Machine Learning for Design

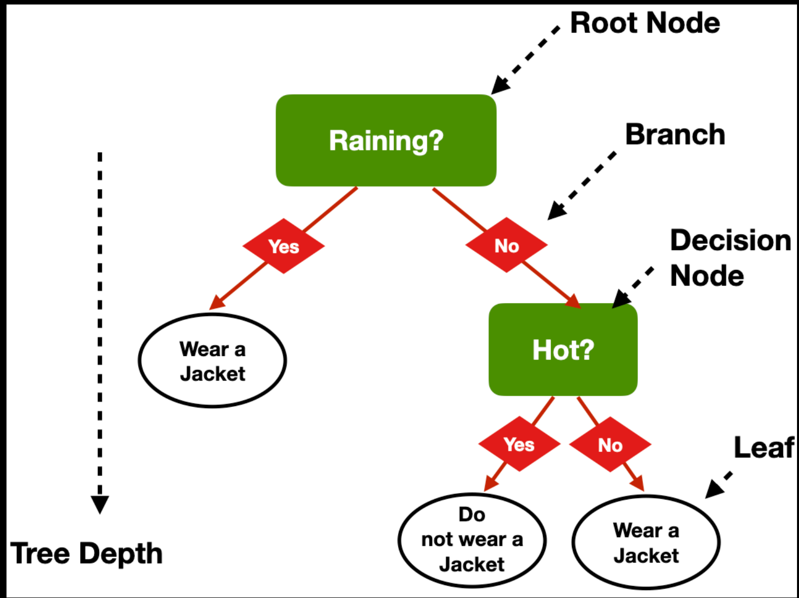
Lecture 8

Design and Develop Machine Learning Models - *Part 2*

ML Algorithms on Structured Data

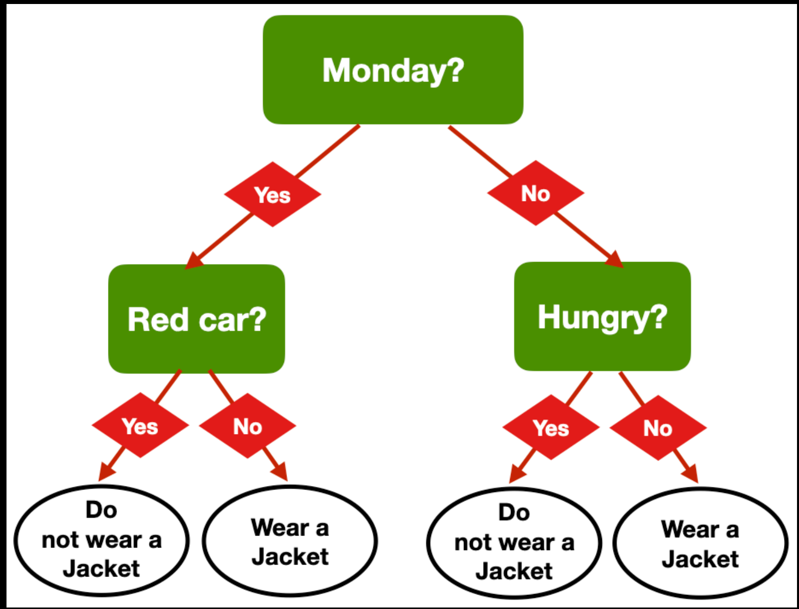
Decision Trees

- Trained with *labelled* data (supervised learning)
  - *classes* → **classification**
  - *values* → **regression**
- Simple model that resembles human reasoning:
  - Answering a lot of *yes/no* questions based on *feature values*



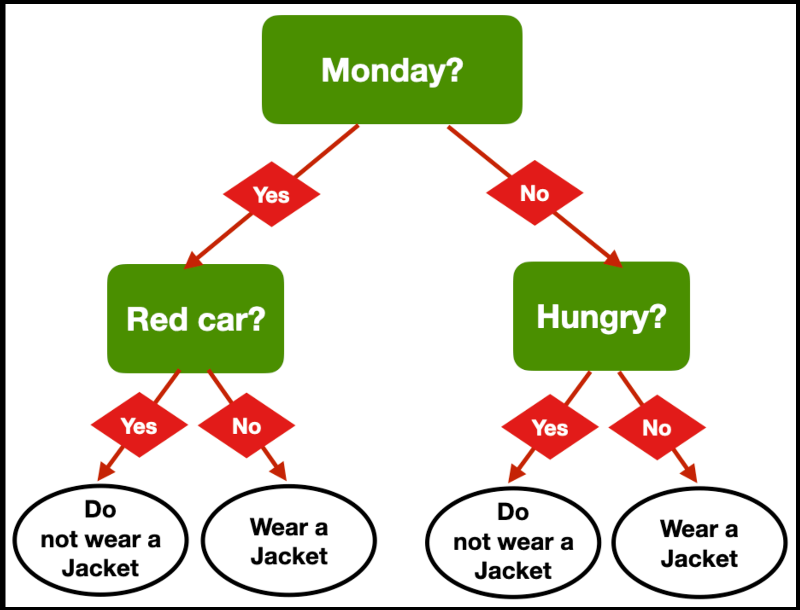
Problems

- Which questions to answer?
- How many questions? (Tree depth)
- In which order?



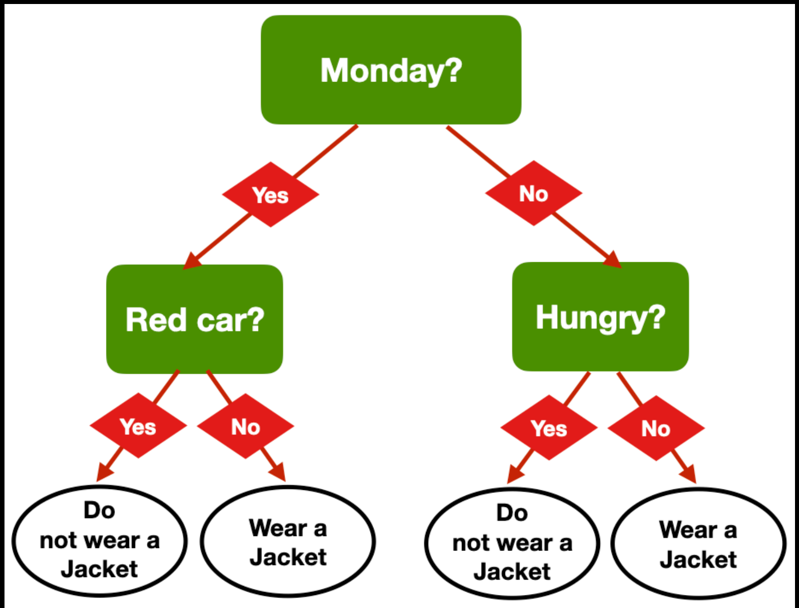
Same Problem, Multiple Trees

- Am I hungry?
- Is there a red car outside?
- Is it Monday?
- Is it raining?
- Is it cold outside?



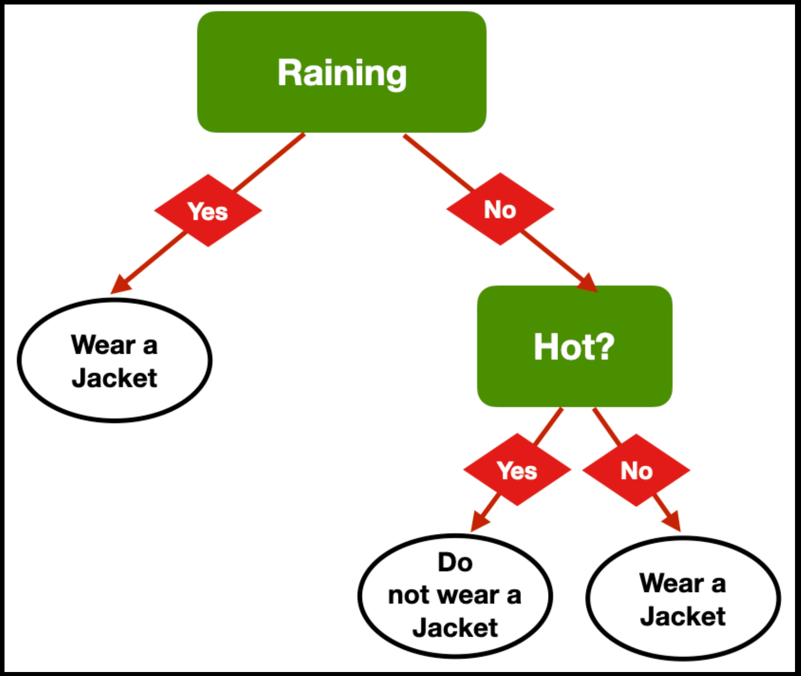
Same Problem, Multiple Trees

- ~~Am I hungry?~~
- ~~Is there a red car outside?~~
- ~~Is it Monday?~~
- Is it raining?
- Is it cold outside?

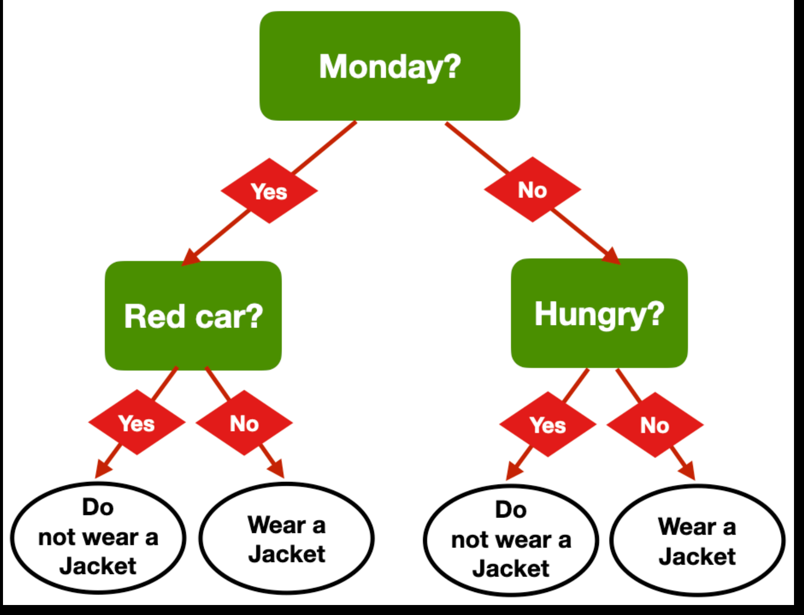


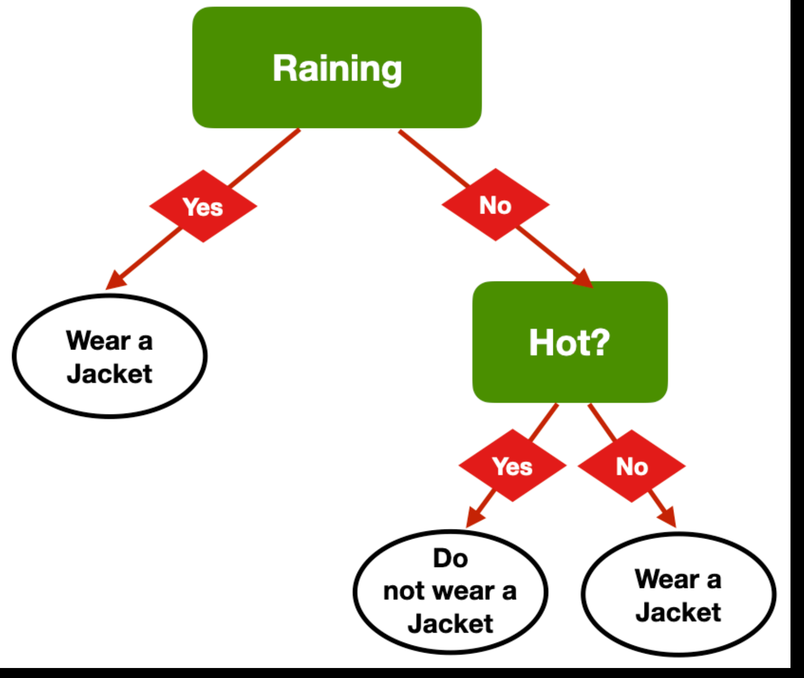
Same Problem, Multiple Trees

- ~~Am I hungry?~~
- ~~Is there a red car outside?~~
- ~~Is it Monday?~~
- Is it raining?
- Is it cold outside?



Same Decision, different tress





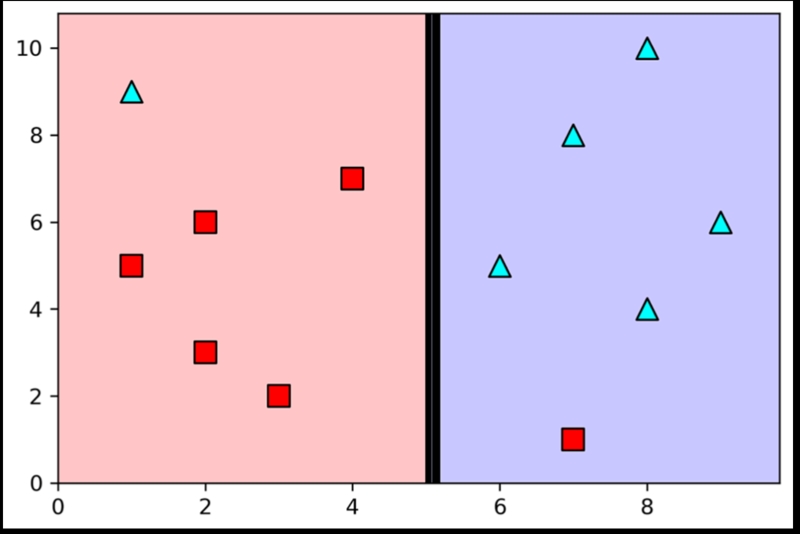
How to decide the best question to ask?

- **Accuracy**
  - Which question helps me be correct more often?
- **Gini Impurity Index**
  - A measure of diversity in a dataset $\longrightarrow$ diversity of classes in a given leaf node
    - index = 0 means that all the items in a leaf node have the same class
  - Which question helps me obtain the *lowest average Gini impurity Index*?
- **Entropy**
  - Another measure of diversity linked to information theory
  - Which question helps me obtain the lowest average **entropy**?

Building the tree (pseudo-code)

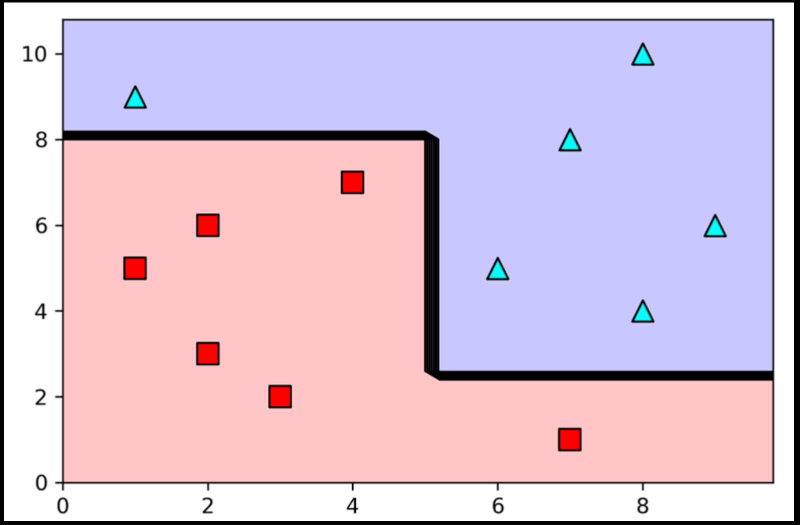
- **Add a root node, and associate it with the entire dataset**
  - This node has level 0. Call it a leaf node
- **Repeat until the stopping conditions are met at every leaf node**
  - Pick one of the leaf nodes at the highest level
  - Go through all the features, and select the one that splits the samples corresponding to that node in an optimal way, according to the selected metric.
    - Associate that feature to the node
  - This feature splits the dataset into two branches
    - Create two new leaf nodes, one for each branch
    - Associate the corresponding samples to each of the nodes
  - If the stopping conditions allow a split, turn the node into a decision node, and add two new leaf nodes underneath it
    - If the level of the node is i, the two new leaf nodes are at level $i + 1$
  - If the stopping conditions don't allow a split, the node becomes a leaf node
    - Associate the most common label among its samples
    - That label is the prediction at the leaf

A geometrical perspective



- *Step 1* - Select the first question
- $X >= 5$
  - Best possible prediction accuracy with one feature

A geometrical perspective



- *Step 2* - Iterate
- $x < 5 \& y < 8;$
- $x >= 5 \& y >= 2$
  - Perfect split of the feature space

Decision Trees: **Pros**

- Simple to understand and interpret.
  - Trees can be visualized
- Requires little data preparation
  - Other techniques often require data normalisation, dummy variables need to be created, and blank values need to be removed
- Able to handle both numerical and categorical data

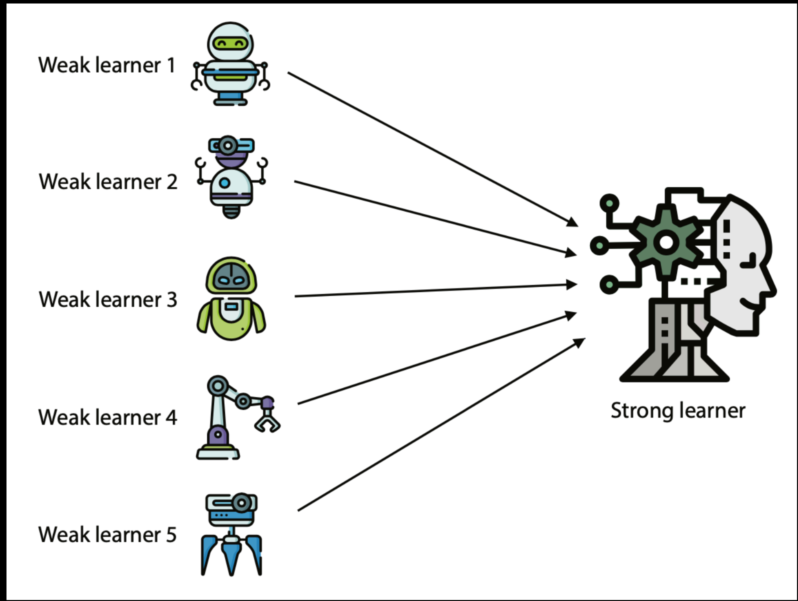
Decision Trees: **Cons**

- Possible to create over-complex trees that do not generalize the data well
  - **overfitting**
- **Unstable** $\longrightarrow$ small variations in the data might result in a completely different tree being generated
- Biased trees if some classes dominate

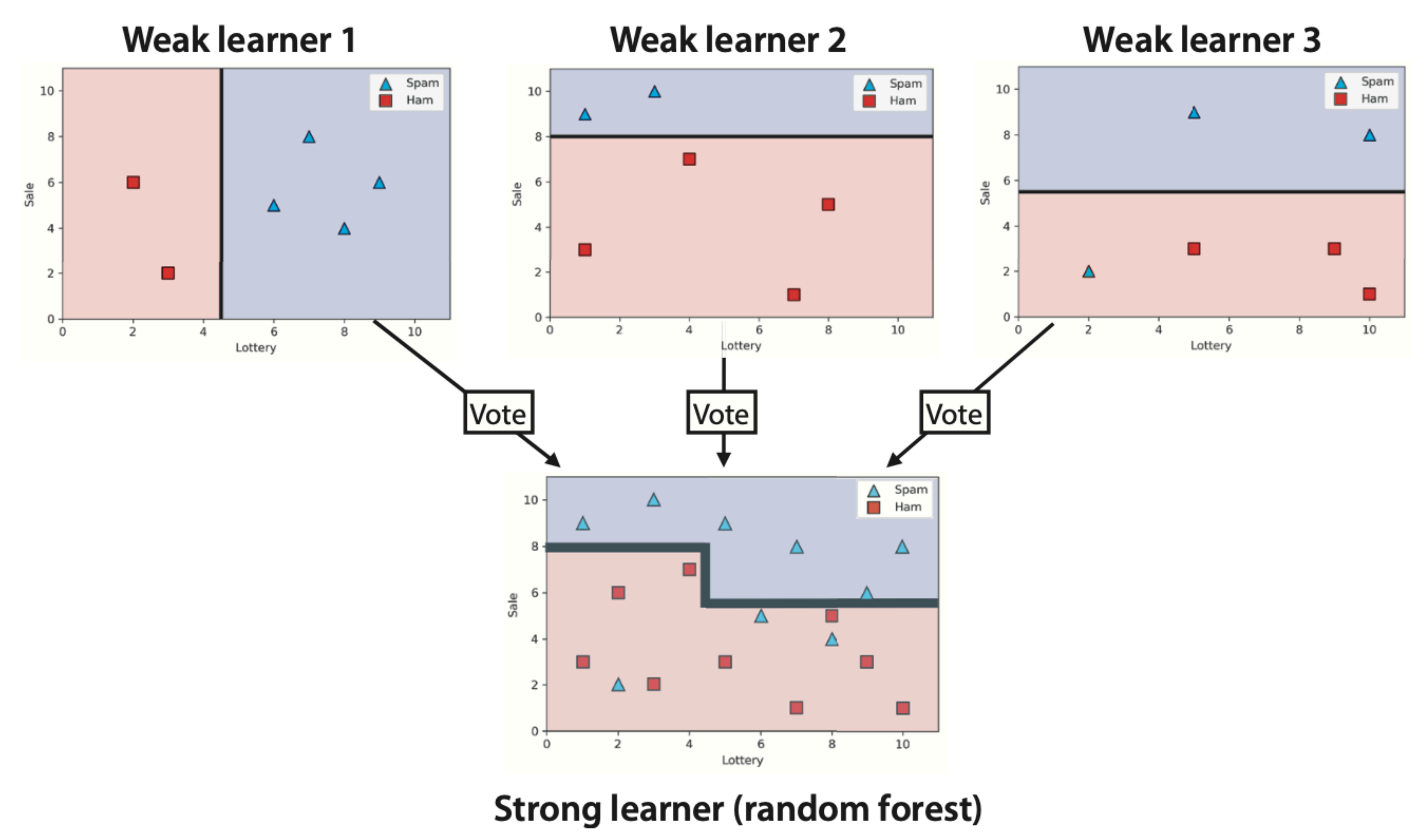
Ensemble Learning

Idea: combine several "weak" learners to build a strong learner

Random Forest: Weak learners are decision trees



- Build random training sets from the dataset
- Train a different model on each of the sets
  - weak learners
- Combination the weak models by voting (if it is a classification model) or averaging the predictions (if it is a regression model)
  - For any input, each of the weak learners predicts a value
  - The most common output (or the average) is the output of the strong learner


Weak learner 1
Weak learner 2
Weak learner 3
Spam
Ham
Sale
Lottery
Vote
Vote
Vote
Strong learner (random forest)

Clustering

What is clustering?

- Grouping items that "belong together" (i.e. have similar features)
- **Unsupervised learning**: we only use data features, not the labels

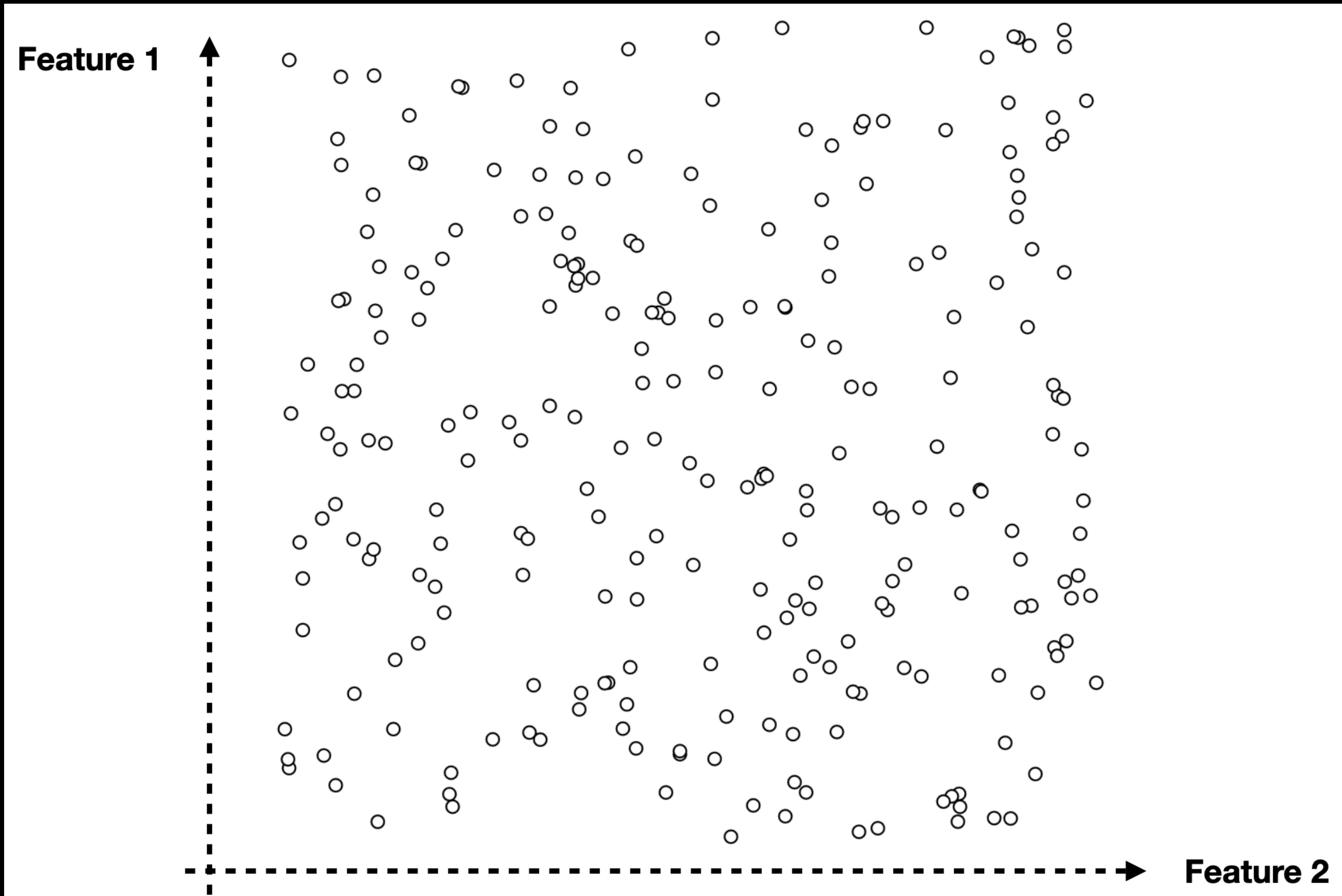
- We can detect patterns
  - Group emails or search results
  - Customer shopping patterns
  - Regions of images
- Useful when you don’t know what you’re looking for
  - But: can give you gibberish
- If the goal is classification, we can later ask a human to label each group (cluster)

Why do we cluster?

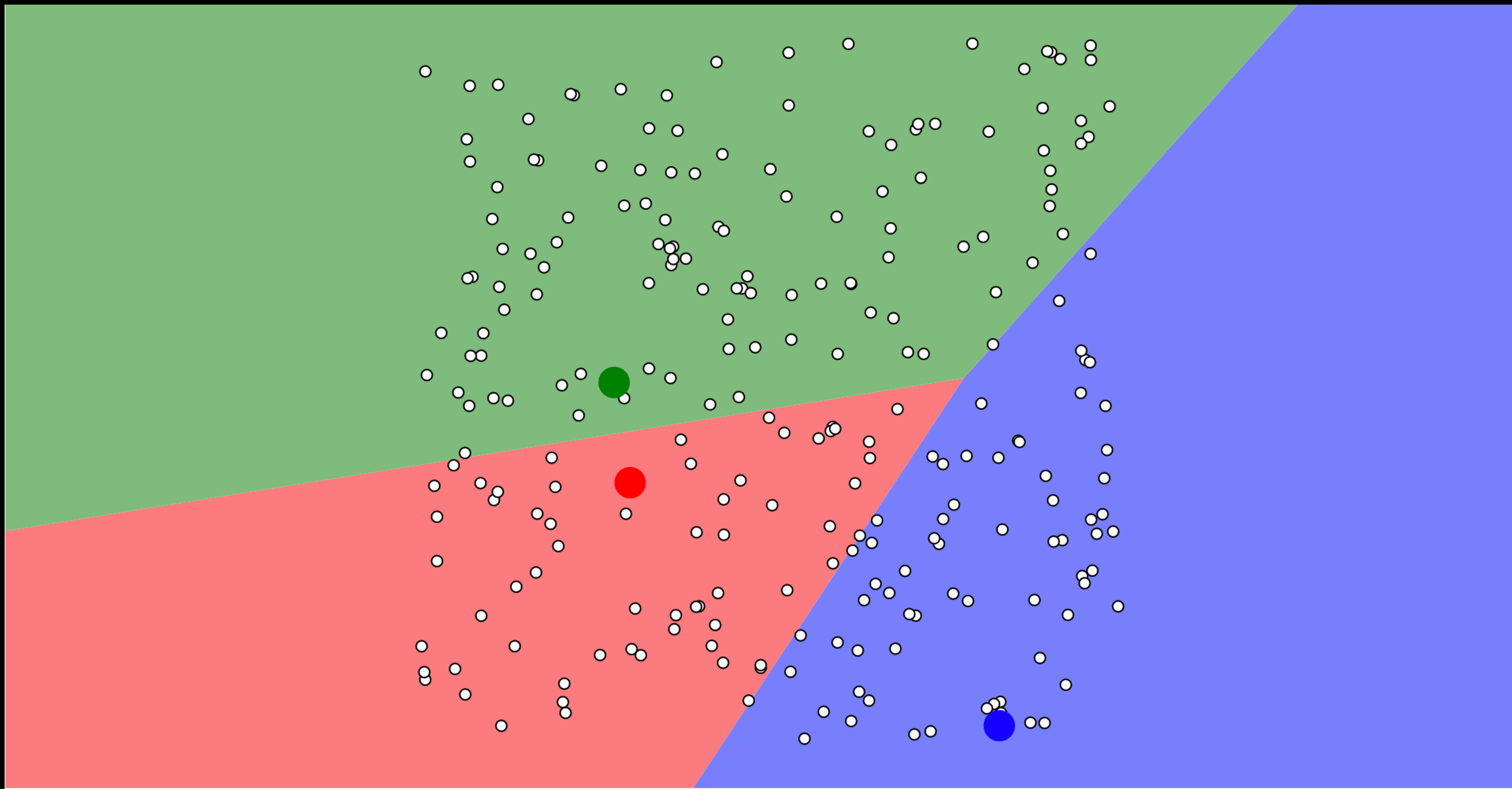
- Summarizing data
  - Look at large amounts of data
  - Represent a large continuous vector with the cluster number
- Counting
  - Computing feature histograms
- Prediction
  - Images in the same cluster may have the same labels
- Segmentation
  - Separate the image into different regions

K-Means

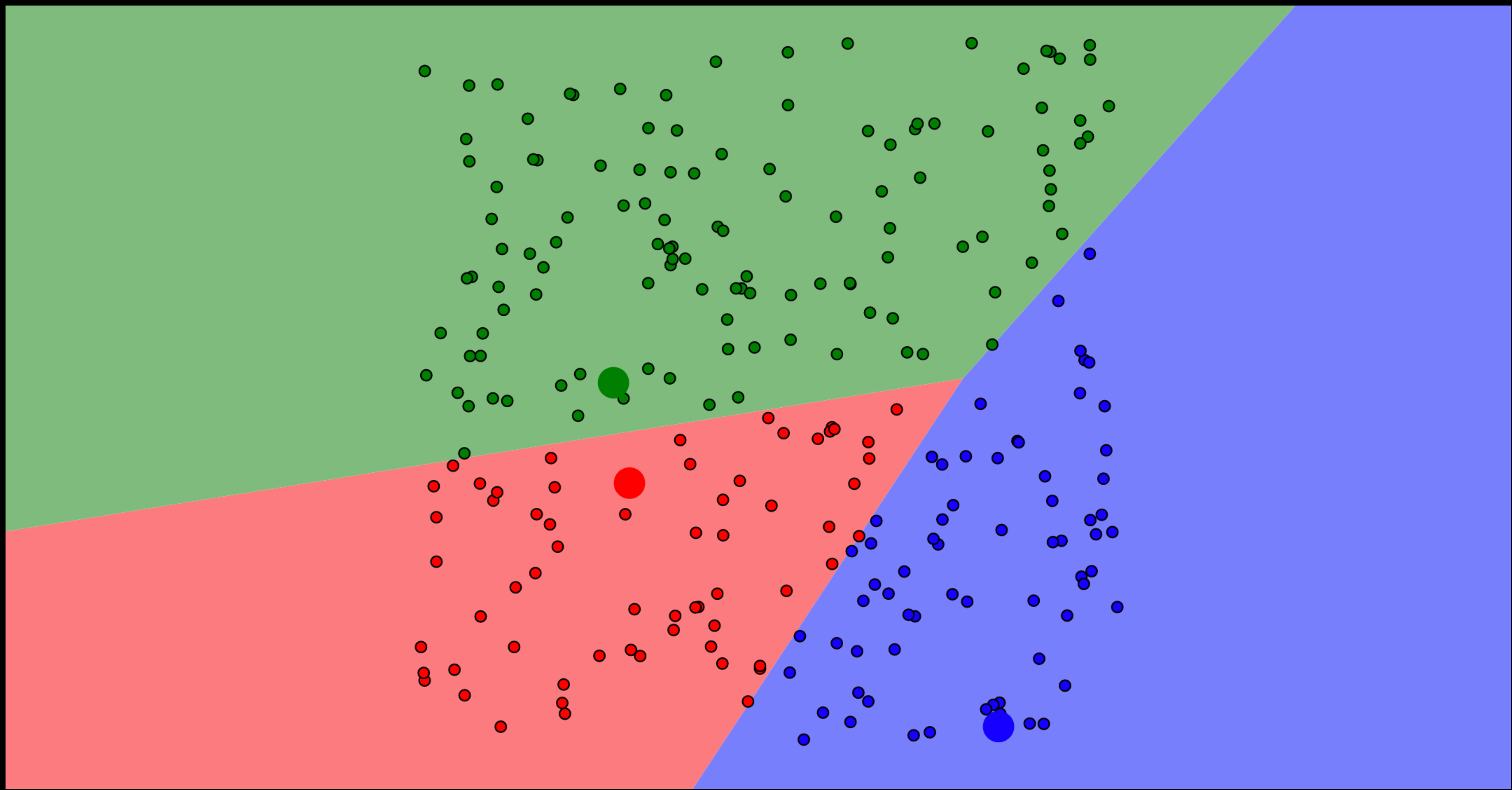
- An iterative clustering algorithm
  - **Initialize**: Pick K random points as cluster centres
  - **Alternate**:
    - Assign data points to the closest cluster centre
    - Change the cluster centre to the average of its assigned points
  - **Stop** when no points' assignments change


Feature 1
Feature 2

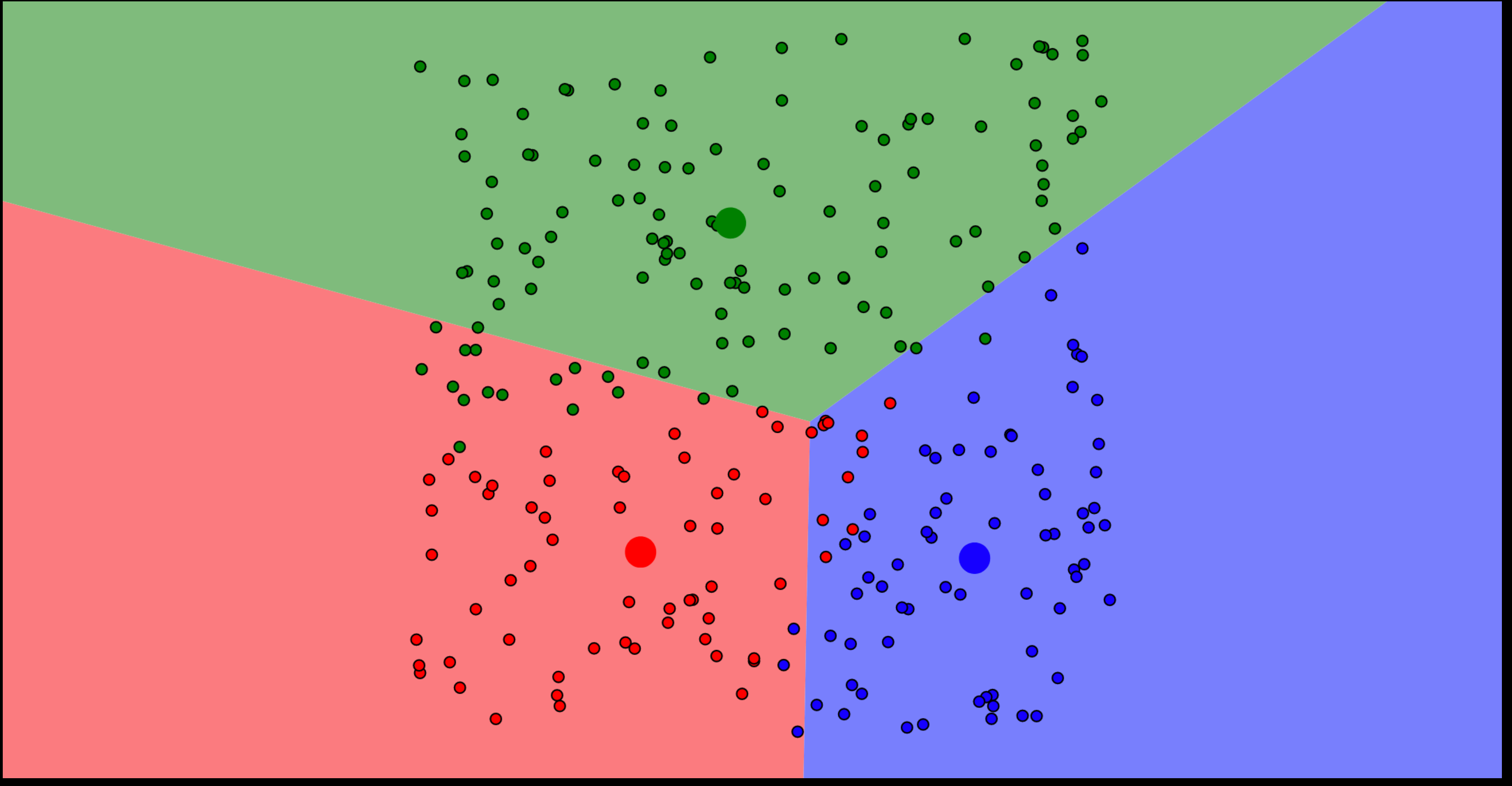
Add 3 Centroids (randomly)



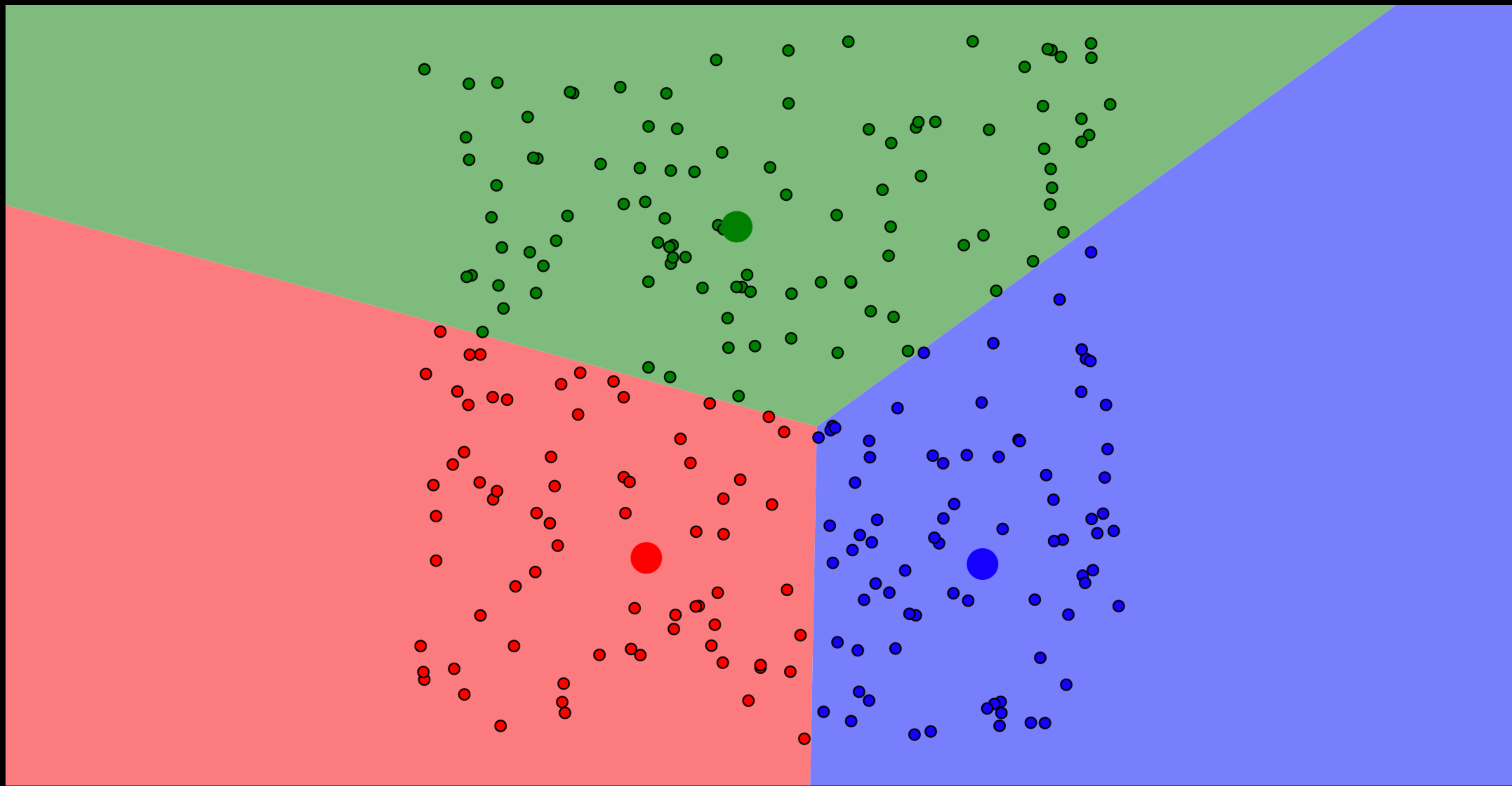
Assign Data Points



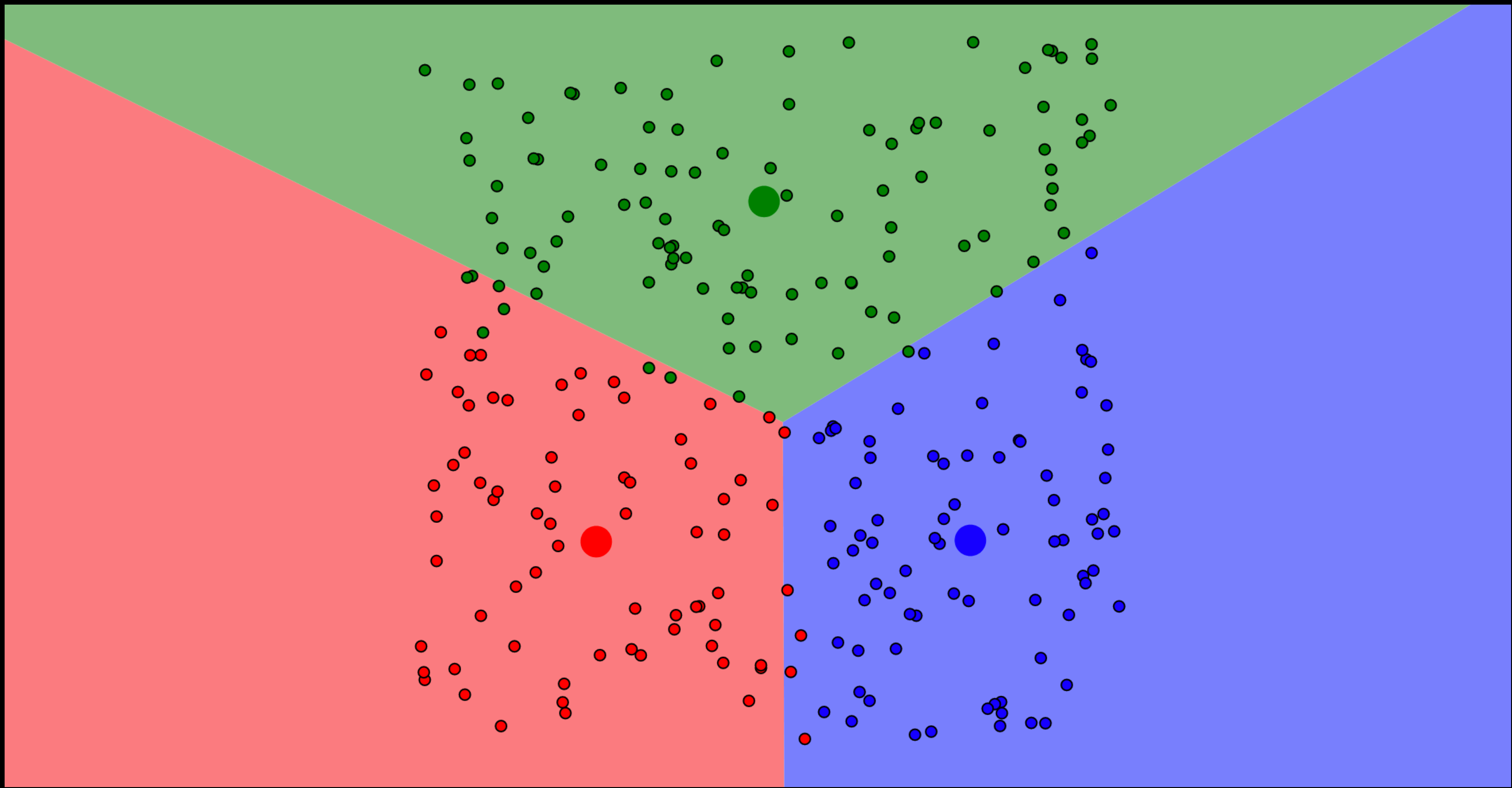
Update Centroids



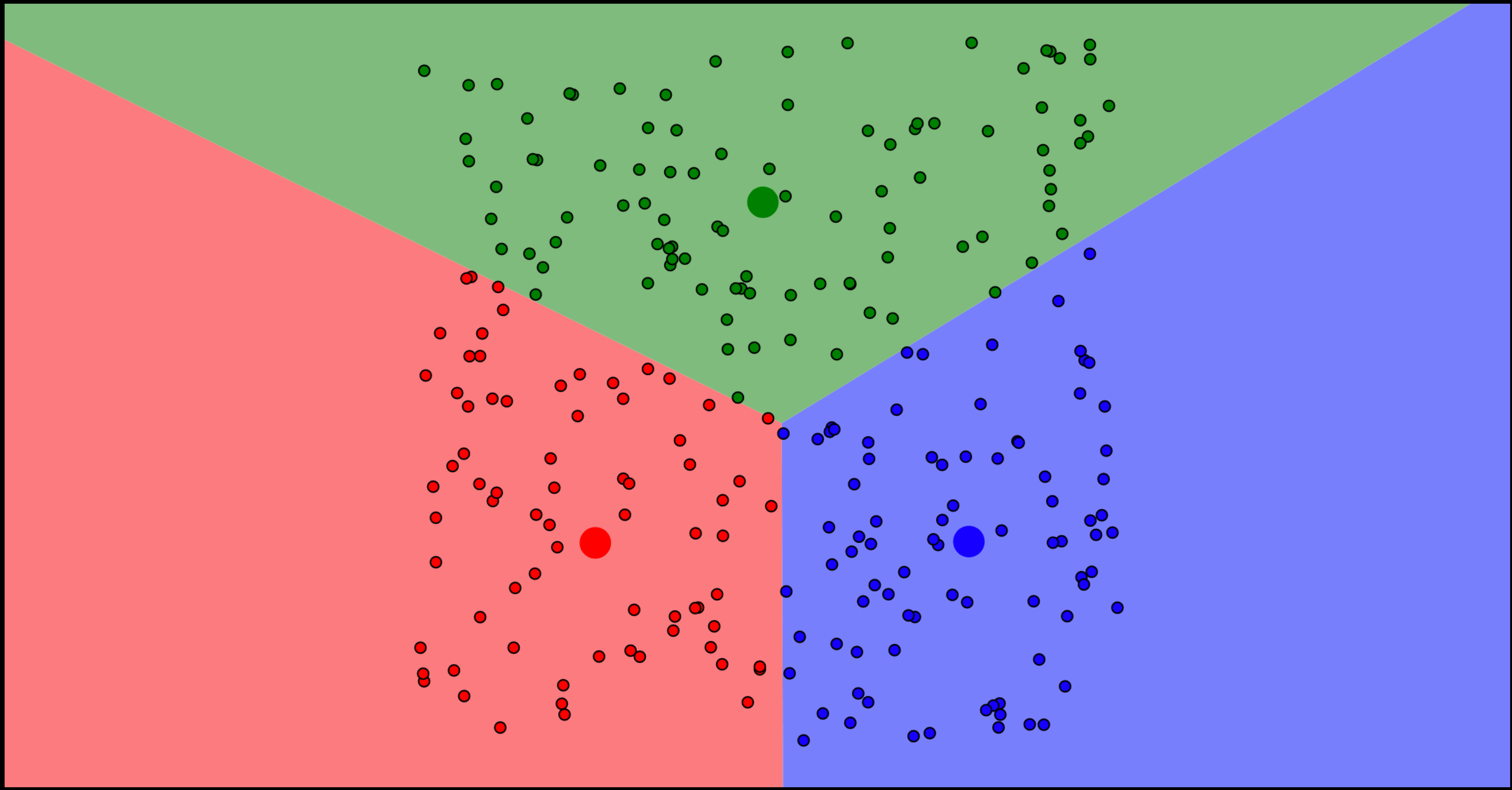
Re-Assign Data Points



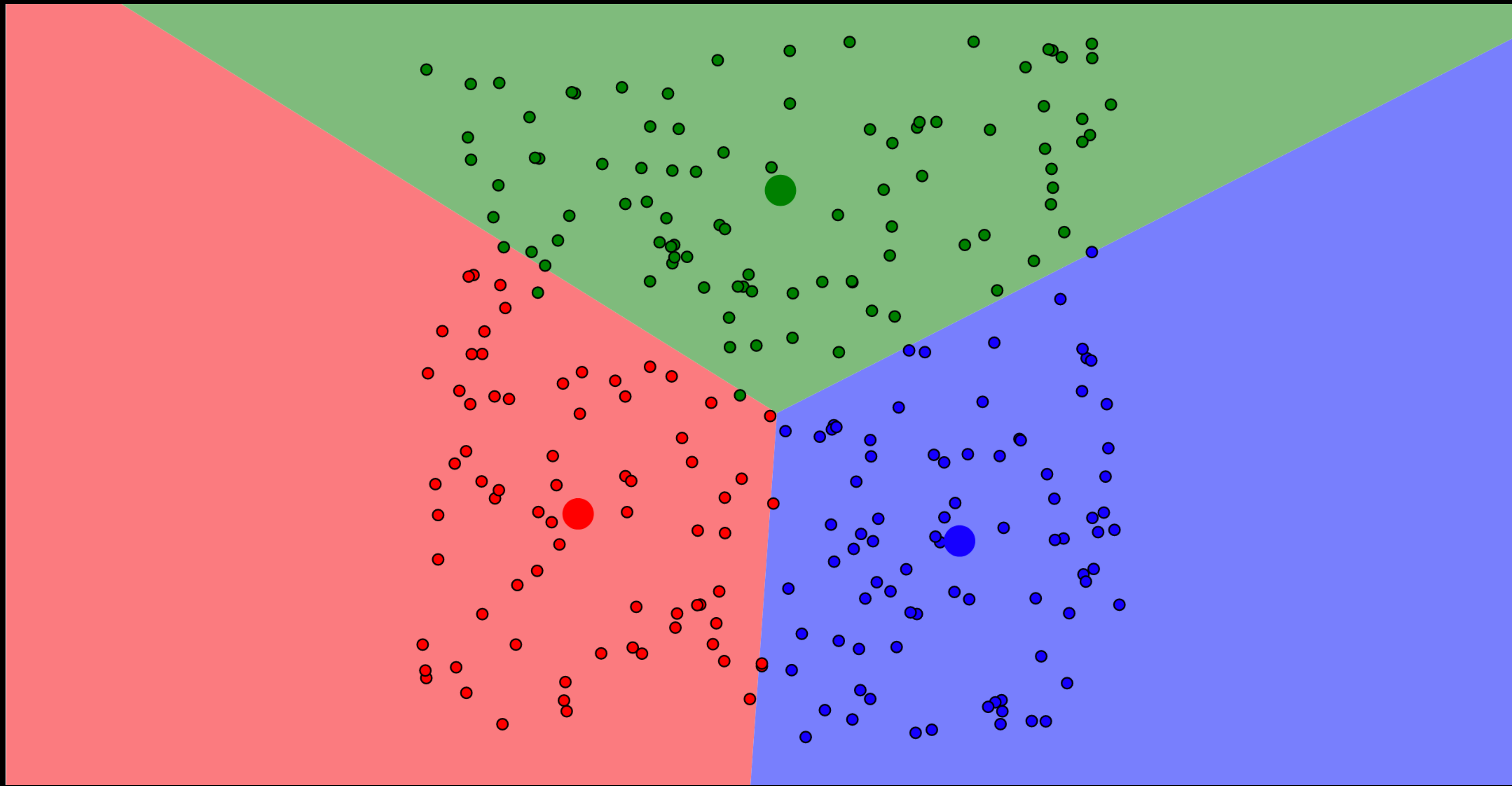
Update Centroids



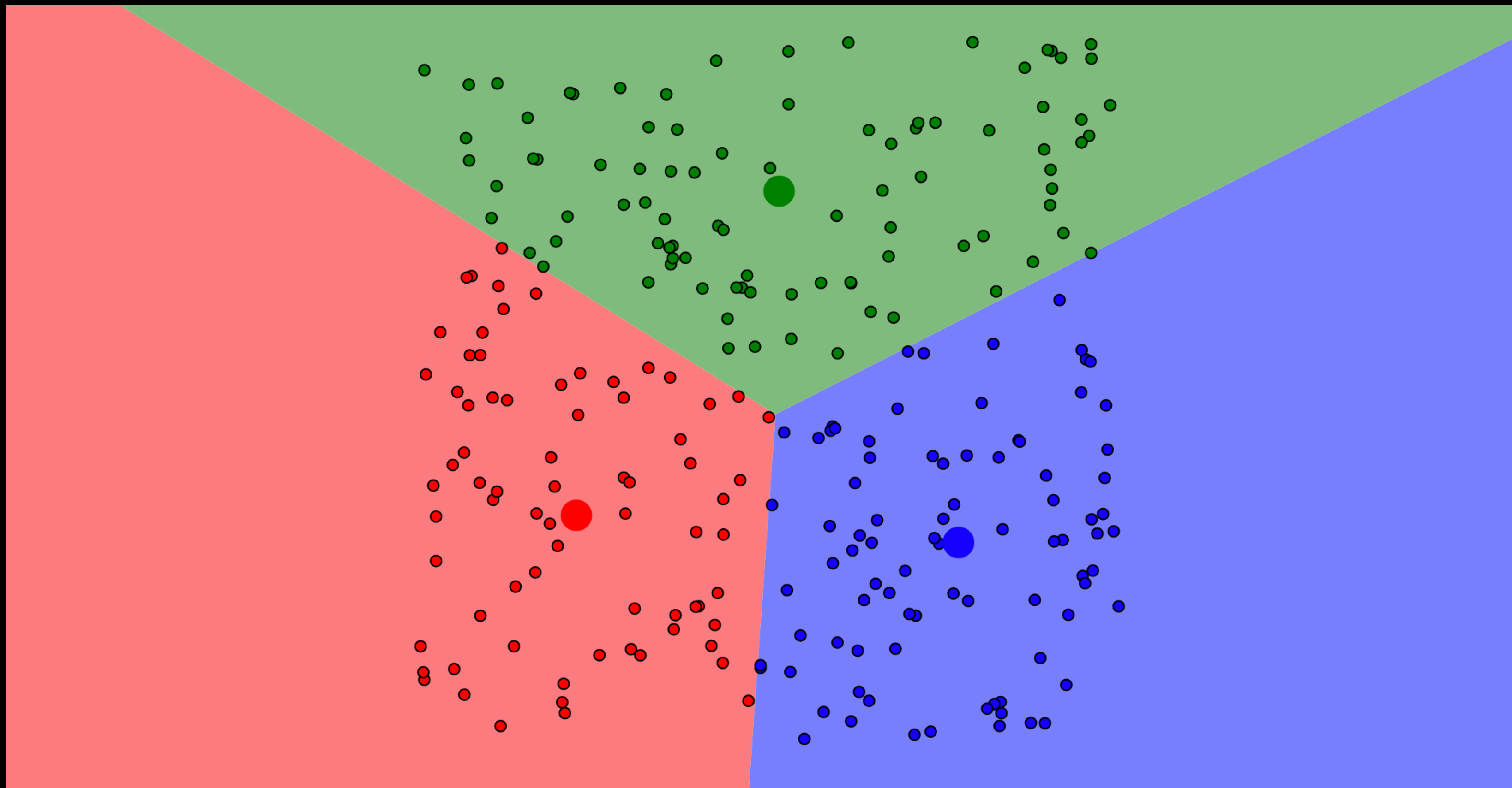
Re-Assign Data Points



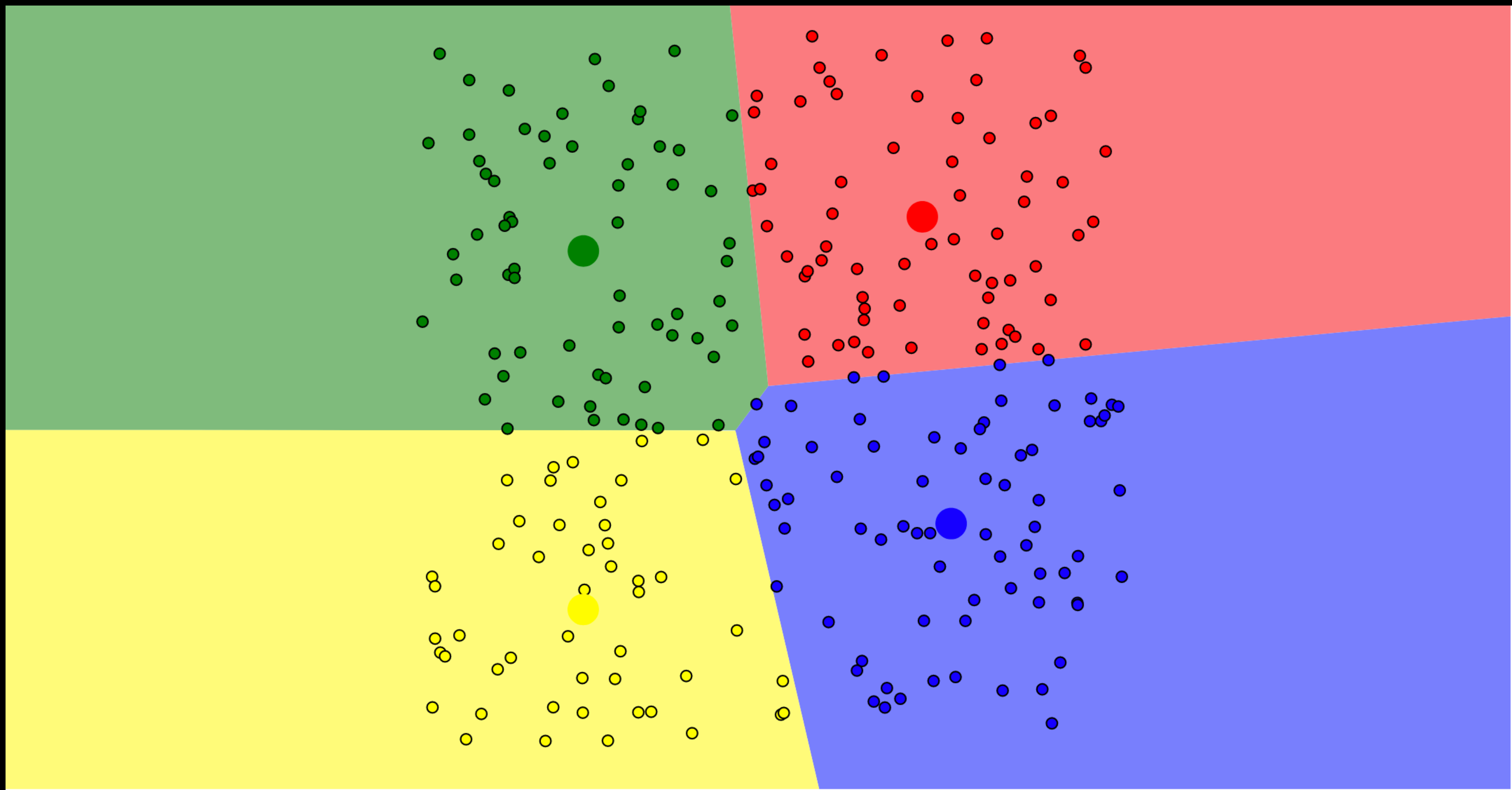
Update Centroids



Re-Assign Data Points - Stop



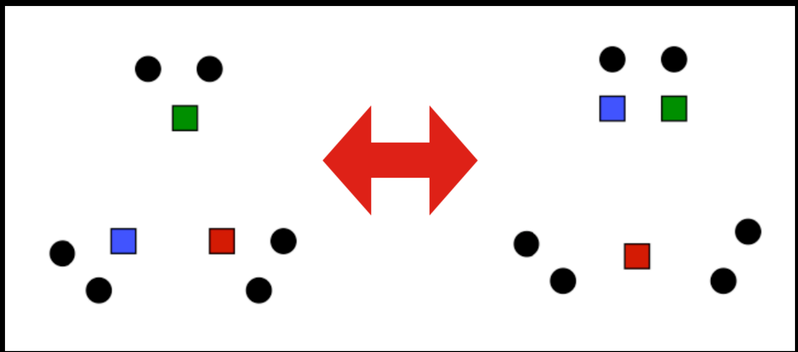
Add 4 Centroids (randomly)



K-Means Pros

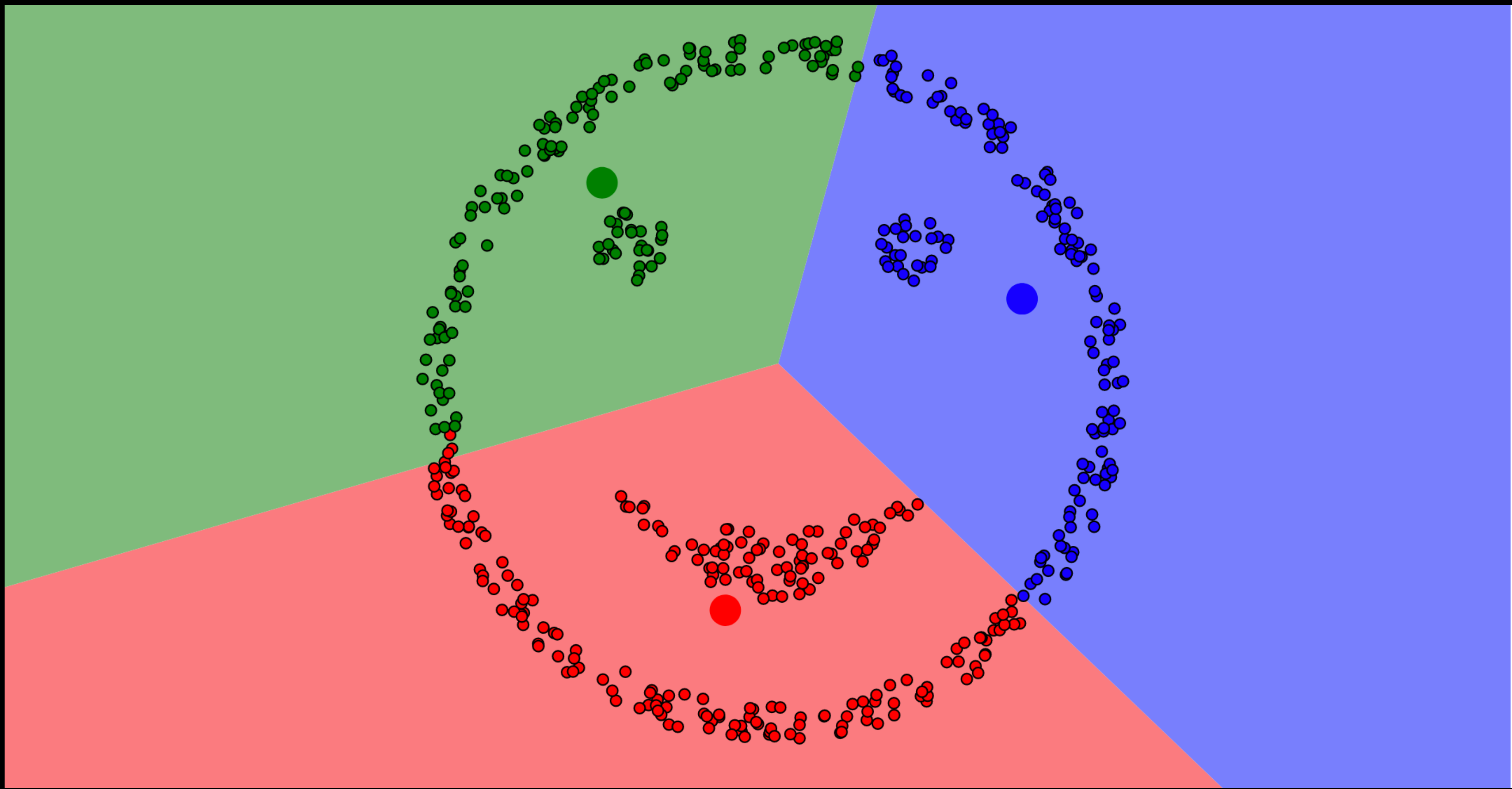
- Simple, fast to compute
  - Guaranteed to converge in a finite number of iterations

K-Means Cons



- Setting k?
  - One way: silhouette coefficient
- Algorithm is **heuristic**
  - It does matter what random points you pick!
  - Sensitive to outliers

Example of K-means not working

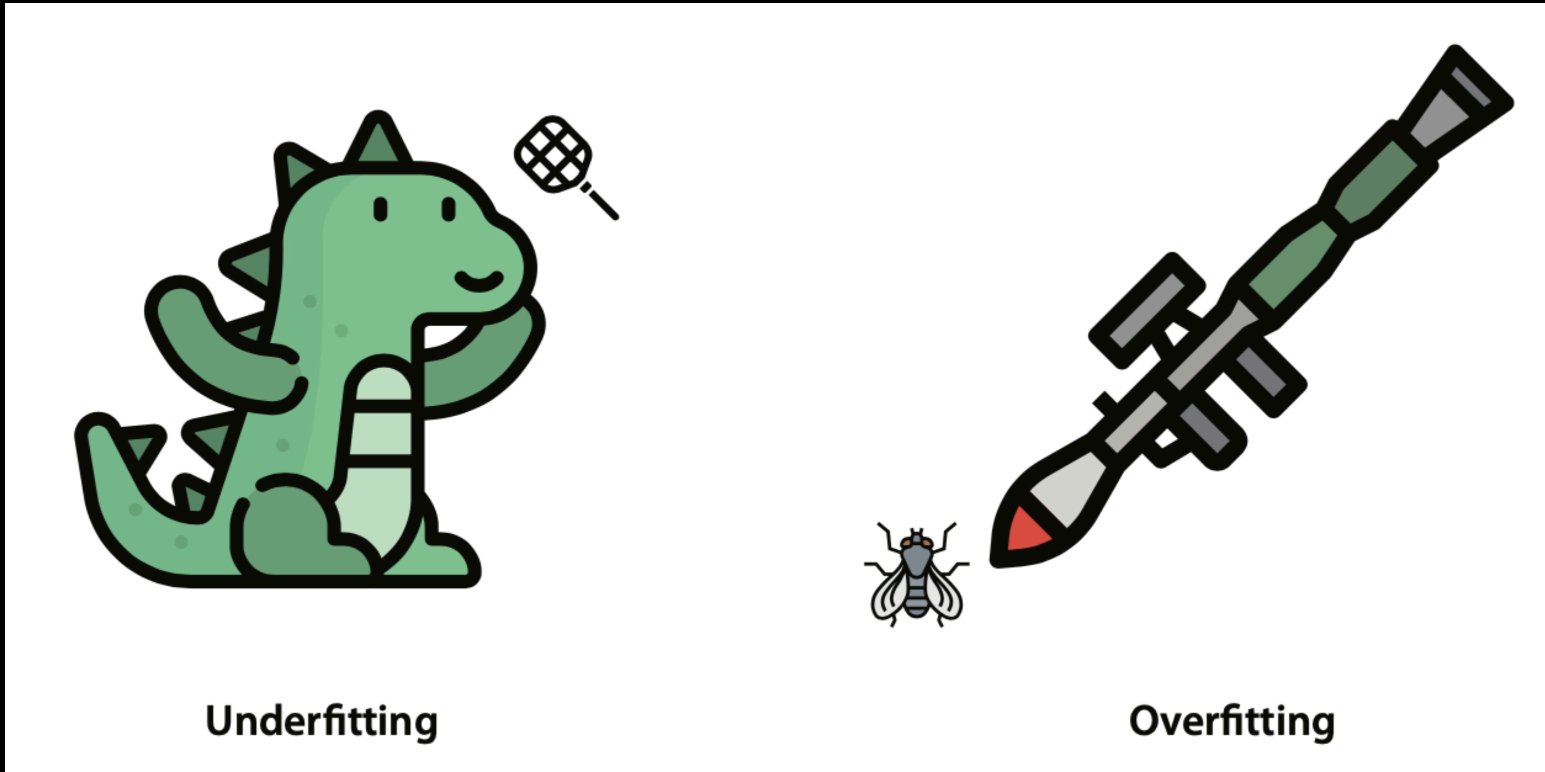


Back to Evaluation

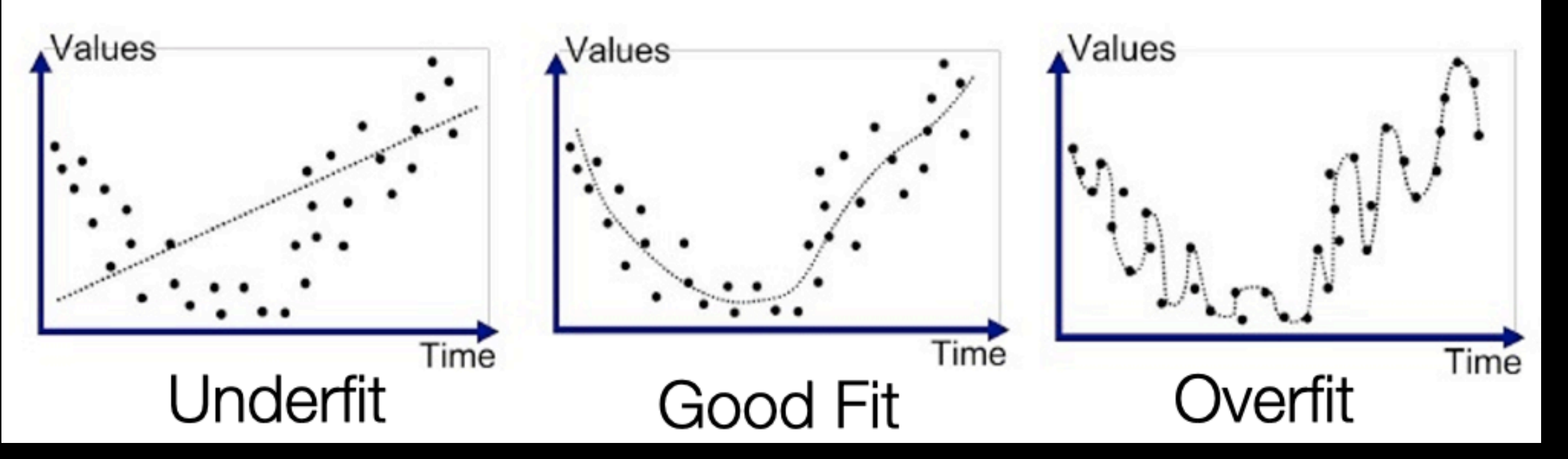
- **No free-lunch**: there is no one best machine learning algorithm for all problems and datasets

- How well does a learned model **generalize** to a new *evaluation* set?
- Challenge: achieving good generalization and a small error

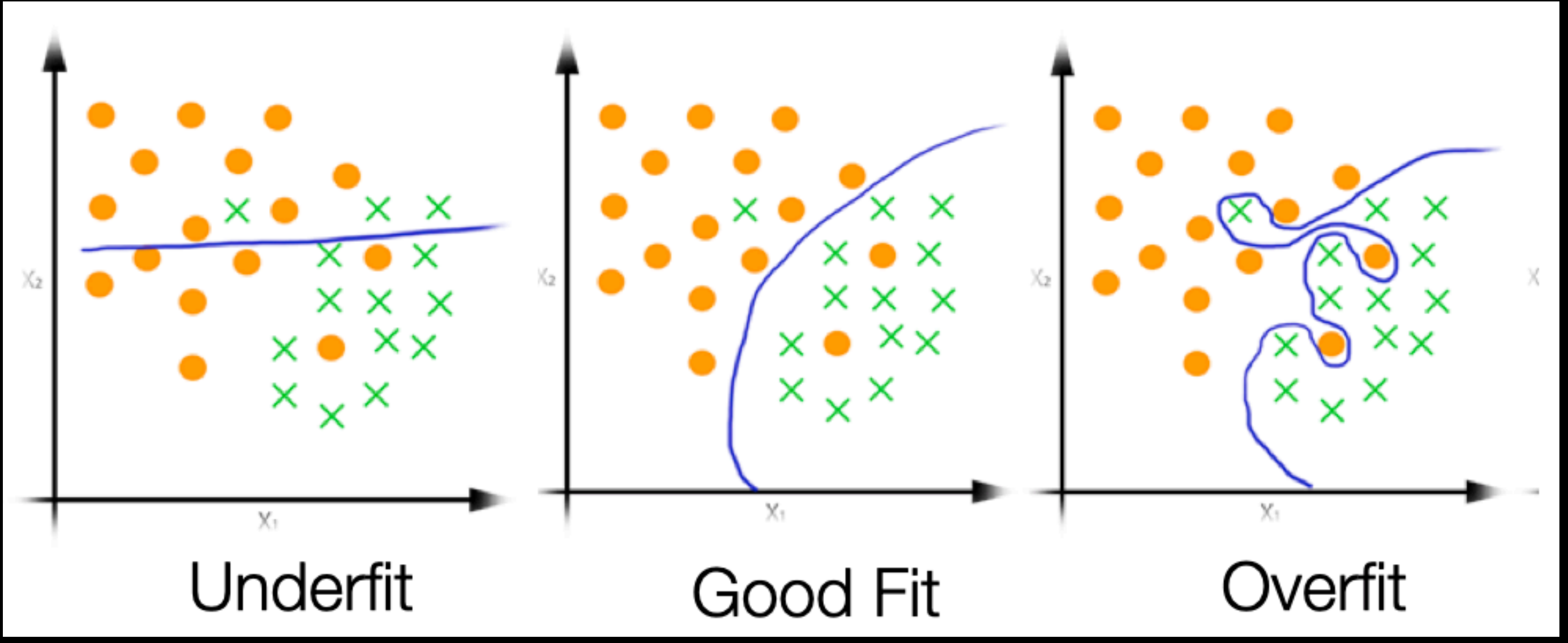
Underfitting vs. Overfitting



Regression

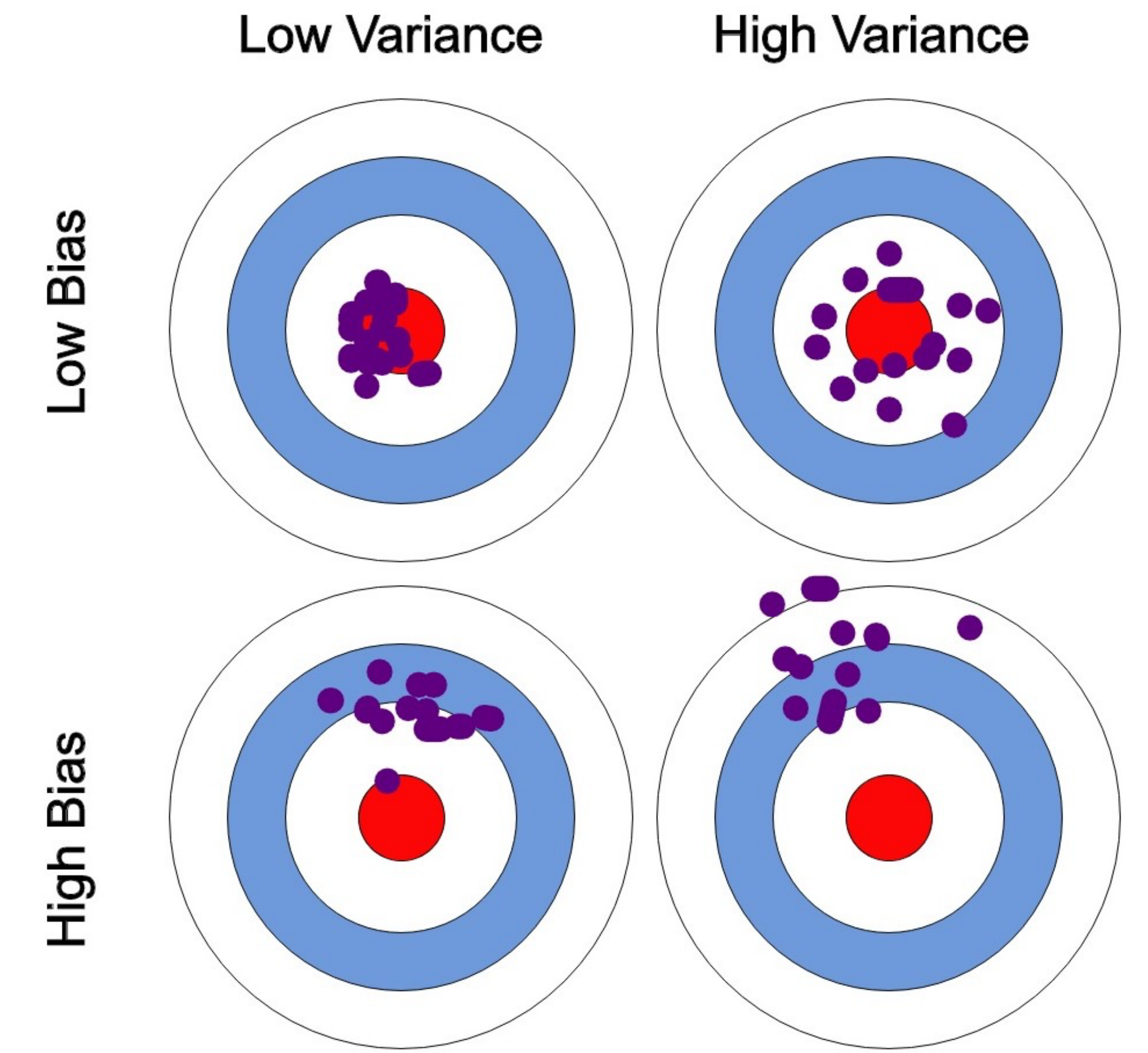

Values
Time
Underfit
Values
Time
Good Fit
Values
Time
Overfit

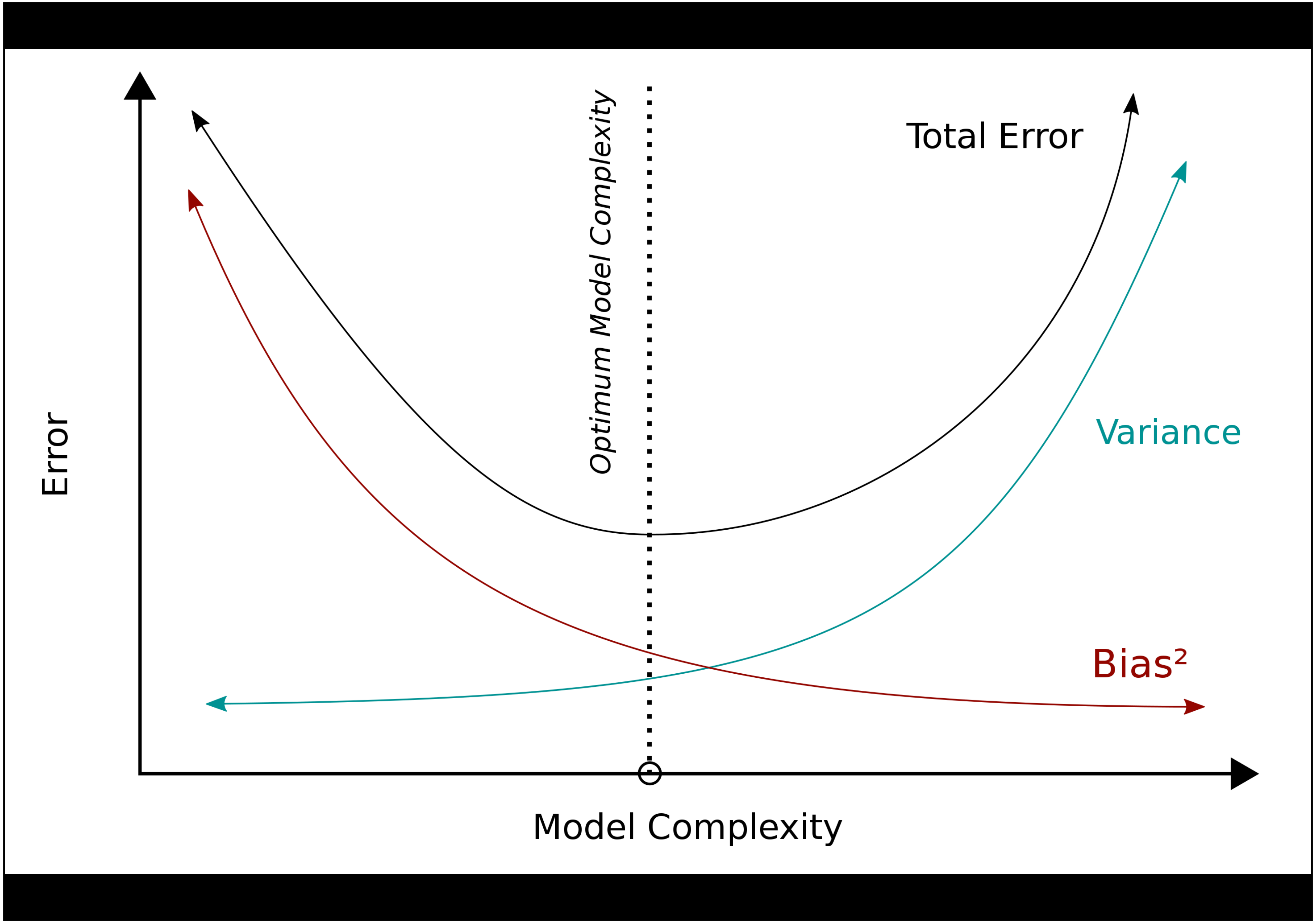
Classification



Components of expected loss

- **Noise** in data: *unavoidable*
- **Bias**: how much the average model differs from the true model
  - Error due to inaccurate assumptions/simplifications made by the model
- **Variance**: how much models estimated from different training sets differ from each other
  - Too much sensitivity to the samples


Low Variance
High Variance
Low Bias
High Bias


Error
Optimum Model Complexity
Total Error
Variance
Bias²
Model Complexity

Protect Against overfitting

Low bias and high variance

Low training error and high test error

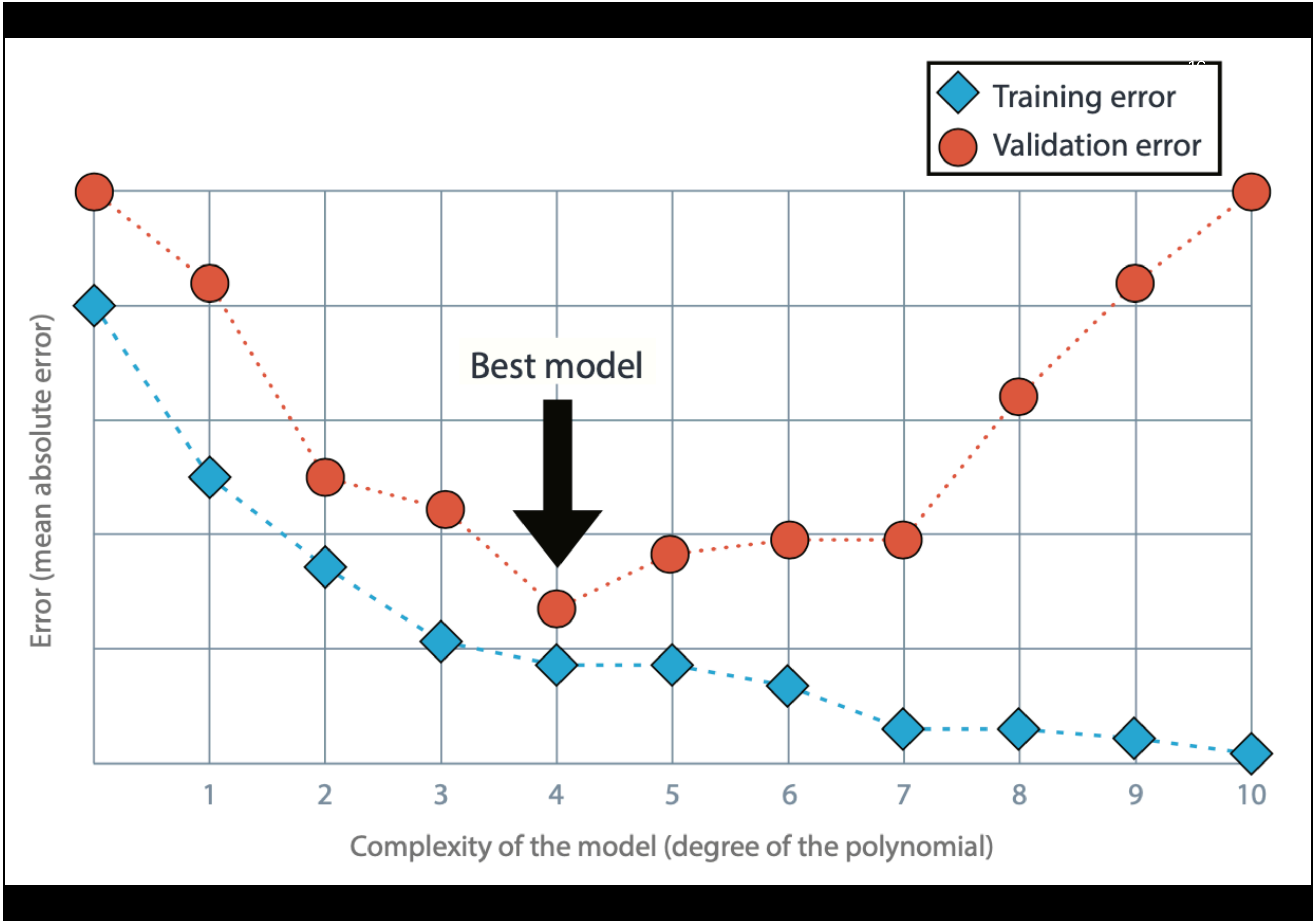
- The model
  - is too complex
  - matches too closely the idiosyncrasies (noise) of the training data

Protect Against underfitting

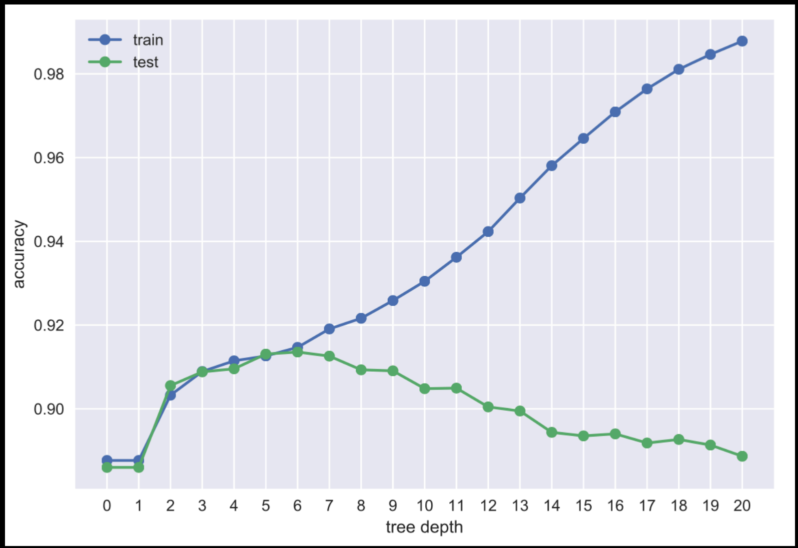
High bias and low variance

High training error and high test error

- The model
  - is too simple
  - does not adequately capture the patterns in the training data

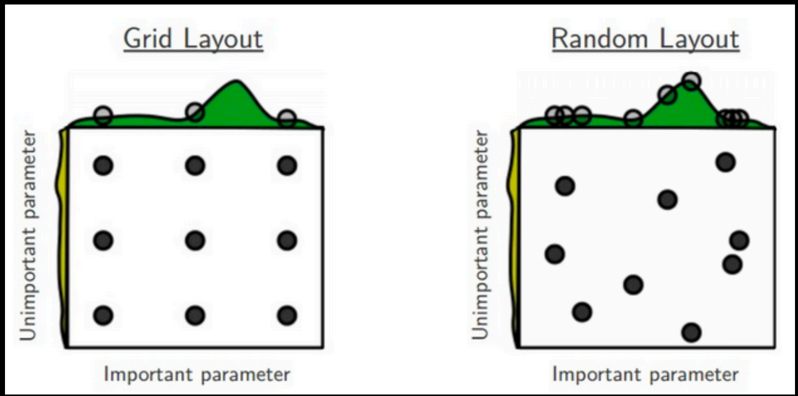

Training error
Validation error
Best model
Error (mean absolute error)
1
2
3
4
5
6
7
8
9
10
Complexity of the model (degree of the polynomial)

Tuning Hyper-parameters



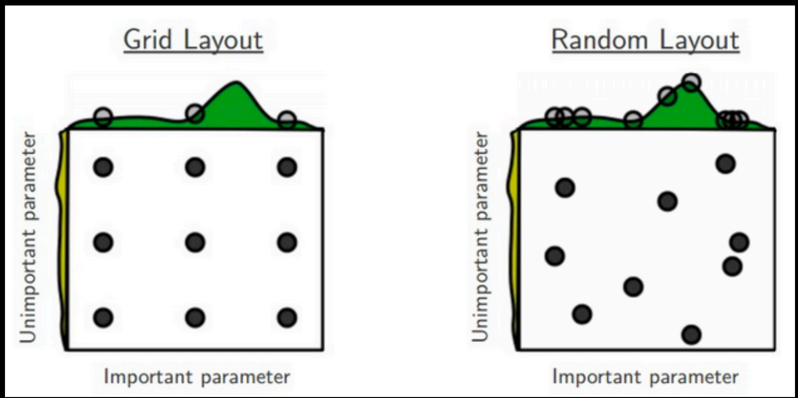
- **Hyper-parameter**: Inputs to the learning algorithms that control their behavior
- Examples:
  - maximum tree depth in decision trees
  - number of neighbors k in k-nearest neighbor
  - Neural networks: architecture, learning rate

Tuning Hyper-parameters



- For a model to work well, they often need to be tuned carefully
  - Huge search space! may be inefficient to search exhaustively

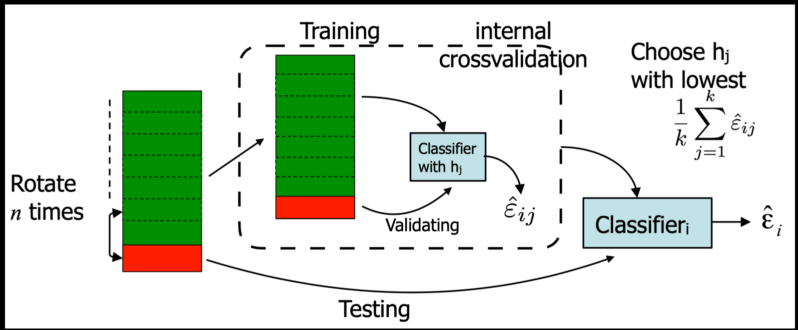
Tuning Hyper-parameters: Approaches



- DON'T optimise these numbers by looking at the test set!That is CHEATING!

- **Grid search**: brute-force exhaustive search among a finite set of hyper-parameter settings
  - All combinations are tried, then the best setting selected
- **Random search**: for each hyper-parameter, define a distribution (e.g., normal, uniform)
  - In the search loop, we sample randomly from these distributions

Double Cross-Validation



- Cross-validation inside another cross-validation
  - To optimise over the hyperparameter
- The minimum error is often not the most interesting. Try to understand the advantages/disadvantages
  - What errors are made? (inspect objects, inspect labels)
  - What classes are problematic? (confusion matrix)
  - Does adding training data help? (learning curve)
  - How robust is the model?

Machine Learning for Design

Lecture 8

Design and Develop Machine Learning Models - *Part 2*

Credits

Grokking Machine Learning. Luis G. Serrano. Manning, 2021

[CIS 419/519 Applied Machine Learning]. Eric Eaton, Dinesh Jayaraman.

https://scikit-learn.org/stable/modules/tree.html

Deep Learning Patterns and Practices - Andrew Ferlitsch, Maanning, 2021

Machine Learning Design Patterns - Lakshmanan, Robinson, Munn, 2020