COMP9321:
Data services engineering

Week 9: Hierarchal Clustering and ML Model Evaluation

Term 1, 2020

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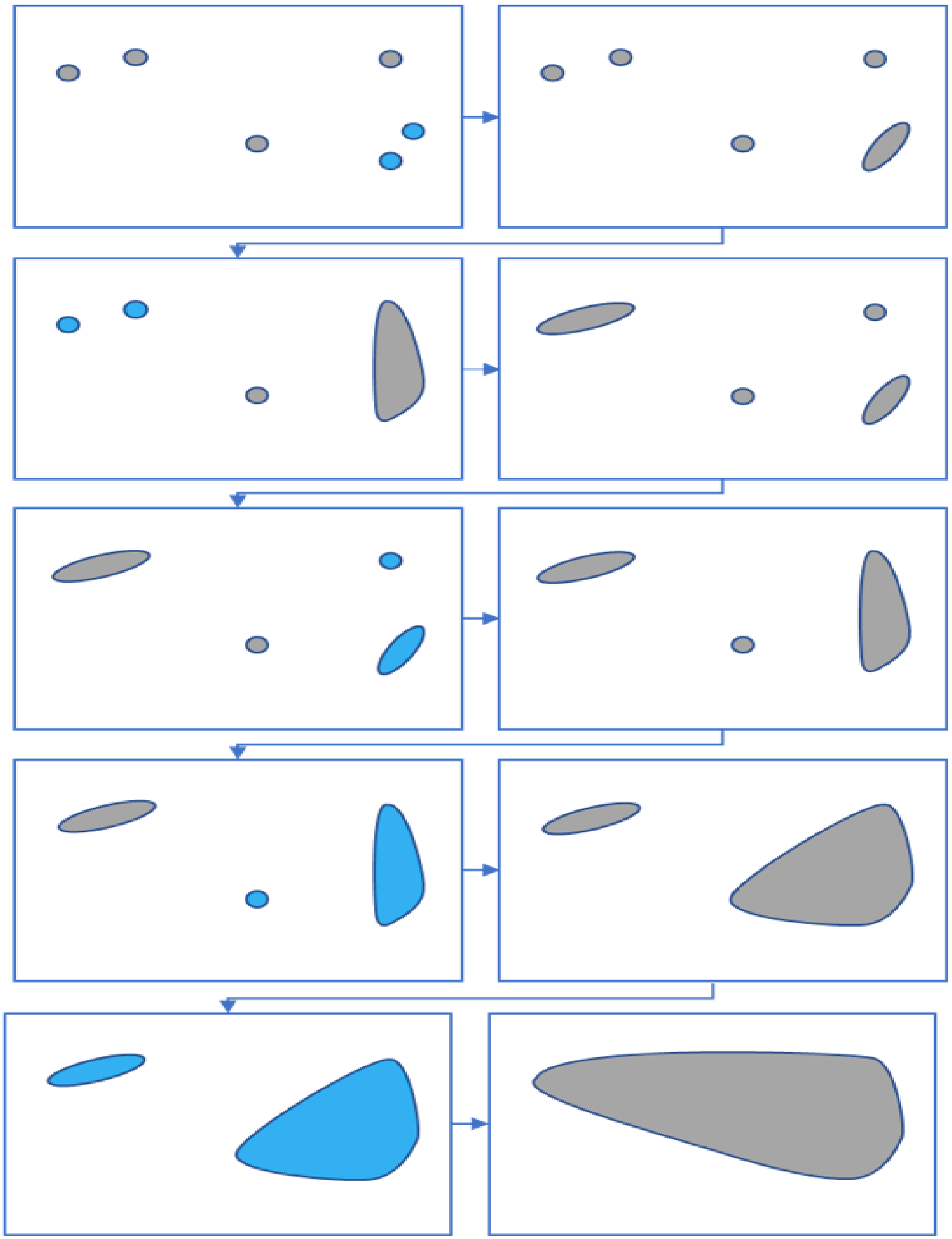
Hierarchal Clustering

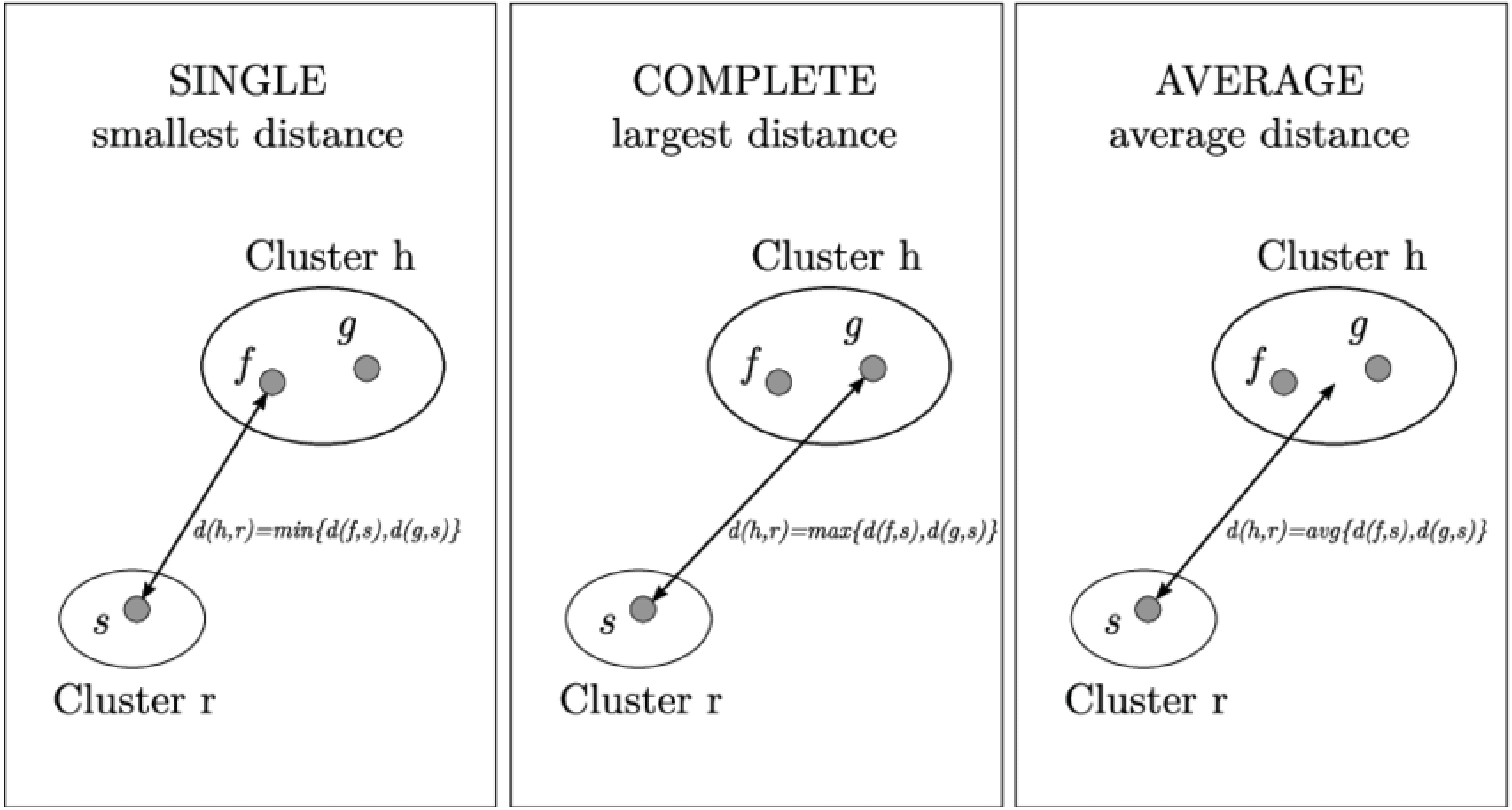
- What is it?
  - Unsupervised machine learning.
  - It is essentially building a hierarchy of clusters
- Types of Hierarchal Clustering
  - Agglomerative hierarchical clustering
  - Divisive Hierarchical clustering



Linkage Criteria

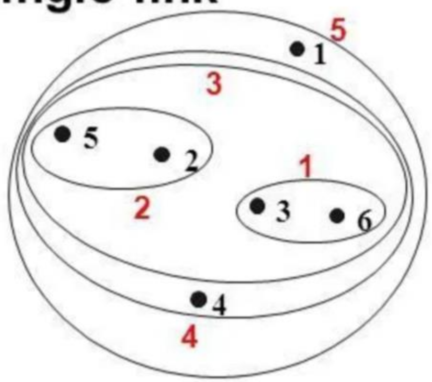
- It is necessary to determine from where distance is computed in cluster.
- Your options
  - ➢It can be computed between the two most similar parts of a cluster (*single-linkage*)
  - ➢the two least similar bits of a cluster (*complete-linkage*)
  - ➢the center of the clusters (*mean* or *average-linkage*)
  - ➢or some other criterion

Linkage Criteria

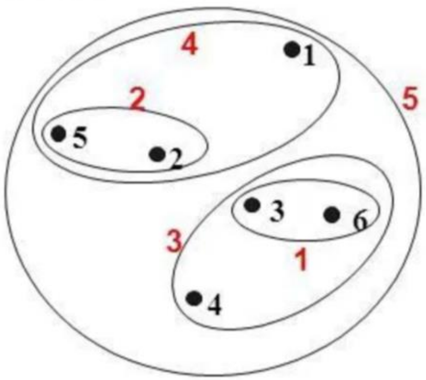


Linkage Criteria Comparison

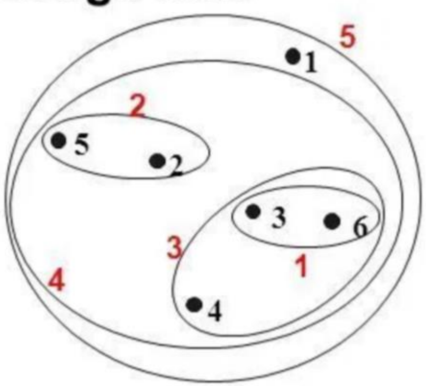
Single-link



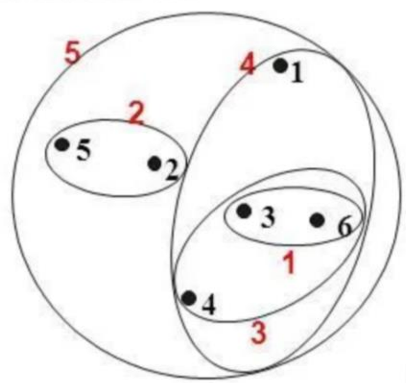
Complete-link



Average-link



Centroid distance



Agglomerative Clustering Algorithm

1. Compute the proximity matrix
2. Let each data point be a cluster
3. Repeat: Merge the two closest clusters and update the proximity matrix
4. Until only a single cluster remains

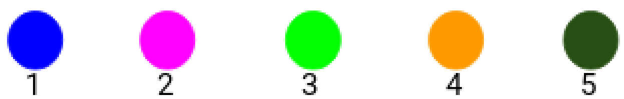
Agglomerative Clustering Example

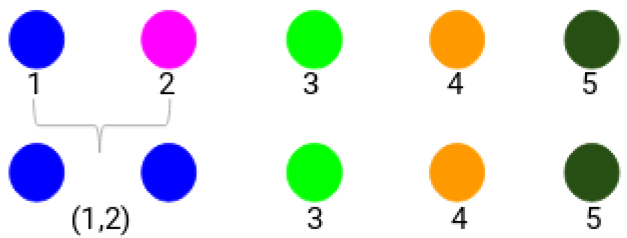
Student_ID	Marks
1	10
2	7
3	28
4	20
5	35

ID	1	2	3	4	5
1	0	3	18	10	25
2	3	0	21	13	28
3	18	21	0	8	7
4	10	13	8	0	15
5	25	28	7	15	0

Proximity Matrix

Agglomerative Clustering Example



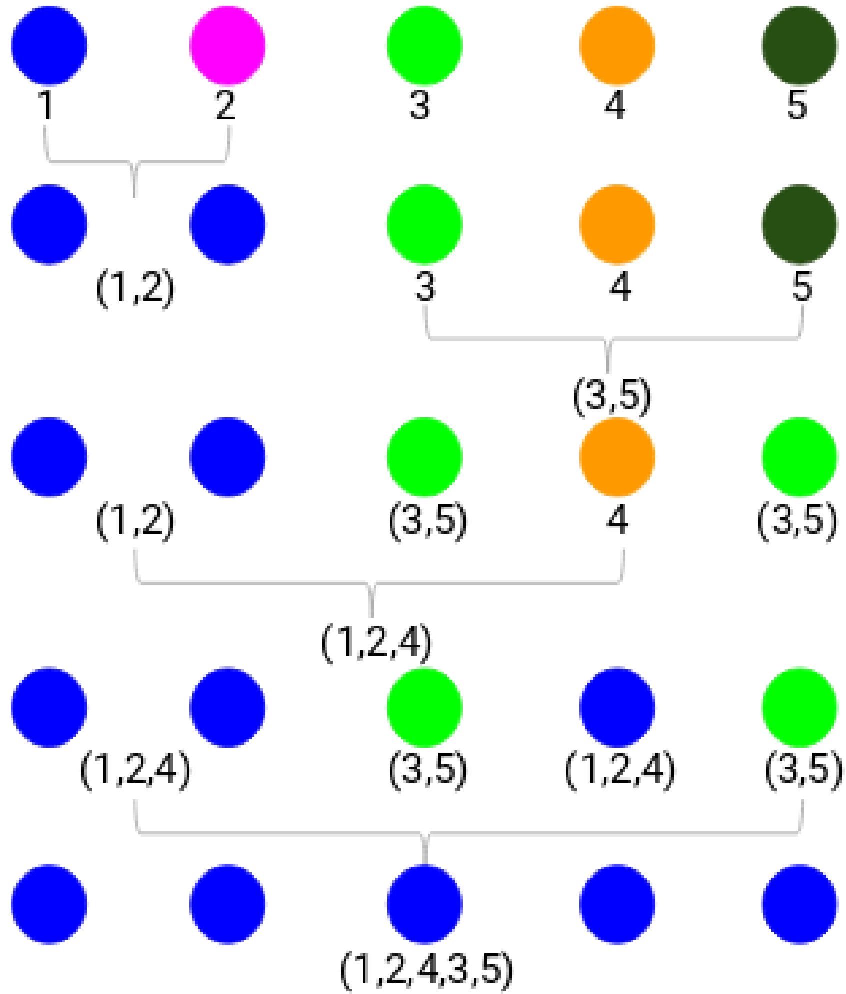


ID	1	2	3	4	5
1	0	3	18	10	25
2	3	0	21	13	28
3	18	21	0	8	7
4	10	13	8	0	15
5	25	28	7	15	0

Student_ID	Marks
(1,2)	10
3	28
4	20
5	35

Agglomerative Clustering Example

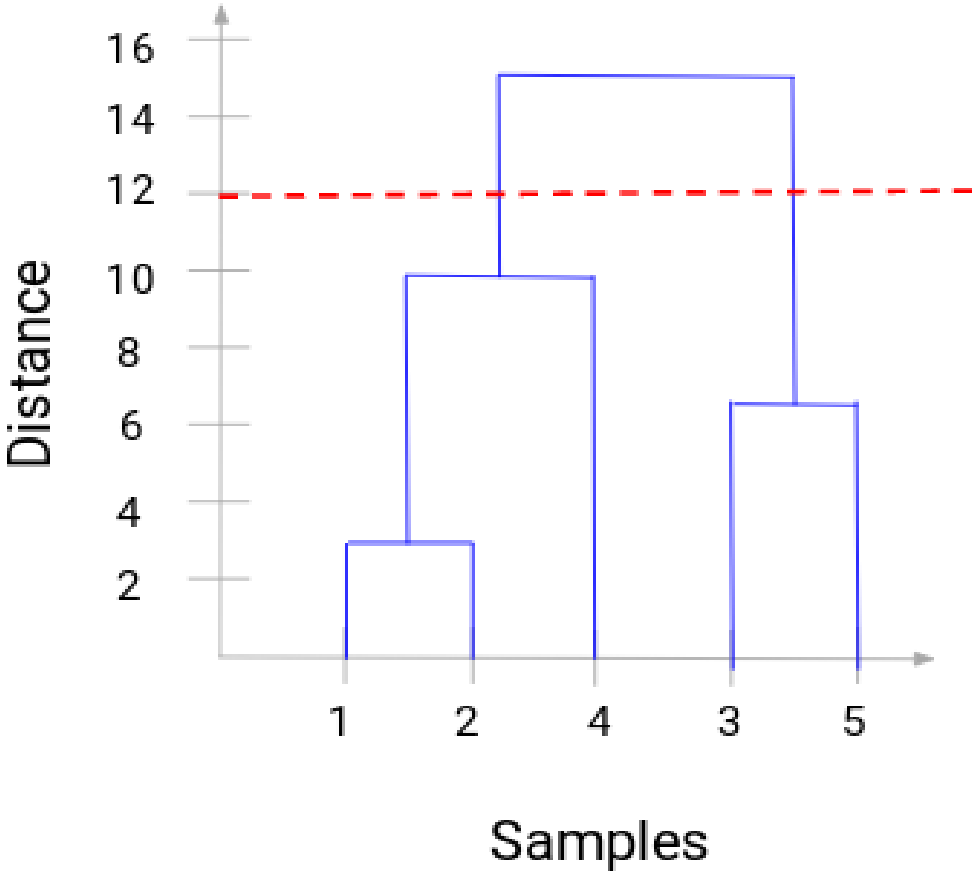
ID	(1,2)	3	4	5
(1,2)	0	18	10	25
3	18	0	8	7
4	10	8	0	15
5	25	7	15	0



How Can we Choose the Number of Clusters?

- Using a Dendrogram
- A dendrogram is a tree-like diagram that records the sequences of merges or splits
- Whenever two clusters are merged, we will join them in this dendrogram and the height of the join will be the distance between these points
- We set a threshold distance and draw a horizontal line (try to set the threshold in such a way that it cuts the tallest vertical line)
- The number of clusters will be the number of vertical lines which are being intersected by the line drawn using the threshold

How Can we Choose the Number of Clusters?

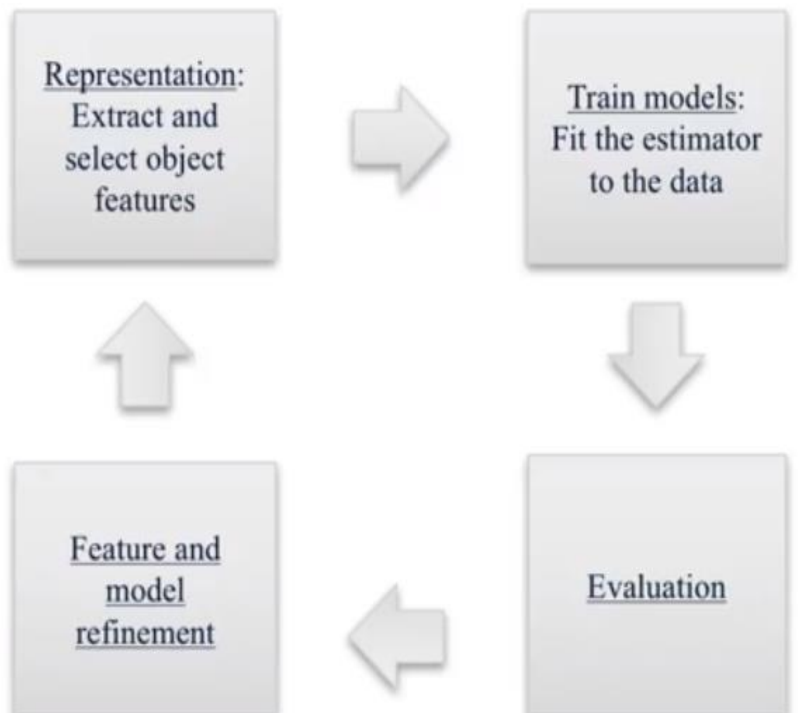


Advantages and Disadvantages of Hierarchal Clustering

- Advantages
  - Easy to Implement
  - No Need to decide the number of clusters beforehand.
- Disadvantages
  - Not suitable for large datasets
  - Sensitive to Outliers
  - Initial Seeds have strong impact of final results
  - Linkage criteria and Distance measure are selected most of the time arbitrary.

Refresher

Represent / Train / Evaluate / Refine Cycle



Machine Learning Evaluation

- There are various metrics and methods to evaluate machine learning algorithms
- They differ according to the algorithm being supervised or unsupervised and they differ according to the task
- Let’s look at some of the metrics and concepts regarding evaluation

Accuracy

- This is the simplest metric
- Number of correct predictions divided by the total number of predictions, multiplied by 100.

$$\text{Accuracy} = \frac{\#\text{correct predictions}}{\#\text{total instances}}$$

Accuracy with Imbalanced Classes

- Suppose you have two classes:
  - The positive class
  - The negative class
- Out of 1000 randomly selected items, on average:
- One item belong to the positive class
- The rest of items (999 of them) belong to the negative class
- The Accuracy will be

$$\text{Accuracy} = \frac{\#\text{correct predictions}}{\#\text{total instances}}$$

Accuracy with Imbalanced Classes

- When you build a classifier to predict the items (positive or negative), you may find out that the accuracy on the test set is 99.9%.
- Be aware that this is not an actually presentation of how good your classifier is.
- For comparison, if we have a “dummy” classifier that do not consider the features at all but rather blindly predict according to the most frequent class

Accuracy with Imbalanced Classes

- If we use the same dataset mentioned in the previous slide (the 1000 data instance with 999 negative and 1 positive). What do you think the accuracy of the dummy classifier would be?

Answer:

$$\text{Accuracy}_{\text{Dummy}} = 999/1000 = 99.9\%$$

- Hence the accuracy alone sometime not a good metric to measure how good the model is

Dealing with Imbalanced Classes

- Data pre-processing
  - ➢ Random Under Sampling
  - ➢ Random Over Sampling
  - ➢ Cluster-Based Over Sampling
  - ➢ Synthetic Minority Over-sampling
- Select More suitable Metrics to Evaluate Imbalanced Classes
  - ➢ Precession and Recall
  - ➢ F1-Score
  - ➢ Log-Loss

Precision and Recall

Precision

Precision attempts to answer the following question:

> What proportion of positive identifications was actually correct?

Precision is defined as follows:

$$\text{Precision} = \frac{TP}{TP + FP}$$

TP: True Positive

FP: False Positive

FN: False Negative

Recall

Recall attempts to answer the following question:

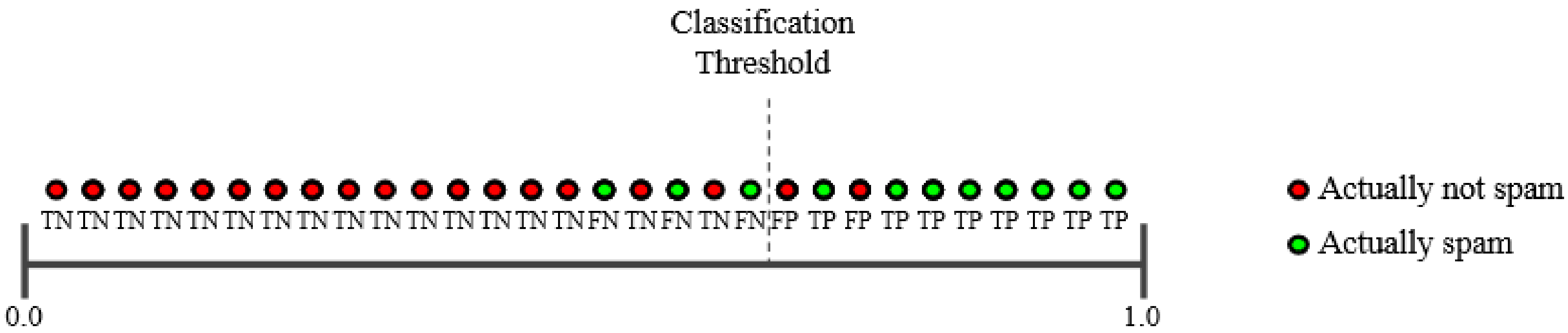
> What proportion of actual positives was identified correctly?

Mathematically, recall is defined as follows:

$$\text{Recall} = \frac{TP}{TP + FN}$$

https://developers.google.com/machine-learning/crash-course/classification/precision-and-recall

Precision and Recall



True Positives (TP): 8	False Positives (FP): 2
False Negatives (FN): 3	True Negatives (TN): 17

Precision measures the percentage of **emails flagged as spam** that were correctly classified—that is, the percentage of dots to the right of the threshold line that are green

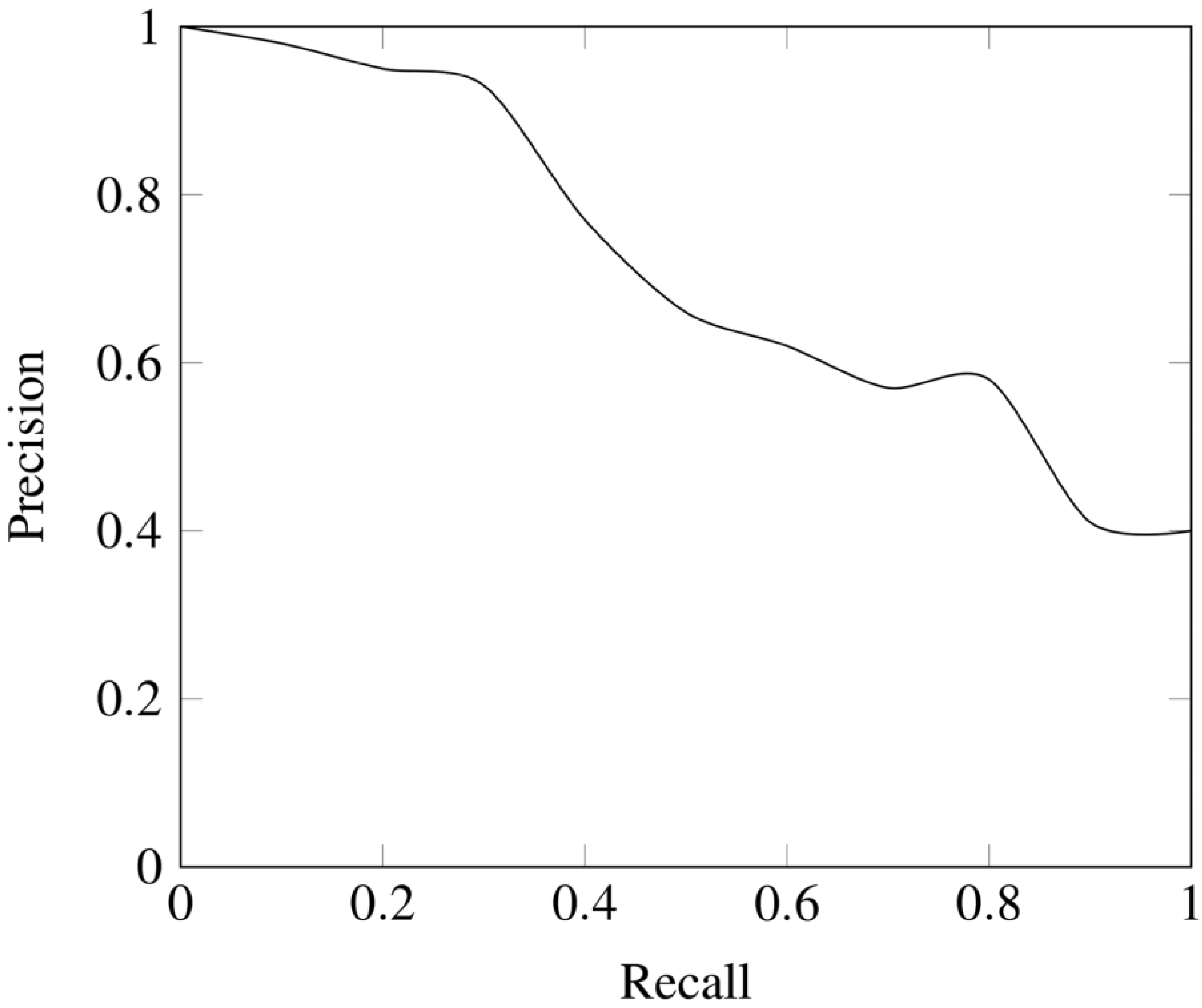
$$\text{Precision} = \frac{TP}{TP + FP} = \frac{8}{8+2} = 0.8$$

Recall measures the percentage of **actual spam emails** that were correctly classified—that is, the percentage of green dots that are to the right of the threshold line

$$\text{Recall} = \frac{TP}{TP + FN} = \frac{8}{8+3} = 0.73$$

https://developers.google.com/machine-learning/crash-course/classification/precision-and-recall

Precision and Recall



https://towardsdatascience.com/beyond-accuracy-precision-and-recall-3da06bea9f6c

F1 Score

- A metric which combines precision and recall
- Harmonic mean of precision and recall

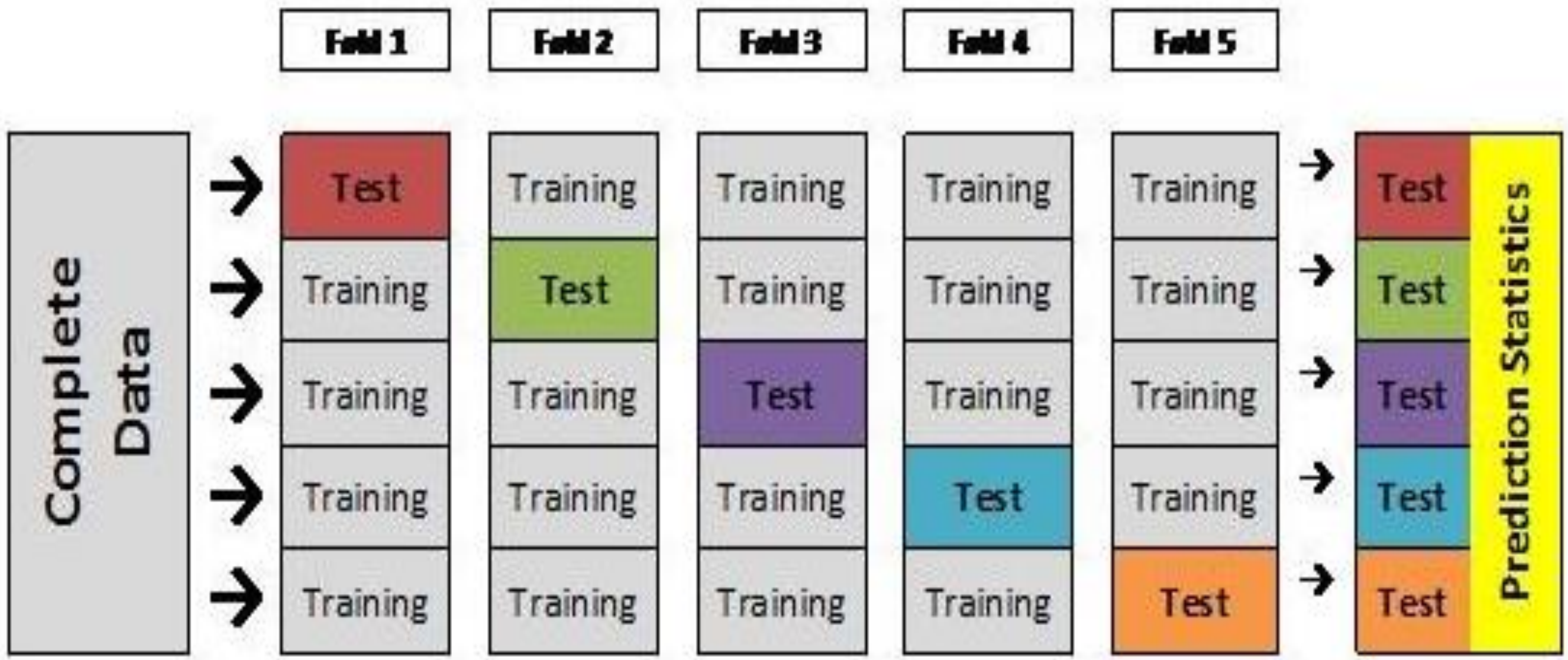
F1-score= 2*Precision*Recall/(Precision+Recall)

Cross-validation

- Cross-validation is a resampling procedure used to evaluate machine learning models on a limited data sample.
- The procedure has a single parameter called k that refers to the number of groups that a given data sample is to be split into. As such, the procedure is often called k-fold cross-validation.
- When a specific value for k is chosen, it may be used in place of k in the reference to the model, such as k=5 becoming 5-fold cross-validation.

https://machinelearningmastery.com/k-fold-cross-validation/

Cross Validation Examples (5-fold)



https://www.datasciencecentral.com/profiles/blogs/14-great-articles-about-cross-validation-model-fitting-and-select

Stratified Cross-validation

fruit_label	fruit_name
1	Apple
1	Apple
1	Apple
1	Apple
1	Apple
2	Mandarin
...	...
3	Orange
...	...
4	Lemon
4	Lemon
4	Lemon
4	Lemon
4	Lemon

(Folds and dataset shortened for illustration purposes.)

Example has 20 data samples
= 4 classes with 5 samples each.

5-fold CV: 5 folds of 4 samples each.

Fold 1 uses the first 20% of the dataset as the test set, which only contains samples from class 1.

Classes 2, 3, 4 are missing entirely from test set and so will be missing from the evaluation.

https://www.coursera.org/learn/python-machine-learning

Stratified Cross-validation

- Stratification is a technique where we rearrange the data in a way that each fold has a good representation of the whole dataset
- It forces each fold to have at least m instances of each class. T
- his approach ensures that one class of data is not overrepresented especially when the target variable is unbalanced.

https://medium.com/datadriveninvestor/k-fold-and-other-cross-validation-techniques-6c03a2563f1e

Useful Resources

https://towardsdatascience.com/understanding-the-concept-of-hierarchical-clustering-technique-c6e8243758ec

https://heartbeat.fritz.ai/introduction-to-machine-learning-model-evaluation-fa859e1b2d7f

https://machinelearningmastery.com/tour-of-evaluation-metrics-for-imbalanced-classification/

https://www.analyticsvidhya.com/blog/2017/03/imbalanced-data-classification/

https://medium.com/james-blogs/handling-imbalanced-data-in-classification-problems-7de598c1059f

https://medium.com/datadriveninvestor/k-fold-and-other-cross-validation-techniques-6c03a2563f1e

Q&A