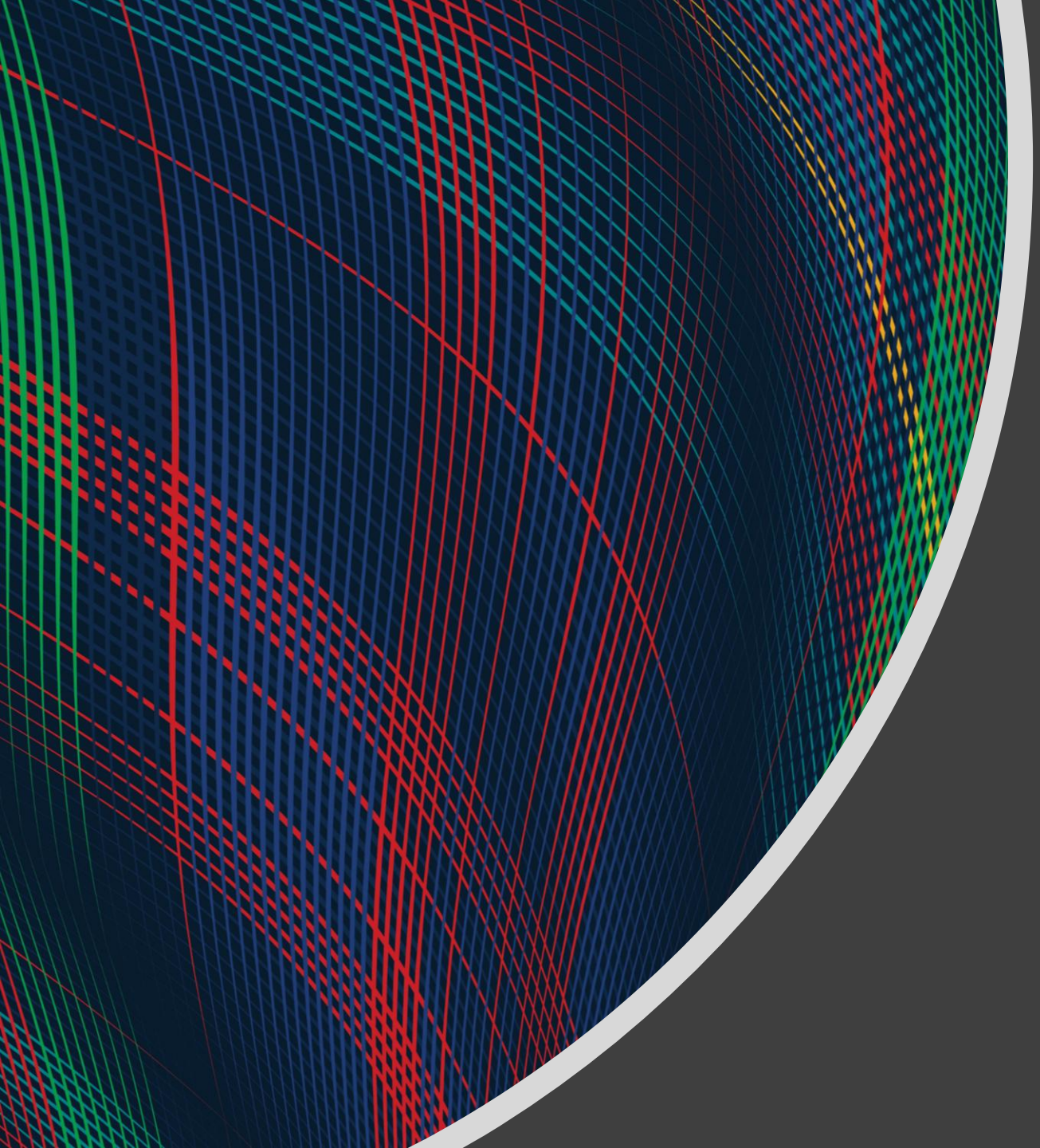


10-315 Introduction to ML

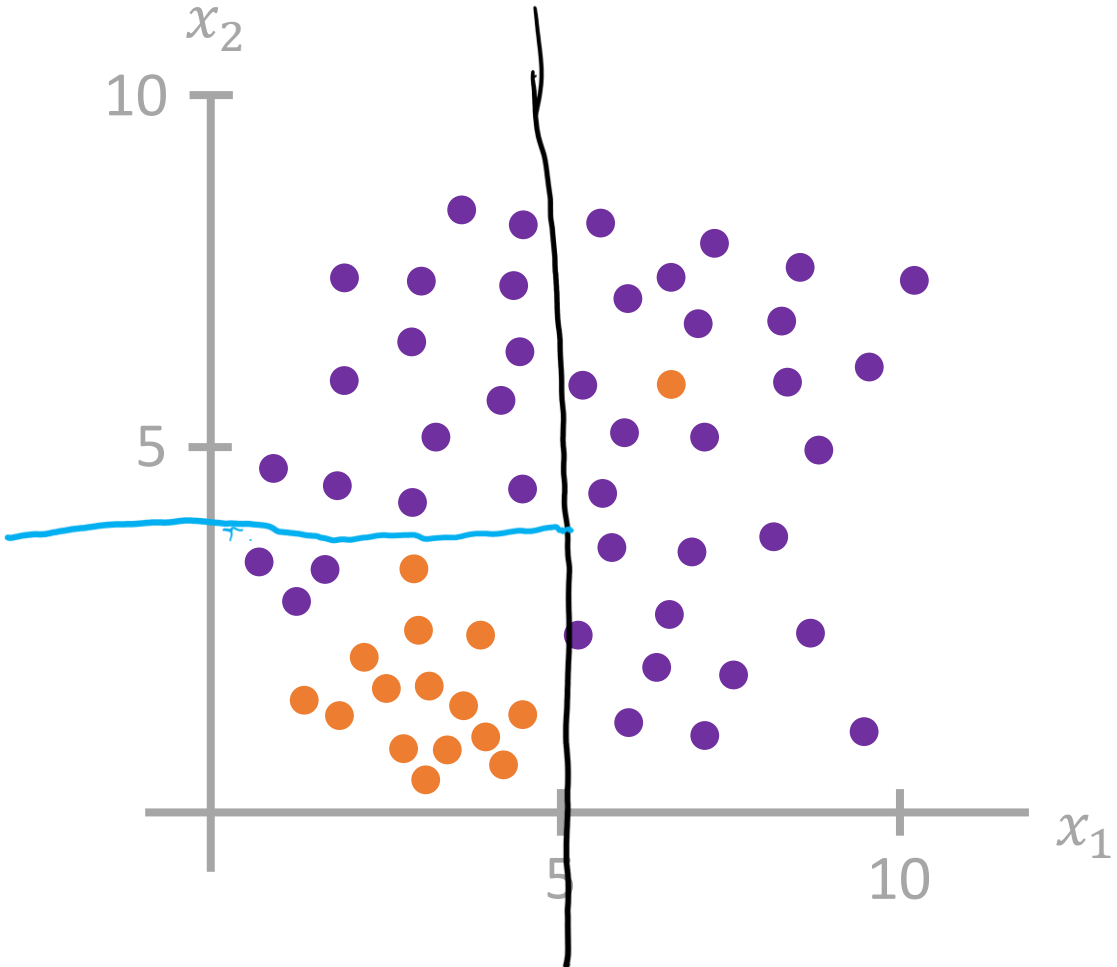
Model Selection

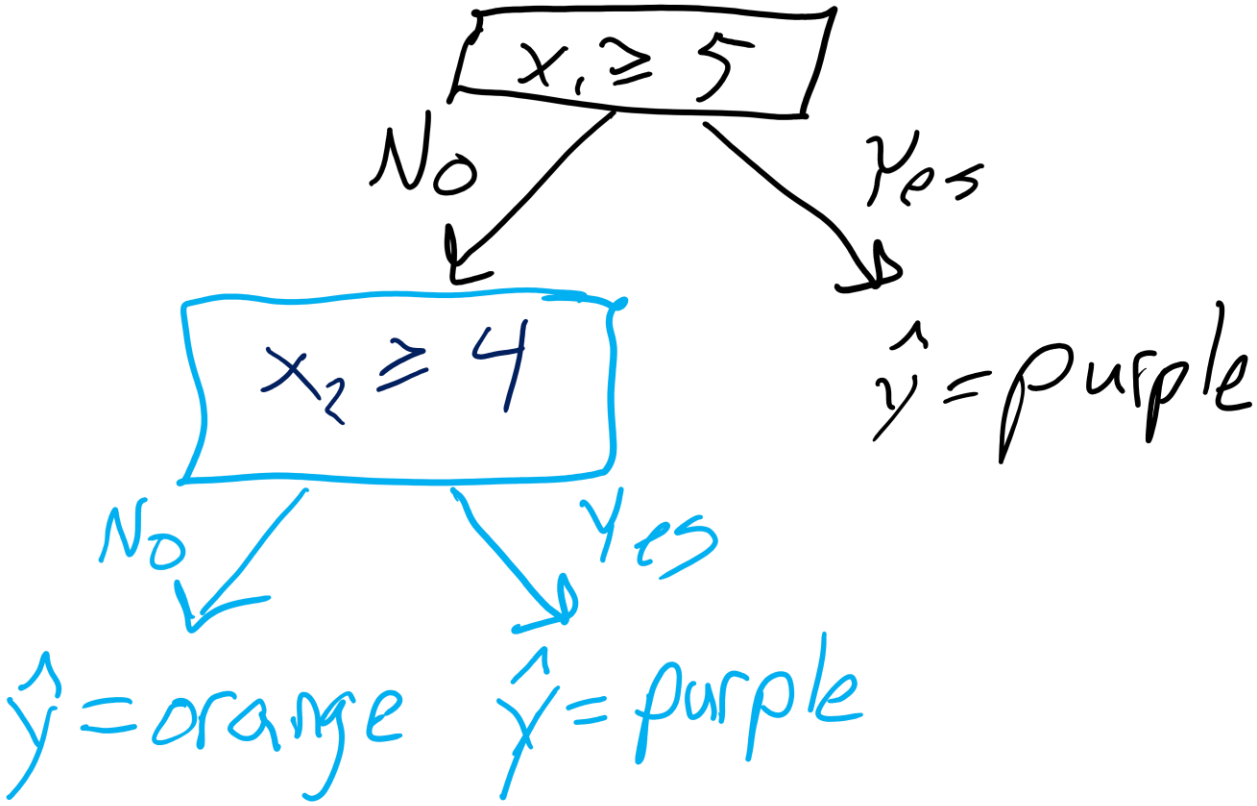
Instructor: Pat Virtue

Reminder: Decision Tree Worksheet

Consider input features $x \in \mathbb{R}^2$.

Draw a reasonable decision tree.





Poll 2

Decision tree generalization

Which of the following generalize best to unseen examples?

A. Small tree with low training accuracy
B. Large tree with low training accuracy
C. Small tree with high training accuracy
D. Large tree with high training accuracy

Underfitting and Overfitting

Underfitting occurs when model:

- is too simple
- can't capture the actual pattern of interest in the training dataset
- has too much inductive bias

Overfitting occurs when model:

- is too complex
- fits noise or "outliers" in the training dataset as opposed to the actual pattern of interest
- doesn't have enough inductive bias pushing it to generalize

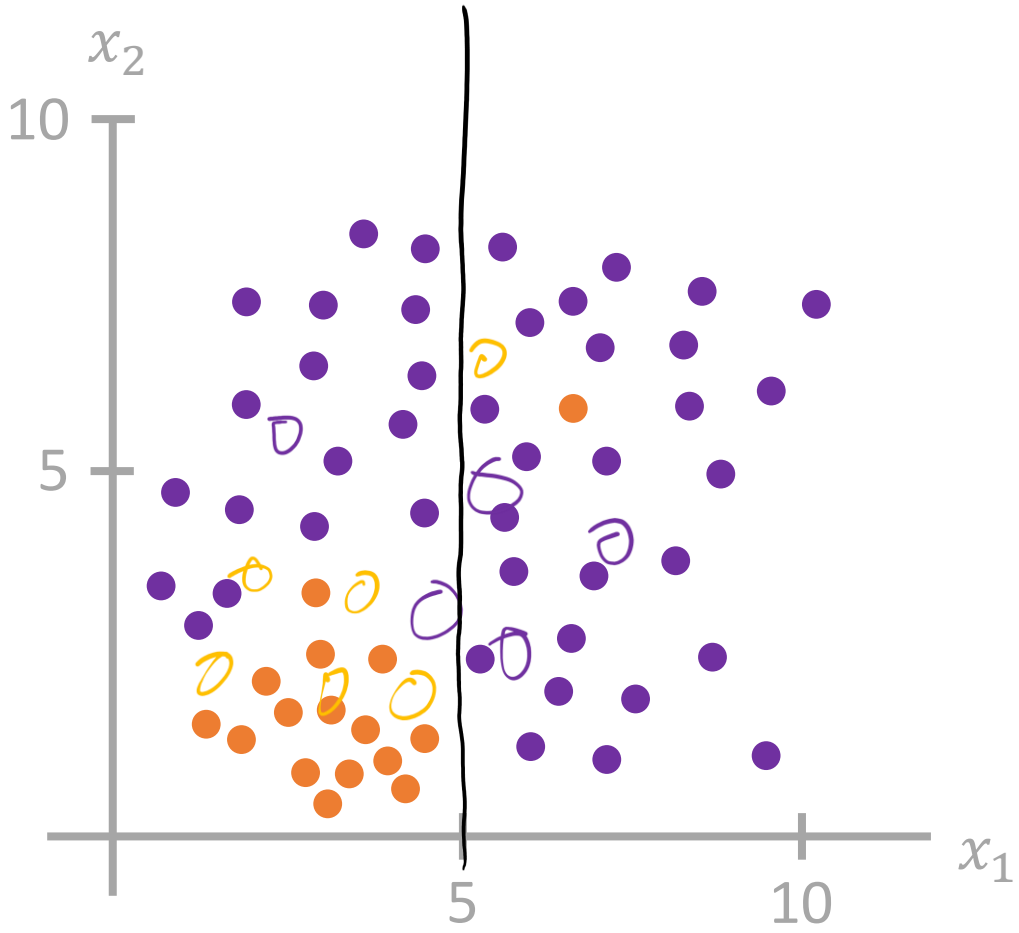
Slide credit: CMU MLD Henry Chai

Underfitting and Overfitting: Classification

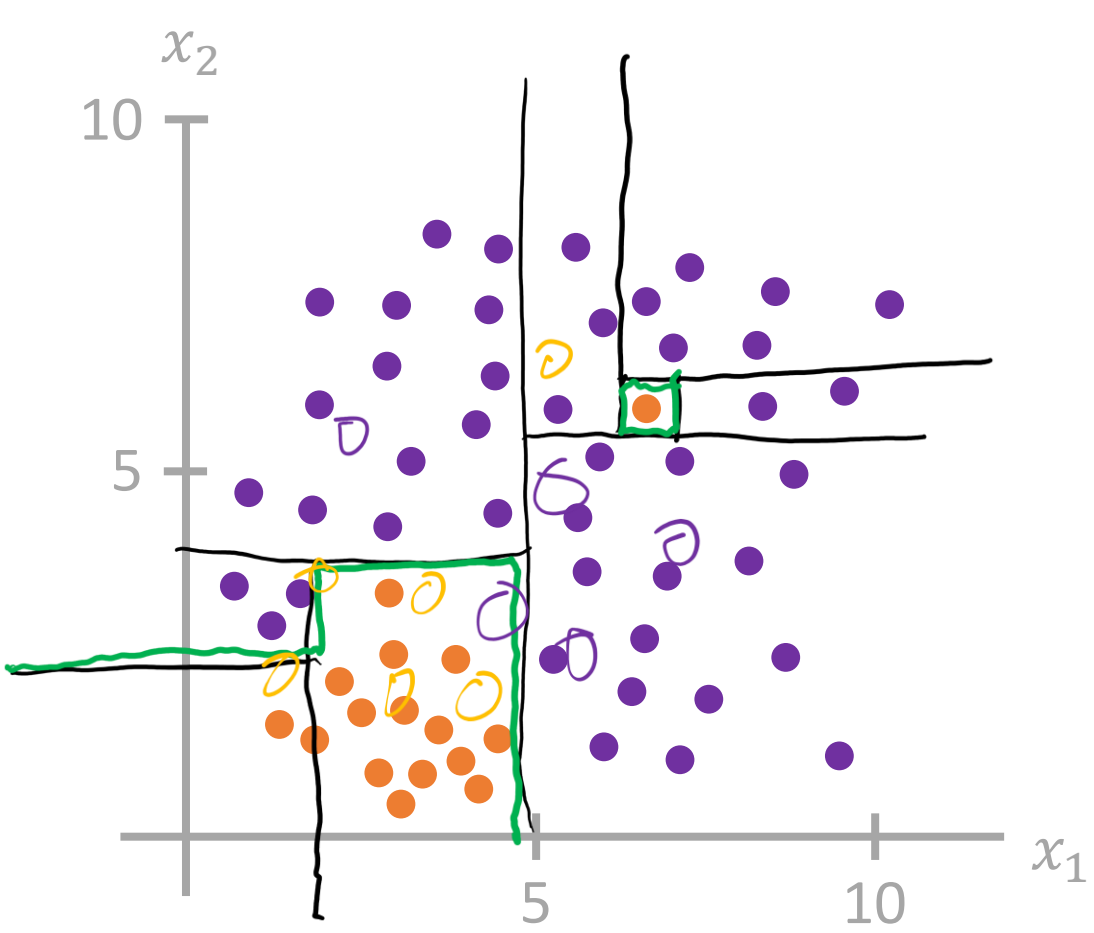
● train data

○ test data

Underfitting

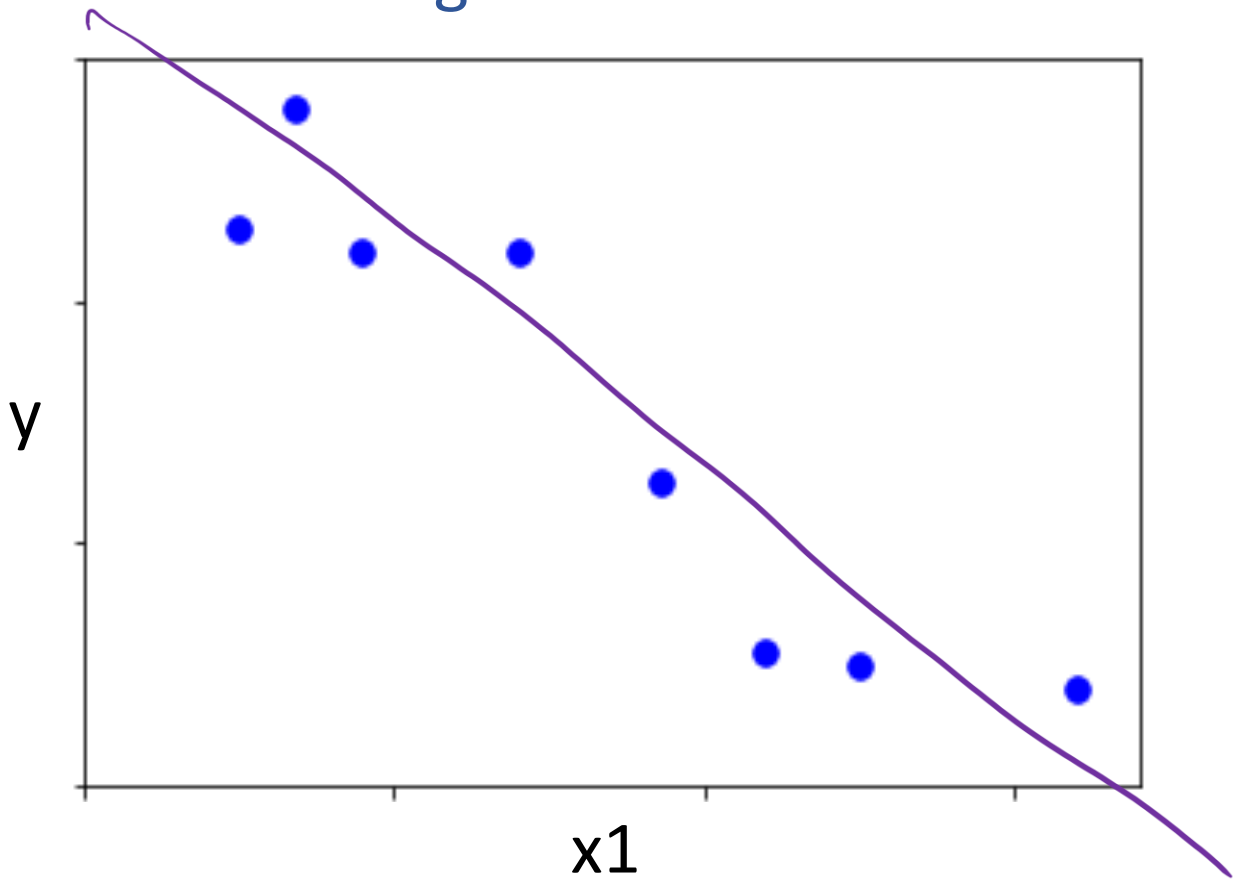


Overfitting

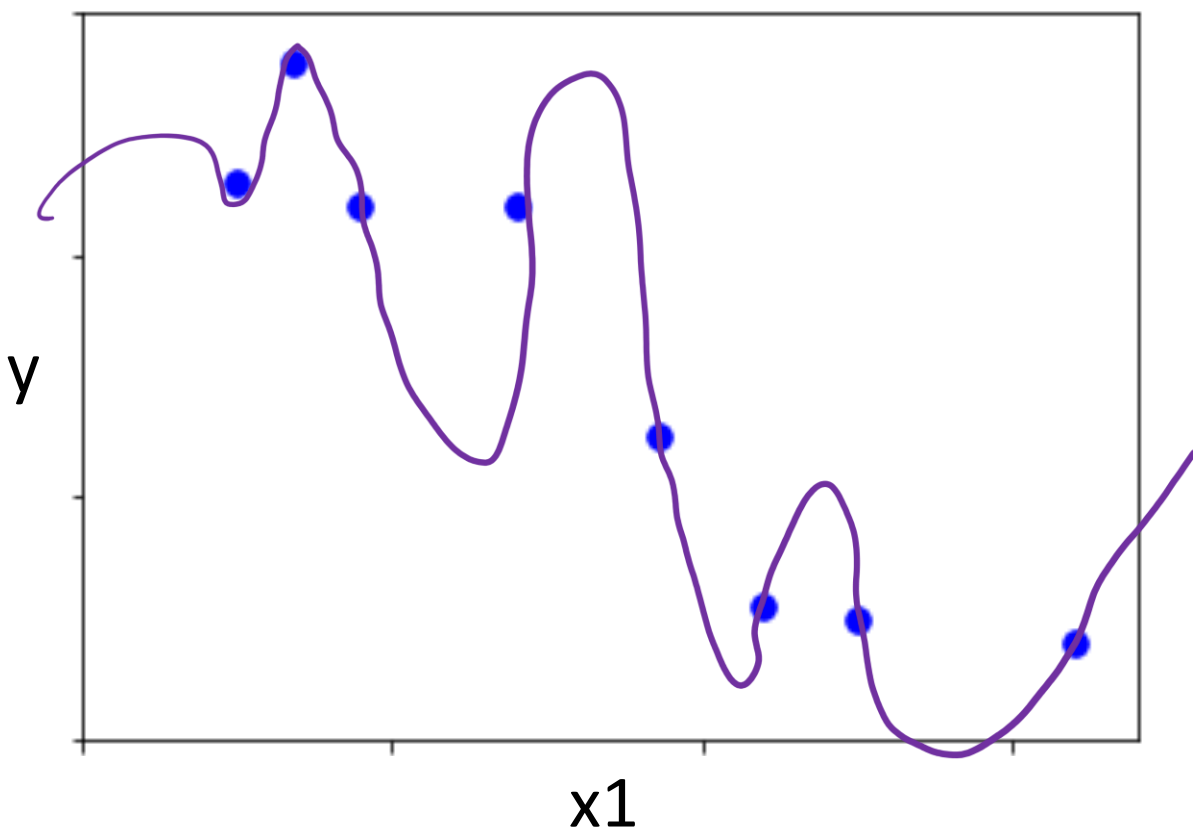


Underfitting and Overfitting: Regression

Underfitting

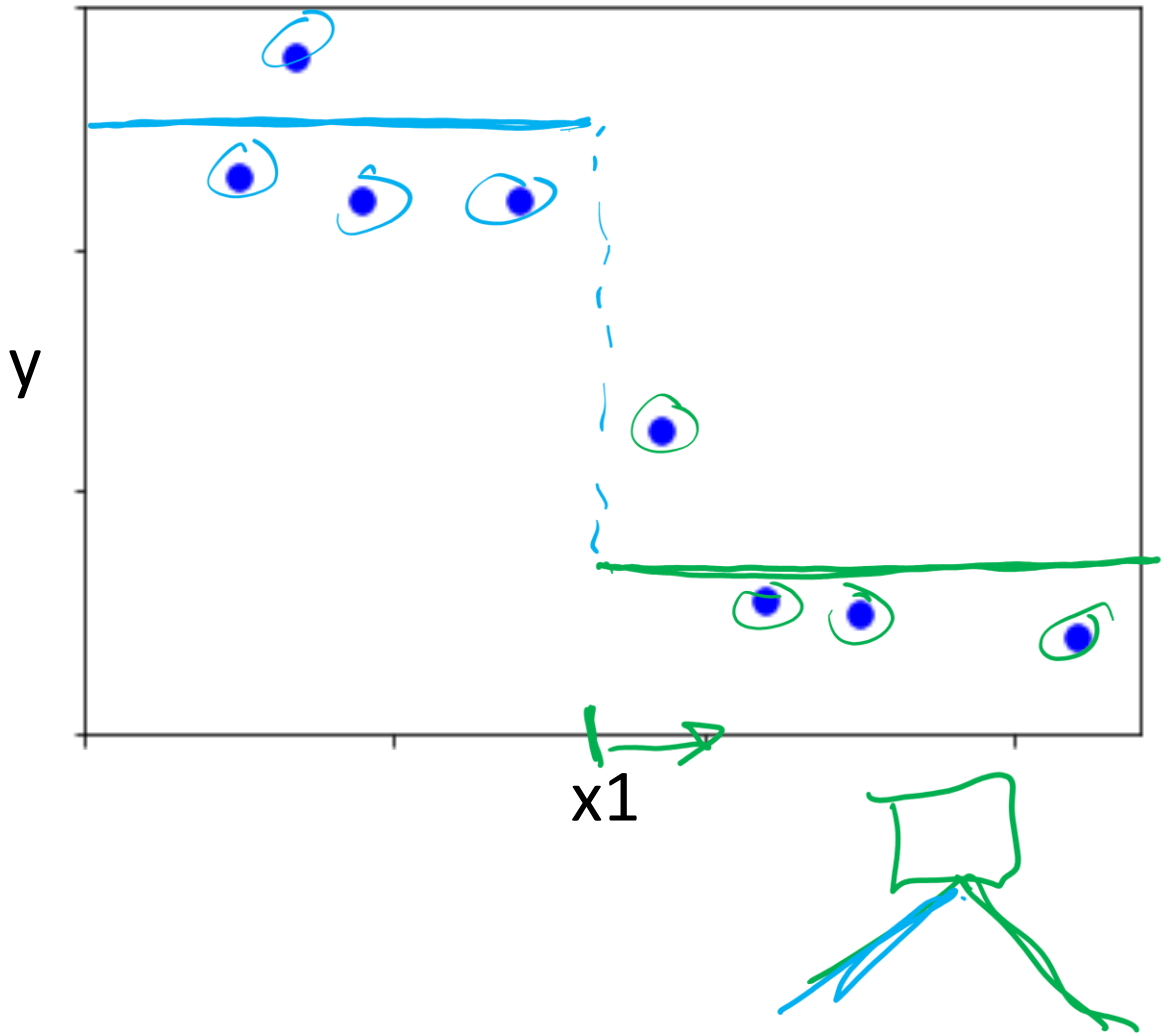


Overfitting

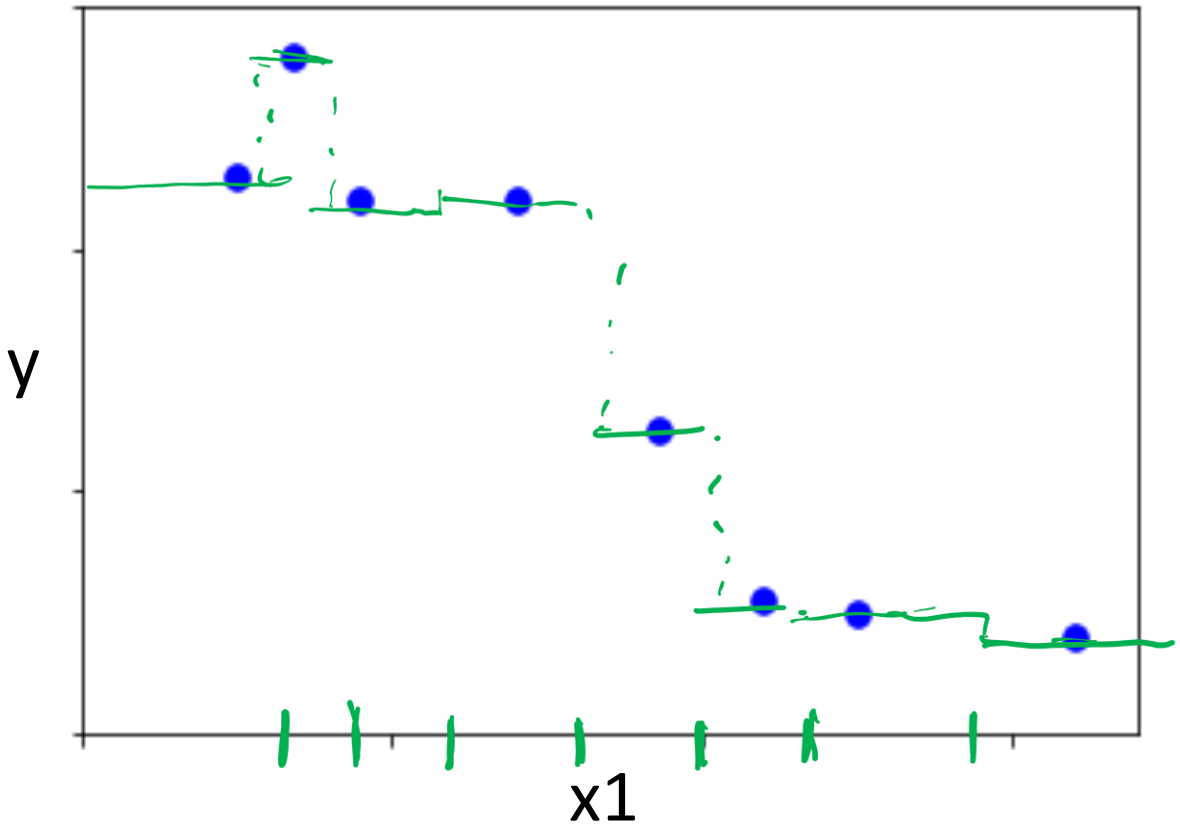


Underfitting and Overfitting: Regression

Underfitting



Overfitting



Reminder: Decision Trees

When do we stop (base case)?

When leaves are “pure”, i.e., output values are all the same

- Likely to overfit

Limit

- Tree depth
- Total number of leaves
- Splitting criteria threshold, e.g. splitting criteria <= τ
- Minimum number of datapoints in a leaf

But how do we choose all of those limits?!?

Answer: Model selection

Model selection is the process to choose the “best” among a set of (trained) models

Today

k-Nearest Neighbor

- 1-NN, k-NN (mostly notation)
- Practical details

Underfitting and Overfitting

- Decision Tree stopping criteria
- Classification and regression examples

Model Selection

- Define terms
- Stress importance
- Cross-validation techniques

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.

Slide credit: CMU MLD Matt Gormley

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

Slide credit: CMU MLD Matt Gormley

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
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Slide credit: CMU MLD Matt Gormley

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

- *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)
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Slide credit: CMU MLD Matt Gormley

Model Selection

Statistics

- *Def*: a **model** defines the data generation process (i.e. a set or family of probability distributions)
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- *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

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

Machine Learning

- *Def*: (loosely) a **model** defines the hypothesis ... which learning performs its ...
- ... **parameters** are the numeric ... ructure selected by the learning ... hat give rise to a hypothesis
- *Def*: the **learning algorithm** defines the data-driven search ... ver the hypothesis space (i.e. search for goo... arameters)
- *Def*: **hyperparameters** are the tunable aspects of the model, that the learning algorithm does *not* select

Slide credit: CMU MLD Matt Gormley

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

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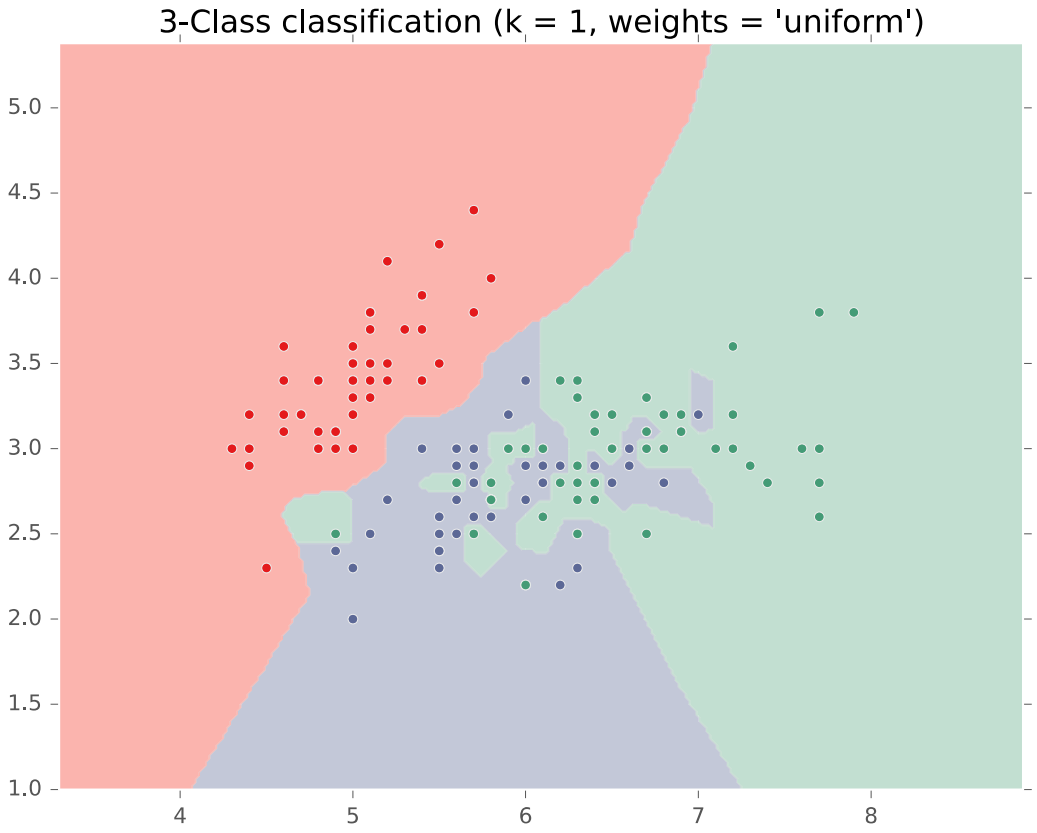
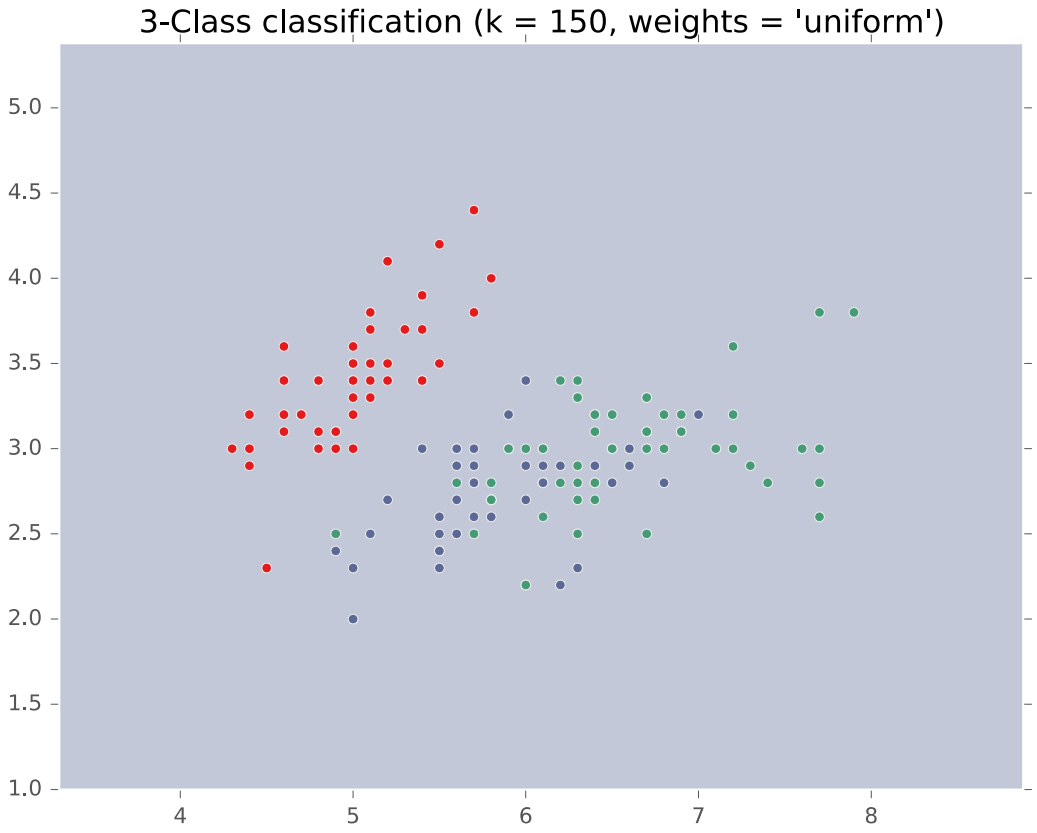
Special Cases of k-NN

k=1: Nearest Neighbor



k=N: Majority Vote



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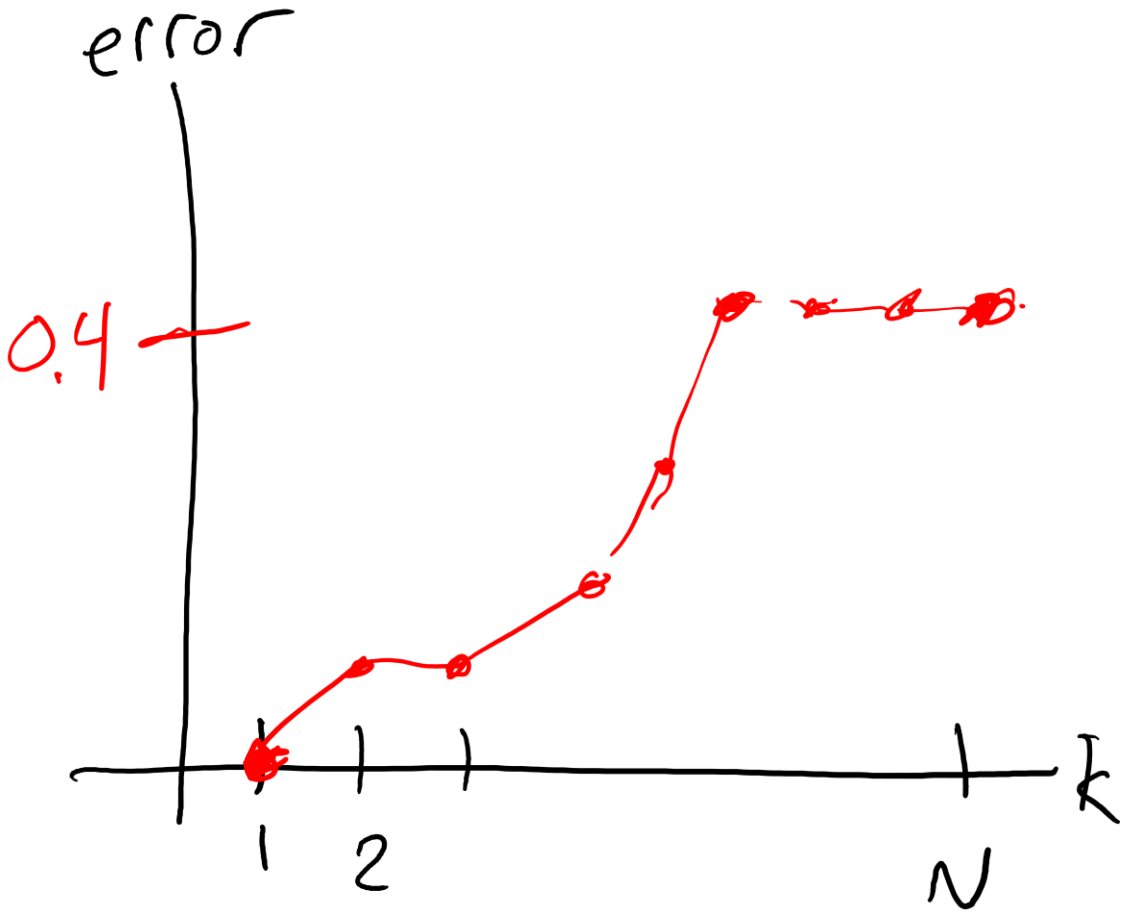
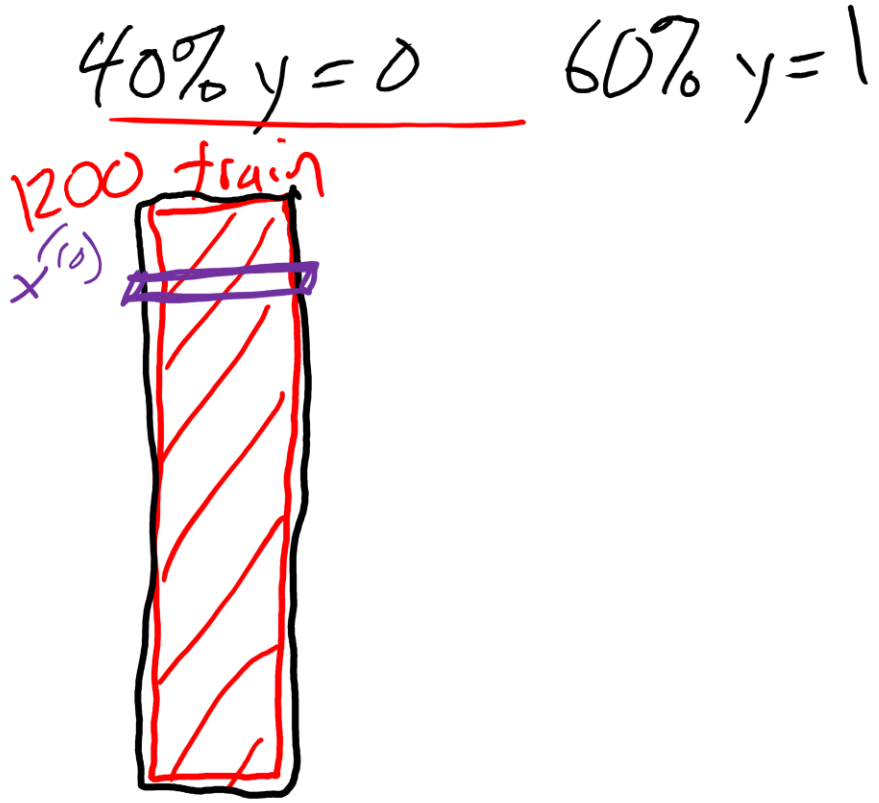
Example of Hyperparameter Optimization

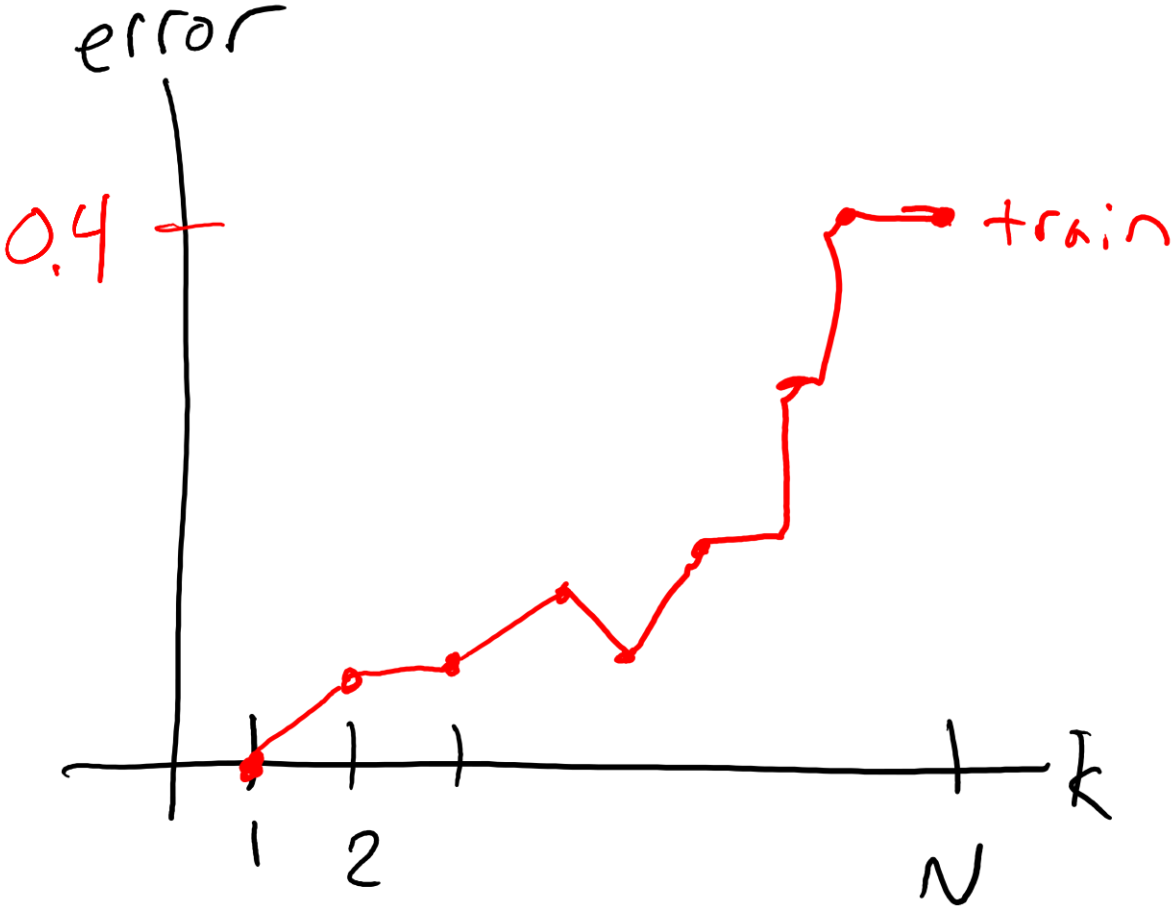
Choosing k for k-NN

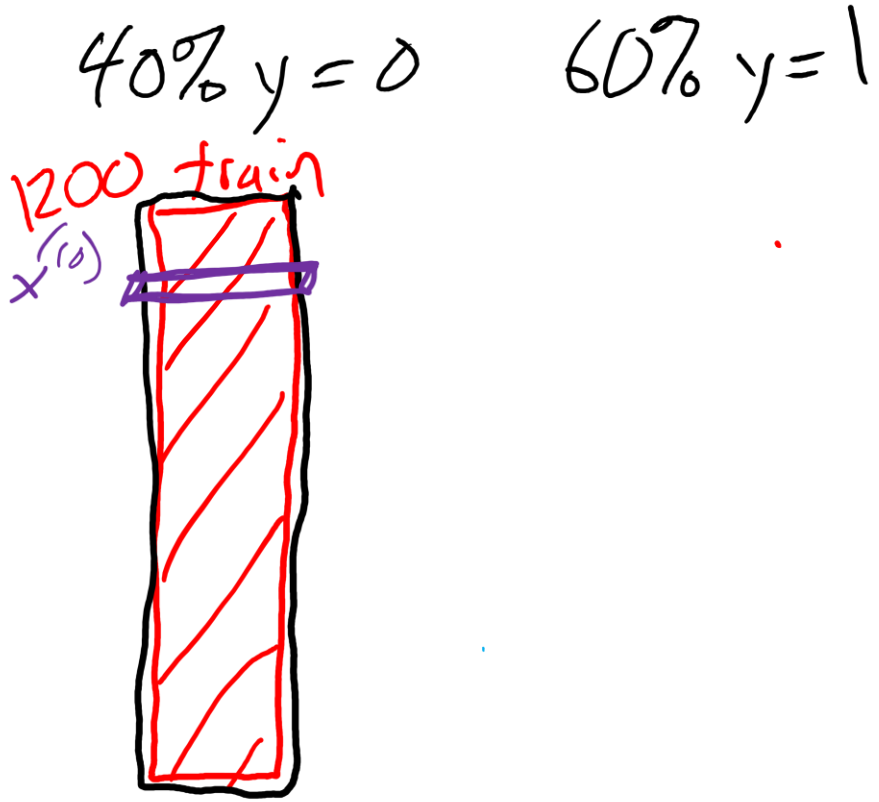




Example of Hyperparameter Optimization

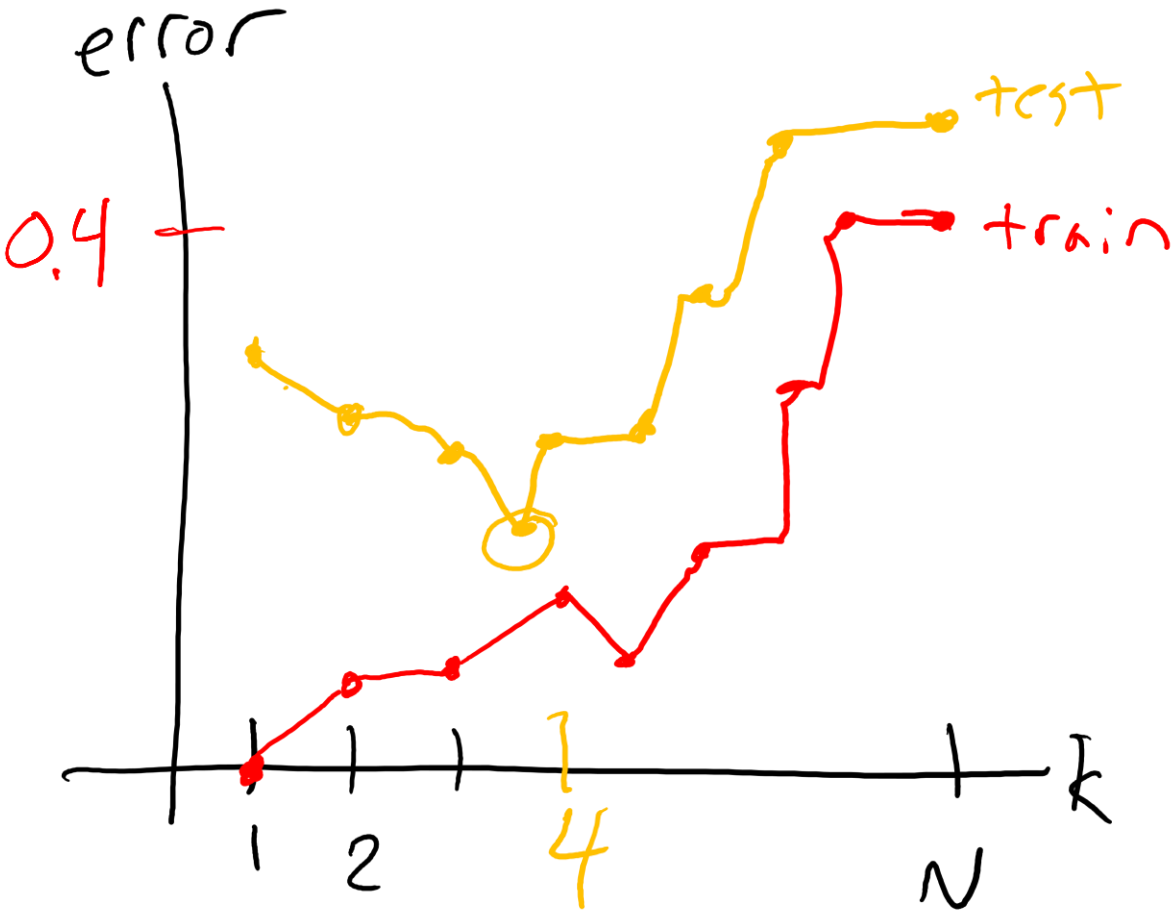
Choosing k for k-NN

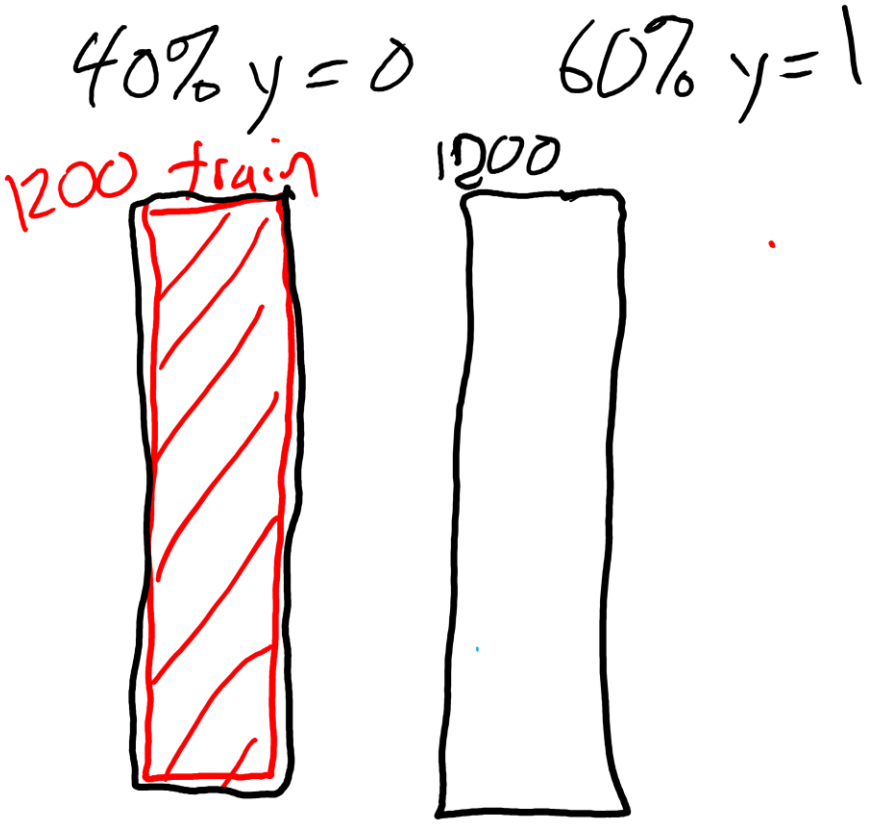




Example of Hyperparameter Optimization

Choosing k for k-NN





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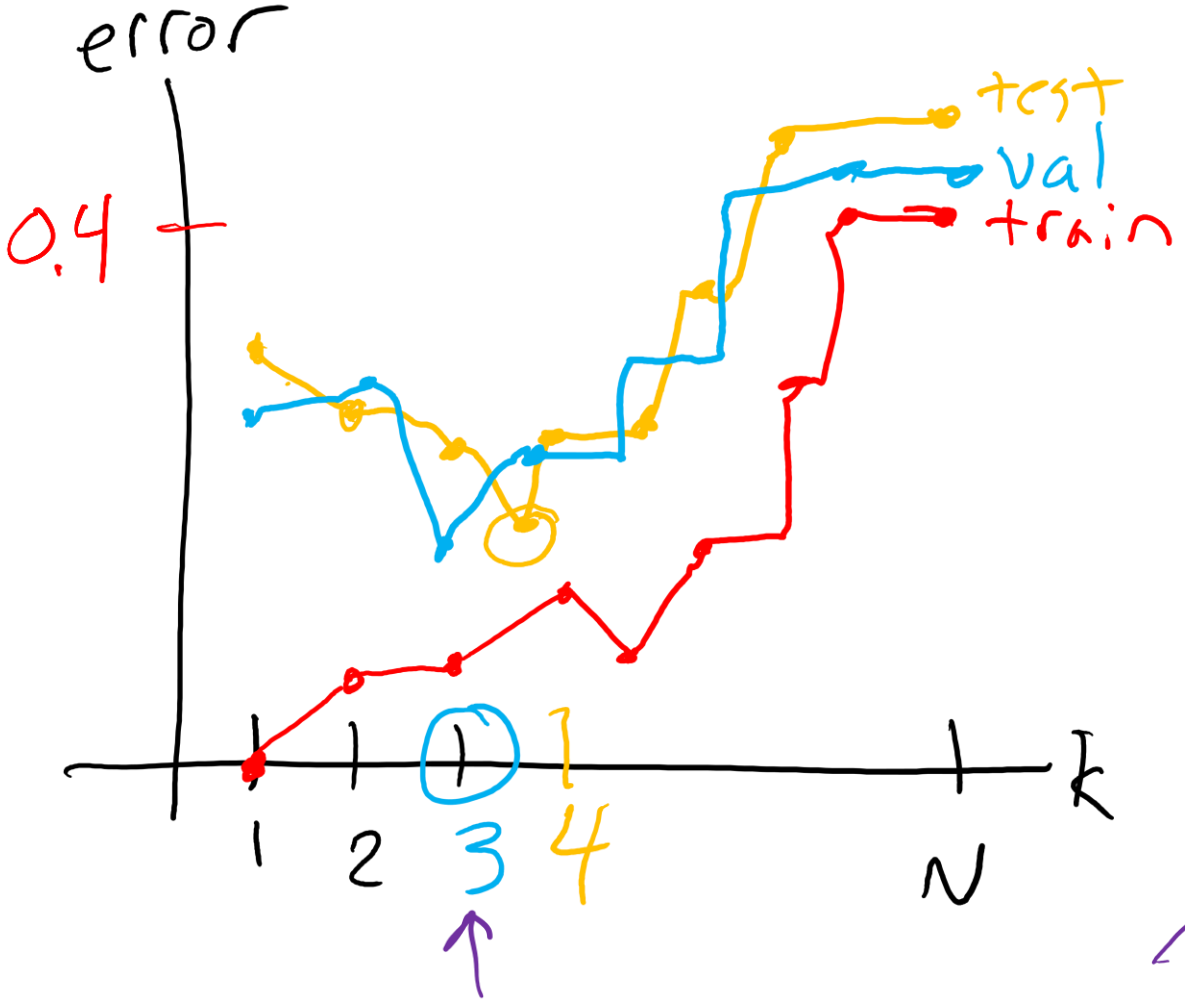
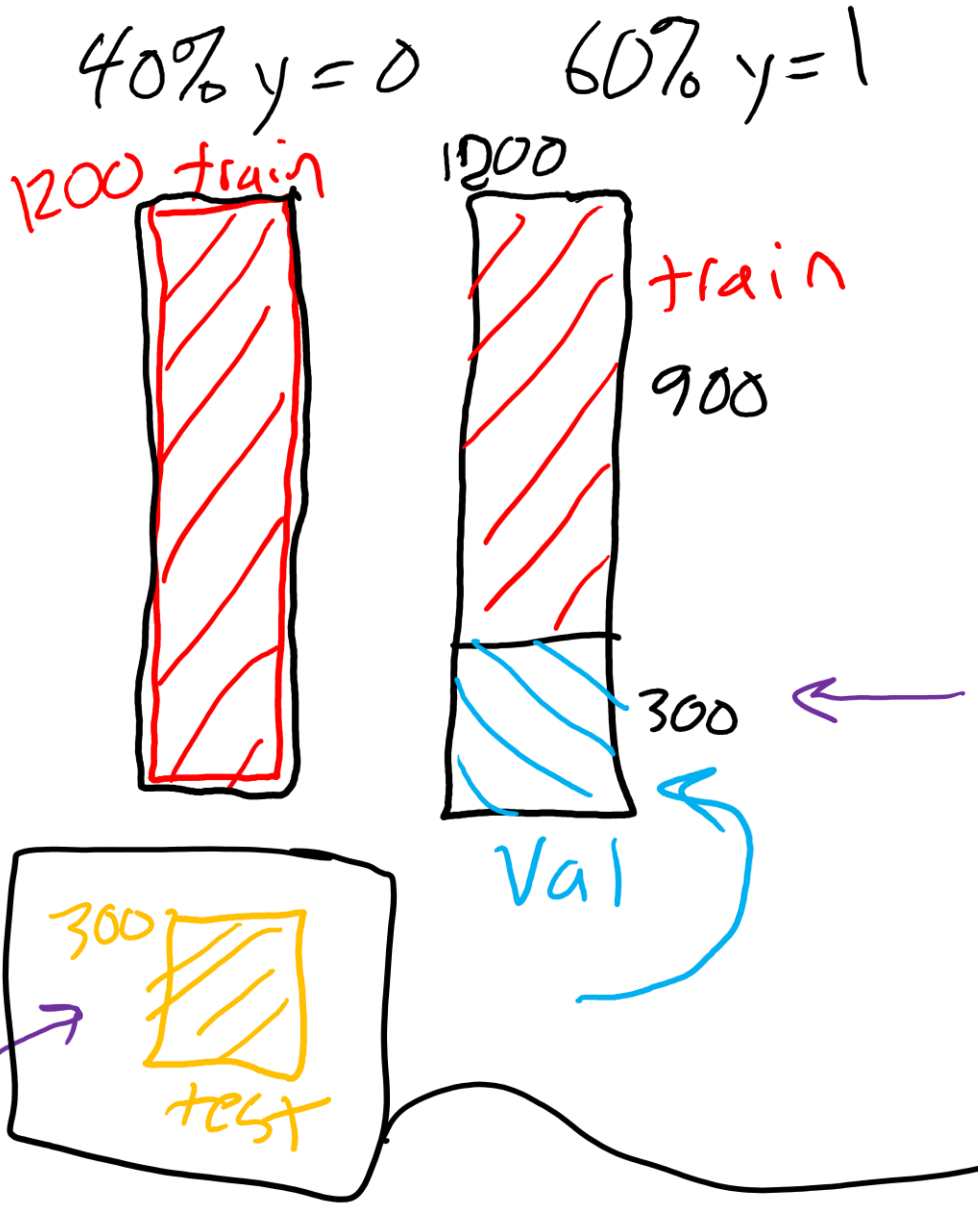
Example of Hyperparameter Optimization

Choosing k for k-NN





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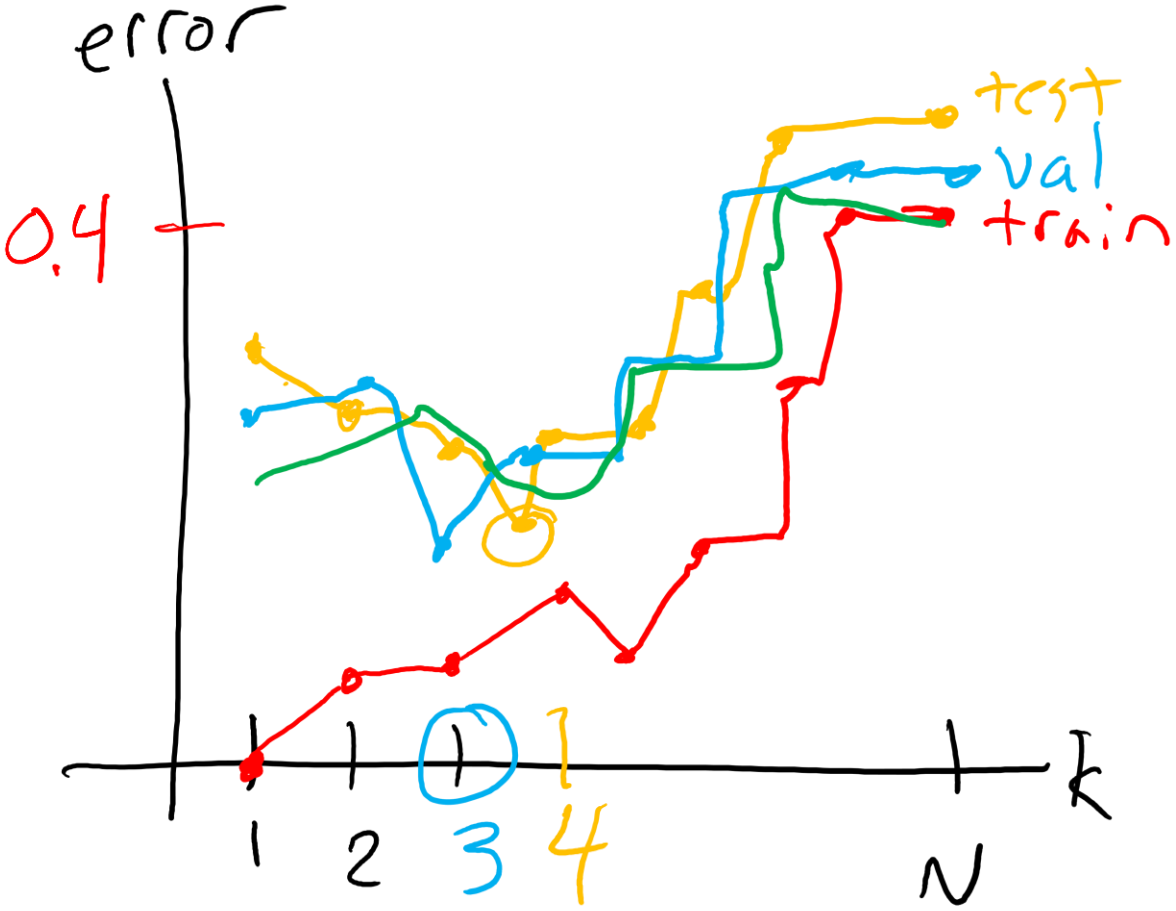
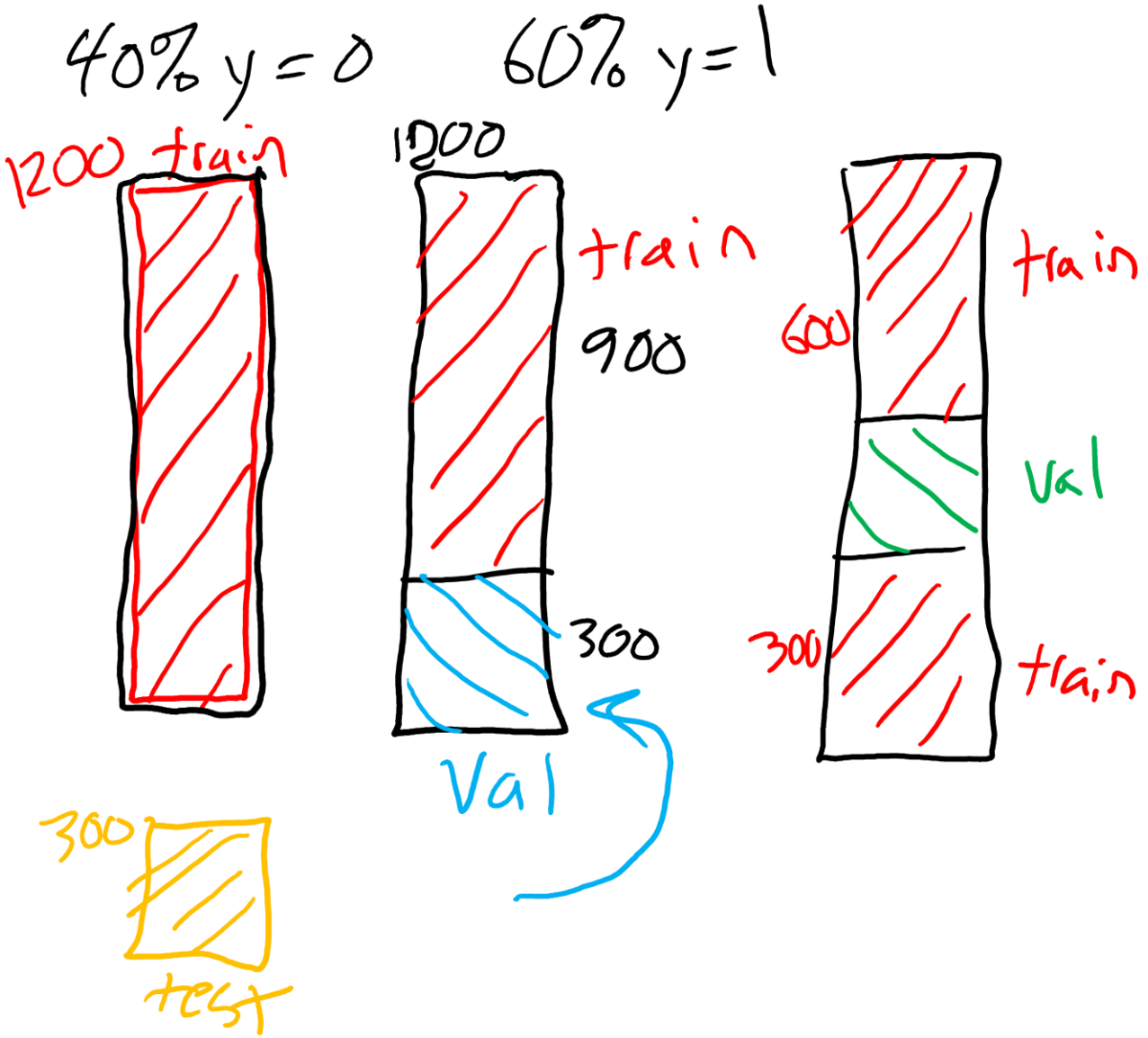
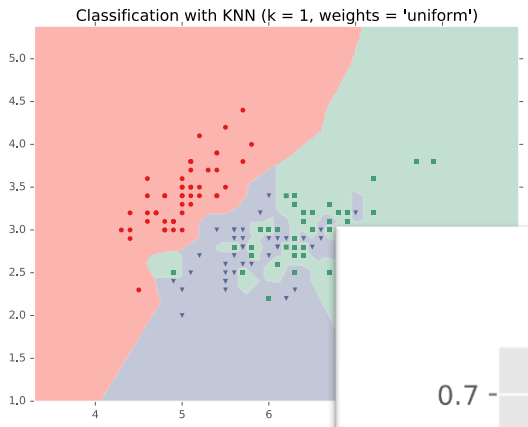
Example of Hyperparameter Optimization

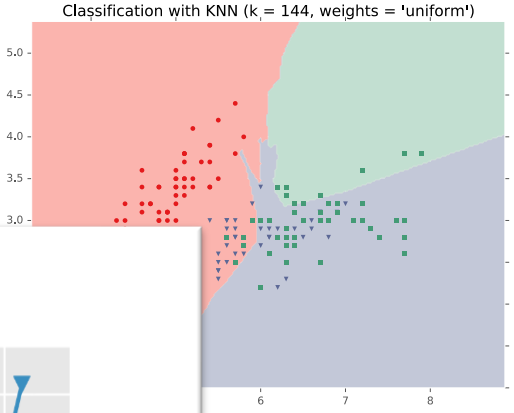
Choosing k for k-NN

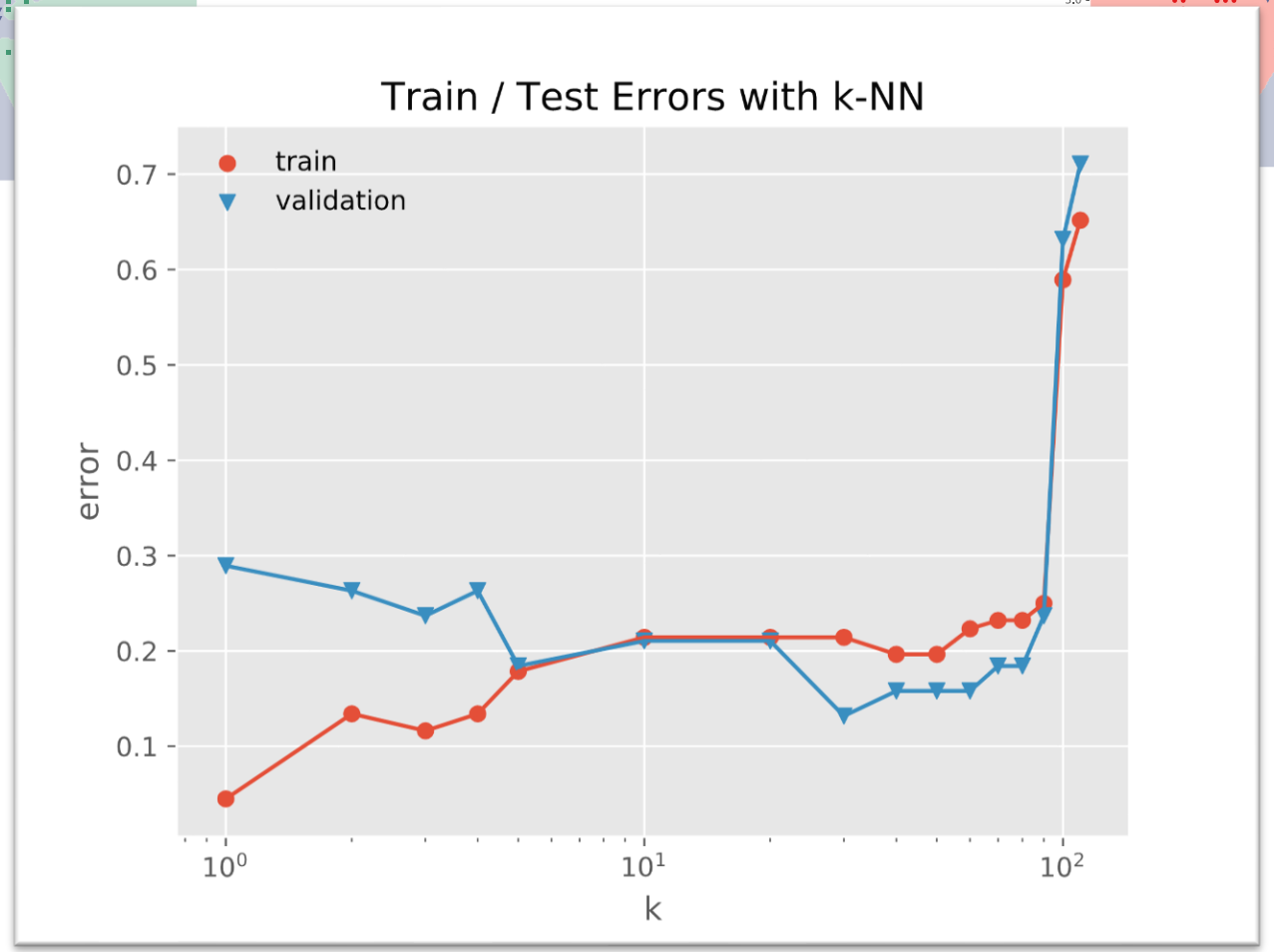




k-NN: Choosing k







Fisher Iris Data: varying the value of k

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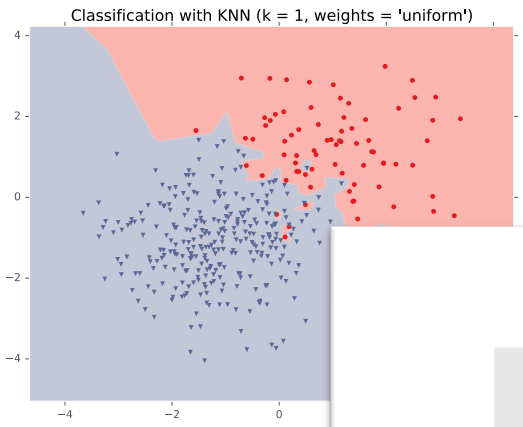
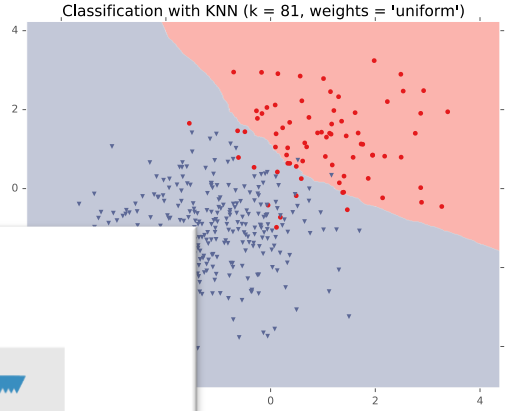
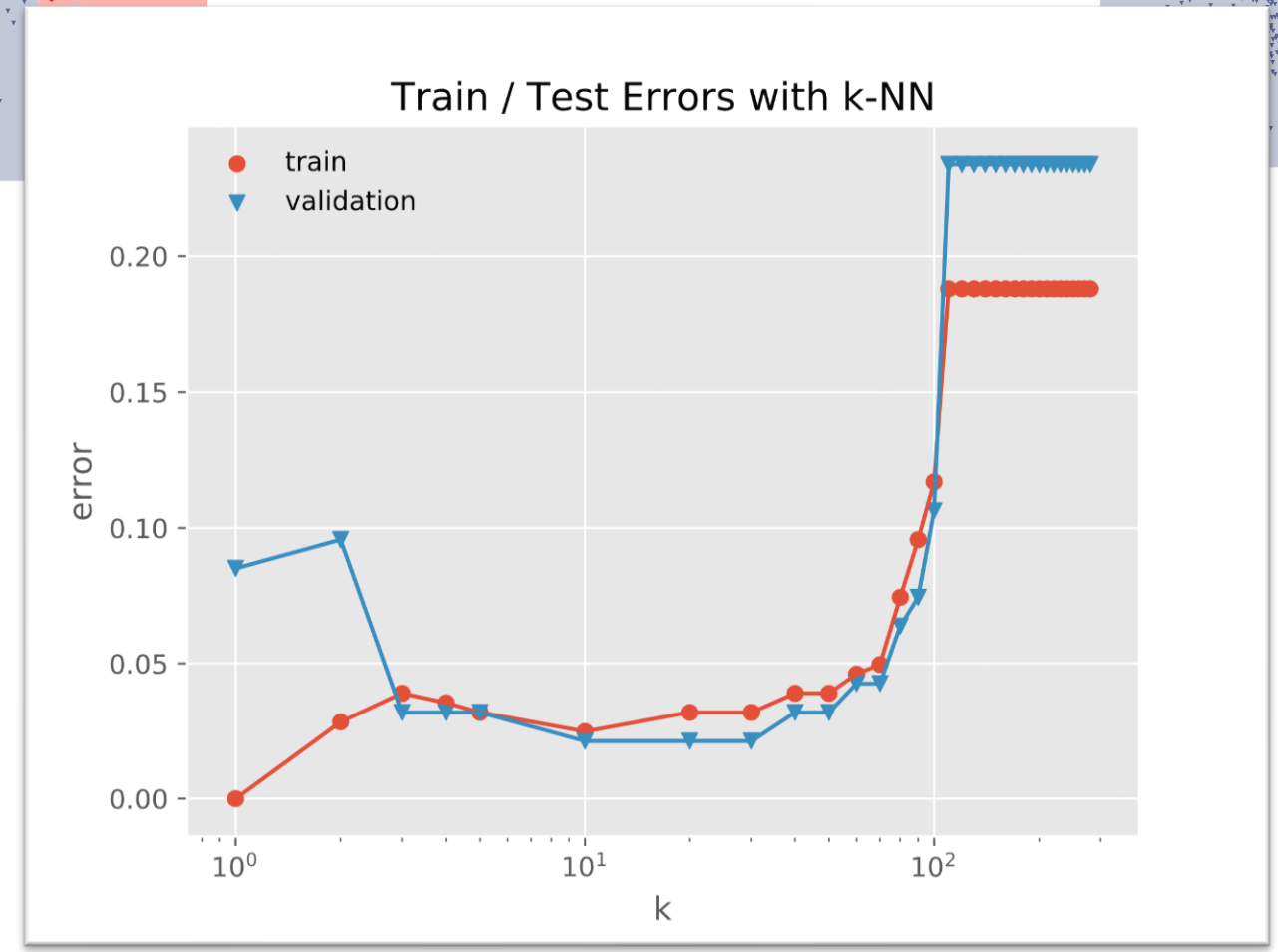
k-NN: Choosing k







Gaussian Data: varying the value of k

Slide credit: CMU MLD Matt Gormley

Cross-validation

Why do we need cross-validation?

- Choose hyperparameters
- Choose technique
- Help make any choices beyond our parameters

But now, we have another choice to make!

- How do we split training and validation?

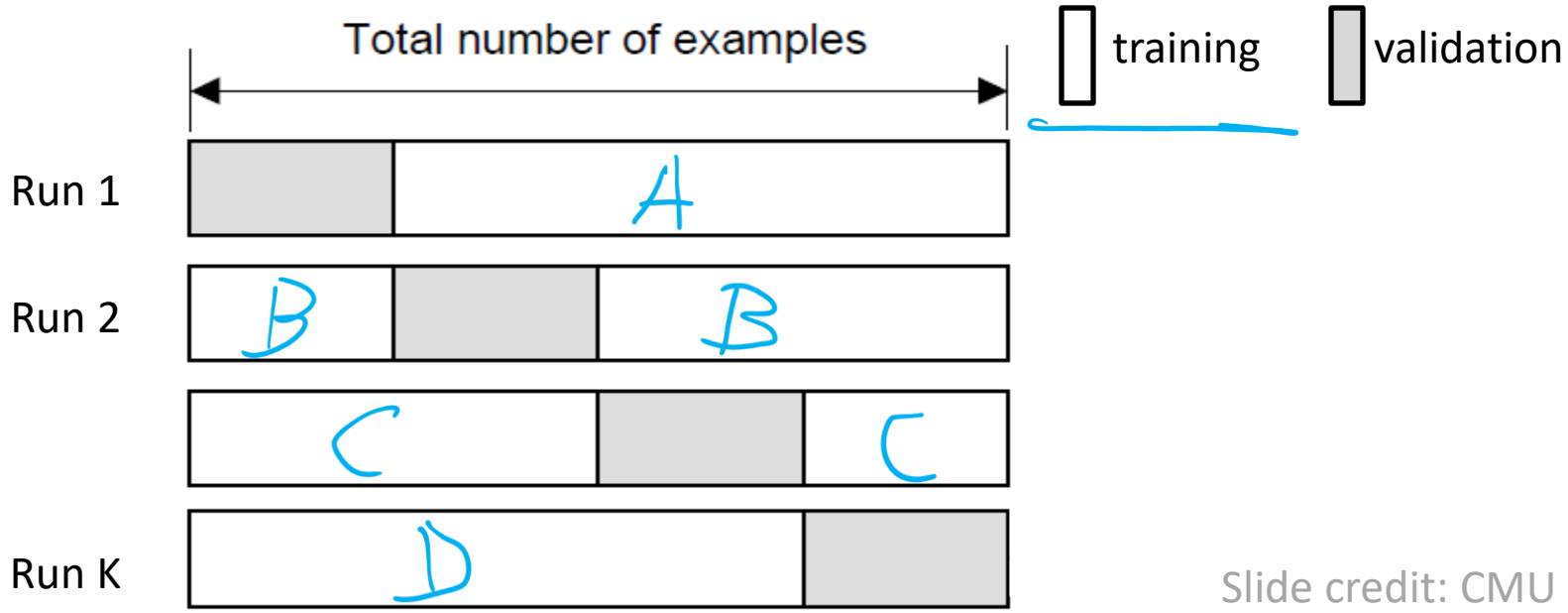
Trade-offs

- More held-out data, better meaning behind validation numbers
- More held-out data, less data to train on!

Cross-validation

K-fold cross-validation

Create K-fold partition of the dataset.
Do K runs: train using K-1 partitions and calculate validation error on remaining partition (rotating validation partition on each run).
Report average validation error

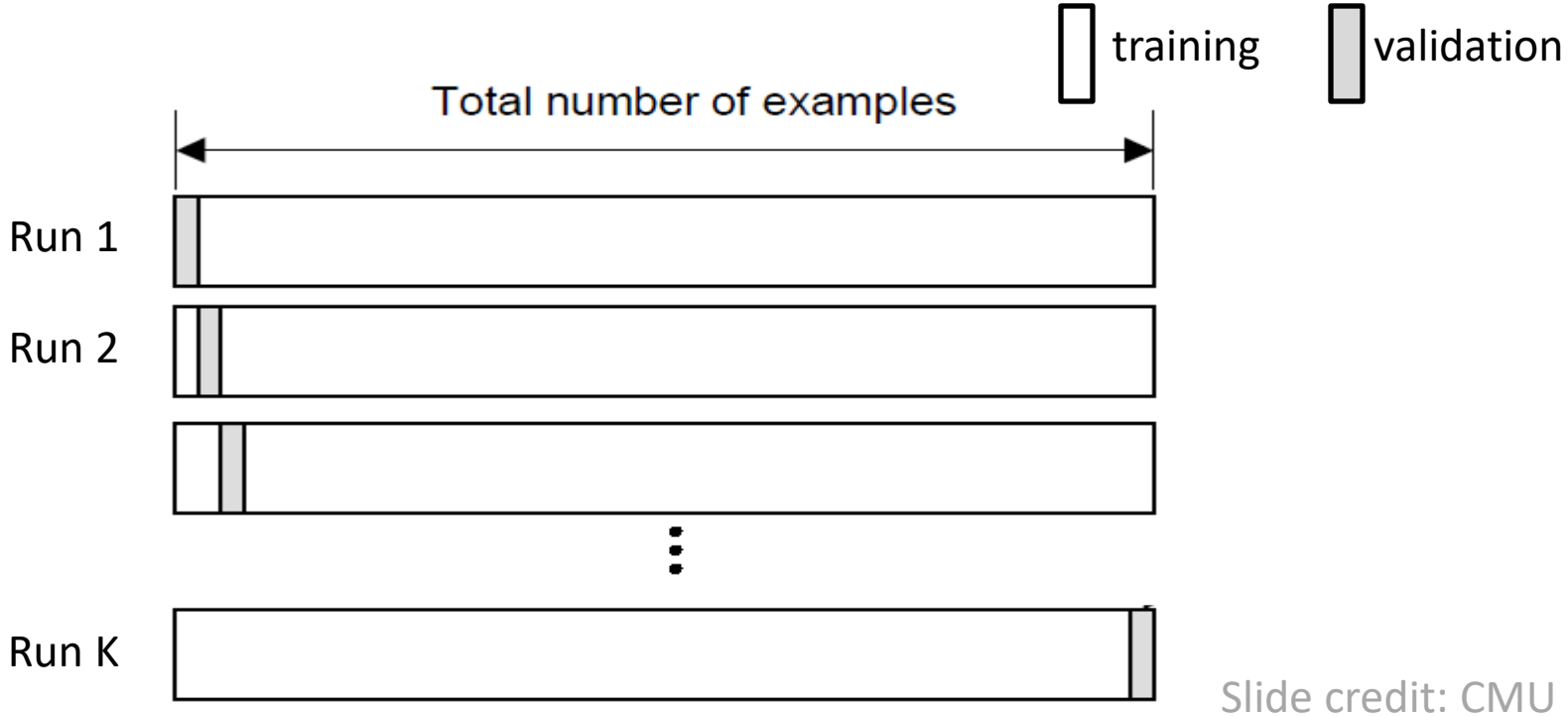


Slide credit: CMU MLD Aarti Singh

Cross-validation

Leave-one-out (LOO) cross-validation

Special case of K-fold with K=N partitions
Equivalently, train on N-1 samples and validate on only one sample per run for N runs



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Cross-validation

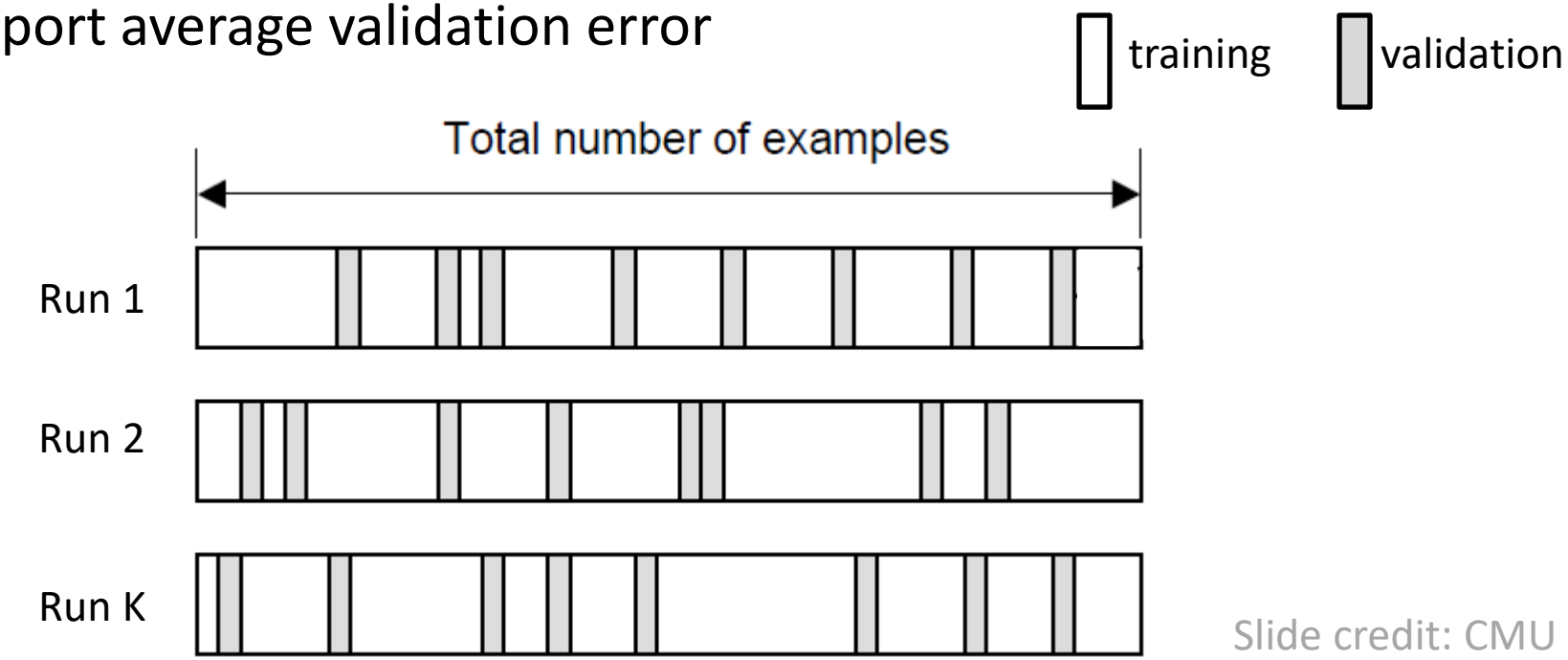
Random subsampling

Randomly subsample a fixed fraction αN ($0 < \alpha < 1$) of the dataset for validation.

Compute validation error with remaining data as training data.

Repeat K times

Report average validation error



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Poll 3

Say you are choosing amongst 7 discrete values of a decision tree *mutual information threshold*, and you want to do K=5-fold cross-validation.

How many times do I have to train my model?

A. 1
B. 5
C. 7
D. 12
E. 35
F. 5^7

Poll 3

Say you are choosing amongst 7 discrete values of a decision tree *mutual information threshold*, and you want to do K=5-fold cross-validation.

How many times do I have to train my model?

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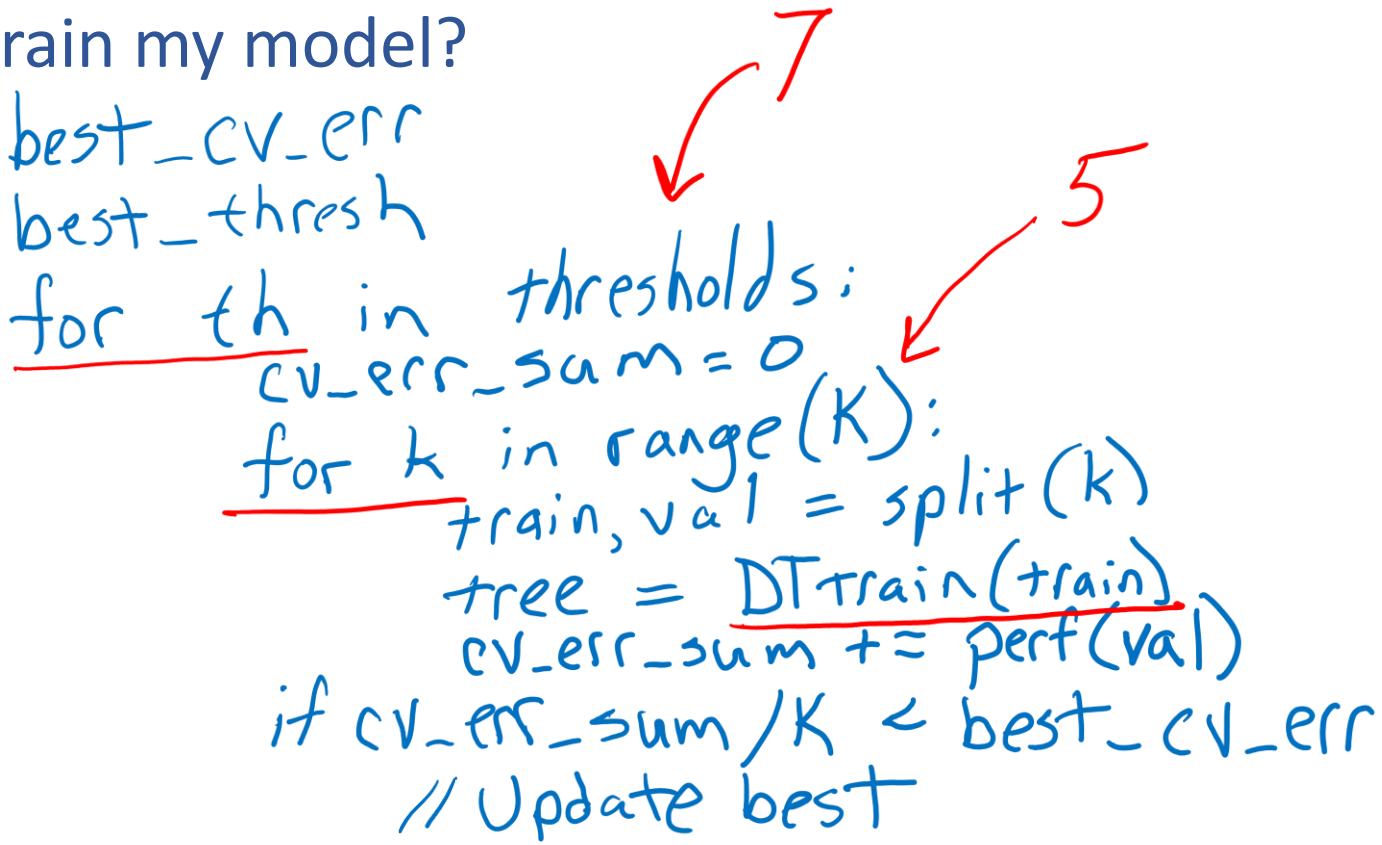

Experimental Design

	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

Slide credit: CMU MLD Matt Gormley