# Classification and Regression: In a Weekend

By
Ajit Jaokar Dan Howarth

With contributions from **Ayse Mutlu** 

## **Contents**

| Introduction and approach                               | 4  |
|---|----|
| Background  | 4  |
| Tools   | 6  |
| Philosophy  | 8  |
| What you will learn from this book?                     | 9  |
| Components for book                                     | 11 |
| Big Picture Diagram                                     | 13 |
| Code outline  | 15 |
| Regression code outline                                 | 15 |
| Classification Code Outline                             | 16 |
| Exploratory data analysis                               | 16 |
| Numeric Descriptive statistics                          | 16 |
| Graphical descriptive statistics                        | 18 |
| Analysing the target variable                           | 22 |
| Pre-processing data                                     | 22 |
| Dealing with missing values                             | 22 |
| Treatment of categorical values                         | 23 |
| Normalise the data                                      | 23 |
| Split the data  | 27 |
| Choose a Baseline algorithm                             |    |
| Defining / instantiating the baseline model             | 30 |
| Fitting the model we have developed to our training set | 30 |

| Define the evaluation metric                                  | 31 |
|---|----|
| Predict scores against our test set and assess how good it is | 33 |
| Evaluation metrics for classification                         | 33 |
| Improving a model – from baseline models to final models      | 38 |
| Understanding cross validation                                | 39 |
| Feature engineering   | 42 |
| Regularization to prevent overfitting                         | 42 |
| Ensembles – typically for classification                      | 45 |
| Test alternative models                                       | 46 |
| Hyperparameter tuning   | 47 |
| Conclusion  | 48 |
| Appendix  | 51 |
| Regression Code   | 51 |
| Classification Code   | 64 |

## Introduction and approach

## **Background**

This book began as a series of weekend workshops created by Ajit Jaokar and Dan Howarth in the "Data Science for Internet of

Things" meetup in London. The idea was to work with a specific (longish) program such that we explore as much of it as possible in one weekend. This book is an attempt to take this idea online. We first experimented on Data Science Central in a small way and continued to expand and learn from our experience. The best way to use this book is to work with the code as much as you can. The code has comments. But you can extend the comments by the concepts explained here. The code is

## Regression

https://colab.research.google.com/drive/14m95e5A3AtzM\_3e7IZLs2dd0M4Gr1y1W

#### Classification

https://colab.research.google.com/drive/1qrj5B5XkI-PkDN-S8XOddlvqOBEggnA9

This document also includes the code in a plain text format in the appendix. The book also includes an online forum where you are free to post questions relating to this book **link of forum** 

## **Community for the book**

https://www.datasciencecentral.com/group/ai-deep-learningmachine-learning-coding-in-a-week

Finally, the book is part of a series. Future books planned in the same style are

"AI as a service: An introduction through Azure in a weekend"
"AI as a service: An introduction through Google Cloud Platform

in a weekend"

## **Tools**

We use <u>Colab</u> from Google. The code should also work on Anaconda. There are four main Python libraries that you should know: numpy, pandas, mathplotlib and sklearn

## **NumPy**

The Python built-in list type does not allow for efficient array manipulation. The NumPy package is concerned with manipulation of multi-dimensional arrays. NumPy is at the foundation of almost all the other packages covering the Data Science aspects of Python.

Classification and Regression: In a Weekend

From a Data Science perspective, collections of Data types like Documents, Images, Sound etc. can be represented as an array of numbers. Hence, the first step in analysing data is to transform data into an array of numbers. NumPy functions are used for transformation and manipulation of data as numbers – especially before the model building stage – but also in the overall process of data science.

#### **Pandas**

The Pandas library in Python provides two data structures: The **DataFrame and the Series** object. The Pandas Series Object is a one-dimensional array of indexed data which can be created from a

list or array. The Pandas DataFrames objects are essentially multidimensional arrays with attached row and column labels. A DataFrame is roughly equivalent to a 'Table' in SQL or a spreadsheet. Through the Pandas library, Python implements a number of powerful data operations similar to database frameworks and spreadsheets. While the NumPy's ndarray data structure provides features for numerical computing tasks, it does not provide flexibility that we see in Tale structures (such as attaching labels to data, working with missing data, etc.). The Pandas library thus provides features for data manipulation tasks.

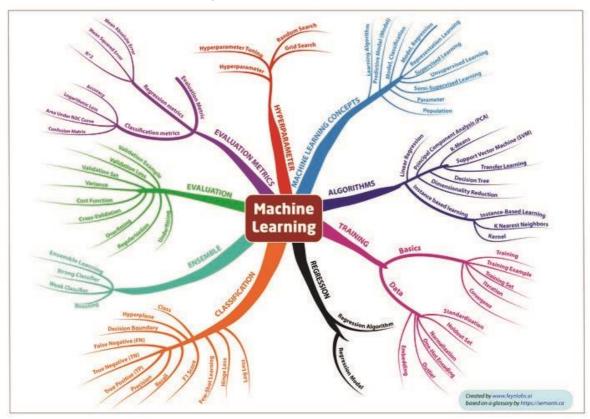
## **Matplotlib**

The Matplotlib library is used for data visualization in Python built on numpy. Matplotlib works with multiple operating systems and graphics backends.

#### Scikit-Learn

The Scikit-Learn package provides efficient implementations of a number of common machine learning algorithms. It also includes modules for cross validation, grid search and feature engineering

Ajit Jaokar – Dan Howarth



(original pdf in attached zip)

## **Philosophy**

The book is based on the philosophy of deliberate practise to learn coding. This concept originated in the old Soviet Union athletes. It is also associated with a diverse range of people including Golf (Ben Hogan), Shaolin Monks, Benjamin Franklin etc. For the purposes of learning coding for machine learning, we apply the following elements of deliberate practice

Classification and Regression: In a Weekend

- Break down key ideas in simple, small steps. In this case, using a mindmap and a glossary
- Work with micro steps
- Keep the big picture in mind

• Encourage reflection/feedback

## What you will learn from this book?

This book covers regression and classification in an end-to-end mode. We first start with explaining specific elements of regression. Then we move to classification where we cover elements of classification which differ (for example evaluation metrics). We then discuss a set of techniques that help to improve a baseline model for both regression and classification.

## Follow me on LinkedIn for more Resources:

https://www.linkedin.com/in/stevenouri/

## **Components for book**

The book comprises of the following components as part of the online zip

## **Regression:**

 $\frac{https://colab.research.google.com/drive/14m95e5A3AtzM\_3e7IZL}{s2dd0M4Gr1y1W}$ 

### **Classification:**

https://colab.research.google.com/drive/1qrj5B5XkI-PkDNS8XOddlvqOBEggnA9

## **Community for book:**

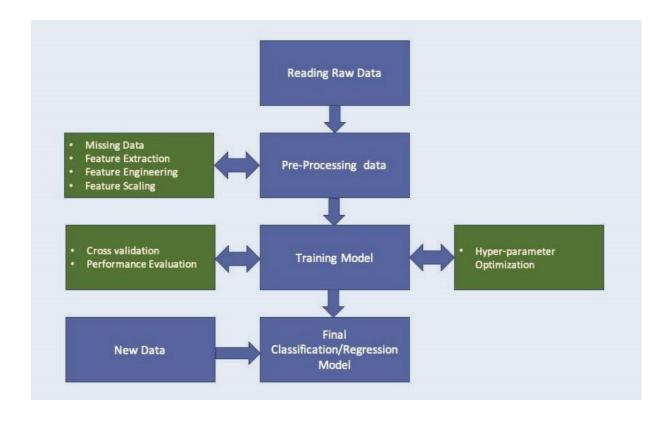
https://www.datasciencecentral.com/group/ai-deep-learningmachine-learning-coding-in-a-week

Glossary: Attached as part of zip also HERE

**Mindmap:** Attached as part of the zip also <u>HERE</u>

## **Big Picture Diagram**

## As below



## **Code outline**

## Regression code outline

https://colab.research.google.com/drive/14m95e5A3AtzM\_3e7IZL s2dd0M4Gr1y1W

The steps for the code are

Load and describe the data

**Exploratory Data Analysis** 

Exploratory data analysis – numerical

Exploratory data analysis - visual

Analyse the target variable

compute the correlation

Pre-process the data

Dealing with missing values

Treatment of categorical values

Remove the outliers

Normalise the data Split

the data

Choose a Baseline algorithm defining /

instantiating the baseline model

fitting the model we have developed to our training set

Define the evaluation metric

predict scores against our test set and assess how good it is

Refine our dataset with additional columns

**Test Alternative Models** 

Choose the best model and optimise its parameters

#### Gridsearch

## **Classification Code Outline**

https://colab.research.google.com/drive/1qrj5B5XkI-PkDNS8XOddlvqOBEggnA9

Load the data
Exploratory data analysis
 Analyse the target variable
 Check if the data is balanced
 Check the co-relations
Split the data
Choose a Baseline algorithm
Train and Test the Model
Choose an evaluation metric
Refine our dataset
Feature engineering
Test Alternative Models
Ensemble models
Choose the best model and optimise its parameters

## **Exploratory data analysis**

## **Numeric Descriptive statistics**

#### Overview

The pandas dataframe structure is a way of storing and operating on tabular data. Pandas has a lot of functionality to assist with exploratory data analysis. describe() provides summary statistics on all numeric columns. describe() function gives descriptive statistics for any numeric columns using describe. For each feature, we can see the 'count', or number of data entries, the 'mean' value, and the 'standard deviation', 'min', 'max' and 'quartile' values. describe() function excludes the character columns. To include both numeric and character columns, we add include='all'. We can also see the shape of the data using the .shape attribute. Keys() method in Python Dictionary, returns a view object that displays a list of all the keys in the dictionary

### **Numeric descriptive statistics**

Standard deviation represents how measurements for a group are spread out from the average (mean). A low standard deviation implies that most of numbers are close to the average. A high standard deviation means that the numbers are spread out. The standard deviation is affected by outliers because the standard deviation is based on the distance from the mean. The mean is also affected by outliers.

## **Interpreting descriptive statistics**

What actions can you take from the output of the describe function at regression problem?

For each feature, we can see the count, or number of data entries, the mean value, and the standard deviation, min, max and quartile values. We can see that the range of values for each feature differs quite a lot, so we can start to think about whether to apply normalization to the data. We can also see that the CHAS feature is either a (1,0) value. If we look back at our description, we can see that this is an example of a categorical variable. These are values

used to describe non-numeric data. In this case, a 1 indicates the house borders near the river, and a 0 that it doesn't.

#### **Source:**

- <a href="http://www.datasciencemadesimple.com/descriptivesummary">http://www.datasciencemadesimple.com/descriptivesummary</a>
   <a href="http://www.datasciencemadesimple.com/descriptivesummary">http://www.datascienc
- <a href="https://pandas.pydata.org/pandas-docs/stable/reference/api/pandas.Series.describe.htmlSource">https://pandas.pydata.org/pandas-docs/stable/reference/api/pandas.Series.describe.htmlSource</a>
- https://www.dataz.io/display/Public/2013/03/20/Describing+ Data%3A+Why+median+and+IQR+are+often+better+ than+mean+and+standard+deviation
- <a href="https://www.quora.com/What-is-the-relation-between-theRange-IQR-and-standard-deviation">https://www.quora.com/What-is-the-relation-between-theRange-IQR-and-standard-deviation</a>

We can build on this analysis by plotting the distribution and boxplots for each column

Classification and Regression: In a Weekend

## **Graphical descriptive statistics**

## Histogram and Boxplots – understanding the distribution

Histograms are used to represent data which is in groups. X-axis represents bin ranges. The Y-axis represents the frequency of the bins. For example, to represent age-wise population in form of graph, then the histogram represents the number of people in age buckets. The bins parameter represents the number of buckets that your data will be divided into. You can specify it as an integer or as a list of bin edges. Interpretation of histograms and box plots and the action taken from it A 'histogram' tells is the number of times, or frequency, a value occurs within a 'bin', or bucket, that splits the data (and which we defined). A histogram shows the frequency with

which values occur within each of these bins, and can tell us about the distribution of data. A 'boxplot' captures within the box the 'interquartile range', the range of values from Q1/25th percentile to Q3/75th percentile, and the median value. It also captures the 'min' and 'max' values of each feature. Together, these charts show us the distribution of values for each feature. We can start to make judgements about how to treat the data, for example whether we want to deal with outliers; or whether we want to normalize the data. The subplot is a utility wrapper that makes it convenient to create common layouts in a single call.

#### **References:**

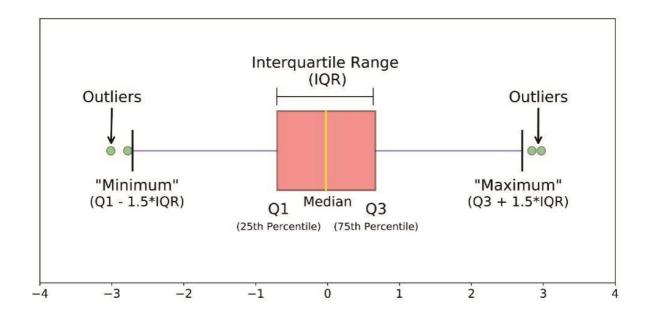
https://matplotlib.org/api/pyplot\_api.html#matplotlib.pyplot.subplots

https://towardsdatascience.com/understandingboxplots5e2df7bcbd51

## **Boxplots and IQR**

An alternative to mean and standard deviation are median and interquartile range (IQR). IQR is the difference between the third and first quartiles (75th and 25th quantiles). IQR is often reported using the "five-number summary," which includes: minimum, first quartile, median, third quartile and maximum. IQR tells you where the middle 50% of the data is located while Standard Deviation tells you about the spread of the data. Median and IQR measure the central tendency and spread, respectively, but are robust against outliers and non-normal data. IQR makes outlier identification easy to do an initial estimate of outliers by looking at values more than one-and-a-half times the IQR distance below the first quartile or

above the third quartile. Skewness: Comparing the median to the quartile values shows whether data is skewed.



https://towardsdatascience.com/understandingboxplots-5e2df7bcbd51?gi=730efa1b7da5

Classification and Regression: In a Weekend

#### Correlation

Correlation is a statistical measure that describes the association between random variables. There are several methods for calculating the correlation coefficient, each measuring different types of strength of association. Correlation values range between - 1 and 1. Pandas dataframe.corr() gives the pairwise correlation of all columns in the dataframe. Three of the most widely used methods.

- 1. Pearson Correlation Coefficient
- 2. Spearman's Correlation
- 3. Kendall's Tau

**Pearson** is the most widely used correlation coefficient. Pearson correlation measures the linear association between continuous variables. In other words, this coefficient quantifies the degree to

which a relationship between two variables can be described by a line.

$$r = \frac{Covariance(x,y)}{S.D.(x)S.D.(y)}$$

$$r = \frac{n\sum xy - (\sum x)(\sum y)}{\sqrt{[n\sum x^2 - (\sum x)^2][n\sum y^2 - (\sum y)^2]}}$$

In this formulation, raw observations are centered by subtracting their means and re-scaled by a measure of standard deviations.

#### Source:

- <a href="https://www.datascience.com/blog/introduction-tocorrelation-learn-data-science-tutorials">https://www.datascience.com/blog/introduction-tocorrelation-learn-data-science-tutorials</a>
- https://www.geeksforgeeks.org/python-pandasdataframecorr/

## heatmaps for co-relation

A heatmap is a two-dimensional graphical representation of data where the individual values are represented as colors. The seaborn python package enables the creation of annotated heatmaps. This heat map works by correlation. This shows you which variables are correlated to each other from a scale of 1 being the most correlated and -1 is not correlated at all. However, you cannot correlate strings. You can only correlate numerical features.

Range from -1 to 1:

- +1.00 means perfect positive relationship (Both variables are moving in the same direction) 0.00 means no relationship
- -1.00 means perfect negative relationship (As one variable increases the other decreases) **Source:**
- https://seaborn.pydata.org/generated/seaborn.heatmap.html
- <a href="https://statisticsbyjim.com/basics/correlations/">https://statisticsbyjim.com/basics/correlations/</a> Source:
- <a href="https://www.datascience.com/blog/introduction-tocorrelation-learn-data-science-tutorials">https://www.datascience.com/blog/introduction-tocorrelation-learn-data-science-tutorials</a>

## Analysing the target variable

There are a number of ways to analyse the target variable we can plot a histogram using binning to find the grouping of the house prices we can plot a boxplot of the target variable we can do is plot a boxplot of one variable against the target variable we can extend the analysis by creating a heatmap this shows the correlation between the features and target

## **Pre-processing data**

## **Dealing with missing values**

Dealing with missing values, where we identify what, if, any missing data we have and how to deal with it. For example, we may replace missing values with the mean value for that feature, or by the average of the neighbouring values. pandas' has a number of

options for filling in missing data that is worth exploring. We can also use `k-nearest neighbour`to help us predict what the missing values should be, or `sklearn Imputer` function (amongst other ways)

## **Treatment of categorical values**

Treat categorical values, by converting them into a numerical representation that can be modelled. There are a number of different ways to do this in 'sklearn' and 'pandas'

### Normalise the data

The terms normalization and standardization are sometimes used interchangeably, but they usually refer to different things. Normalization usually means to scale a variable to have a value between 0 and 1, while standardization transforms data to have a mean of zero and a standard deviation of 1. (source: statisticshowto). Rescaling data in this way is a common pre-processing task in machine learning because many of algorithms assume that all features are on the same scale, typically 0 to 1 or -1 to 1. We need to rescale the values of numerical feature to be between two values. We have several methods to do that. In skicit learn, the commonly used methods are MinMaxScaler and StandardScaler.

**MinMaxScaler:** Normalization shrinks the range of the data such that the range is fixed between 0 and 1. It works better for cases in which the standardization might not work so well. If the distribution is not Gaussian or the standard deviation is very small, the min-max

scaler works better. Normalization makes training less sensitive to the scale of features, so we can better solve for coefficients.

Normalization is typically done via the following equation:

$$z = \frac{x - \min(x)}{\max(x) - \min(x)}$$

**The StandardScaler:** Standardization is used to transform the data such that it has a mean of 0 and a standard deviation of 1. Specifically, each element in the feature is transformed. The mean and standard deviation are separately calculated for the feature, and the feature is then scaled based on:

$$\frac{x_i - mean(x)}{stdev(x)}$$

Classification and Regression: In a Weekend

#### Source:

- <a href="https://www.statisticshowto.datasciencecentral.com/normalized/">https://www.statisticshowto.datasciencecentral.com/normalized/</a>
- <a href="https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.StandardScaler.html">https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.StandardScaler.html</a>
- <u>https://datascience.stackexchange.com/questions/12321/difference-between-fit-and-fit-transform-in-scikit-learn-models</u>
- <a href="https://medium.com/@zaidalissa/standardization-vsnormalization-da7a3a308c64">https://medium.com/@zaidalissa/standardization-vsnormalization-da7a3a308c64</a>
- <a href="https://pandas.pydata.org/pandas-docs/stable/reference/api/pandas.DataFrame.drop.html">https://pandas.pydata.org/pandas-docs/stable/reference/api/pandas.DataFrame.drop.html</a>
- <a href="https://docs.scipy.org/doc/numpy/reference/generated/numpy.ravel.html">https://docs.scipy.org/doc/numpy/reference/generated/numpy.ravel.html</a>

- https://jovianlin.io/feature-scaling/
- <a href="https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.StandardScaler.html">https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.StandardScaler.html</a>
- https://jovianlin.io/feature-scaling/
- <a href="https://scikitlearn.org/stable/modules/generated/sklearn.pre">https://scikitlearn.org/stable/modules/generated/sklearn.pre</a>
  <a href="processing.StandardScaler.html">processing.StandardScaler.html</a>
- <a href="https://scikitlearn.org/stable/modules/generated/sklearn.pre">https://scikitlearn.org/stable/modules/generated/sklearn.pre</a>
  <a href="processing.StandardScaler.html">processing.StandardScaler.html</a>
- <a href="https://datascience.stackexchange.com/questions/12321/diffe">https://datascience.stackexchange.com/questions/12321/diffe</a> rence-between-fit-and-fit-transform-in-scikit-learn-models
- <a href="https://medium.com/@zaidalissa/standardization-vsnormalization-da7a3a308c64">https://medium.com/@zaidalissa/standardization-vsnormalization-da7a3a308c64</a>

## Follow me on LinkedIn for more Resources:

https://www.linkedin.com/in/stevenouri/

## Split the data

Training: This data is used to build your model. E.g. finding the optimal coefficients in a Linear Regression model; or using the CART algorithm to create a Decision Tree. **Testing:** This data is used to see how the model performs on unseen data, as it would in a real-world situation. This data should be left completely unseen until you would like to test your model to evaluate performance.

Model Selection contains 4 groups of lists. You can check the links (<a href="https://scikit-learn.org/stable/modules/classes.html#module-sklearn.model\_selection">https://scikit-learn.org/stable/modules/classes.html#module-sklearn.model\_selection</a>) for details. Splitter Classes, Splitter Functions, Hyper-parameter optimizers and Model validation. The module is mainly used for splitting the dataset. It includes 14 different classes and two functions for that purpose. It also provides some functions for model validation and hyper-parameter optimization.

#### Source

https://scikit-learn.org/stable/modules/generated/ sklearn.model\_selection.ShuffleSplit.html#sklearn.model\_selection.ShuffleSplit

## **Choose a Baseline algorithm**

## Defining / instantiating the baseline model

A baseline is a method that uses heuristics, simple summary statistics, randomness, or machine learning to create predictions for a dataset. You can use these predictions to measure the baseline's performance (e.g., accuracy). This metric will then become what you compare any other machine learning algorithm against. For example, your algorithm may be 75% accurate. You would want your 75% accuracy to be higher than any baseline you have run on the same data.

#### Source:

https://datascience.stackexchange.com/questions/30912/whatdoes-baseline-mean-in-the-context-of-machine-learning

## Fitting the model we have developed to our training set

Linear models are among the oldest and most interpretable modelling methods. A linear model uses a linear function to map a set of values to a set of normal distributions. Linear models are widely useful because the normal distribution occurs frequently in the natural world and any continuous function can be approximated well with a straight line over a short distance.

Fitting your model to (i.e. using the fit() method on the training data is the training part of the modelling process. After it is trained, the model can be used to make predictions, with a predict() method call. Model fitting is a procedure that takes three steps:

- 1. First you need a function that takes in a set of parameters and returns a predicted data set.
- 2. Second you need an 'error function' that provides a number representing the difference between your data and the model's prediction for any given set of model parameters. This is usually either the sums of squared error (SSE) or maximum likelihood.
- 3. Third you need to find the parameters that minimize this difference.

#### Source:

https://courses.washington.edu/matlab1/ModelFitting.html http://garrettgman.github.io/model-fitting/ **Source:** https://courses.washington.edu/matlab1/ModelFitting.html

## Define the evaluation metric

The most commonly used metric for regression tasks is RMSE (root-mean-square error). This is defined as the square root of the average squared distance between the actual score and the predicted score:

Classification and Regression: In a Weekend

$$\text{RMSE} = \sqrt{\frac{\sum_{i} (y_i - \hat{y}_i)^2}{n}}$$

Here, yi denotes the true score for the ith data point, and yi denotes the predicted value. One intuitive way to understand this formula is that it is the Euclidean distance between the vector of the true scores and the vector of the predicted scores, averaged by n, where n is the number of data points.

**Mean Squared Error** is difference between of the estimated values and what you get as a result. The predicted value is based on some equation and tell what you will expect as an average but the result you get might differ from this prediction which is a slight error from the estimated value. This difference is called MSE. This determines how good is the estimation based on your equation.

Mean Absolute Error is the measure of the difference between the two continuous variables. The MAE is the average vertical distance between each actual value and the line that best matches the data. MAE is also the average horizontal distance between each data point and the best matching line.

**R^2** is (coefficient of determination) regression score function. It is also called as coefficient of determination. R<sup>2</sup> gives us a measure of how well the actual outcomes are replicated by the model or the regression line. This is based on the total variation of prediction explained by the model. R<sup>2</sup> is always between 0 and 1 or between 0% to 100%.

| Mean squared error             | MSE  | -              | $\frac{1}{n} \sum_{t=1}^{n} e_t^2$                              |
|--------------------------------|------|----------------|---|
| Root mean squared error        | RMSE | =              | $\sqrt{\frac{1}{n}\sum_{t=1}^{n}e_t^2}$                         |
| Mean absolute error            | MAE  | 05 <b>—</b> 28 | $\frac{1}{n}\sum_{t=1}^{n} e_t $                                |
| Mean absolute percentage error | MAPE | =              | $\frac{100\%}{n} \sum_{t=1}^{n} \left  \frac{e_t}{y_t} \right $ |

#### **Source:**

- <a href="https://stats.stackexchange.com/questions/131267/how-tointerpret-error-measures">https://stats.stackexchange.com/questions/131267/how-tointerpret-error-measures</a>
- <a href="https://stats.stackexchange.com/questions/118/why-squarethe-difference-instead-of-taking-the-absolute-value-instandard-devia">https://stats.stackexchange.com/questions/118/why-squarethe-difference-instead-of-taking-the-absolute-value-instandard-devia</a>

## Predict scores against our test set and assess how good it is

as above

## **Evaluation metrics for classification**

Previously, we considered evaluation metrics for Regression. In this section, we consider the evaluation metrics for Classification.

Evaluating the performance of a machine learning model is a fundamental requirement. Essentially, we are exploring two questions: How can I measure the success of this algorithm and when do I know that I have succeeded i.e. should not improve the algorithm more. Different machine learning algorithms have varying evaluation metrics. We have seen evaluation metrics for regression — we now explore the evaluation metrics for classification

For classification, the most common metric is **Accuracy**. Accuracy simply measures how often the classifier makes the correct prediction. It's the ratio between the number of correct predictions and the total number of predictions

While accuracy is easy to understand, the accuracy metric is not suited for unbalanced classes. Hence, we also need to explore other metrics for classification. A **confusion matrix** is a structure to represent classification and it forms the basis of many classification metrics.

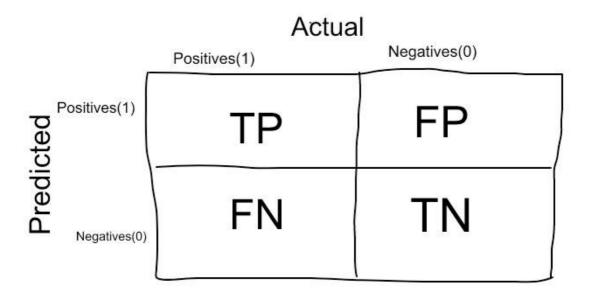


Image source: thalus-ai

There are 4 important terms:

True Positives: The cases in which we predicted YES and the actual output was also YES.

True Negatives: The cases in which we predicted NO and the actual output was NO.

False Positives: The cases in which we predicted YES and the actual output was NO.

False Negatives: The cases in which we predicted NO and the actual output was YES.

Accuracy for the matrix can be calculated by taking average of the values lying across the "main diagonal" i.e.

$$Accuracy = \frac{TruePositives \dotplus FalseNegatives}{TotalNumber of Samples}$$

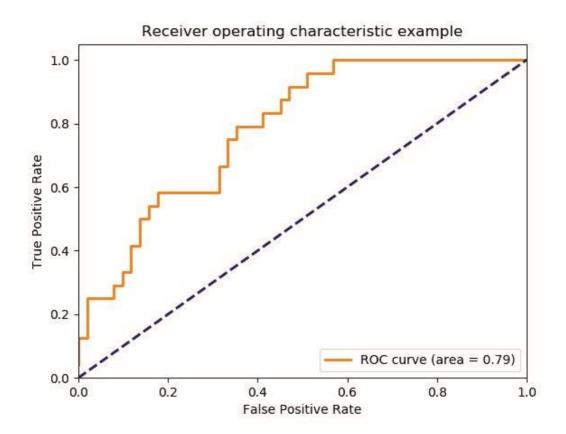
Classification and Regression: In a Weekend

#### **Area Under Curve**

One of the widely used metrics for binary classification is the **Area Under Curve(AUC)** AUC represents the probability that the classifier will rank a randomly chosen positive example higher than a randomly chosen negative example. The AUC is based on a plot of the false positive rate vs the true positive rate which are defined as:

$$TruePositiveRate = rac{TruePositive}{FalseNegative + TruePositive}$$
 
$$FalsePositiveRate = rac{FalsePositive}{FalsePositive + TrueNegative}$$

The area under the curve represents the area under the curve when the false positive rate is plotted against the True positive rate as below.



AUC has a range of [0, 1]. The greater the value, the better is the performance of the model because the closer the curve is towards the True positive rate. The AUC shows the correct positive classifications can be gained as a trade-off between more false positives. The advantage of considering the AUC i.e. the area under a curve .. as opposed to the whole curve is that – it is easier to compare the area (a number) with other similar scenarios. Another metric commonly used is Precision-Recall. The Precision metric represents "Out of the items that the classifier predicted to be relevant, how many are truly relevant? The recall answers the question, "Out of all the items that are truly relevant, how many are found by the ranker/classifier?". Similar to the AUC, we need a numeric value to compare similar scenarios. A single number that combines the precision and recall is the F1 score which is represented by the harmonic mean of the precision and recall.

$$F_1 = 2 \frac{\text{precision*recall}}{\text{precision} + \text{recall}}$$

For unbalanced classes and outliers, we need other considerations which are explained <u>HERE</u>

#### Source:

- 1. Evaluating machine learning models by Alice Zheng <a href="https://www.oreilly.com/ideas/evaluating-machine-learningmodels">https://www.oreilly.com/ideas/evaluating-machine-learningmodels</a>
- 2. <a href="https://towardsdatascience.com/metrics-to-evaluate-yourmachine-learning-algorithm-f10ba6e38234">https://towardsdatascience.com/metrics-to-evaluate-yourmachine-learning-algorithm-f10ba6e38234</a>
- 3. <a href="https://medium.com/thalus-ai/performance-metrics-forclassification-problems-in-machine-learning-part-ib085d432082b">https://medium.com/thalus-ai/performance-metrics-forclassification-problems-in-machine-learning-part-ib085d432082b</a>

# Improving a model – from baseline models to final models

Once we have a baseline model, we can enhance it further. There are a number of steps we could take to achieve this. The baseline model represents the simplest possible prediction. From this point on, you employ a series of techniques to improve the algorithm evaluation metrics. The baseline may be a poor result but it should be seen as a starting point for improvement.

In this document, the strategies we use to improve the baseline model are:

- a) Feature engineering by adding extra columns and trying to understand if it improves the model
- b) Regularization to prevent overfitting
- c) Ensembles typically for classification
- d) Test alternative models
- e) Hyperparameter tuning

### **References:**

https://machinelearningmastery.com/how-to-get-baseline-resultsand-why-they-matter/

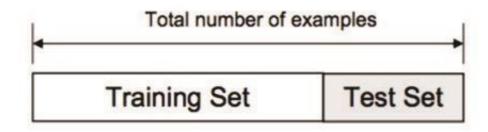
# **Understanding cross validation**

Cross validation is a technique commonly used In Data Science. Most people think that it plays a small part in the data science pipeline, i.e. while training the model. However, it has a broader application in model selection and hyperparameter tuning.

Let us first explore the process of cross validation itself and then see how it applies to different parts of the data science pipeline.

Cross-validation is a resampling procedure used to evaluate machine learning models on a limited data sample. In **k-fold cross-validation**, the original sample is randomly partitioned into **k** equal sized subsamples. Of the **k** subsamples, a single subsample is retained as the **validation** data for testing the model, and the remaining  $\mathbf{k} - 1$  subsamples are used as training data.

In the model training phase, Cross-validation is primarily used in applied machine learning to estimate the skill of a machine learning model on unseen data to overcome situations like overfitting. The choice of k is usually 5 or 10, but there is no formal rule. Cross validation is implemented through KFold() scikit-learn class. Taken to one extreme, for k = 1, we get a single train/test split is created to evaluate the model. There are also other forms of cross validation ex stratified cross validation



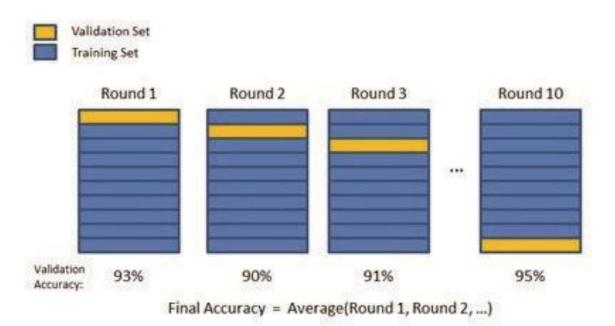


Image source

https://towardsdatascience.com/cross-validation-70289113a072

Now, let's recap the end to end steps for classification based on <u>THIS classification code</u> which we use in the <u>learn machinelearning coding basics in a weekend</u>

## Classification code outline

Load the data

Exploratory data analysis Analyse

the target variable

Check if the data is balanced

Check the co-relations Split

the data

Choose a Baseline algorithm

Train and Test the Model

Choose an evaluation metric

Refine our dataset

Feature engineering

**Test Alternative Models** 

Ensemble models

Choose the best model and optimise its parameters

In this context, we outline below two more cases where we can use cross validation

- 1. In choice of alternate models and
- 2. In hyperparameter tuning we explain these below

## 1) Choosing alternate models:

If we have two models, and we want to see which one is better, we can use cross validation to compare the two for a given dataset. For the code listed above, this is shown in the following section.

```
"""### Test Alternative Models
logistic = LogisticRegression()
cross_val_score(logistic, X, y, cv=5, scoring="accuracy").mean()
rnd_clf = RandomForestClassifier()
cross_val_score(rnd_clf, X, y, cv=5, scoring="accuracy").mean()
```

## 2) hyperparameter tuning

Finally, cross validation is also used in hyperparameter tuning As per cross validation parameter tuning grid search

"In machine learning, two tasks are commonly done at the same time in data pipelines: cross validation and (hyper)parameter tuning. Cross validation is the process of training learners using one set of data and testing it using a different set. Parameter tuning is the process to selecting the values for a model's parameters that maximize the accuracy of the model."

So, to conclude, cross validation is a technique used in multiple parts of the data science pipeline

## **Feature engineering**

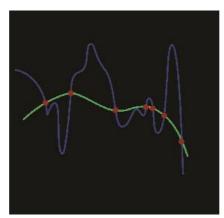
Feature engineering is a key part of the machine learning pipeline. We refine our dataset with additional columns with the objective that some combination of features better represents the problems space and so is an indicator of the target variable. we are using pandas functionality to add a new column called LSTAT 2, which will square of LSTAT feature values that the are values boston\_X['LSTAT\_2'] = boston\_X['LSTAT'].map(lambda x: x\*\*2) we can now run the same code as before on our refined dataset to see if things have improved

```
lm.fit(X_train, Y_train)
Y_pred = lm.predict(X_test)
evaluate(Y_test, Y_pred)
```

lambda operator or lambda function is used for creating small, onetime and anonymous function objects in Python.

# Regularization to prevent overfitting

In machine learning, regularization is the process of adding information in order to solve an ill-posed problem or to prevent overfitting. Regularization applies to objective functions in ill-posed optimization problems. It can be depicted as below.



https://en.wikipedia.org/wiki/Regularization (mathematics)

The green and blue functions both incur zero loss on the given data points. A learned model can be induced to prefer the green function, which may generalize better to more points drawn from the underlying unknown distribution, by adjusting lambda, the weight of the regularization term.

A regularization term R(f) is added to a loss function:

$$\min_{f} \sum_{i=1}^{n} V(f(x_i), y_i) + \lambda R(f)$$

where V is an underlying loss function that describes the cost of predicting f(x) when the label is y.  $^{\lambda}$  is a parameter which controls the importance of the regularization term. The regularization function is typically chosen to impose a penalty on the complexity of f(x). A theoretical justification for regularization is that it attempts to impose Occam's razor (i.e. the simplest feasible solution) (as depicted in the figure above, where the green function, the simpler one, may be preferred). From a Bayesian point of view, many regularization techniques correspond to imposing certain prior

distributions on model parameters. Regularization helps in avoiding overfitting and also increasing model interpretability.

Regularization, significantly reduces the variance of the model, without substantial increase in its bias. So, the tuning parameter  $\lambda$ , used in the regularization techniques described above, controls the impact on bias and variance. As the value of  $\lambda$  rises, it reduces the value of coefficients and thus reducing the variance.

Regularization is particularly important in deep learning where we have a large number of parameters to optimise. Ian Goodfellow describes regularization as "any modification we make to the learning algorithm that is intended to reduce the generalization error, but not its training error".

Generalization in machine learning refers to how well the concepts learned by the model apply to examples which were not seen during training. The goal of most machine learning models is to generalize well from the training data, in order to make good predictions in the future for unseen data. Overfitting happens when the models learns too well the details and the noise from training data, but it doesn't generalize well, so the performance is poor for testing data. A number of regularization techniques are used in deep learning including Dataset augmentation, Early stopping, Dropout layer, Weight penalty L1 and L2

## **Sources:**

https://towardsdatascience.com/regularization-an-

importantconcept-in-machine-learning-5891628907ea

https://chatbotslife.com/regularization-in-deep-

learningf649a45d6e0

https://en.wikipedia.org/wiki/Regularization\_(mathematics)

# **Ensembles – typically for classification**

What is ensemble learning?

Ensemble learning is a machine learning paradigm where multiple models (often called "weak learners") are trained to solve the same problem and combined to get better results. The main hypothesis is that when weak models are correctly combined we can obtain more accurate and/or robust models.

Then, the idea of ensemble methods is to try reducing bias and/or variance of such weak learners by combining several of them together in order to create a strong learner (or ensemble model) that achieves better performances.

In order to set up an ensemble learning method, we first need to select our base models to be aggregated. One important point is that our choice of weak learners should be coherent with the way we aggregate these models. If we choose base models with low bias but high variance, it should be with an aggregating method that tends to reduce variance whereas if we choose base models with low variance but high bias, it should be with an aggregating method that tends to reduce bias.

There are three major kinds of meta-algorithms that aims at combining weak learners:

**bagging**, that often considers homogeneous weak learners, learns them independently from each other in parallel and combines them following some kind of deterministic averaging process

**boosting**, that often considers homogeneous weak learners, learns them sequentially in an adaptive way (a base model depends on the

previous ones) and combines them following a deterministic strategy

**stacking**, that often considers heterogeneous weak learners, learns them in parallel and combines them by training a meta-model to output a prediction based on the different weak models predictions

Weak learners can be combined to get a model with better performances. The way to combine base models should be adapted to their types. Low bias and high variance weak models should be combined in a way that makes the strong model more robust whereas low variance and high bias base models better be combined in a way that makes the ensemble model less biased.

#### **Source:**

https://towardsdatascience.com/ensemble-methods-baggingboosting-and-stacking-c9214a10a205

## **Test alternative models**

As per the section on cross validation, if we have two models, and we want to see which one is better, we can use cross validation to compare the two for a given dataset. For the code listed above, this is shown in the following section.

```
"""### Test Alternative Models logistic
= LogisticRegression()
cross_val_score(logistic, X, y, cv=5,
scoring="accuracy").mean() rnd_clf =
RandomForestClassifier()
cross_val_score(rnd_clf, X, y, cv=5,
scoring="accuracy").mean()
```

# Hyperparameter tuning

In this section, we introduce Hyperparameters and how they determine a model's performance. The process of learning Parameters involves taking the input data and using a function to generate a model. In this case, the model parameters tell how to transform input data into desired output whereas, hyperparameters of the model are used to determine the structure of the model itself. The performance of the model depends heavily on the hyperparameter values selected. The goal of hyperparameter tuning is to search across various hyperparameter configurations to find a configuration that will result in the best performance. Hyperparameters help answer questions like: the depth of the decision tree or how many layers should a neural network have etc. There are mainly three methods to perform hyperparameter tuning: Grid search, Random search and Bayesian optimisation

#### **Source:**

https://www.analyticsindiamag.com/what-are-hyperparametersand-how-do-they-determine-a-models-performance/

https://towardsdatascience.com/hyperparameter-tuning-therandom-forest-in-python-using-scikit-learn-28d2aa77dd74

# **Conclusion**

We hope you have learnt from this book. Please post your comments at Community for the book:

https://www.datasciencecentral.com/group/ai-deep-learningmachine-learning-coding-in-a-week

# Follow me on LinkedIn for more Resources:

https://www.linkedin.com/in/stevenouri/

# **Appendix**

In this section, the code is provided in a python text format based on a .py file exported and simplified from colab

## **Regression Code**

import pandas as pd import

```
numpy as np import
matplotlib.pyplot as plt
import seaborn as sns
# rather than importing the whole sklearn library,
we will import certain modules
from sklearn.linear model import LinearRegression
from sklearn.ensemble import RandomForestRegressor
from sklearn.datasets import load boston from
sklearn import model selection from
sklearn.preprocessing import StandardScaler
from sklearn import metrics
# we load the dataset and save it as the variable
boston
boston = load boston()
# if we want to know what sort of detail is
provided with this dataset, we can call .keys()
boston.keys()
```

# the info at the .DESCR key will tell us more
print(boston.DESCR)
# we can use pandas
to create a
dataframe, which is
basically a way of
storing and
operating on tabular
data
# here we pass in both the data and the column
names as variables
boston\_X = pd.DataFrame(boston.data, columns =
boston.feature\_names)
# we can then look at the top of the dataframe to

# we can then look at the top of the dataframe to see the sort of values it contains boston\_X.head()

# pandas has a lot of functionality to assist with
exploratory data analysis
# .describe() provide summary statistics on all
numeric columns
print(boston X.describe())

# we can also see the shape of the data
print(boston X.shape)

"""\* For each feature, we can see the `count`, or number of data entries, the `mean` value, and the `standard deviation`, `min`, `max` and `quartile` values.

- \* We can see that the range of values for each feature differs quite a lot, so we can start to think about whether to apply normalization to the data.
- \* We can also see that the `CHAS` faeture is either

a (1,0) value. If we look back at our description, we can see that this is an example of a `categorical` variable. These are values used to describe non-numeric data. In this case, a `1` indicates the house borders near the river, and a `0` that it doesn't.

# we can build on this analysis by plotting the distribution and boxplots for each column

# we loop through all the columns for col in boston X.columns:

# and for each column we create space for one row with 2 charts

f, axes = plt.subplots(1, 2, figsize=(12, 6)) # our first chart is a histogram and we set the title

boston X[col].hist(bins = 30, ax = axes[0]) axes[0].set title('Distribution of '+ col)

# our second column is the boxplot boston X.boxplot(column =  $col_{,}$  ax = axes[1]) # we then use this to command to display the charts plt.show()

"""\* A `histogram` tells is the number of times, or frequency, a value occurs within a `bin`, or bucket, that splits the data (and which we defined). A histogram shows the frequency with which values occur within each of these bins, and can tell us about the distribution of data. \* A `boxplot` captures within the box the `interquartile range`, the range of values from Q1/25th percentile to Q3/75th percentile, and the median value. It also captures the `min` and `max` values of each feature.

\* Together, these charts show us the distribution

of values for each feature. We can start to make judgements about how to treat the data, for example whether we want to deal with outliers; or whether we want to normalize the data. # we can now look at our target variable boston y = boston.target # we can plot a histogram in a slightly different way plt.hist(boston y, bins = 40) plt.title('Housing price distribution, \$K') plt.show() # and the same for the boxplot plt.boxplot(boston y) plt.title('Box plot for housing price.') plt.show() # another thing we can do is plot a boxplot of one variable against the target variable # it is interesting to see how house value distribution differs by CHAS, the categorical variable # here we create a grouped dataframe that includes the target variable grouped df = boston X.copy() # note we create a copy of the data here so that any changes don't impact the original data grouped df['target'] = boston y.copy() # we then plot it here f, axes = plt.subplots(1, 1, figsize=(10, 5)) grouped df.boxplot(column='target', by = 'CHAS',

ax = axes) plt.show()

"""\* The `interquartile range`for houses next to the river is higher than for those houses not next to the river, and the `min` and `max` values differ too.

\* This suggests this could be an important variable for us to include in our model, given that as it differs, the target value distribution changes.

# we can extend this sort of analysis by creating a heatmap

# this shows the correlation between the features and target

# first we compute the correlation corr

= grouped df.corr(method='pearson')

# and plot our figure size plt.figure(figsize

= (15, 10)

# and use seaborn to fill this figure with a
heatmap

sns.heatmap(corr, annot = True)

"""\* We will let you review this heatmap to see what features are important for modelling and why."""

# OPTIONAL: below is code that generate a pairplot using seaborn

# look up what a pairplot is and see if you can interpret the output of the code below

#sns.pairplot(grouped\_df)

"""#### Preprocess the data

- \* We proprocess the data to ensure it is a suitable state for modelling. The sort of things that we do to preprocess the data includes:
- \* \*Dealing with missing values\*, where we identify what, if, any missing data we have and how to deal with it. For example, we may replace missing values with the mean value for that feature, or by the average of the neighbouring values.
- \* `pandas` has a number of options for filling in missing data that is worth exploring
- \* We can also use `k-nearest neighbour`to help us predict what the missing values should be, or `sklearn Imputer` function (amongst other ways)
- \* \*Treat categorical values\*, by converting them into a numerical representation that can be modelled.
- \* There are a number of different ways to do this in `sklearn` and `pandas`
- \* \*Normalise the data\*, for example by ensuring the data is, for example all on the scale (such as within two defined values); normally distributed; has a zero-mean, etc. This is sometimes necessary for the ML models to work, and can also help speed up the time it takes for the models to run. 

  \* Again, `sklearn` and `pandas` have in-built functions to help you do this.
- \* In this notebook, we will look to remove `outliers`, which are values that might be erroneous and which can over-influence the model,

and `normalize` the data

# lets start by removing outliers

```
Classification and Regression: In a Weekend – Appendix
```

```
# here we define the columns where we have
identified there could be outliers
numeric columns = ['CRIM', 'ZN', 'INDUS', 'NOX',
'RM', 'AGE', 'DIS', 'RAD', 'TAX', 'PTRATIO', 'B',
'LSTAT']
# this function can be used on any dataset to
return a list of index values for the outliers def
get outliers(data, columns):
    # we create an empty list
outlier idxs = [] for col
in columns:
        elements = data[col]
        # we get the mean value for each column
        mean = elements.mean()
        # and the standard deviation of the column
        sd = elements.std()
        # we then get the index values of all
values higher or lower than the mean +/- 2 standard
deviations
        outliers mask = data[(data[col] > mean +
3*sd) \mid (data[col] < mean - 3*sd) \mid .index
# and add those values to our list
outlier idxs += [x for x in outliers mask]
    return list(set(outlier idxs))
# we call the function we just created on the
boston dataset
boston outliers = get outliers (boston X,
numeric columns)
# and drop those values from our feature and target
boston X = boston X.drop(boston outliers, axis = 0)
boston y =
pd.DataFrame(boston y).drop(boston outliers, axis =
0).values.ravel()
```

```
# we can check that this code has worked by looking
at the shape of our data print
(boston X.shape) print
(boston y.shape)
# we can also create a function to normalize our
data
# first lets look at the data before normalisation
boston X[0:10]
# this function loops through columns in a data set
and defines a predefined scaler to each def
scale numeric (data, numeric columns, scaler):
for col in numeric columns:
                               data[col] =
scaler.fit transform(data[col].values.reshape(-1,
1))
    return data
# we can now define the scaler we want to use and
apply it to our dataset
# a good exercise would be to research waht
StandardScaler does - it is from the scikit learn
library
scaler = StandardScaler()
boston X = scale numeric(boston X, numeric columns,
scaler)
# here we can see the result
boston X[0:10]
"""### : Split the data
     In order to train our model and see how well
it performs, we need to split our data into
training and testing sets.
```

- \* We can then train our model on the training set, and test how well it has generalised to the data on the test set.
- \* There are a number of options for how we can split the data, and for what proportion of our original data we set aside for the test set.

# a common way for splitting our dataset is using
train test split

# as an exercise, go to the scikit learn
documentation to learn more about this function and
the parameters available

X\_train, X\_test, Y\_train, Y\_test =
model\_selection.train\_test\_split(boston\_X,
boston\_y, test\_size = 0.2, random\_state = 5)

# get shape of test and training sets
print('Training Set:')
print('Number of datapoints: ', X\_train.shape[0])
print('Number of features: ', X\_train.shape[1])
print('\n') print('Test
Set:')
print('Number of datapoints: ', X\_test.shape[0])
print('Number of features: ', X test.shape[1])

"""### Choose a Baseline algorithm

# linear regression is a fairly simple algorithm

compared to more complicate regression options, so

provides a good baseline lm

= LinearRegression()

"""### Train and Test the Model"""

# fitting the model to the data means to train our model on the data

# the fit function takes both the X and y variables
of the training data lm.fit(X\_train,
Y train)

# from this, we can generate a set of predictions
on our unseen features, X\_test
Y pred = lm.predict(X test)

"""### : Choose an evaluation metric

- \* We then need to compare these predictions with the actual result and measure them in some way.
- \* This is where the selection of evaluation metric is important. For regression, we measure the distance between the predicted and actual answers in some way. The shorter the distance, the more correct the model is. \* We cover three common metrics below:
- \* `Mean Absolute Error`: which provides a mean score for all the predicted versus actual values as

an absolute value

- \* `Means Squared Error`: which provides a mean score for all the predicted versus actual values as
- a square of the absolute value
- \* `R2`: which we recommend you research as an exercise to grow your knowledge. WIkipedia and `sklearn` document are a great place to start!

def evaluate(Y\_test,
Y pred):

# this block of code returns all the metrics we
are interested in

mse = metrics.mean\_squared\_error(Y\_test,
Y pred)

msa = metrics.mean\_absolute\_error(Y\_test,
Y pred)

```
r2 = metrics.r2 score(Y test, Y pred)
    print("Mean squared error: ", mse)
print("Mean absolute error: ", msa)
    print("R^2 : ", r2)
    # this creates a chart plotting predicted and
actual
    plt.scatter(Y test, Y pred)
plt.xlabel("Prices: $Y i$")
    plt.ylabel("Predicted prices: $\hat{Y} i$")
plt.title("Prices vs Predicted prices: $Y i$ vs
$\hat{Y} i$")
evaluate(Y test, Y pred)
# we can explore how metrics are dervied in a
little more detail by looking at MAE
# here we will implement MAE using numpy, building
it up step by step
# with MAE, we get the absolute values of the error
- as you can see this is of the difference between
the actual and predicted values np.abs(Y test
- Y pred)
# we will then sum them up np.sum(np.abs(Y test
- Y pred))
# then divide by the total number of
predictions/actual values
# as you will see, we get to the same score
implemented above
np.sum(np.abs(Y test - Y pred))/len(Y test)
"""### : Refine our dataset
```

- \* This step allows us to add or modify features of the dataset. We might do this if, for example, some combination of features better represents the problems space and so is an indicator of the target variable.
- \* Here, we create one additional feature as an example, but you should reflect on our EDA earlier and see whether there are other features that can be added to our dataset.

# here we are using pandas functionality to add a
new column called LSTAT\_2, which will feature
values that are the square of LSTAT values
boston\_X['LSTAT\_2'] = boston\_X['LSTAT'].map(lambda
x: x\*\*2)

# we can run our train\_test\_split function and see
that we have an additional features X\_train,
X\_test, Y\_train, Y\_test =
model\_selection.train\_test\_split(boston\_X,
boston\_y, test\_size = 0.2, random\_state = 5)
print('Number of features after dataset refinement:
', X\_train.shape[1])

# we can now run the same code as before on our refined dataset to see if things have improved lm.fit(X train, Y train)

Y\_pred = lm.predict(X\_test)

evaluate(Y\_test, Y\_pred)

"""### Step 8: Test Alternative Models
\* Once we got a nice baseline model working for
this dataset, we also can try something more
sophisticated and rather different, e.g.

RandomForest Regressor. So, let's do so and also evaluate the result.

\*\* \*\* \*\*

# as you can see, its very similar code to
instantiate the model

# we are able to pass in additional parameters as the model is created, so optionally you can view the documentation and play with these values

rfr = RandomForestRegressor() rfr.fit(X\_train,
Y\_train)
Y pred = rfr.predict(X test)

evaluate (Y test, Y pred)

"""### : Choose the best model and optimise its parameters \* We can see that we have improved our model as we have added features and trained new models.

- \* At the point that we feel comfortable with a good model, we can start to tune the parameters of the model.
- \* There are a number of ways to do this, and a common way is shown below

## grid search is a 'brute force' search, one that
will explore every possible combination of
parameters that you provide it

# we first define the parameters we want to search
as a dictionary. Explore the documentation to what
other options are avaiable params =
{'n\_estimators': [100, 200], 'max\_depth':
[2, 10, 20]}

# we then create a grid search object with our
chosen model and paramters. We also use cross
validation here - explored more in Day 2
grid = model\_selection.GridSearchCV(rfr, params,
cv=5)

# we fit our model to the data as before
grid.fit(X\_train, Y\_train)

# one output of the grid search function is that we
can get the best\_estimator - the model and
parameters that scored best on the training data # and save it as a new a model best\_model
= grid.best\_estimator\_

# and use it to predict and evaluate as before
Y\_pred = best\_model.predict(X\_test)
 evaluate(Y\_test,
Y pred)

## **Classification Code**

# -\*- coding: utf-8 -\*-

# import main data analysis libraries
import pandas as pd
import numpy as np import
seaborn as sns
import matplotlib.pyplot as plt
# note we use scipy for generating a uniform
distribution in the model optimization step
from scipy.stats import uniform

# note that because of the different dataset and algorithms, we use different sklearn libraries from Day 1

```
from sklearn.datasets import load breast cancer
from sklearn.linear model import LogisticRegression
from sklearn.ensemble import RandomForestClassifier
from sklearn.ensemble import VotingClassifier from
sklearn.tree import DecisionTreeClassifier
from sklearn.model selection import
train test split
from sklearn.model selection import
RandomizedSearchCV
from sklearn.model selection import cross val score
from sklearn.dummy import DummyClassifier
from sklearn import metrics
from sklearn.metrics import accuracy score
from sklearn.svm import SVC
# hide warnings import
warnings
warnings.filterwarnings('ignore')
# we load the dataset and save it as the variable
data = load breast cancer()
# if we want to know what sort of detail is
provided with this dataset, we can call .keys()
data.keys()
# the info at the .DESCR key will tell us more
print (data.DESCR)
#### Analyze the Data
X = pd.DataFrame(data.data, columns =
data.feature names)
# we can then look at the top of the dataframe to
see the sort of values it contains
X.describe(include = 'all')
```

# we can now look at our target variable
y = data.target

# we can see that it is a list of 0s and 1s, with 1s matching to the Benign class y

# we can analyse the data in more detail by understanding how the features and target variables interact.

# we can do this by grouping the features and the target into the same dataframe

# note we create a copy of the data here so that any changes don't impact the original data

full\_dataset = X.copy()
full dataset['target'] = y.copy()

# let's take a look at the first few lines of the
dataset
full dataset.head()

# lets see how balanced the classes are (and if
that matches to our expectation)
full dataset['target'].value counts()

# let's evaluate visually how well our classes are
differentiable on the pairplots # can see
two classes being present on a two variables
charts?

# the pairplot function is an excellent way of seeing how variables inter-relate, but 30 feature can make studying each combination difficult! sns.pairplot(full dataset, hue = 'target')

"""\* We can clearly see the presence of two clouds with different colors, representing our target classes.

\* Of course, they are still mixed to some extent, but if we were to visualise the variables in multidimentional space they would become more separable. \* Now let's check the Pearson's correlation between pairs of our features and also between the features and our target.

# we can again use seaborn to easily create a
visually interesting chart plt.figure(figsize
= (15, 10))

# we can add the annot=True parameter to the
sns.heatmap arguments if we want to show the
correlation values
sns.heatmap(full dataset.corr(method='pearson'))

"""\* Dark red colours are positilvey correlated with the corresponding feature, dark blue features are negatively correlated. \* We can see that some values are negatively correlated with our target variable.

\* This information could help us with feature engineering.

#### ### Split the data

- \* In order to train our model and see how well it performs, we need to split our data into training and testing sets.
- \* We can then train our model on the training set, and test how well it has generalised to the data on the test set.
- \* There are a number of options for how we can split the data, and for what proportion of our original data we set aside for the test set.

```
# Because our classes are not absolutely equal in
number, we can apply stratification to the split
# and be sure that the ratio of the classes in both
train and test will be the same
# you can learn about the other parameters by
looking at the documentation
X train, X test, y train, y test =
train test split(X, y, test size = 0.2, stratify =
y, shuffle=True)
# as with Day 1, we can get shape of test and
training sets print ('Training
Set: ')
print('Number of datapoints: ', X train.shape[0])
print('Number of features: ', X train.shape[1])
print('\n') print('Test
Set:')
print('Number of datapoints: ', X test.shape[0])
print('Number of features: ', X test.shape[1])
# and we can verify the stratifications using
np.bincount
print('Labels counts in y:', np.bincount(y))
print('Percentage of class zeroes in
class y', np.round(np.bincount(y)[0]/len(y)*100))
print("\n")
print('Labels counts in y train:',
np.bincount(y train))
print('Percentage of class zeroes in
y train',np.round(np.bincount(y_train)[0]/len(y_tra
in) *100))
print("\n")
print('Labels counts in y test:',
np.bincount(y test))
print('Percentage of class zeroes in
y test',np.round(np.bincount(y test)[0]/len(y test)
*100))
```

"""### : Choose a Baseline algorithm \*
Building a model in `sklearn` involves:
## we can create a baseline model to benchmark our
other estimators against
## this can be a simple estimator or we can use a
dummy estimator to make predictions in a random
manner
# this creates our dummy classifier, and the value
we pass in to the strategy parameter dtermn dummy
= DummyClassifier(strategy='uniform',
random\_state=1)

"""### : Train and Test the Model"""
# "Train" model
dummy.fit(X\_train, y\_train)
# from this, we can generate a set of predictions

"""### : Choose an evaluation metric

dummy predictions = dummy.predict(X test)

on our unseen features, X test

- \* We then need to compare these predictions with the actual result and measure them in some way. This is where the selection of evaluation metric is important.
- \* Classification metrics include:
- \* `accuracy`: this assess how often the model selects the best class. This can be more useful when there are balanced classes (i.e. there are a similar number of instances of each class we are trying to predict).
- \* There are some limits to this metric. For example, if we think about something like credit card fraud, where the instances of fraudulent transactions might be 0.5%, then a model that \*always\* predicts that a transaction is not

fraudulent will be 99.5% accurate! So we often need metrics that can tell us how a model performs in more detail. \* `f1 score`:

- \* `roc auc`:
- \* `recall`:
- \* We recommend you research these metrics to improve your understanding of how they work. Try to look up an explanation or two (for example on wikipedia and scikit-learn documentation) and write a one line summary in the space provided above.

Then, below, when we implement a scoring function, select these different metrics and try to explain what is happening. This will help cement you knowledge.

\*\* \*\* \*\*

|def evaluate(y\_test,
y pred):

# this block of code returns all the metrics we
are interested in

accuracy = metrics.accuracy\_score(y\_test,
y pred)

f1 = metrics.f1\_score(y\_test, y\_pred)
auc = metrics.roc\_auc\_score(y\_test, y\_pred)

# we can call the function on the actual results
versus the predictions

# we will see that the metrics are what we'd expect from a random model

evaluate(y\_test, dummy\_predictions)

"""### Test Alternative Models

## here we fit a new estimator and use
cross\_val\_score to get a score based on a defined
metric

# instantiate logistic regression classifier
logistic = LogisticRegression()

# we pass our estimator and data to the method. we
also specify the number of folds (default is 3)
# the default scoring method is the one associated
with the estimator we pass in # we can use the
scoring parameter to pass in different scoring
methods. Here we use f1. cross\_val\_score(logistic,
X, y, cv=5, scoring="f1")

# we can see that this returns a score for all the
five folds of the cross\_validation
# if we want to return a mean, we can store as a
variable and calculate the mean, or do it directly
on the function
# this time we will use accuracy
cross\_val\_score(logistic, X, y, cv=5,
scoring="accuracy").mean()

# lets do this again with a different model rnd\_clf
= RandomForestClassifier()

# and pass that in
cross\_val\_score(rnd\_clf, X, y, cv=5,
scoring="accuracy").mean()

"""#### Ensemble models

\* Let's take this opportunity to explore ensemble methods.

- \* The goal of ensemble methods is to combine different classifiers into a meta-classifier that has better generalization performance than each individual classifier alone.
- \* There are several different approaches to achieve this, including \*\*majority voting\*\* ensemble methods, which we select the class label that has been predicted by the majority of classifiers.
- \* The ensemble can be built from different classification algorithms, such as decision trees, support vector machines, logistic regression classifiers, and so on. Alternatively, we can also use the same base classification algorithm, fitting different subsets of the training set.
- \* Indeed, Majority voting will work best if the classifiers used are different from each other and/or trained on different datasets (or subsets of the same data) in order for their errors to be uncorrelated.

\*\* \*\* \*\*

# lets instantiate an additional model to make an
ensemble of three models dt\_clf =
DecisionTreeClassifier()

voting='soft')

# here we can cycle through the individual
estimators # for clf in (log\_clf, rnd\_clf,
svm\_clf, voting\_clf): for clf in (log\_clf,
rnd clf, dt clf, voting clf):

```
# fit them to the training data
clf.fit(X_train, y_train)

# get a prediction
y_pred = clf.predict(X_test)

# and print the prediction
print(clf.__class__.__name__,
accuracy_score(y_test, y_pred))
```

"""\* We can see that `voting classifier` in this the case does have a slight edge on the other models (note that this could vary depending on how the data is split at training time).

\* This is an interesting approach and one to consider when you are developing your models.

### Step 9: Choose the best model and optimise its parameters \* We can see that we have improved our model as we have added features and trained new models.

- \* At the point that we feel comfortable with a good model, we can start to tune the parameters of the model.
- \* There are a number of ways to do this. We applied `GridSearchCV` to identify the best hyperparameters for our models on Day 1.
- \* There are other methods available to use that don't take the brute force approach of `GridSearchCV`.
- \* We will cover an implementation of `RandomizedSearchCV` below, and use the exercise for you to implement it on the other datatset.
- \* We use this method to search over defined hyperparameters, like `GridSearchCV`, however a

fixed number of parameters are sampled, as defined by `n iter` parameter. # we will optimise logistics regression # we can create hyperparameters as a list, as in type regularization penalty penalty = ['11', '12'] # or as a distribution of values to sample from -'C' is the hyperparameter controlling the size of the regularisation penelty C = uniform(loc=0, scale=4) # we need to pass these parameters as a dictionary of {param name: values} hyperparameters = dict(C=C, penalty=penalty) # we instantiate our model randomizedsearch = RandomizedSearchCV(logistic, hyperparameters, random\_state=1, n iter=100, cv=5, verbose=0, n jobs=-1) # and fit it to the data best model = randomizedsearch.fit(X, y) # from this, we can generate a set of predictions on our unseen features, X test best predictions = best model.predict(X test) # and evaluate model performance evaluate(y test, best predictions) # and we can call this method to return the best parameters the search returned best model.best estimator

# and - we can evaluate the model using the cross

validation method discussed above
cross\_val\_score(best\_model, X, y, cv=5,
scoring="accuracy").mean()

"""\* evaluation of the scores