COMP47490

Evaluation in Machine Learning

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Introduction

- Evaluation is a central task in machine learning. Two common types of evaluation experiment in classification:
    1. Verify a trained classifier on unseen data.
    2. Compare the performance of two or more classifiers on similar problems.
- These experiments generally include the following steps:
    1. Choose one or more appropriate evaluation measures.
    2. Run the classifier one or more times on a dataset or selection of datasets.
    3. Compare the performance of the classifier with existing benchmark classifiers, based on the evaluation measure(s).
- The exact experimental setup depends on the hypothesis that we wish to test.

Hypothesis Testing

- Goal of hypothesis testing: formally examine two opposing hypotheses H_0 and H_A. These two hypotheses are mutually exclusive, so one is true to the exclusion of the other.
- Null Hypothesis H_0: States the assumption to be tested.
  e.g. There is no difference between the performance of two machine learning algorithms.
- *Type I error*: Rejecting H_0 when it is in fact true.
  This is a “false alarm” or "false positive" - detecting a difference, when none actually exists.
- *Type II error*: Failing to reject H_0 when it is in fact false.
  This is a "false negative" - concluding there is no difference, when there really is a difference.

Type I and Type II Errors

- *Type I error*: Rejecting H_0 when it is in fact true.
  i.e. "false positive" - detecting a difference, when none exists.

- *Type II error*: Failing to reject H_0 when it is in fact false.
  i.e. "false negative" - concluding there is no difference, when there is.

Statistical Test Result

Real World	H_0 Rejected	H_0 Not Rejected
There is a real difference	**Correct** A Hit	**Type II Error** Missed a real difference
There is in fact no difference	**Type I Error** False alarm	**Correct** Right to be sceptical of H_A

Type I and Type II Errors

Depending on the hypothesis being tested, these errors will have different costs associated with them.

Null Hypothesis	**Type I Error "False Positive"**	**Type II Error "False Negative"**
"*The email X is a spam email*"	X is a legitimate email, but is wrongly marked as spam.	X is a spam email, but is not detected as spam.
Cost of the error	The user misses out on a potentially important email.	Spam email appears in the user's inbox.

Null Hypothesis	**Type I Error "False Positive"**	**Type II Error "False Negative"**
"*Person X is not guilty of the crime*"	X is found guilty of a crime, when they are actually innocent.	X is found not-guilty of a crime, when they did actually commit the crime.
Cost of the error	Social cost of sending an innocent person to prison.	Risk of letting a guilty criminal go free.

Classifier Accuracy

When making predictions, we need a quantitative measure to capture how often the model makes correct or incorrect predictions, and how severe the mistakes are.

Misclassification Rate:
Fraction of incorrect predictions made by the classifier.

$$MR = \frac{\#\ \text{incorrect predictions}}{\text{total predictions}}$$

Accuracy:
Fraction of correct predictions made by the classifier.

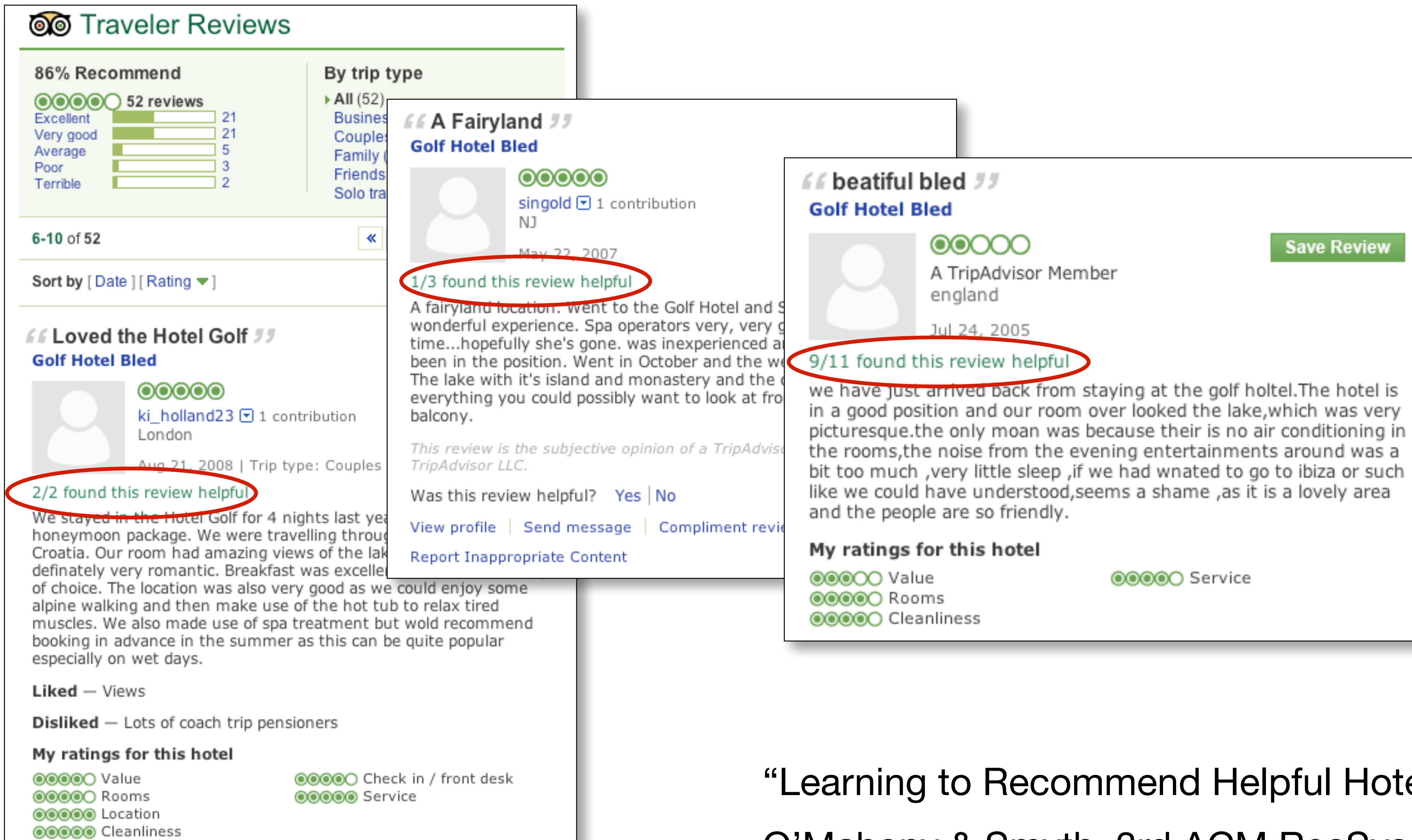
$$ACC = \frac{\#\ \text{correct predictions}}{\text{total predictions}}$$

Email	Label	Prediction	Correct?
1	spam	non-spam	✗
2	spam	spam	✓
3	non-spam	non-spam	✓
4	spam	spam	✓
5	non-spam	spam	✗
6	non-spam	non-spam	✓
7	spam	spam	✓
8	non-spam	spam	✗
9	non-spam	non-spam	✓
10	spam	spam	✓

$$MR = \frac{3}{10} = 0.3 \qquad ACC = \frac{7}{10} = 0.7$$

Example: Hotel Reviews

Q. Can we predict the "helpfulness" of TripAdvisor hotel reviews?



"Learning to Recommend Helpful Hotel Reviews"

O'Mahony & Smyth, 3rd ACM RecSys Conference, 2009

http://dl.acm.org/citation.cfm?id=1639774

Example: Hotel Reviews

- Compare performance of Naïve Bayes and Support Vector Machine (SVM) classifiers on review data using Weka.
- Test set: 105 “Helpful”, 60 “Unhelpful” reviews
- Testing option: Hold-out validation with 66/33% hold-out split.

SVM classifier

```
Correctly Classified Instances         117               70.9091 %
Incorrectly Classified Instances        48               29.0909 %
Kappa statistic                          0.3071
Mean absolute error                      0.2909
Root mean squared error                  0.5394
Relative absolute error                 62.6804 %
Root relative squared error            112.1168 %
Total Number of Instances              165

=== Detailed Accuracy By Class ===

               TP Rate   FP Rate   Precision   Recall  F-Measure   ROC Area  Class
                 0.895     0.617      0.718     0.895     0.797      0.639    good
                 0.383     0.105      0.676     0.383     0.489      0.639    bad
Weighted Avg.    0.709     0.431      0.703     0.709     0.685      0.639

=== Confusion Matrix ===

  a  b   <-- classified as
 94 11 |  a = good
 37 23 |  b = bad
```

Naïve Bayes classifier

```
Correctly Classified Instances         103               62.4242 %
Incorrectly Classified Instances        62               37.5758 %
Kappa statistic                          0.1995
Mean absolute error                      0.3793
Root mean squared error                  0.5316
Relative absolute error                 81.7353 %
Root relative squared error            110.5048 %
Total Number of Instances              165

=== Detailed Accuracy By Class ===

               TP Rate   FP Rate   Precision   Recall  F-Measure   ROC Area  Class
                 0.686     0.483      0.713     0.686     0.699      0.674    good
                 0.517     0.314      0.484     0.517     0.5        0.674    bad
Weighted Avg.    0.624     0.422      0.63      0.624     0.627      0.674

=== Confusion Matrix ===

  a  b   <-- classified as
 72 33 |  a = good
 29 31 |  b = bad
```

Example: Hotel Reviews

- Compare performance of Naïve Bayes and Support Vector Machine (SVM) classifiers on review data using Weka.
- Test set: 105 “Helpful”, 60 “Unhelpful” reviews
- Testing option: Hold-out validation with 66/33% hold-out split.

SVM

Accuracy = 70.9%

Prediction: H	Prediction: U	Real World
94	**11**	H
37	**23**	U

SVM biased toward majority class (H)

Naïve Bayes

Accuracy = 62.4%

Prediction: H	Prediction: U	Real World
72	**33**	H
29	**31**	U

What if this is important?

Confusion Matrices

Confusion matrix summarises the performance of an algorithm, when compared with the real classes (“ground truth”).

		Predicted Class	
		Positive	**Negative**
Real Class	**Positive**	**TP** **True positive** Correct!	**FN** **False Negative** (Type II error)
	Negative	**FP** **False Positive** (Type I error)	**TN** **True Negative** Correct!

Clinical Example: Predict a case as *positive* (person has the disease) or *negative* (person does not have the disease)

- **TP** = Sick people correctly predicted as sick
- **FP** = Healthy people incorrectly predicted as sick
- **TN** = Healthy people correctly predicted as healthy
- **FN** = Sick people incorrectly predicted as healthy

Confusion Matrices

Spam Filtering Example: Predict emails as *spam* or *non-spam*…

- **TP** = Spam emails correctly predicted as spam
- **FP** = Non-spam emails incorrectly predicted as spam
- **TN** = Non-spam emails correctly predicted as non-spam
- **FN** = Spam emails incorrectly predicted as non-spam

Email	Label	Prediction	Correct?	Outcome
1	spam	non-spam	✗	FN
2	spam	spam	✓	TP
3	non-spam	non-spam	✓	TN
4	spam	spam	✓	TP
5	non-spam	spam	✗	FP
6	non-spam	non-spam	✓	TN
7	spam	spam	✓	TP
8	non-spam	spam	✗	FP
9	non-spam	non-spam	✓	TN
10	spam	spam	✓	TP

Predicted Class

Spam	Non	
TP=4	**FN=1**	Spam
FP=2	**TN=3**	Non

Real Class

Evaluation Measures

- Accuracy: Fraction of predictions correct

$$\text{Accuracy} = \frac{TP + TN}{TP + FP + TN + FN}$$

- True Positive Rate:
  Focus on TPs
  Also called *Sensitivity*

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

Predicted

	Pos	Neg	
P	TP	FN	Pos
N	FP	TN	Neg

Real

- False Positive Rate:
  Focus on FPs

$$\text{FPRate} = \frac{FP}{FP + TN}$$

Predicted

	Pos	Neg	
P	TP	FN	Pos
N	FP	TN	Neg

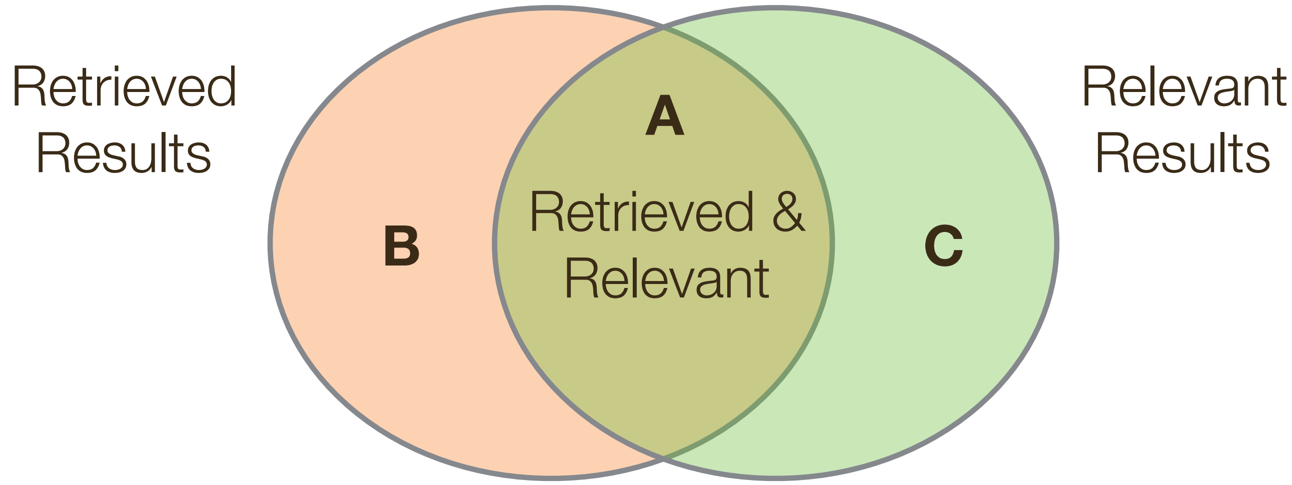
Real

- True Negative Rate:
  Focus on TNs
  Also called *Specificity*

$$\text{TNRate} = \frac{TN}{FP + TN}$$

Precision & Recall

- Measures from information retrieval, but used in ML evaluation.
- Precision: proportion of retrieved results that are relevant.
- Recall: proportion of relevant results that are retrieved.



$$\text{Precision} = \frac{A}{A+B}$$

$$\text{Recall} = \frac{A}{A+C}$$

Search Example: Given a collection of 100k documents, we want to find all documents on "water charges". In fact, 45 relevant documents actually exist.

Perform a search, 9 out of 10 results on first page are relevant documents.

➡ Precision = 9/10 = 90% of retrieved results were relevant.

➡ Recall = 9/45 = 20% of all possible relevant results were retrieved.

Precision & Recall

- Precision and Recall are also used as measures to evaluate machine learning algorithms.

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

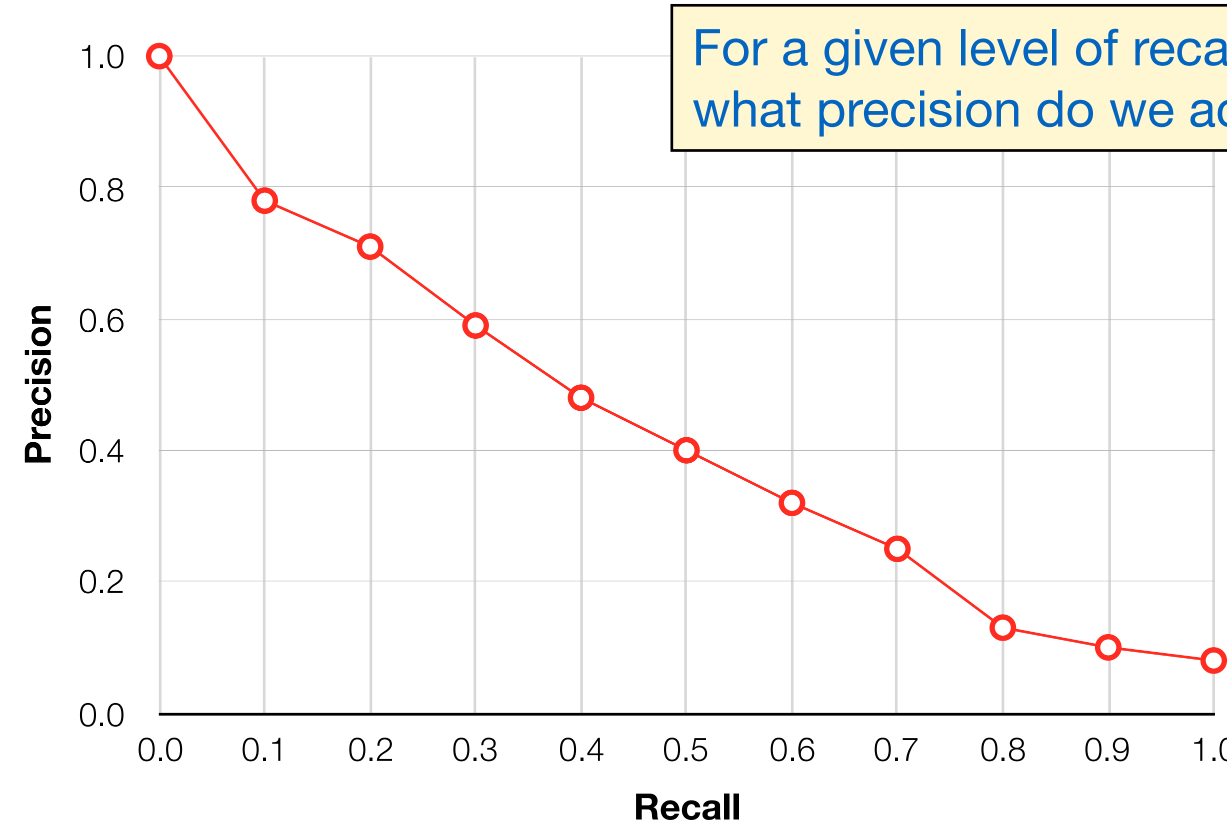
	Predicted Pos	Predicted Neg	
P	TP	FN	Real Pos
N	FP	TN	Real Neg

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

	Predicted Pos	Predicted Neg	
P	TP	FN	Real Pos
N	FP	TN	Real Neg

- Plot the trade-off between the two measures using a Precision-Recall (PR) curve.
- Used to study the output of a binary classifier.
- Measure precision at fixed recall intervals.

For a given level of recall, what precision do we achieve?



Example Calculations

$$\text{Accuracy} = \frac{TP + TN}{TP + FP + TN + FN}$$

$$= \frac{4+3}{10} = 0.7$$

$$\text{TPRate} = \frac{TP}{TP + FN} = \frac{4}{4+1} = 0.8$$

$$\text{FPRate} = \frac{FP}{FP + TN} = \frac{2}{2+3} = 0.4$$

$$\text{TNRate} = \frac{TN}{FP + TN} = \frac{3}{2+3} = 0.6$$

$$\text{Precision} = \frac{TP}{TP + FP} = \frac{4}{4+2} = 0.667$$

$$\text{Recall} = \frac{TP}{TP + FN} = \frac{4}{4+1} = 0.8$$

	Label	Prediction	Correct?	Outcome
1	spam	non-spam	✗	FN
2	spam	spam	✓	TP
3	non-spam	non-spam	✓	TN
4	spam	spam	✓	TP
5	non-spam	spam	✗	FP
6	non-spam	non-spam	✓	TN
7	spam	spam	✓	TP
8	non-spam	spam	✗	FP
9	non-spam	non-spam	✓	TN
10	spam	spam	✓	TP

Predicted Class

Spam	Non	
TP=4	**FN=1**	Spam
FP=2	**TN=3**	Non

Real Class

Imbalanced Data

- Imbalanced data: Refers to a problem in classification where the classes in the data are not represented equally (i.e. the distribution of class sizes is skewed).
- **Example:** In a binary classification problem, we have a dataset of 100 items. 80 items belong to Class A, 20 belong to Class B. This is an imbalanced dataset, where the ratio A:B is 4:1. We call A the majority class and B the minority class.
- This phenomenon occurs in many real-world problems:
  - Fraud detection: Vast majority of financial transactions are legitimate, a small minority are fraudulent.
  - Churn analysis: Vast majority of customers stay with their mobile operator, a small minority cancel their subscription.
  - Other examples: medical diagnosis, e-commerce, security.

Balanced Accuracy

- When evaluating classifiers applied to imbalanced datasets, some evaluation measures can be misleading.
- High accuracy can be achieved by biased (or trivial) classifiers which just predict the majority class.

$\Rightarrow$ Accuracy = 90%

Classified as

Pos	Neg	
0	**10**	Pos
0	**90**	Neg

Real World

- To deal with skewed classes, use a balanced evaluation measure. Measures include:
  - Balance Accuracy Rate (BAR): Mean of TP Rate and TN Rate
  - Balance Error Rate (BER): Mean of FP Rate and FN Rate

Balanced Accuracy

- F-Measure: A single measure that trades off precision against recall, for a given level of balance.

$$\mathrm{F} = \frac{(1+\beta^2) \times \mathrm{Precision} \times \mathrm{Recall}}{\beta^2 \times \mathrm{Precision} + \mathrm{Recall}}$$

- The Beta parameter controls the trade-off:
  - $\beta < 1$ Focus more on Precision
  - $\beta = 1$ Harmonic mean of Precision and Recall.
  - $\beta > 1$ Focus more on Recall

- F1-Measure: Most widely-used variant, sets $\beta = 1$

$$\mathrm{F1} = \frac{2 \times \mathrm{Precision} \times \mathrm{Recall}}{\mathrm{Precision} + \mathrm{Recall}}$$

harmonic mean of precision and recall

Example: Measure Calculations

$$\text{Accuracy} = \frac{TP + TN}{TP + FP + TN + FN}$$

$$= \frac{4+3}{10} = 0.7$$

$$\text{TPRate} = \frac{TP}{TP + FN} = \frac{4}{4+1} = 0.8$$

$$\text{FPRate} = \frac{FP}{FP + TN} = \frac{2}{2+3} = 0.4$$

$$\text{TNRate} = \frac{TN}{FP + TN} = \frac{3}{2+3} = 0.6$$

$$\text{Precision} = \frac{TP}{TP + FP} = \frac{4}{4+2} = 0.667$$

$$\text{Recall} = \frac{TP}{TP + FN} = \frac{4}{4+1} = 0.8$$

	Label	Prediction	Correct?	Outcome
1	spam	non-spam	✗	FN
2	spam	spam	✓	TP
3	non-spam	non-spam	✓	TN
4	spam	spam	✓	TP
5	non-spam	spam	✗	FP
6	non-spam	non-spam	✓	TN
7	spam	spam	✓	TP
8	non-spam	spam	✗	FP
9	non-spam	non-spam	✓	TN
10	spam	spam	✓	TP

$$\text{F1} = \frac{2 \times \text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

$$F1 = \frac{2 \times 0.667 \times 0.8}{0.667 + 0.8} = 0.727$$

Decision Thresholds

- Many binary classifiers, such as Naïve Bayes, return the probability of belonging to the positive class.
  e.g. A Naïve Bayes spam classifier returning P(spam)=0.8
- Often we say that if the probability is > 0.5, assign the input to the positive class. Otherwise assign it to the negative class.
- However, in some applications the cost of a false positive or false negative is very high, so we need to be more sure.
  e.g. A clinical decision on cancer diagnosis.
- We can artificially move that threshold from 0.5 to higher or lower values, to change the sensitivity of the model.
- Decision threshold: the value θ used to discriminate when selecting between a positive and negative outcome. The most common value is $\theta = 0.5$

ROC Analysis

- Varying the decision threshold value θ can lead to different results, and so to different confusion matrices.

	Label	Score	> 0.5?	Prediction	Outcome
1	spam	0.1	N	non-spam	FN
2	spam	0.8	Y	spam	TP
3	non-spam	0.6	Y	spam	FP
4	spam	0.9	Y	spam	TP
5	non-spam	0.8	Y	spam	FP
6	non-spam	0.2	N	non-spam	TN
7	spam	0.8	Y	spam	TP
8	non-spam	0.6	Y	spam	FP
9	non-spam	0.1	N	non-spam	TN
10	spam	0.9	Y	spam	TP

	Label	Score	> 0.7?	Prediction	Outcome
1	spam	0.1	N	non-spam	FN
2	spam	0.8	Y	spam	TP
3	non-spam	0.6	N	non-spam	TN
4	spam	0.9	Y	spam	TP
5	non-spam	0.8	Y	spam	FP
6	non-spam	0.2	N	non-spam	TN
7	spam	0.8	Y	spam	TP
8	non-spam	0.6	N	non-spam	TN
9	non-spam	0.1	N	non-spam	TN
10	spam	0.9	Y	spam	TP

Decision Threshold

$\theta = 0.5$

Predicted Class

Spam	Non	Real Class
TP=4	**FN=1**	Spam
FP=3	**TN=2**	Non

Decision Threshold

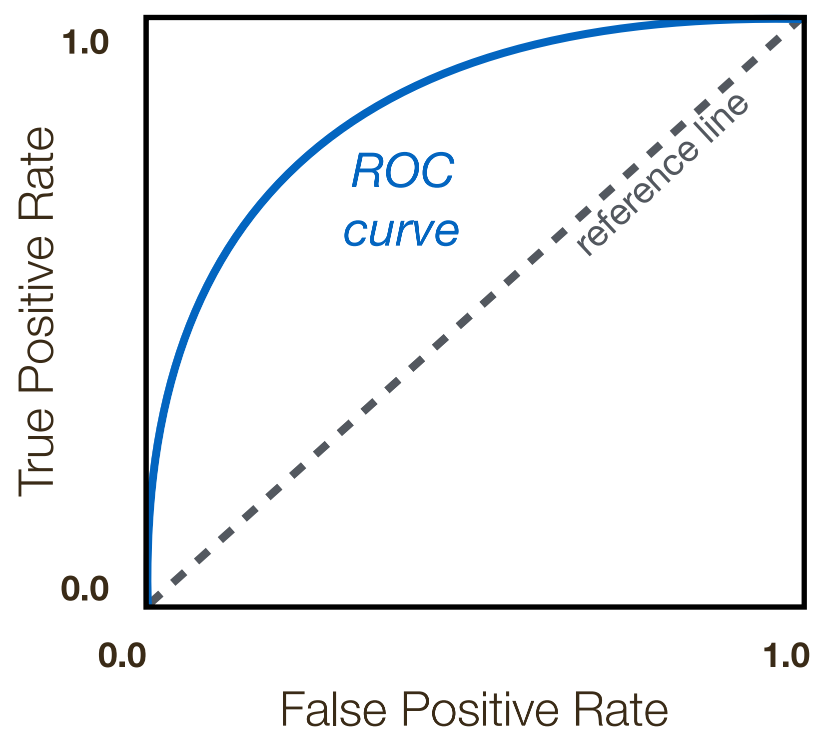
$\theta = 0.7$

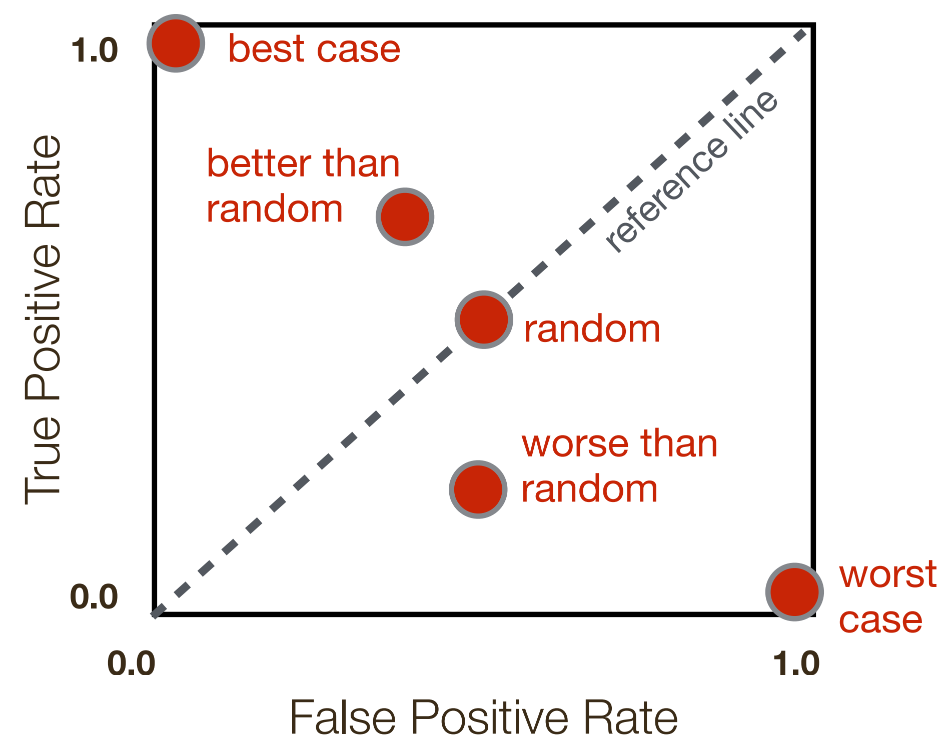
Predicted Class

Spam	Non	Real Class
TP=4	**FN=1**	Spam
FP=1	**TN=4**	Non

ROC Analysis

- Often want to compare the performance of classifiers at many different decision thresholds (i.e. summarise many confusion matrices).
- A Receiver Operating Characteristic (ROC Curve) is a graphical plot of how the true positive rate and false positive rate change over many different thresholds. The curve is drawn by plotting a point for each feasible threshold and joining them.
- A trained classifier should always be above the "random" reference line. The strength of the classifier increases as the ROC curve moves further from the line (i.e. closer to top left corner).



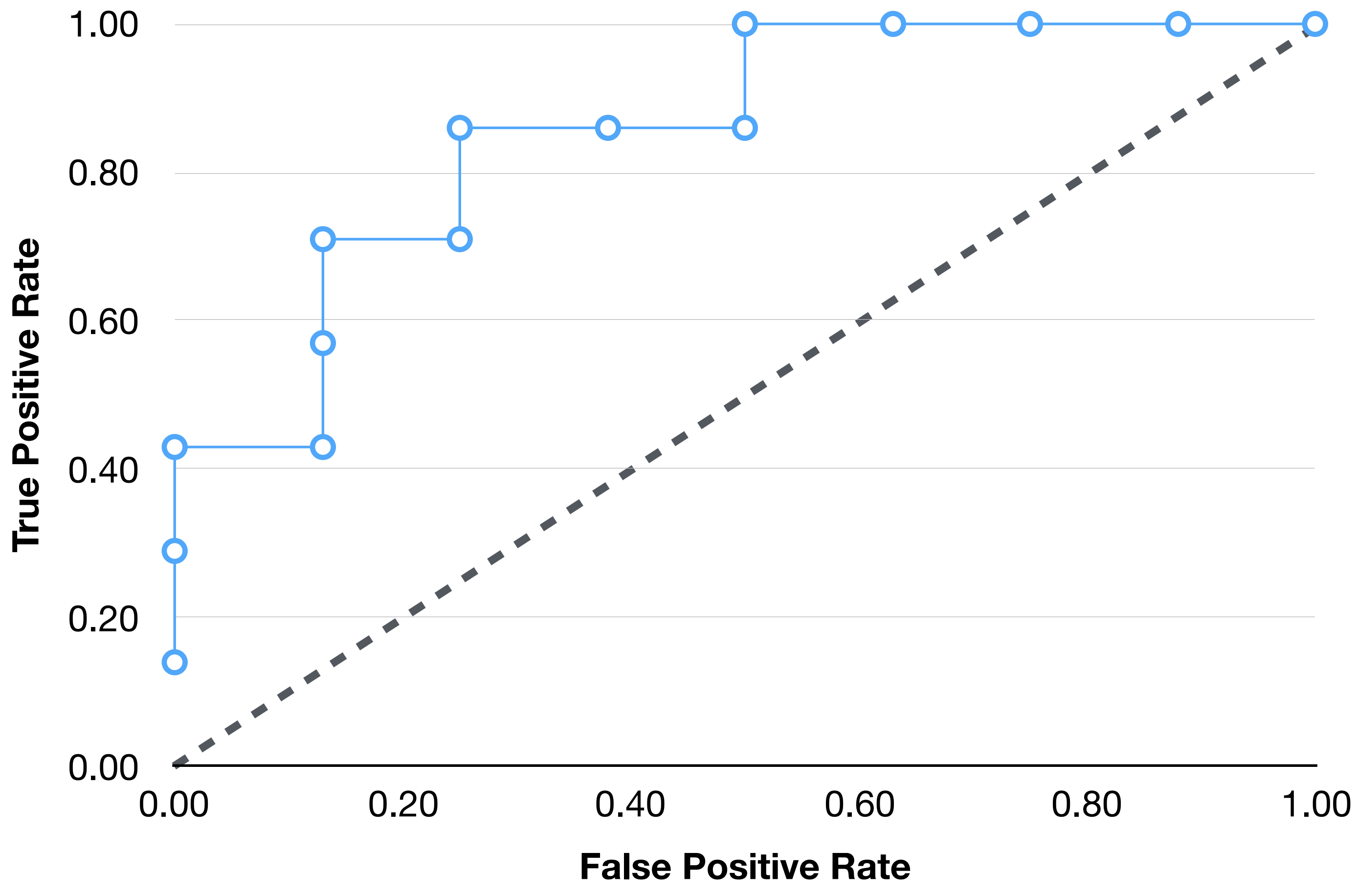


Example: ROC Analysis

- Given a ranking classifier which will score test samples with a probability P of belonging to the positive class.
- Decision threshold θ controls whether a sample will be classified as positive or negative - i.e. $P > \theta$

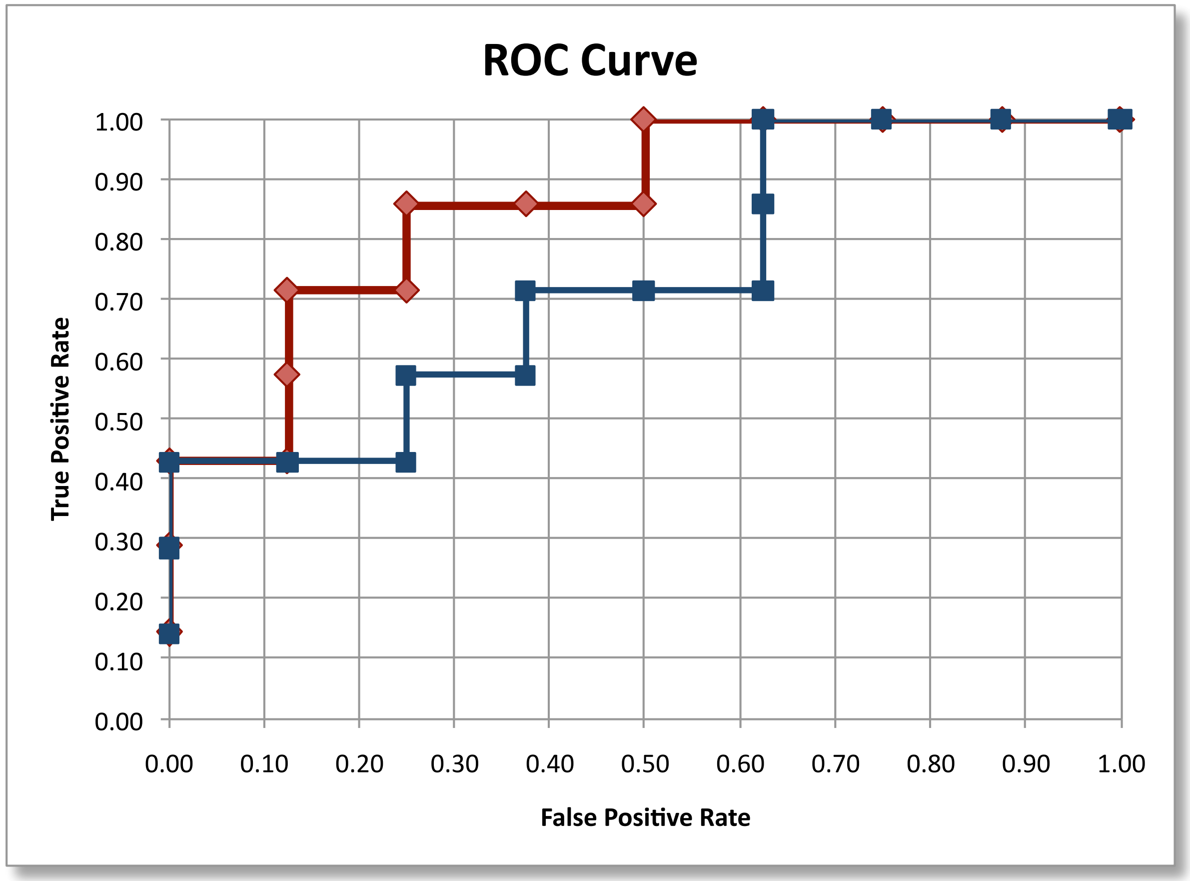
Single example $\theta = 0.5$

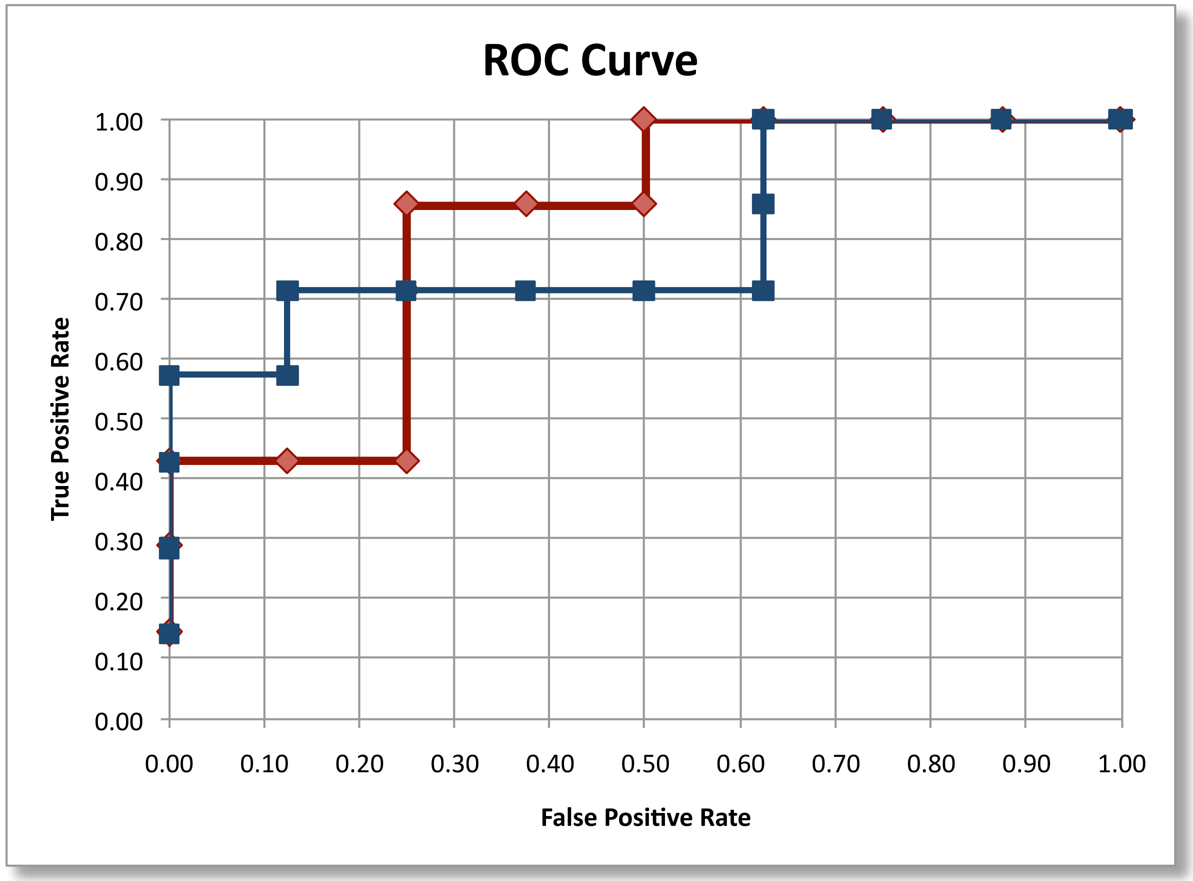
P	> 0.5	Real
0.99	1	1
0.90	1	1
0.80	1	1
0.85	1	0
0.70	1	1
0.70	1	1
0.65	1	0
0.60	1	1
0.45	0	0
0.45	0	0
0.40	0	1
0.30	0	0
0.20	0	0
0.20	0	0
0.20	0	0



Comparing ROC Curves

- Often want to compare the performance of two classifiers at different thresholds → we can look at their ROC curves.
- In some cases, one classifier will always be better than another across all values of θ. In other cases, it will be more complicated…





➡ Make comparisons based on Area Under the Curve (AUC). A better classifier will have a ROC curve closer to top-left corner, giving a larger area under the curve.

Overfitting

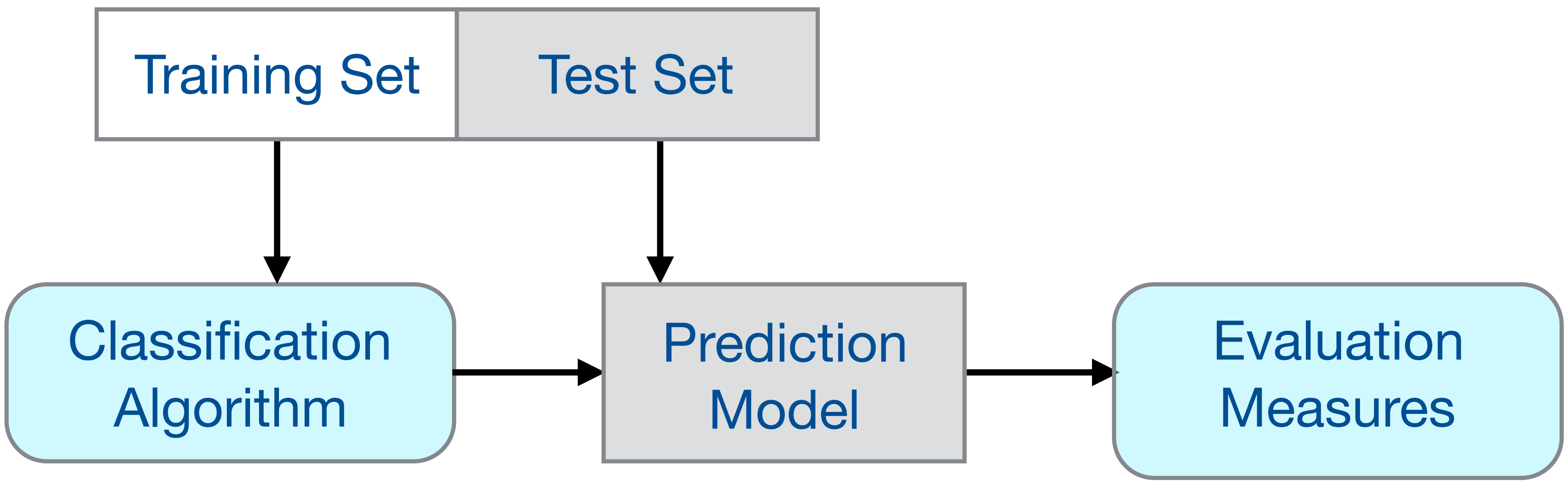
- For real-world tasks, we are interested in generalisation accuracy.
- Overfitting: Model is fitted too closely to the training data (including its noise). The model cannot generalise to situations not presented during training, so it is not useful when applied to unseen data.

- **Possible Causes**
    - *Small training set*: Classifier only given a few examples, may not be representative of the underlying concepts.
    - *Complex model*: Model has too many parameters relative to the number of training examples.
    - *Noise*: Spurious or contradictory patterns in the training data.
    - *High-dimensionality*: Data has many irrelevant features (dimensions) containing noise which leads to a poor model.

➡ A good model must not only fit the training data well, but also accurately classify examples that it has never seen before.

Simple Hold-Out Strategy

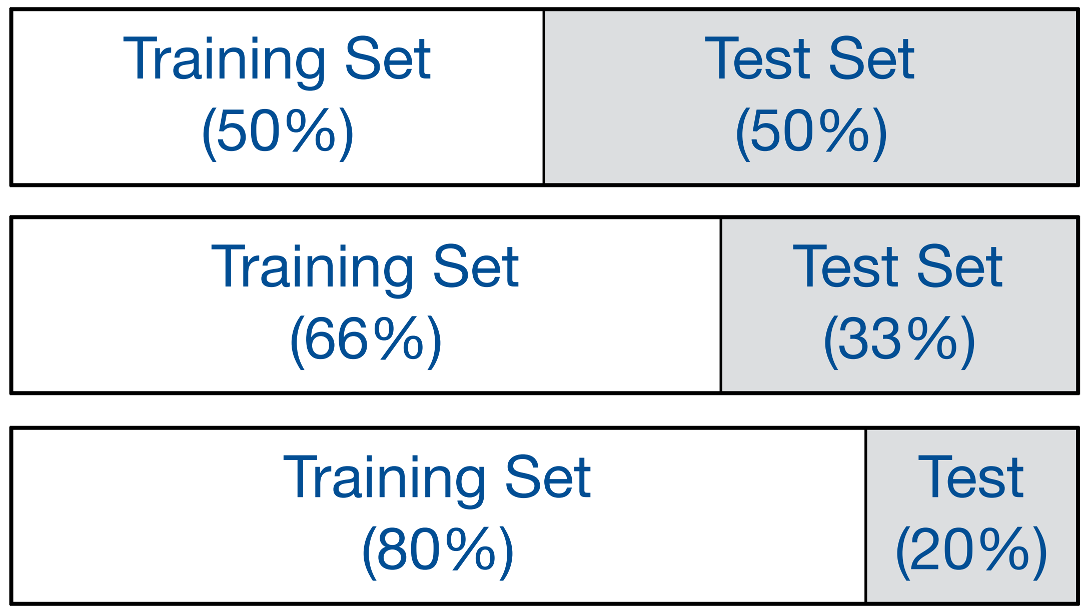
- Keep some training data back (the hold-out set) to use for evaluating the model produced by the classifier.
- Use performance on the hold-out set as a proxy for performance on unseen data (i.e. generalisation accuracy).



- Using a hold-out set avoids peeking - when the performance of a model is evaluated using the same data used to train it.
e.g. Use of same training data for testing in Weka can produce unrealistic accuracy results that are "too good to be true".

Simple Hold-Out Strategy

- **Random Split:** Obtain a hold-out set by randomly assigning examples to either the training or test set with some probability.

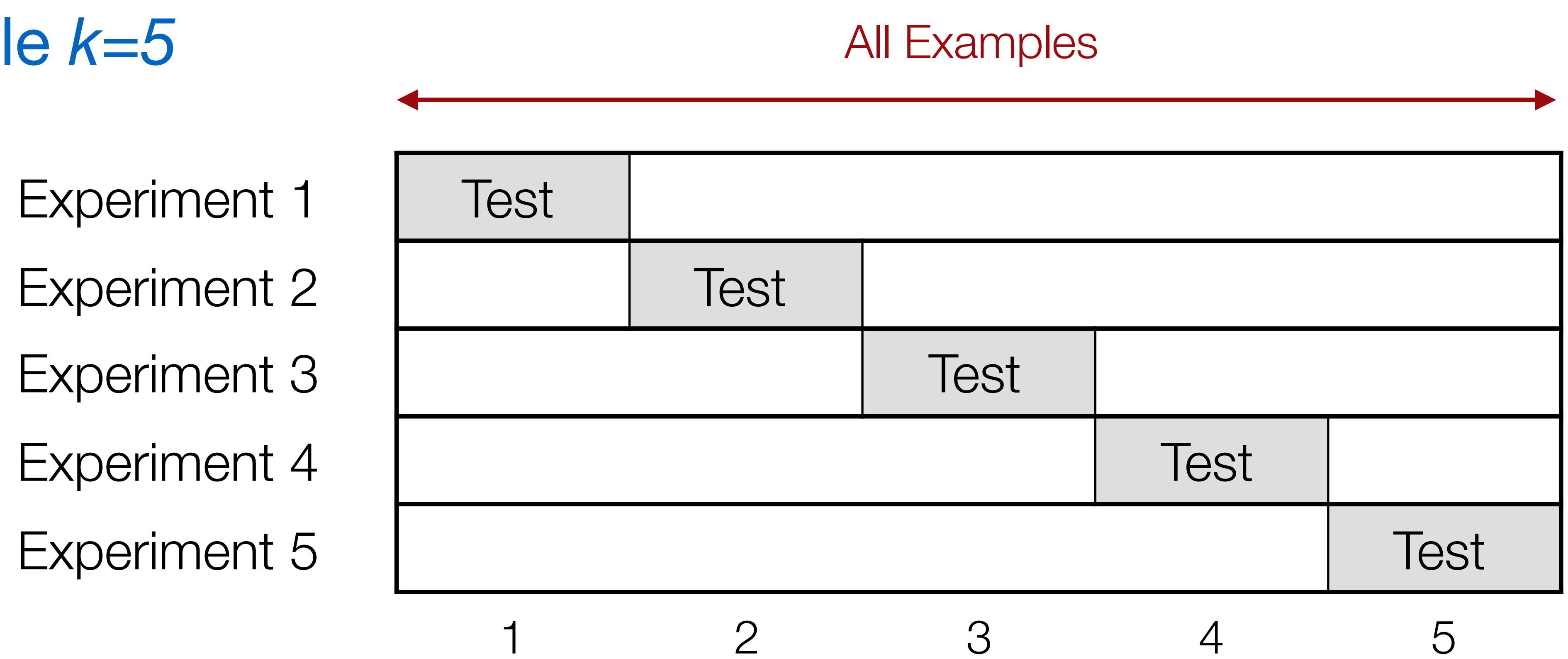


- Sometimes we don't the “luxury” of setting aside data for testing.
- Since it is a single experiment, the hold-out estimate of error rate can be misleading if we get an “unfortunate” split of the data
- Even if we use multiple splits, some examples will never included for training or testing, while others might be selected many times.

Cross Validation

- ***k*-Fold Cross Validation:**
  - Divide the data into *k* disjoint subsets - “folds” (e.g. *k=5* or *10*).
  - For each of *k* experiments, use *k-1* folds for training and the selected one fold for testing.
  - Repeat for all *k* folds, average the accuracy/error rates.

Example *k=5*



Example: Cross Validation

- Number of correct and incorrect predictions made by a spam classifier on 300 emails, when we run 5-fold cross validation.

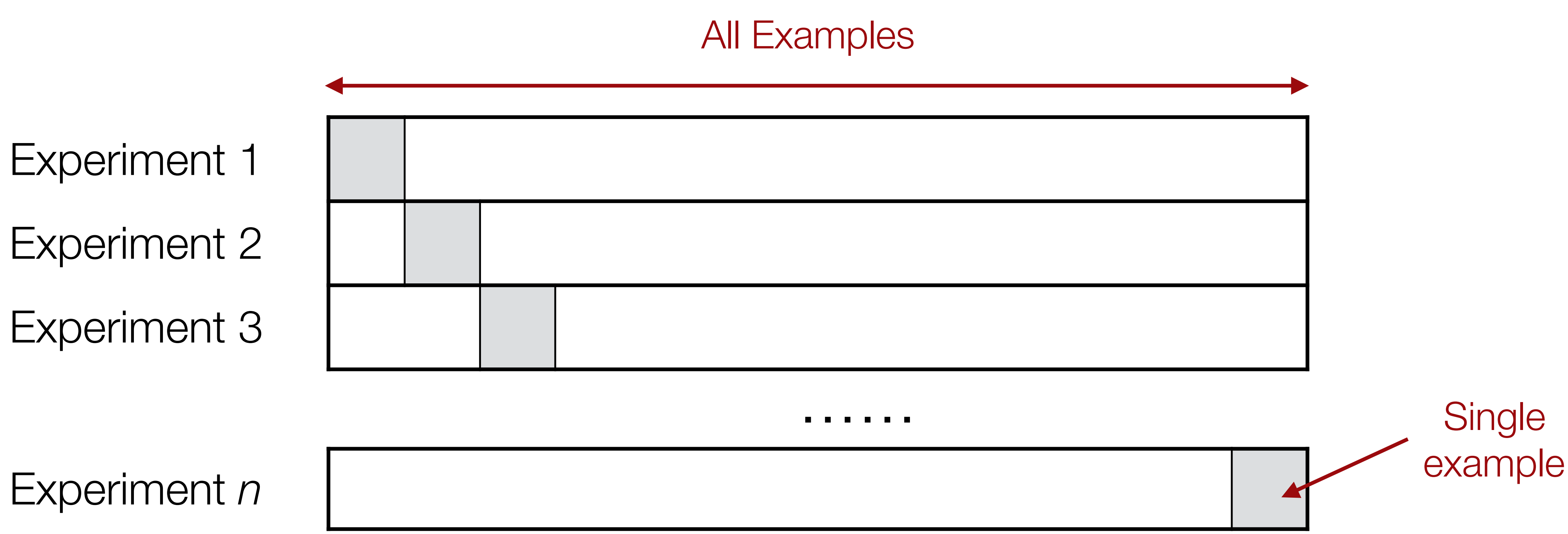
	Class: Non-Spam		**Class: Spam**		
Fold	Correct	Incorrect	Correct	Incorrect	**Accuracy**
1	173	22	87	18	86.67%
2	107	88	71	34	59.33%
3	143	52	80	25	74.33%
4	185	10	59	46	81.33%
5	162	33	71	34	77.67%
Mean	154	41	74	31	**75.87%**

Accuracy for each fold

Average accuracy across all 5 folds

Leave-one-out Cross Validation

- **Leave-one-out:** Extreme case of *k*-Fold Cross Validation where *k* is selected to be the total number of examples in the dataset.
  - For a dataset with *n* examples, perform *n* experiments.
  - For each experiment use *n-1* examples for training and the remaining single example for testing.
  - Average the accuracy/error rates over all *n* experiments.



Experimental Setup

- **Three-Way Hold-Out Strategy:** Divide the full dataset into three different subsets.

  1. Training set: The subset of examples used for learning.
  2. Validation set: The subset of examples used to tune the classifier (e.g. select parameter values).
  3. Test set: The subset of examples used <u>only</u> to assess the performance of a fully-trained classifier.

Training Set (50%)	Validation Set (20%)	Test Set (30%)

Training Set (40%)	Validation Set (20%)	Test Set (40%)

➡ This avoids a bias in evaluation of the model, where reusing examples from the validation set could lead to underestimates of the real error rate.

Comparing Classifiers

- Robust evaluation process: Apply *k*-fold cross validation with a three-way hold-out strategy.

Overall Process

- Divide data set into k folds.
- FOR EACH of the k folds:
  - Create test set T from the k-th fold.
  - Create training set R from the remaining examples.
  - Divide R into R_1 and validation set V.
  - FOR EACH classifer
    - Use V to tune parameters on a model trained with R_1.
    - Use selected parameters to train a model with R.
    - Measure Accuracy on T.
- Collate results, assess significance of differences.

- Significance of proportions of wins and losses across all experiments can be measured statistically (e.g. McNemar's test).
- We can repeat entire process multiple times to further reduce random variance - e.g. 10 x 10-fold cross validation.

References

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