Introduction to Machine Learning part 2

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Outline

- Performance metrics
- Generalisation and overfitting
- Train, validate, test

Performance Metrics: Classification

- True Positives (TP): The class is + and the prediction is +
- True Negatives (TN): The class is - and the prediction is -
- False Positive (FP): The class is - and the prediction is +
- False Negative (FN): The class is + and the prediction is -

Predicted

Actual

	Dog	**Cat**
Dog	TP	FN
Cat	FP	TN

Accuracy

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

$$acc = \frac{n^{\underline{o}}\ \text{correctly classified}}{n}$$

Predicted

		Dog	**Cat**
Actual	**Dog**	TP	FN
	Cat	FP	TN

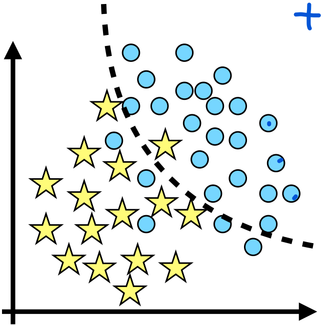
Precision

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

$$\frac{21}{21+1} = \frac{21}{22}$$

Predicted

		Dog	Cat
Actual	Dog	TP	FN
	Cat	FP	TN

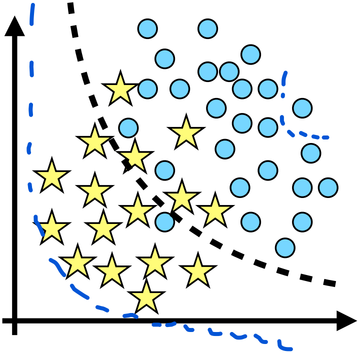


Recall

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

$$\frac{25}{26}$$

		Predicted	
		Dog	**Cat**
Actual	**Dog**	TP	FN
	Cat	FP	TN



F_1-score

The F_1 score is the harmonic mean of precision and recall

$$\begin{aligned} F_1 &= \frac{1}{precision^{-1} + recall^{-1}} \\ &= 2\frac{precision \cdot recall}{precision + recall} \end{aligned}$$

Metrics for more than two classes

$$Accuracy = \frac{\sum_{i=1}^{n} \underline{1}(\underline{y_i} = \underline{f(\vec{x}_i)})}{n} = \frac{\text{Correct class}^{n}}{n}$$

- This is the same as the binary case, even though the equation looks different

Predicted

		Dog	Cat	Bird
Actual	Dog	$\underline{10}$	2	0
	Cat	1	$\underline{5}$	1
	Bird	2	0	$\underline{12}$

$10 + 5 + 12 = 27$

$$acc = \frac{27}{33}$$

Metrics for more than two classes

- Macro-averaging:
  $Precision = \frac{1}{k}\sum_{j=1}^{k} Precision_j \quad Recall = \frac{1}{k}\sum_{j=1}^{k} Recall_j$

		Predicted		
		Dog	**Cat**	**Bird**
Actual	**Dog**	10	2	0
	Cat	1	5	1
	Bird	2	0	12

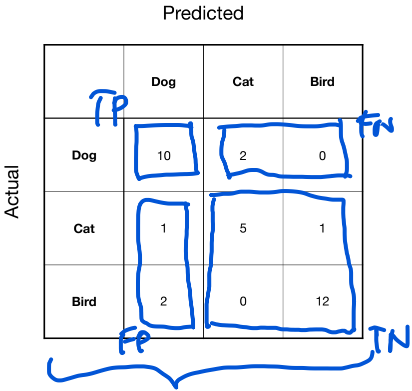
		Predicted		
		Dog	**Cat**	**Bird**
Actual	**Dog**	10	2	0
	Cat	1	5	1
	Bird	2	0	12

$$precision_{dog} = \frac{10}{13}$$

$$Recall_{dog} = \frac{10}{12}$$

Metrics for more than two classes

- Micro-averaging



Predicted

Actual

	Dog	Cat	Bird
Dog	10	2	0
Cat	1	5	1
Bird	2	0	12

Predicted

Actual

	D	**non D**
D	10	2
non D	3	18

Predicted

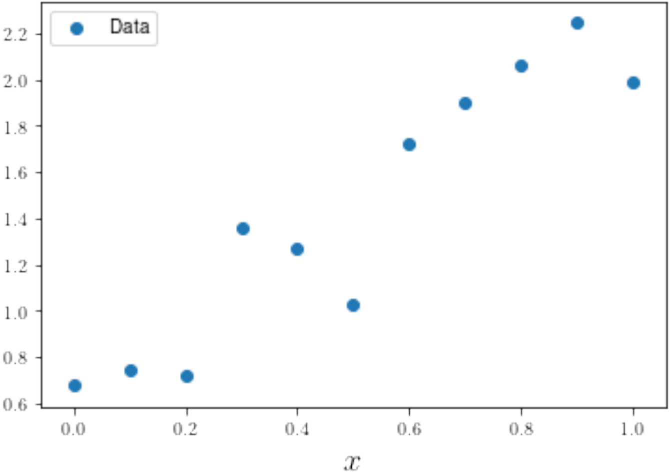
	C	**non C**
C	5	2
non C	2	24

Actual

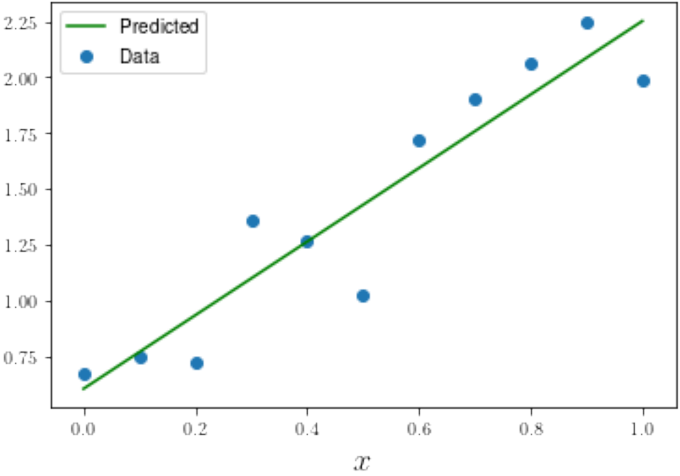
	B	**non B**
B	12	2
non B	1	18

	+	**-**
+	27	6
-	6	60

Performance Metrics: Regression



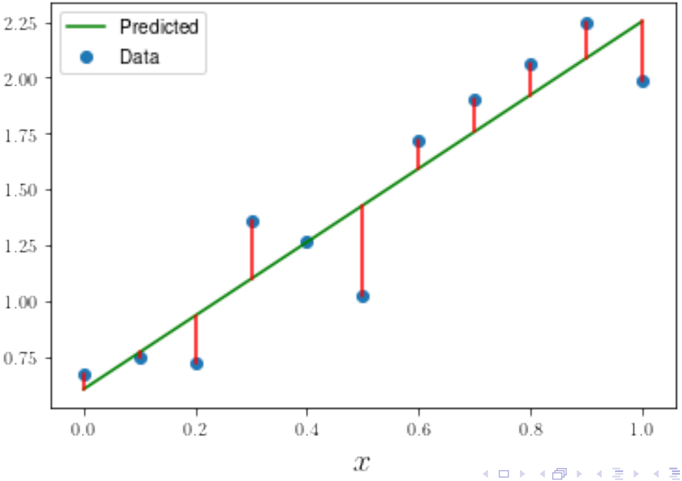
Performance Metrics: Regression



Performance Metrics: Regression

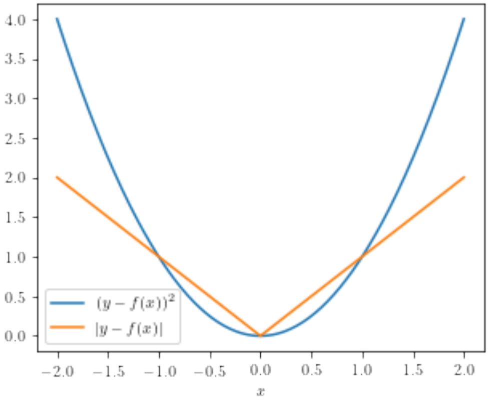
- Mean Squared Error (MSE):

$$\underline{E} = \frac{1}{N} \sum_{(\vec{x},y)} (y - f(\vec{x}))^2$$



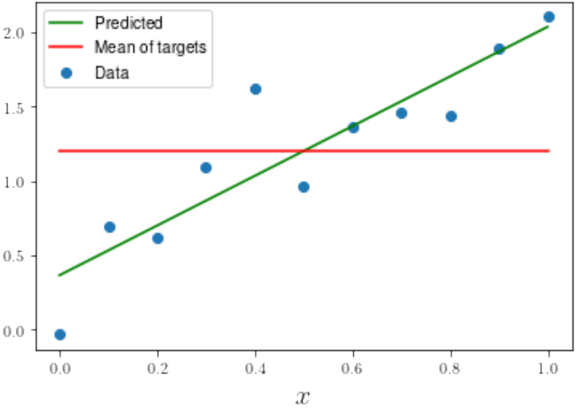
Performance Metrics: Regression

- Root Mean Squared Error (RMSE):
  $E = \sqrt{\frac{1}{N} \sum_{(\vec{x},y)} (y - f(\vec{x}))^2}$
- Mean Absolute Error (MAE): $E = \frac{1}{N} \sum_{(\vec{x},y)} \underline{|y - f(\vec{x})|}$



Performance Metrics: Regression

- $R^2 = 1 - \frac{\sum_{(\vec{x},y)}(y - f(\vec{x}))^2}{\sum_{(\vec{x},y)}(y - \bar{y})^2}$
  where $\bar{y}$ is the mean of the target values y

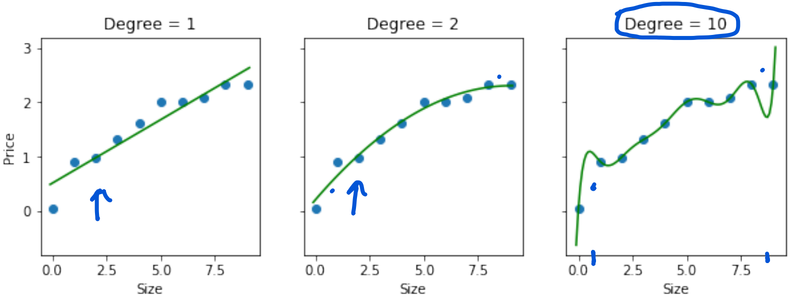


Summary: Performance Metrics

- For classification problems, we can use metrics such as accuracy, precision, recall, or F_1 score.
- These can be used for multi-class problems as well as binary problems
- Mean squared error or absolute error can be used for regression problems
- R^2 is often used for linear regression

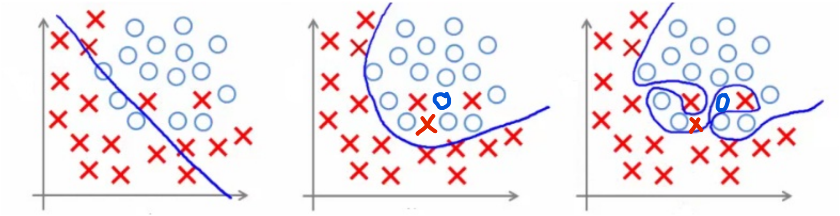
Generalisation

- By fitting an approximation function with a high number of parameters it is possible to obtain very high accuracy for the data on which you train.
- However, this learnt approximation may not then perform well on different, previously unseen, data.
- This is called over-fitting



Over-Fitting in Classification

- For classification problems we must be careful how we model the boundary between different classes in the feature space.



Under-fitting

(too simple to explain the variance)

Appropriate-fitting

Over-fitting

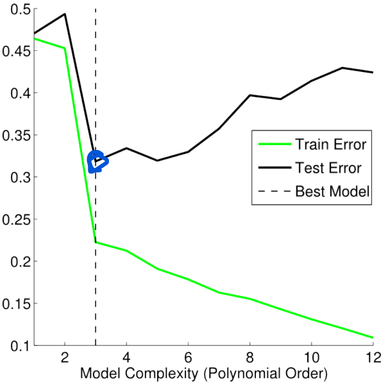
(forcefitting -- too good to be true)

Summary: Generalisation and overfitting

- As well as attaining good scores onour training data, we want our algorithms to generalise well to unseen data
- Both regression and classification problems can overfit to data

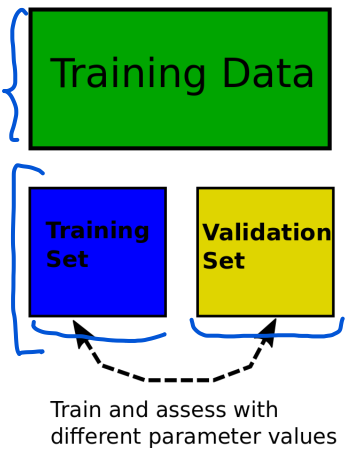
Train and Test Data

- To evaluate the generalisation of a model available data should be divided into training and test sets.



Train, Validation and Test Data

- To fit model parameters the training data is sometimes further divided into train and validation sets.

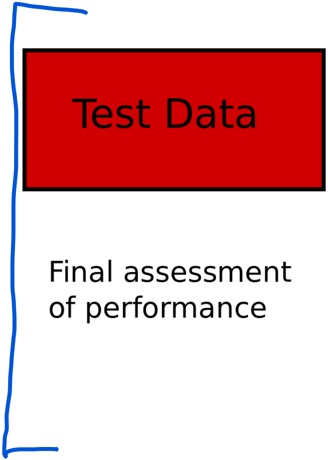


Training Data

Training Set

Validation Set

Train and assess with different parameter values

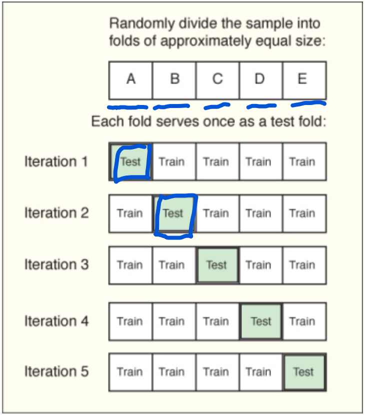


Test Data

Final assessment of performance

n-Folds

- How do you know that you have not just been lucky in your choice of training and test data?
- Answer: Repeat many times with different divisions into training and test.



Randomly divide the sample into folds of approximately equal size:

A	B	C	D	E

Each fold serves once as a test fold:

Iteration 1	Test	Train	Train	Train	Train
Iteration 2	Train	Test	Train	Train	Train
Iteration 3	Train	Train	Test	Train	Train
Iteration 4	Train	Train	Train	Test	Train
Iteration 5	Train	Train	Train	Train	Test

cross-validation can be used with the validation set.

- Splitting data into training and test sets helps ensure that our model can generalise.
- We can further split our training set into training and validation sets, to test the performance of our model on unseen data
- Cross-validation can give a more rounded view of performance

Overall summary

We have looked at:

- Performance metrics
- Generalization and overfitting
- Training and test splits

You can practice working with these concepts in the...

Worksheet

- Available as pdf and also as jupyter notebook
- Covers evaluation metrics, generalisation, overfitting
- If you don't already know Python, please do work through the Introduction to Python available on BlackBoard
- You can ask questions in the lecture or in problem classes

Next time

Simple supervised learning algorithms

- k-Nearest neighbours
- Linear regression
- Naive Bayes classifier