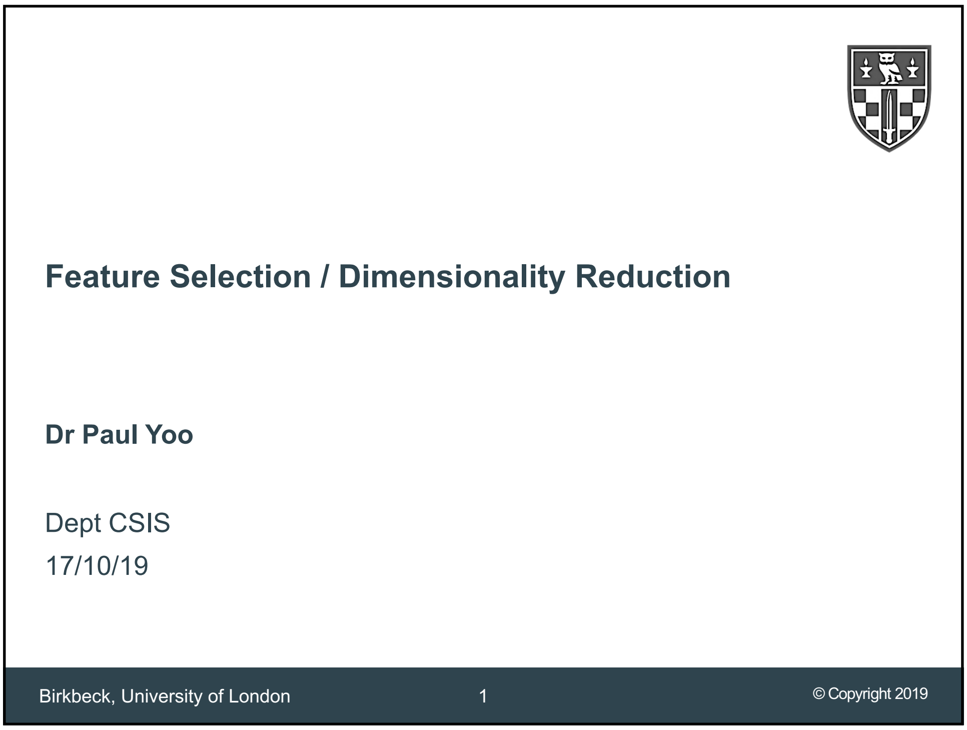

Feature Selection / Dimensionality Reduction

Dr Paul Yoo

Dept CSIS

17/10/19

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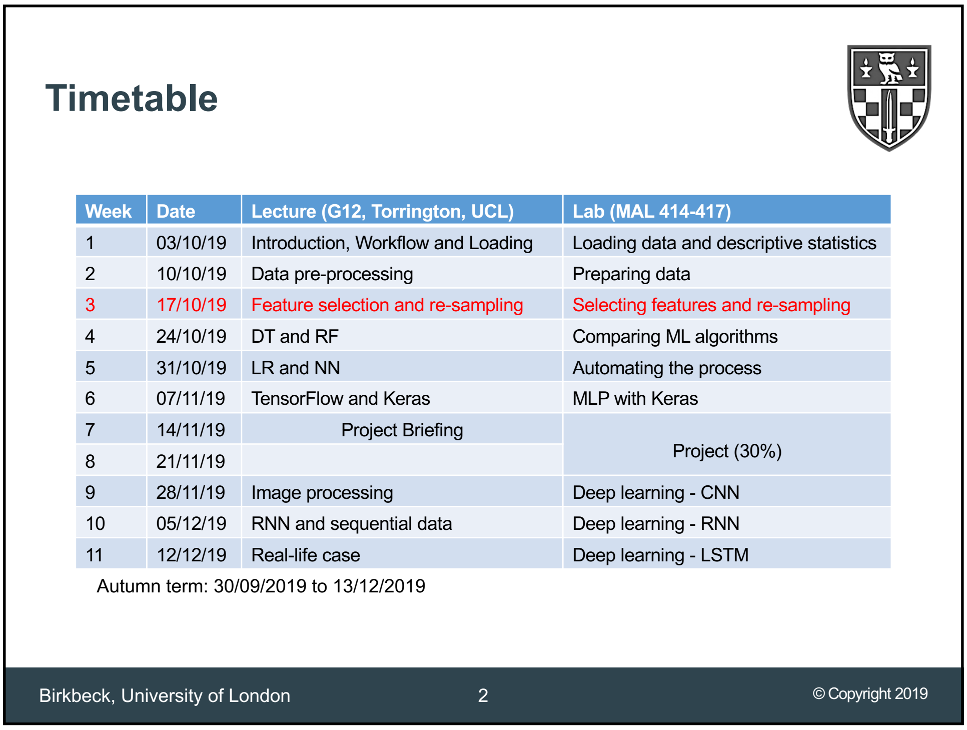

Timetable

Week	Date	Lecture (G12, Torrington, UCL)	Lab (MAL 414-417)
1	03/10/19	Introduction, Workflow and Loading	Loading data and descriptive statistics
2	10/10/19	Data pre-processing	Preparing data
3	17/10/19	Feature selection and re-sampling	Selecting features and re-sampling
4	24/10/19	DT and RF	Comparing ML algorithms
5	31/10/19	LR and NN	Automating the process
6	07/11/19	TensorFlow and Keras	MLP with Keras
7	14/11/19	Project Briefing	Project (30%)
8	21/11/19		
9	28/11/19	Image processing	Deep learning - CNN
10	05/12/19	RNN and sequential data	Deep learning - RNN
11	12/12/19	Real-life case	Deep learning - LSTM

Autumn term: 30/09/2019 to 13/12/2019

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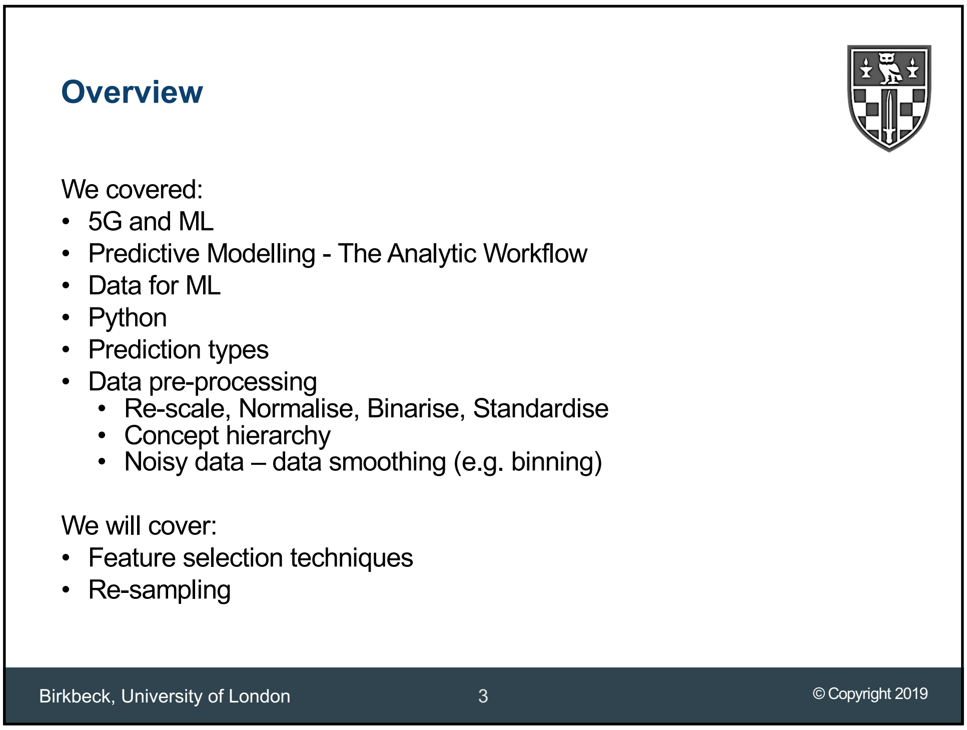


Overview

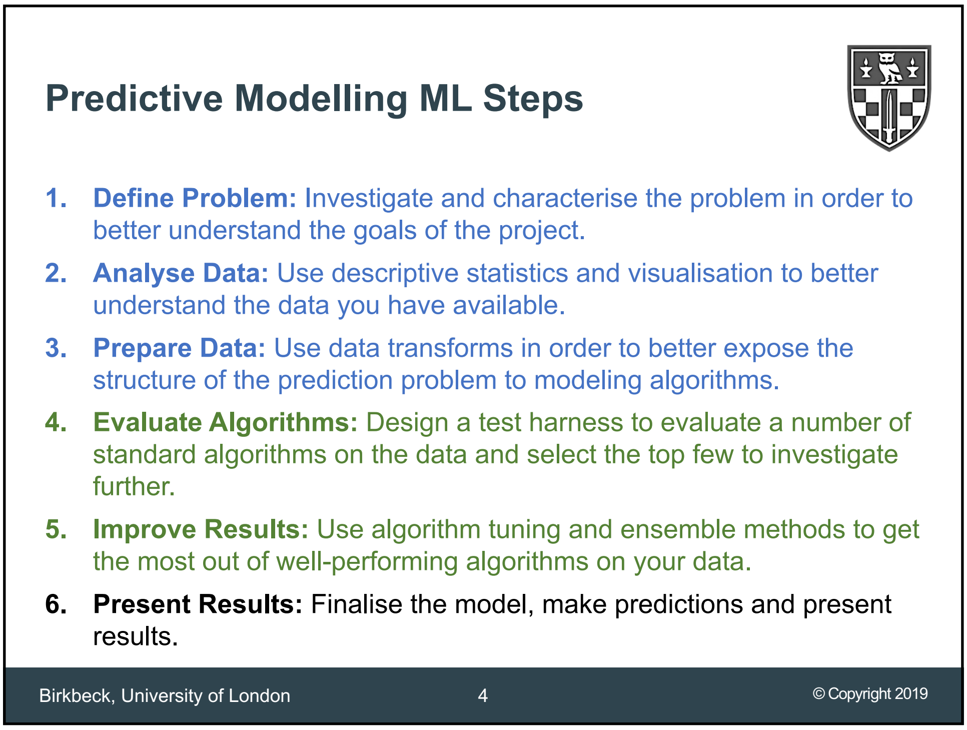
We covered:

- 5G and ML
- Predictive Modelling - The Analytic Workflow
- Data for ML
- Python
- Prediction types
- Data pre-processing
  - Re-scale, Normalise, Binarise, Standardise
  - Concept hierarchy
  - Noisy data – data smoothing (e.g. binning)

We will cover:

- Feature selection techniques
- Re-sampling

3

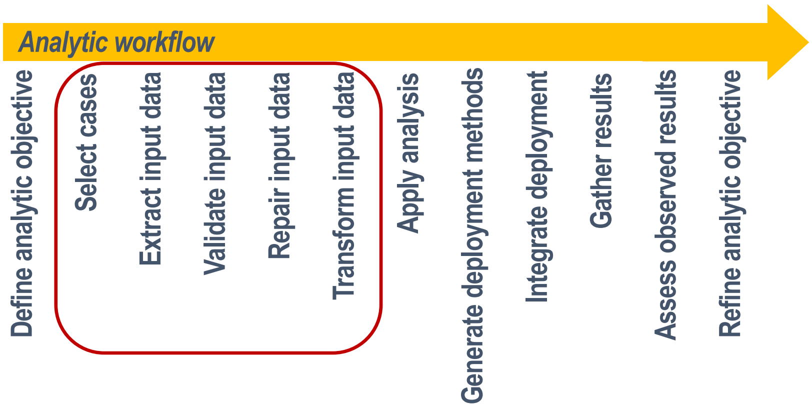


Predictive Modelling ML Steps

1. **Define Problem:** Investigate and characterise the problem in order to better understand the goals of the project.
2. **Analyse Data:** Use descriptive statistics and visualisation to better understand the data you have available.
3. **Prepare Data:** Use data transforms in order to better expose the structure of the prediction problem to modeling algorithms.
4. **Evaluate Algorithms:** Design a test harness to evaluate a number of standard algorithms on the data and select the top few to investigate further.
5. **Improve Results:** Use algorithm tuning and ensemble methods to get the most out of well-performing algorithms on your data.
6. **Present Results:** Finalise the model, make predictions and present results.

4

The Analytic Workflow



Analytic workflow

Define analytic objective

Select cases

Extract input data

Validate input data

Repair input data

Transform input data

Apply analysis

Generate deployment methods

Integrate deployment

Gather results

Assess observed results

Refine analytic objective

Source: SAS.com

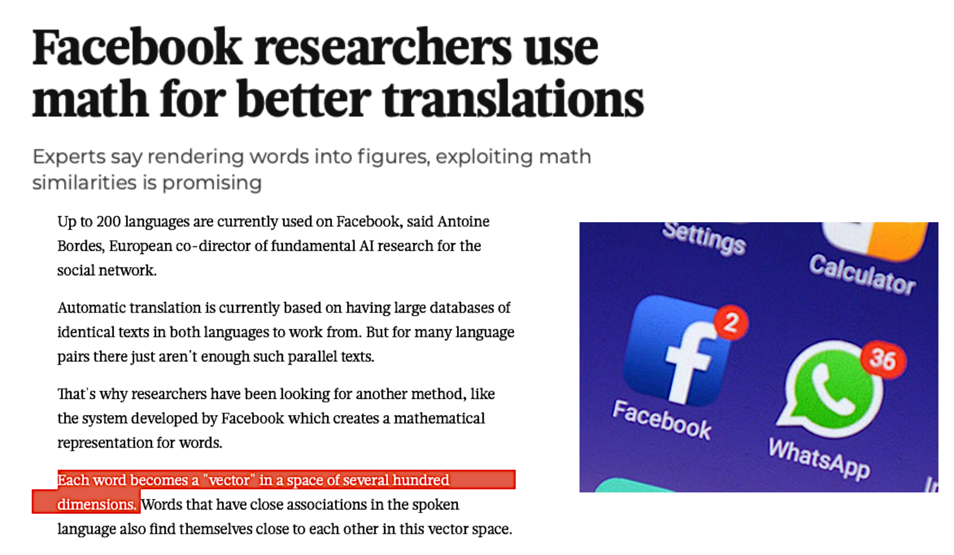
Discussion

"Art is the elimination of the unnecessary." Pablo Picasso

In small groups discuss what FS is and why FS is so important in machine learning (benefits of using FS techniques).

You have **5 minutes** and then we will discuss your answers.

1881 - 1973



Facebook researchers use math for better translations

Experts say rendering words into figures, exploiting math similarities is promising

Up to 200 languages are currently used on Facebook, said Antoine Bordes, European co-director of fundamental AI research for the social network.

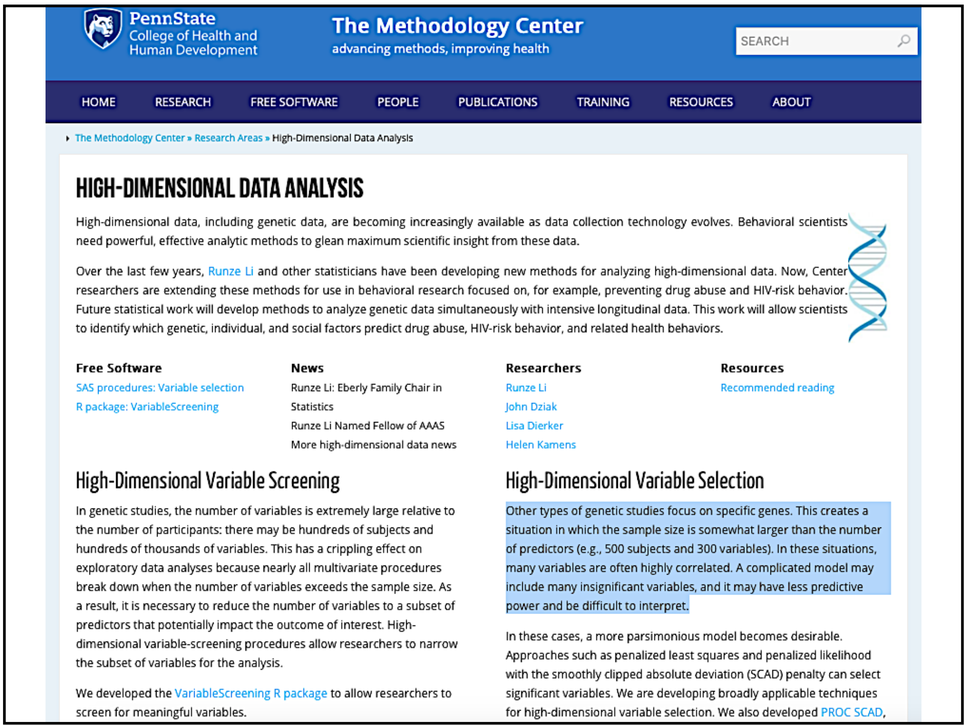
Automatic translation is currently based on having large databases of identical texts in both languages to work from. But for many language pairs there just aren't enough such parallel texts.

That's why researchers have been looking for another method, like the system developed by Facebook which creates a mathematical representation for words.

Each word becomes a "vector" in a space of several hundred dimensions. Words that have close associations in the spoken language also find themselves close to each other in this vector space.

[Source] https://gulfnews.com/world/americas/facebook-researchers-use-math-for-better-translations-1.1570941848964

7



The Methodology Center

advancing methods, improving health

The Methodology Center » Research Areas » High-Dimensional Data Analysis

HIGH-DIMENSIONAL DATA ANALYSIS

High-dimensional data, including genetic data, are becoming increasingly available as data collection technology evolves. Behavioral scientists need powerful, effective analytic methods to glean maximum scientific insight from these data.

Over the last few years, Runze Li and other statisticians have been developing new methods for analyzing high-dimensional data. Now, Center researchers are extending these methods for use in behavioral research focused on, for example, preventing drug abuse and HIV-risk behavior. Future statistical work will develop methods to analyze genetic data simultaneously with intensive longitudinal data. This work will allow scientists to identify which genetic, individual, and social factors predict drug abuse, HIV-risk behavior, and related health behaviors.

Free Software

SAS procedures: Variable selection

R package: VariableScreening

News

Runze Li: Eberly Family Chair in Statistics

Runze Li Named Fellow of AAAS

More high-dimensional data news

Researchers

Runze Li

John Dziak

Lisa Dierker

Helen Kamens

Resources

Recommended reading

High-Dimensional Variable Screening

In genetic studies, the number of variables is extremely large relative to the number of participants: there may be hundreds of subjects and hundreds of thousands of variables. This has a crippling effect on exploratory data analyses because nearly all multivariate procedures break down when the number of variables exceeds the sample size. As a result, it is necessary to reduce the number of variables to a subset of predictors that potentially impact the outcome of interest. High-dimensional variable-screening procedures allow researchers to narrow the subset of variables for the analysis.

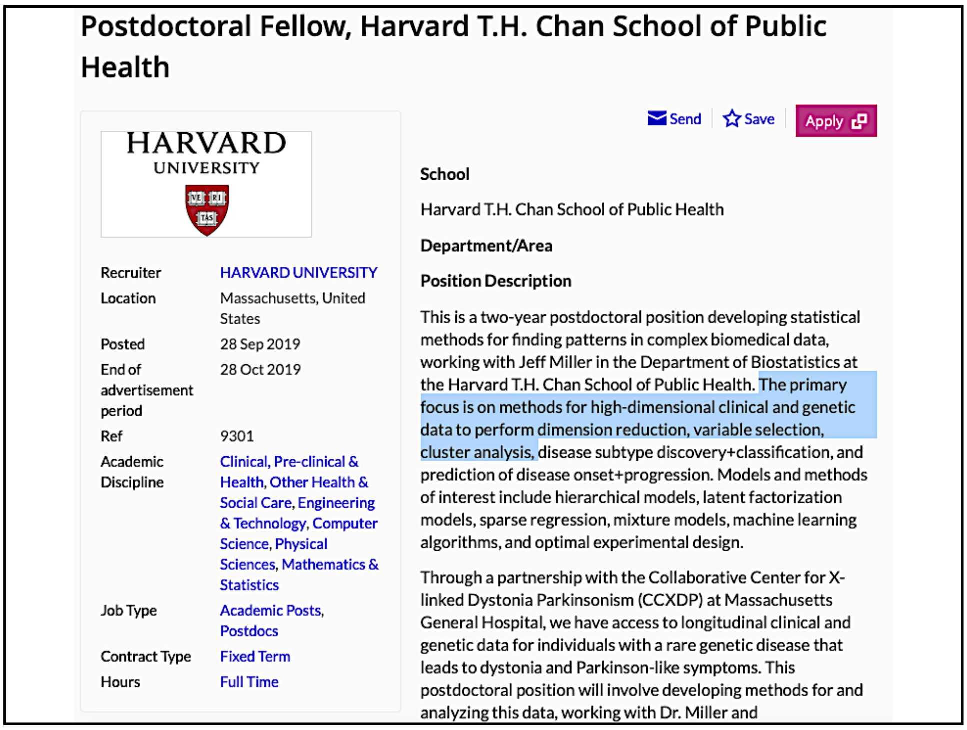
We developed the VariableScreening R package to allow researchers to screen for meaningful variables.

High-Dimensional Variable Selection

Other types of genetic studies focus on specific genes. This creates a situation in which the sample size is somewhat larger than the number of predictors (e.g., 500 subjects and 300 variables). In these situations, many variables are often highly correlated. A complicated model may include many insignificant variables, and it may have less predictive power and be difficult to interpret.

In these cases, a more parsimonious model becomes desirable. Approaches such as penalized least squares and penalized likelihood with the smoothly clipped absolute deviation (SCAD) penalty can select significant variables. We are developing broadly applicable techniques for high-dimensional variable selection. We also developed PROC SCAD,

8



Postdoctoral Fellow, Harvard T.H. Chan School of Public Health

Recruiter	HARVARD UNIVERSITY
Location	Massachusetts, United States
Posted	28 Sep 2019
End of advertisement period	28 Oct 2019
Ref	9301
Academic Discipline	Clinical, Pre-clinical & Health, Other Health & Social Care, Engineering & Technology, Computer Science, Physical Sciences, Mathematics & Statistics
Job Type	Academic Posts, Postdocs
Contract Type	Fixed Term
Hours	Full Time

School

Harvard T.H. Chan School of Public Health

Department/Area

Position Description

This is a two-year postdoctoral position developing statistical methods for finding patterns in complex biomedical data, working with Jeff Miller in the Department of Biostatistics at the Harvard T.H. Chan School of Public Health. The primary focus is on methods for high-dimensional clinical and genetic data to perform dimension reduction, variable selection, cluster analysis, disease subtype discovery+classification, and prediction of disease onset+progression. Models and methods of interest include hierarchical models, latent factorization models, sparse regression, mixture models, machine learning algorithms, and optimal experimental design.

Through a partnership with the Collaborative Center for X-linked Dystonia Parkinsonism (CCXDP) at Massachusetts General Hospital, we have access to longitudinal clinical and genetic data for individuals with a rare genetic disease that leads to dystonia and Parkinson-like symptoms. This postdoctoral position will involve developing methods for and analyzing this data, working with Dr. Miller and

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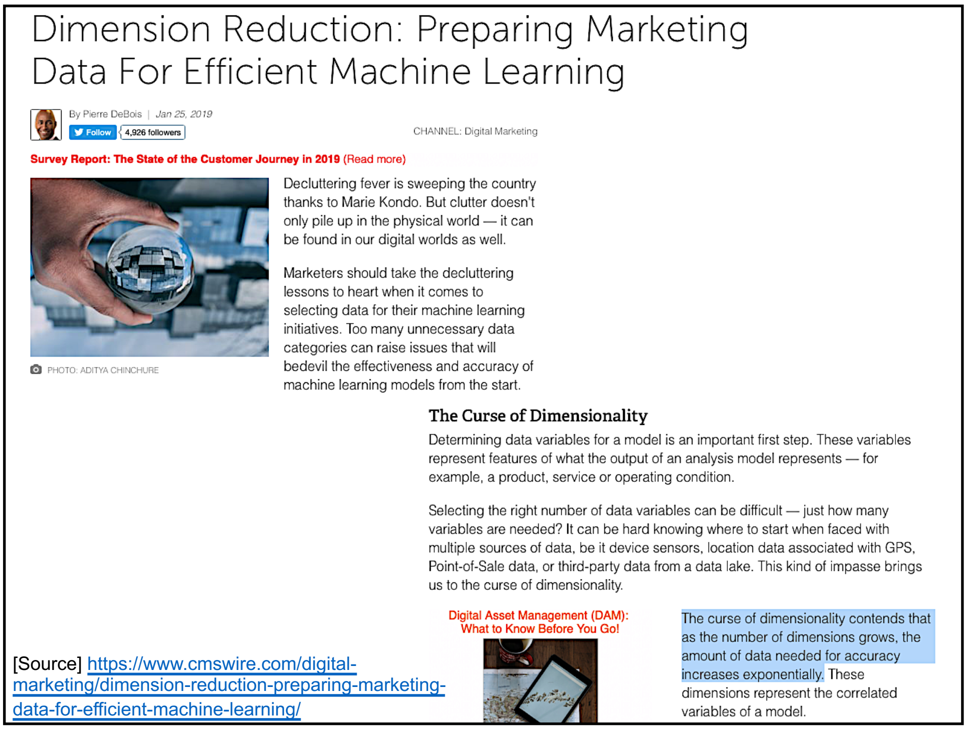


Dimension Reduction: Preparing Marketing Data For Efficient Machine Learning

By Pierre DeBois | Jan 25, 2019

CHANNEL: Digital Marketing

Survey Report: The State of the Customer Journey in 2019 (Read more)

PHOTO: ADITYA CHINCHURE

Decluttering fever is sweeping the country thanks to Marie Kondo. But clutter doesn't only pile up in the physical world — it can be found in our digital worlds as well.

Marketers should take the decluttering lessons to heart when it comes to selecting data for their machine learning initiatives. Too many unnecessary data categories can raise issues that will bedevil the effectiveness and accuracy of machine learning models from the start.

The Curse of Dimensionality

Determining data variables for a model is an important first step. These variables represent features of what the output of an analysis model represents — for example, a product, service or operating condition.

Selecting the right number of data variables can be difficult — just how many variables are needed? It can be hard knowing where to start when faced with multiple sources of data, be it device sensors, location data associated with GPS, Point-of-Sale data, or third-party data from a data lake. This kind of impasse brings us to the curse of dimensionality.

Digital Asset Management (DAM): What to Know Before You Go!

The curse of dimensionality contends that as the number of dimensions grows, the amount of data needed for accuracy increases exponentially. These dimensions represent the correlated variables of a model.

[Source] https://www.cmswire.com/digital-marketing/dimension-reduction-preparing-marketing-data-for-efficient-machine-learning/

10

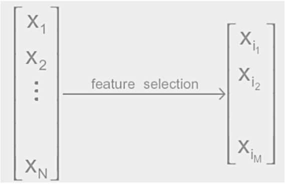
Discussion

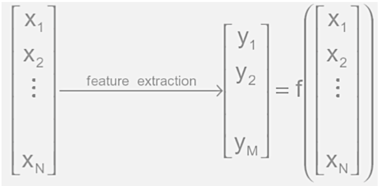
What are the differences between FS, Dimensionality Reduction and Feature Extraction?

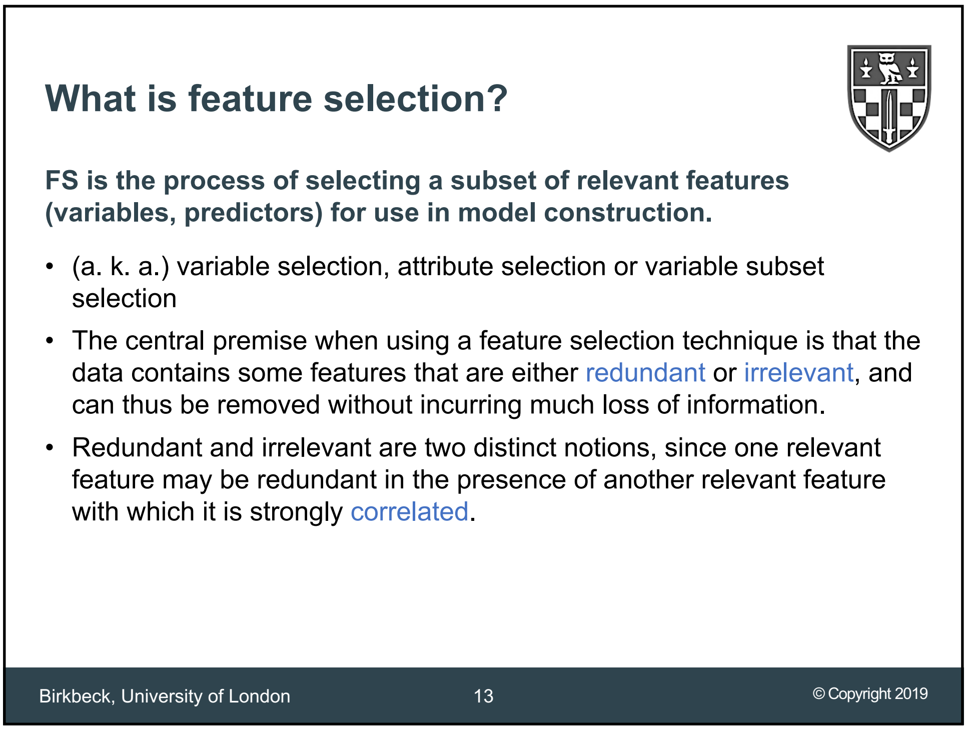
You have **5 minutes** and then we will discuss your answers.

FS, DR and FE

- **Feature selection** is the process of selecting a subset of relevant features for use in model construction.
- **Feature selection** is simply selecting and excluding given features without changing them.
- **Dimensionality reduction** transforms features into a lower dimension
  - It is often not reversible because some information is lost in the process of dimensionality reduction.



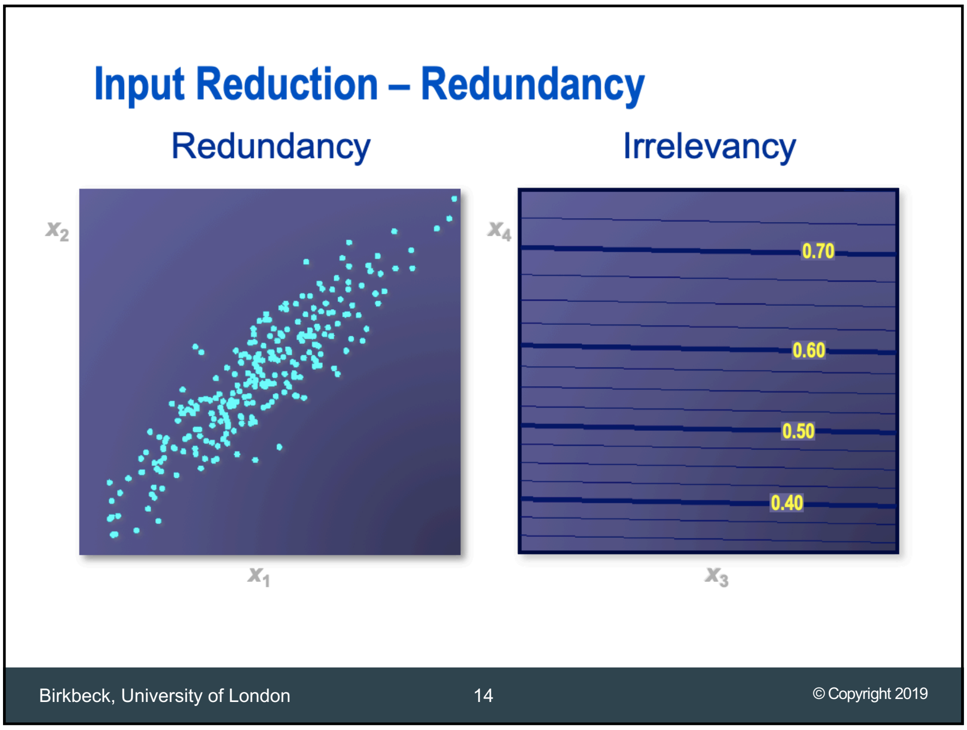




What is feature selection?

FS is the process of selecting a subset of relevant features (variables, predictors) for use in model construction.

- (a. k. a.) variable selection, attribute selection or variable subset selection
- The central premise when using a feature selection technique is that the data contains some features that are either redundant or irrelevant, and can thus be removed without incurring much loss of information.
- Redundant and irrelevant are two distinct notions, since one relevant feature may be redundant in the presence of another relevant feature with which it is strongly correlated.



Input Reduction – Redundancy

Redundancy

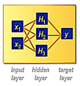
Irrelevancy

Feature selection techniques are used for several reasons

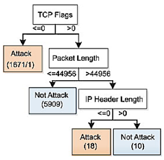
Simplification of models to make them easier to interpret by researchers/users

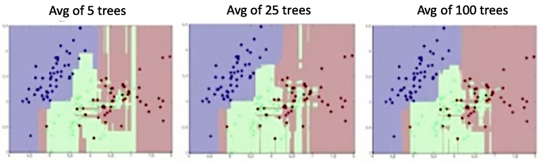
White/Grey Box Modelling

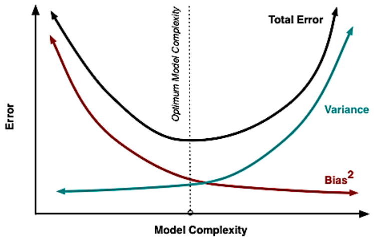
$$\log\left(\frac{\hat{p}}{1-\hat{p}}\right) = \hat{w}_{00} + \hat{w}_{01} \cdot H_1 + \hat{w}_{02} \cdot H_2 + \hat{w}_{03} \cdot H_3$$



$$H_1 = \tanh(\hat{w}_{10} + \hat{w}_{11}\, x_1 + \hat{w}_{12}\, x_2)$$
$$H_2 = \tanh(\hat{w}_{20} + \hat{w}_{21}\, x_1 + \hat{w}_{22}\, x_2)$$
$$H_3 = \tanh(\hat{w}_{30} + \hat{w}_{31}\, x_1 + \hat{w}_{32}\, x_2)$$



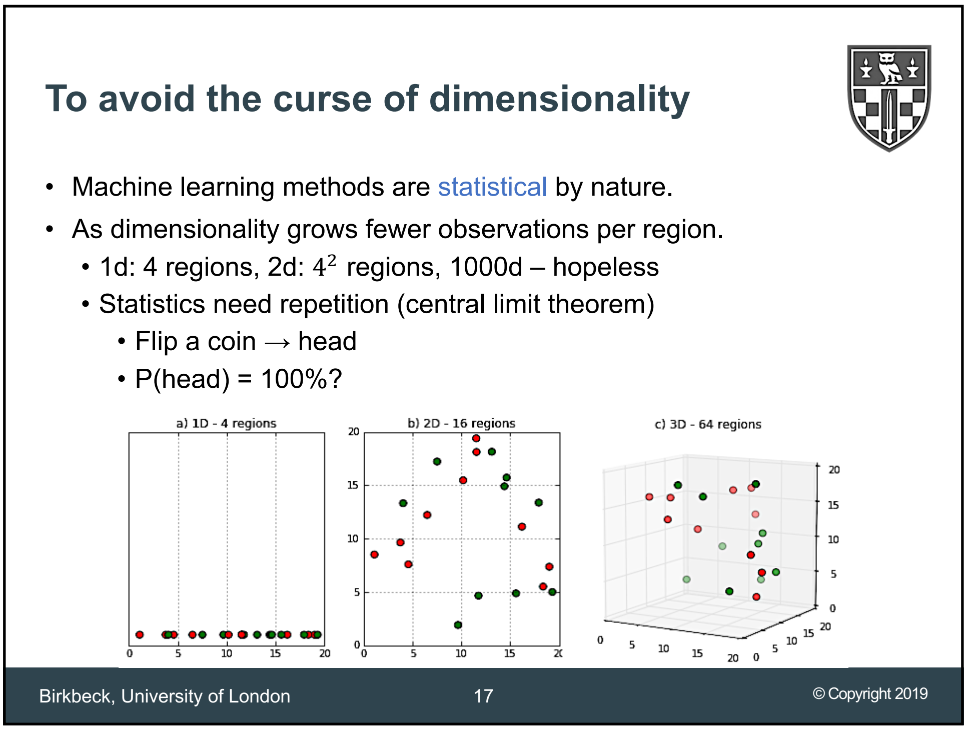

Avg of 5 trees
Avg of 25 trees
Avg of 100 trees



[Source] Gareth James; Daniela Witten; Trevor Hastie; Robert Tibshirani (2013). An Introduction to Statistical Learning. Springer. p. 204.

Shorter training times Vs Better Accuracy

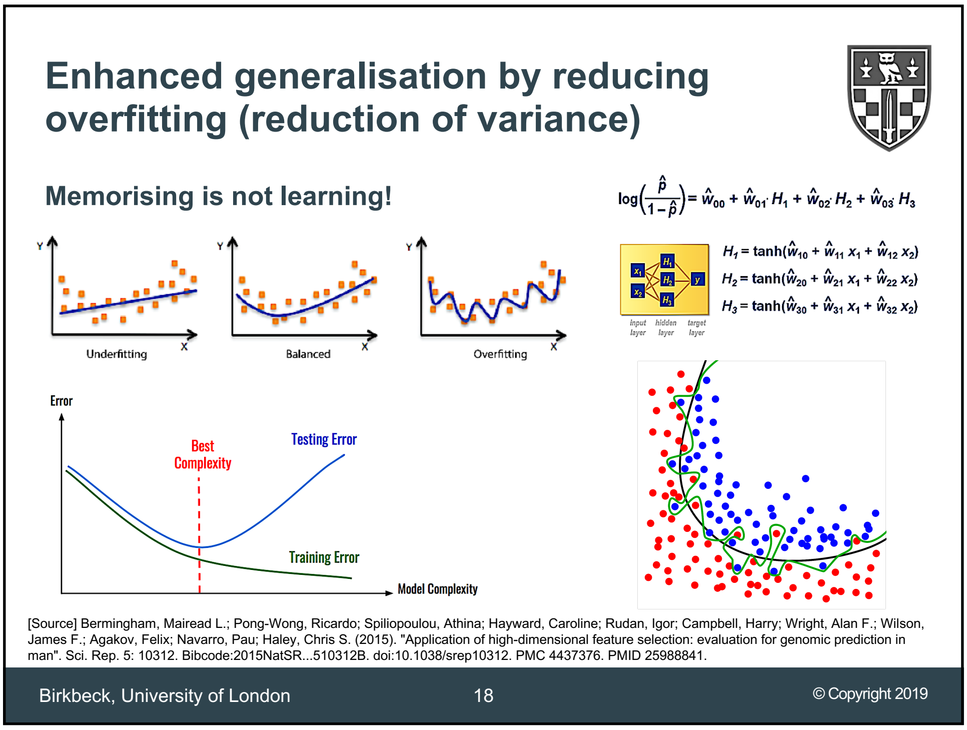
- Reduce the noise → help the model to become less overfit to the noises from the training data → the model will have a better generalisation ability when tested with unseen data points.
- Sometimes FS also results in the loss of predictive accuracy. For example,
  - 100 features = 95% accuracy
  - 50 features = 93% accuracy
- While the dimensionality of the model decreases, the complexity of the model also decreases.
- This eventually leads to a faster model training time and convergence.



To avoid the curse of dimensionality

- Machine learning methods are statistical by nature.
- As dimensionality grows fewer observations per region.
  - 1d: 4 regions, 2d: 4^2 regions, 1000d – hopeless
  - Statistics need repetition (central limit theorem)
    - Flip a coin → head
    - P(head) = 100%?

a) 1D - 4 regions
0
5
10
15
20
b) 2D - 16 regions
0
5
10
15
20
c) 3D - 64 regions
0
5
10
15
20



Enhanced generalisation by reducing overfitting (reduction of variance)

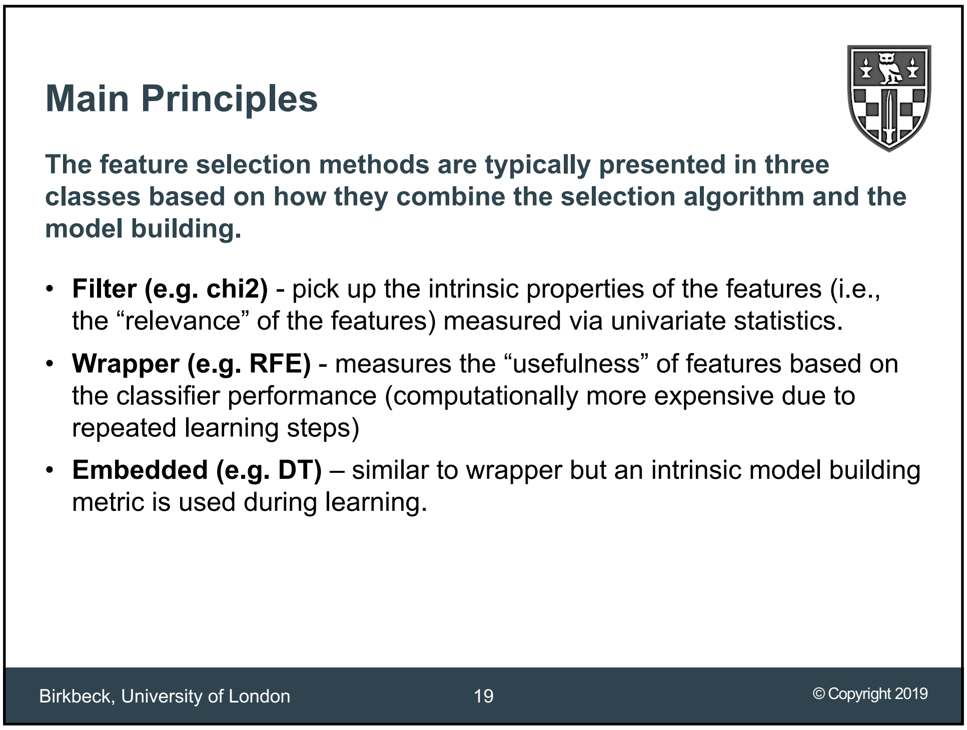
Memorising is not learning!

$$\log\left(\frac{\hat{p}}{1-\hat{p}}\right) = \hat{w}_{00} + \hat{w}_{01} \cdot H_1 + \hat{w}_{02} \cdot H_2 + \hat{w}_{03} \cdot H_3$$

$$H_1 = \tanh(\hat{w}_{10} + \hat{w}_{11}\, x_1 + \hat{w}_{12}\, x_2)$$
$$H_2 = \tanh(\hat{w}_{20} + \hat{w}_{21}\, x_1 + \hat{w}_{22}\, x_2)$$
$$H_3 = \tanh(\hat{w}_{30} + \hat{w}_{31}\, x_1 + \hat{w}_{32}\, x_2)$$

Y
X
Underfitting
Y
X
Balanced
Y
X
Overfitting
x_1
x_2
H_1
H_2
H_3
y
input layer
hidden layer
target layer
Error
Best Complexity
Testing Error
Training Error
Model Complexity

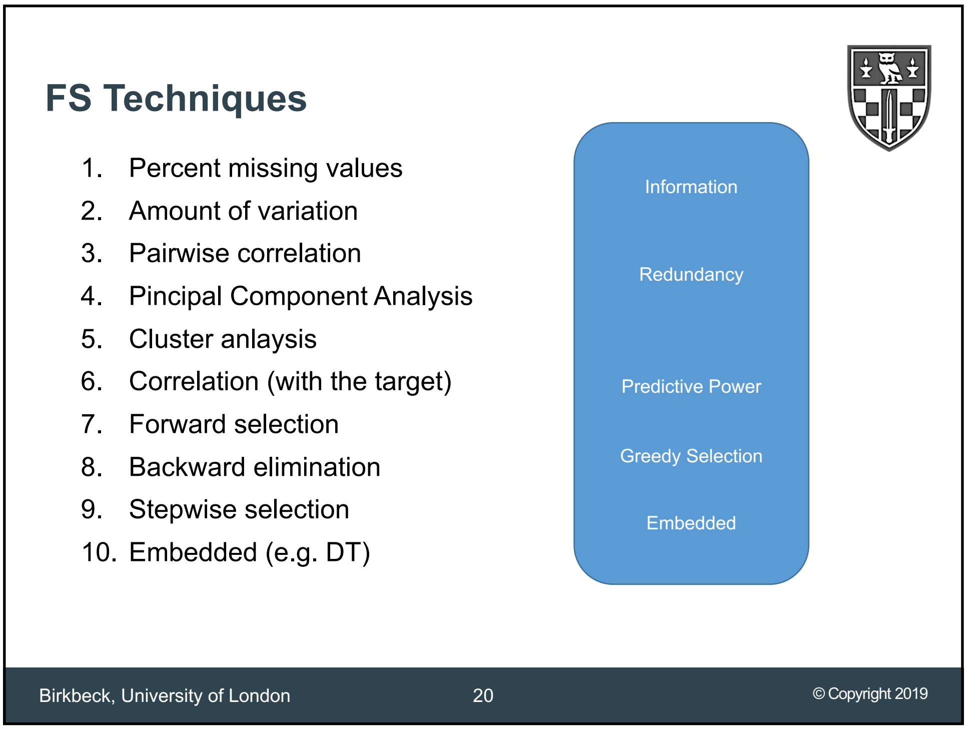
[Source] Bermingham, Mairead L.; Pong-Wong, Ricardo; Spiliopoulou, Athina; Hayward, Caroline; Rudan, Igor; Campbell, Harry; Wright, Alan F.; Wilson, James F.; Agakov, Felix; Navarro, Pau; Haley, Chris S. (2015). "Application of high-dimensional feature selection: evaluation for genomic prediction in man". Sci. Rep. 5: 10312. Bibcode:2015NatSR...510312B. doi:10.1038/srep10312. PMC 4437376. PMID 25988841.



Main Principles

The feature selection methods are typically presented in three classes based on how they combine the selection algorithm and the model building.

- **Filter (e.g. chi2)** - pick up the intrinsic properties of the features (i.e., the "relevance" of the features) measured via univariate statistics.
- **Wrapper (e.g. RFE)** - measures the "usefulness" of features based on the classifier performance (computationally more expensive due to repeated learning steps)
- **Embedded (e.g. DT)** – similar to wrapper but an intrinsic model building metric is used during learning.



FS Techniques

1. Percent missing values
2. Amount of variation
3. Pairwise correlation
4. Pincipal Component Analysis
5. Cluster anlaysis
6. Correlation (with the target)
7. Forward selection
8. Backward elimination
9. Stepwise selection
10. Embedded (e.g. DT)

Information
Redundancy
Predictive Power
Greedy Selection
Embedded

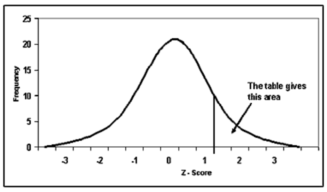
Percent Missing Values

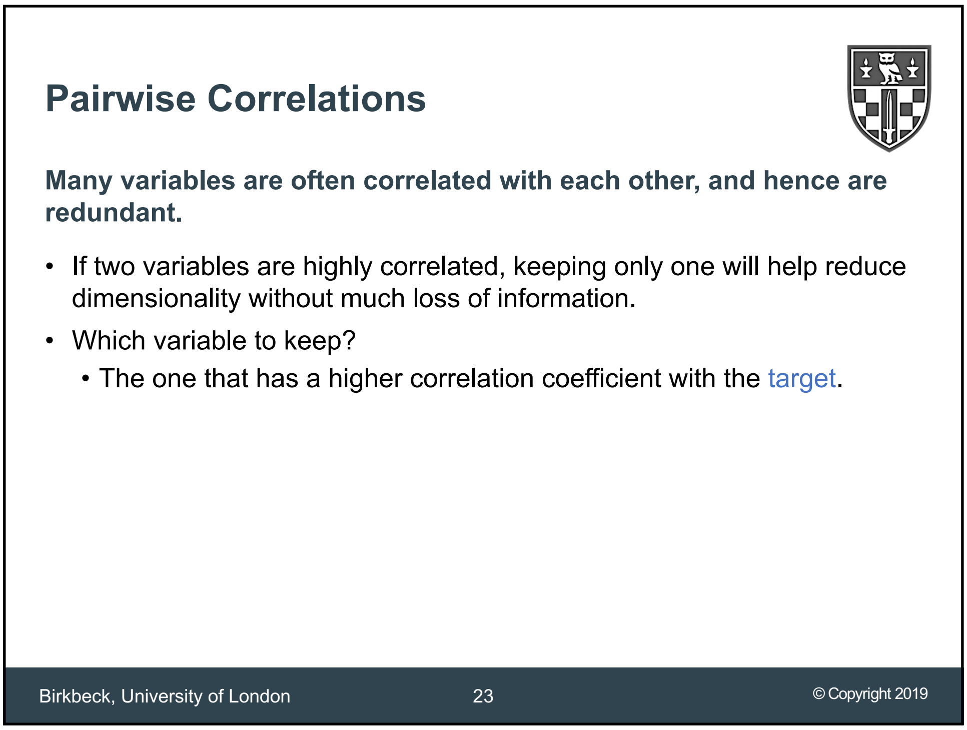
- Drop variables that have a very high % of missing values
  - # of records with missing values / # of total records
- Create binary indicators (encode) to denote missing (or non-missing) values
- Review or visualise variables with high % of missing values. Why?

Amount of Variation

Drop or review variables that have a very low variation

- $VAR(x) = \sigma^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \mu)^2$
- Either standardise all variables, or use standard deviation σ to account for variables with different scales
- Z-scores $(\boldsymbol{z} = (\boldsymbol{x} - \boldsymbol{\mu}) / \boldsymbol{\sigma})$ are a way to compare results from a test to a "normal" population.
- Drop variables with zero variation (unary)

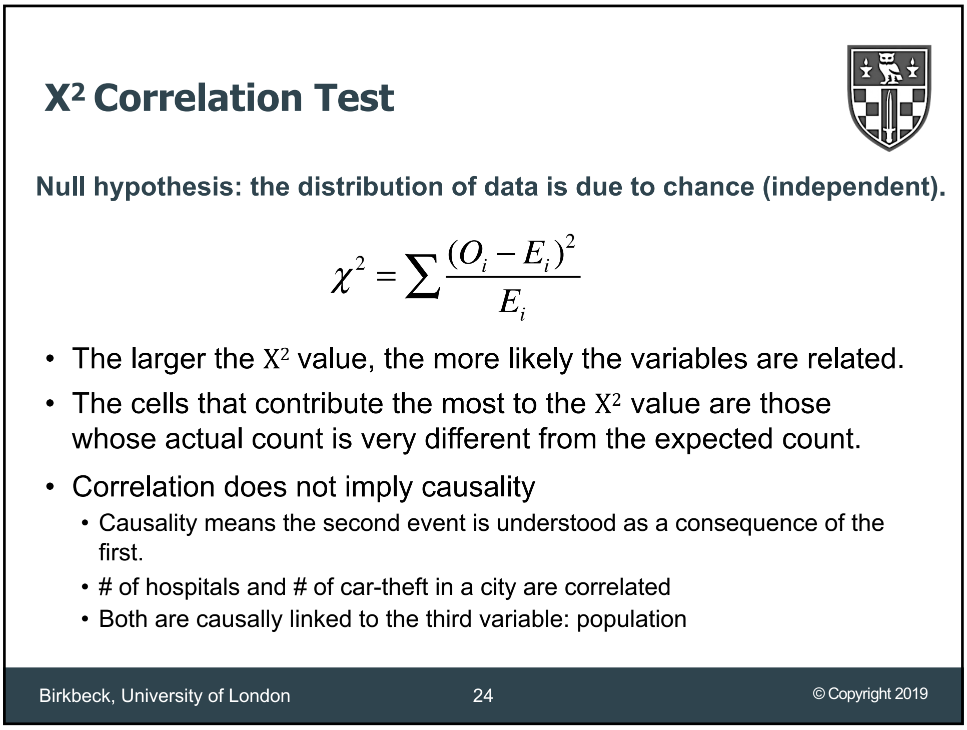




Pairwise Correlations

Many variables are often correlated with each other, and hence are redundant.

- If two variables are highly correlated, keeping only one will help reduce dimensionality without much loss of information.
- Which variable to keep?
  - The one that has a higher correlation coefficient with the target.

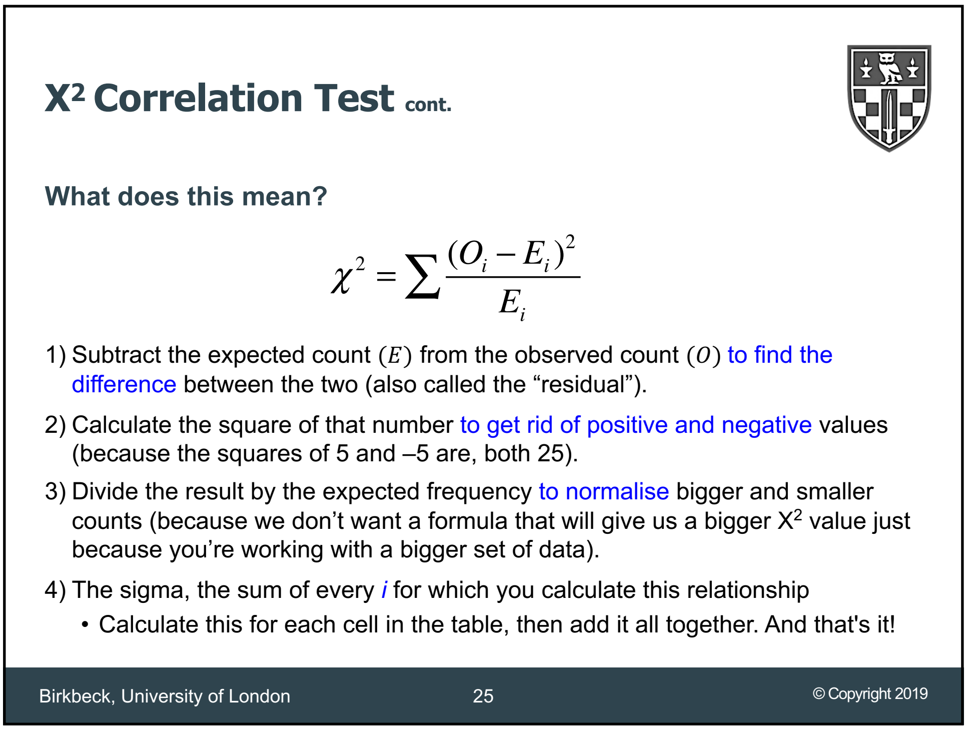


X² Correlation Test

Null hypothesis: the distribution of data is due to chance (independent).

$$\chi^2 = \sum \frac{(O_i - E_i)^2}{E_i}$$

- The larger the X^2 value, the more likely the variables are related.
- The cells that contribute the most to the X^2 value are those whose actual count is very different from the expected count.
- Correlation does not imply causality
  - Causality means the second event is understood as a consequence of the first.
  - # of hospitals and # of car-theft in a city are correlated
  - Both are causally linked to the third variable: population

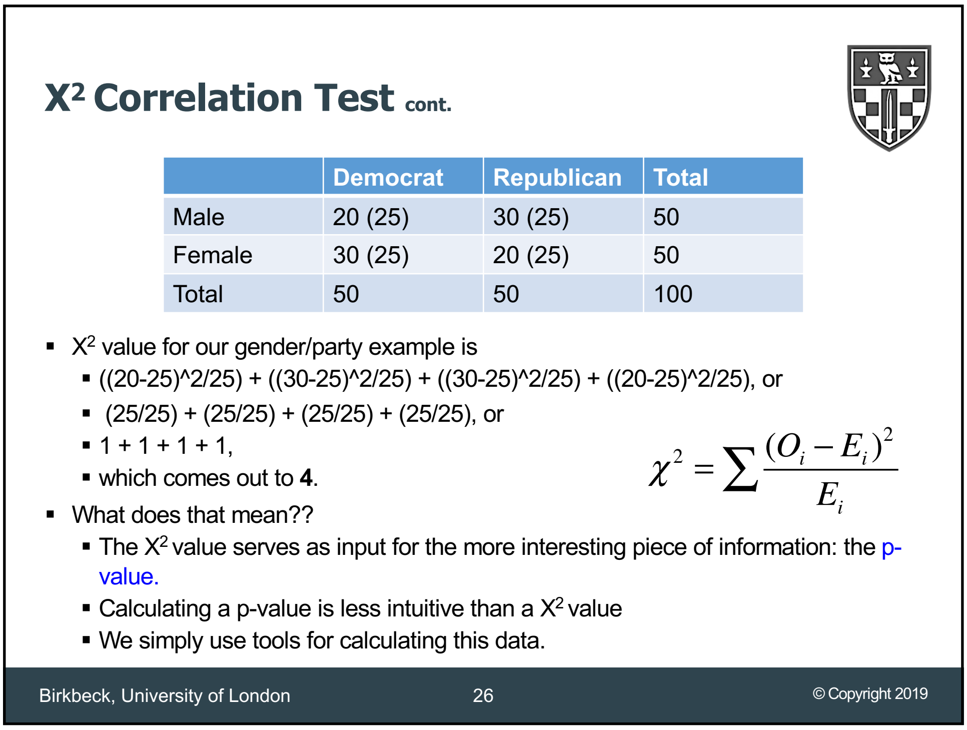


X² Correlation Test cont.

What does this mean?

$$\chi^2 = \sum \frac{(O_i - E_i)^2}{E_i}$$

1) Subtract the expected count (E) from the observed count (O) to find the difference between the two (also called the “residual”).
2) Calculate the square of that number to get rid of positive and negative values (because the squares of 5 and –5 are, both 25).
3) Divide the result by the expected frequency to normalise bigger and smaller counts (because we don’t want a formula that will give us a bigger X^2 value just because you’re working with a bigger set of data).
4) The sigma, the sum of every *i* for which you calculate this relationship
   - Calculate this for each cell in the table, then add it all together. And that's it!



X² Correlation Test cont.

	Democrat	Republican	Total
Male	20 (25)	30 (25)	50
Female	30 (25)	20 (25)	50
Total	50	50	100

- X^2 value for our gender/party example is
  - ((20-25)^2/25) + ((30-25)^2/25) + ((30-25)^2/25) + ((20-25)^2/25), or
  - (25/25) + (25/25) + (25/25) + (25/25), or
  - 1 + 1 + 1 + 1,
  - which comes out to **4**.

$$\chi^2 = \sum \frac{(O_i - E_i)^2}{E_i}$$

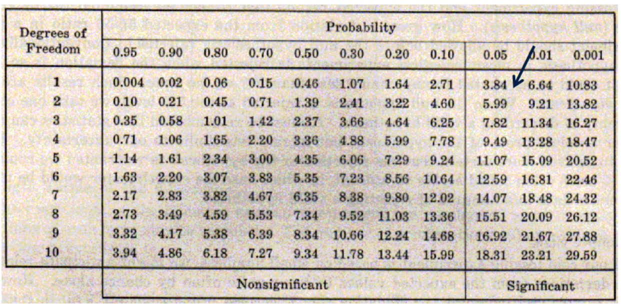
- What does that mean??
  - The X^2 value serves as input for the more interesting piece of information: the p-value.
  - Calculating a p-value is less intuitive than a X^2 value
  - We simply use tools for calculating this data.

X^2 Correlation Test cont.

- X^2 value of 4, and
- Degree of freedon (df) of 1
  - For 2x2 table,
    - df=1=(2-1)(2-1)
- Use the p-value calculator: https://www.socscistatistics.com/pvalues/
- Gives us a p-value of 0.0455.
- This is interpreted as a 4.6% likelihood that the null hypothesis is correct.
- To put it best, if the distribution of this data is due entirely to chance, then you have a 4.6% chance of finding a discrepancy between the observed and expected distributions that is at least this extreme.
- x^2 value needed to reject the hypothesis is 3.84 (95% confidence level)
- Critical value of 3.84 < X^2 of 4
- So reject! The two attributes are dependent

X^2 Correlation Test cont.

- Look up the critical chi-square statistic value for $p = 0.05$ (95% confidence level) with 1 degree of freedom → 3.84



Degrees of Freedom	Probability										
	0.95	0.90	0.80	0.70	0.50	0.30	0.20	0.10	0.05	0.01	0.001
1	0.004	0.02	0.06	0.15	0.46	1.07	1.64	2.71	3.84	6.64	10.83
2	0.10	0.21	0.45	0.71	1.39	2.41	3.22	4.60	5.99	9.21	13.82
3	0.35	0.58	1.01	1.42	2.37	3.66	4.64	6.25	7.82	11.34	16.27
4	0.71	1.06	1.65	2.20	3.36	4.88	5.99	7.78	9.49	13.28	18.47
5	1.14	1.61	2.34	3.00	4.35	6.06	7.29	9.24	11.07	15.09	20.52
6	1.63	2.20	3.07	3.83	5.35	7.23	8.56	10.64	12.59	16.81	22.46
7	2.17	2.83	3.82	4.67	6.35	8.38	9.80	12.02	14.07	18.48	24.32
8	2.73	3.49	4.59	5.53	7.34	9.52	11.03	13.36	15.51	20.09	26.12
9	3.32	4.17	5.38	6.39	8.34	10.66	12.24	14.68	16.92	21.67	27.88
10	3.94	4.86	6.18	7.27	9.34	11.78	13.44	15.99	18.31	23.21	29.59
	Nonsignificant								Significant		

Critical values for the X^2 Distribution

[Source] https://www.itl.nist.gov/div898/handbook/eda/section3/eda3674.htm

Principal Component Analysis (PCA)

Dimensionality reduction technique which emphasises variation.

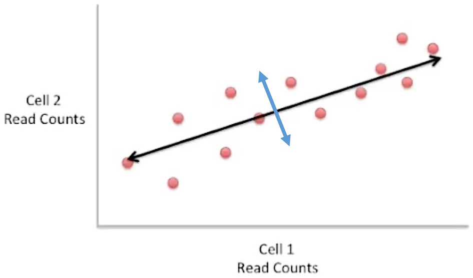
- Uses orthogonal transformation
- When to use:
  - Excessive multicollinearity - high intercorrelations or inter-associations among the independent variables.
  - Explanation of the predictors is not important
  - A light overhead in implementation is okay
  - More suitable for unsupervised learning

A PCA example

We'll start with just two cells.

Gene	Cell1 reads	Cell2 reads
a	10	8
b	0	2
c	14	10
d	33	45
e	50	42
f	80	72
g	95	90
h	44	50
i	60	50
... (etc)	... (etc)	... (etc)

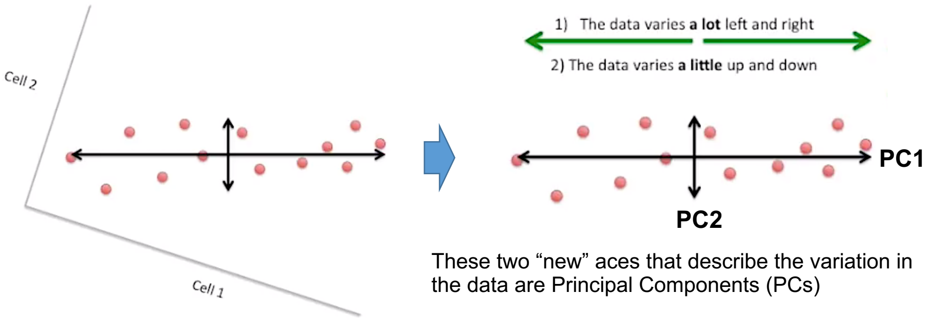
The dots are also spread out a little above and below the first line.



The 2nd largest amount of variation is at the endpoints of the newline.

Rotate the whole graph

The two lines that we drew make new X and Y axes.


Cell 2
Cell 1
1) The data varies **a lot** left and right
2) The data varies **a little** up and down
PC1
PC2

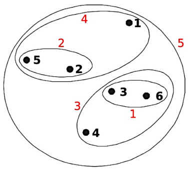
These two “new” aces that describe the variation in the data are Principal Components (PCs)

- PC1 is the axis that spans the most variation
- PC2 is the axis that spans the 2nd most variation.

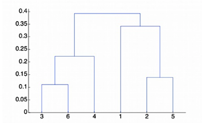
Cluster Analysis

- Dimensionality reduction technique which emphasizes correlation/similarity.
  - Identify groups of variables that are as correlated as possible among themselves and as uncorrelated as possible with variables in other clusters
- Produces a set of nested clusters organised as a hierarchical tree.
- Can be visualised as a dendrogram
- When to use:
  - Excessive multicollinearity
  - Explanation of the predictors is important

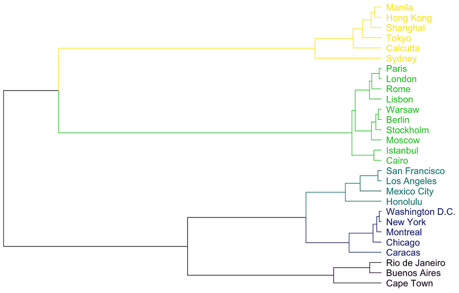
Cluster Analysis



Nested Clusters



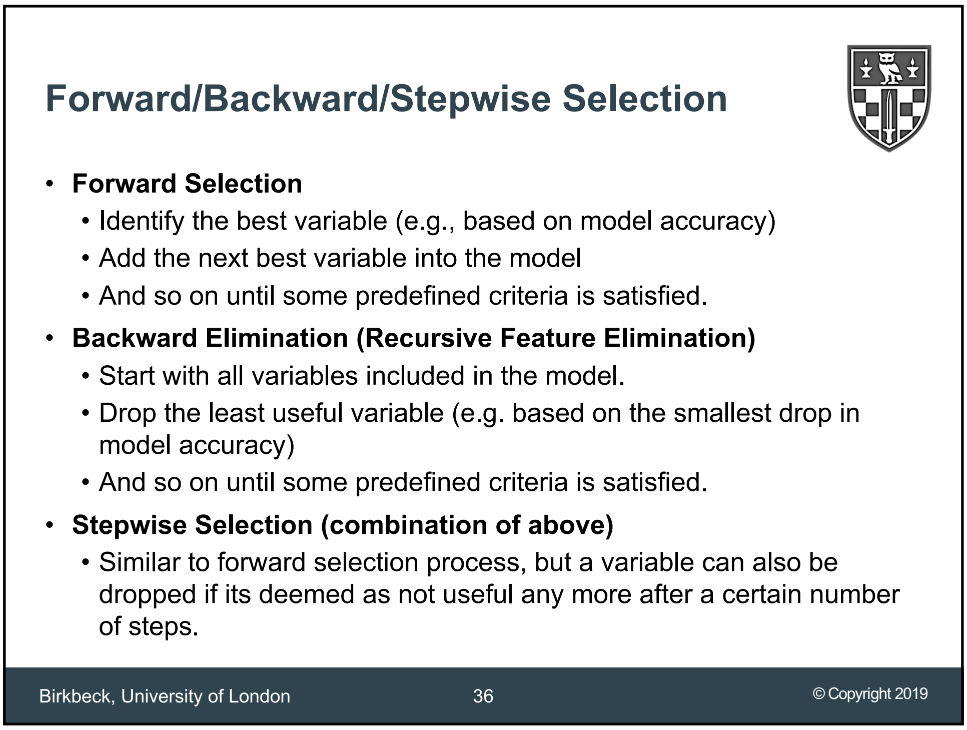
Dendrogram



Correlation with the Target

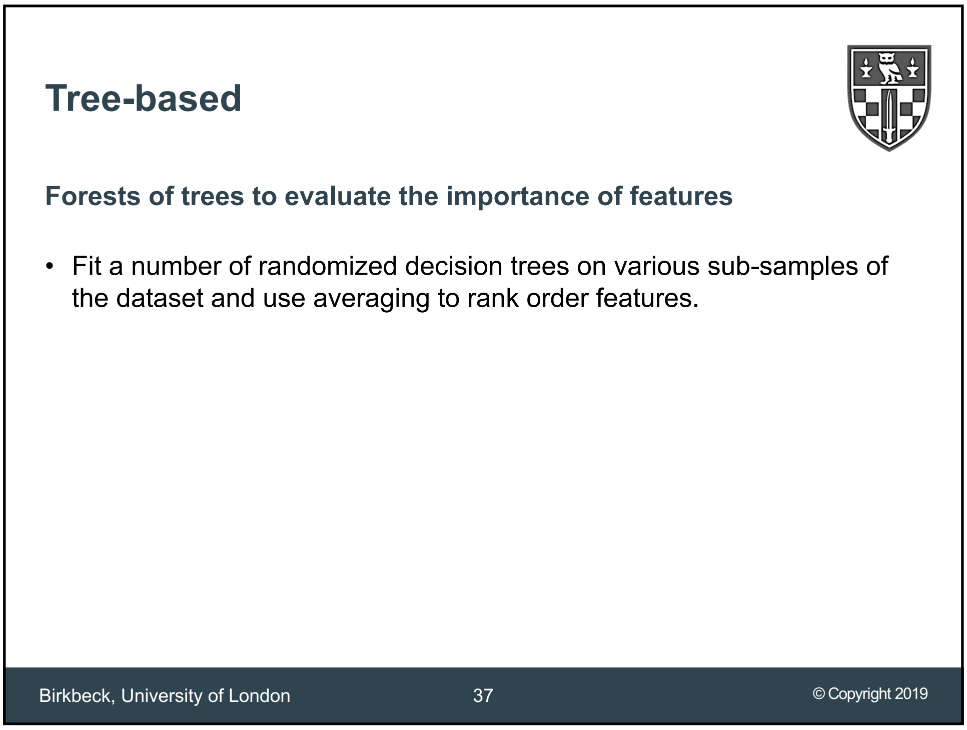
Drop variables that have a very low correlation with the target.

- If a variable has a very low correlation with the target, it’s not going to useful for the model (prediction).



Forward/Backward/Stepwise Selection

- **Forward Selection**
  - Identify the best variable (e.g., based on model accuracy)
  - Add the next best variable into the model
  - And so on until some predefined criteria is satisfied.
- **Backward Elimination (Recursive Feature Elimination)**
  - Start with all variables included in the model.
  - Drop the least useful variable (e.g. based on the smallest drop in model accuracy)
  - And so on until some predefined criteria is satisfied.
- **Stepwise Selection (combination of above)**
  - Similar to forward selection process, but a variable can also be dropped if its deemed as not useful any more after a certain number of steps.



Tree-based

Forests of trees to evaluate the importance of features

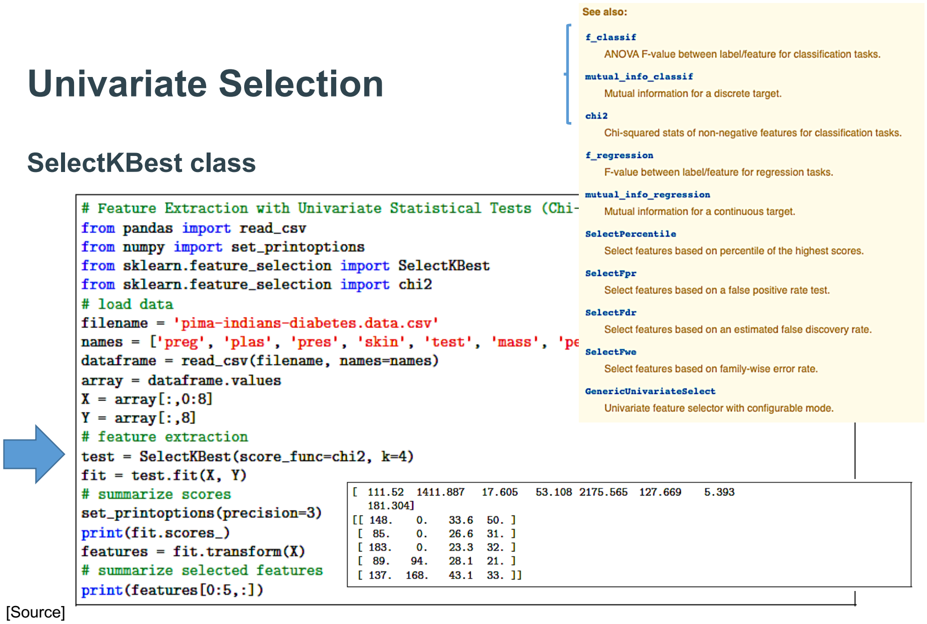
- Fit a number of randomized decision trees on various sub-samples of the dataset and use averaging to rank order features.

Labs (scikit-learn)

- Univariate Selection
- Recursive Feature Elimination
- Principal Component Analysis
- Feature Importance (Tree-based)

Univariate Selection

SelectKBest class



```
# Feature Extraction with Univariate Statistical Tests (Chi-
from pandas import read_csv
from numpy import set_printoptions
from sklearn.feature_selection import SelectKBest
from sklearn.feature_selection import chi2
# load data
filename = 'pima-indians-diabetes.data.csv'
names = ['preg', 'plas', 'pres', 'skin', 'test', 'mass', 'pe
dataframe = read_csv(filename, names=names)
array = dataframe.values
X = array[:,0:8]
Y = array[:,8]
# feature extraction
test = SelectKBest(score_func=chi2, k=4)
fit = test.fit(X, Y)
# summarize scores
set_printoptions(precision=3)
print(fit.scores_)
features = fit.transform(X)
# summarize selected features
print(features[0:5,:])
```

```
[  111.52  1411.887   17.605   53.108 2175.565  127.669    5.393
   181.304]
[[ 148.    0.    33.6   50. ]
 [  85.    0.    26.6   31. ]
 [ 183.    0.    23.3   32. ]
 [  89.   94.    28.1   21. ]
 [ 137.  168.    43.1   33. ]]
```

See also:

`f_classif`
ANOVA F-value between label/feature for classification tasks.

`mutual_info_classif`
Mutual information for a discrete target.

`chi2`
Chi-squared stats of non-negative features for classification tasks.

`f_regression`
F-value between label/feature for regression tasks.

`mutual_info_regression`
Mutual information for a continuous target.

`SelectPercentile`
Select features based on percentile of the highest scores.

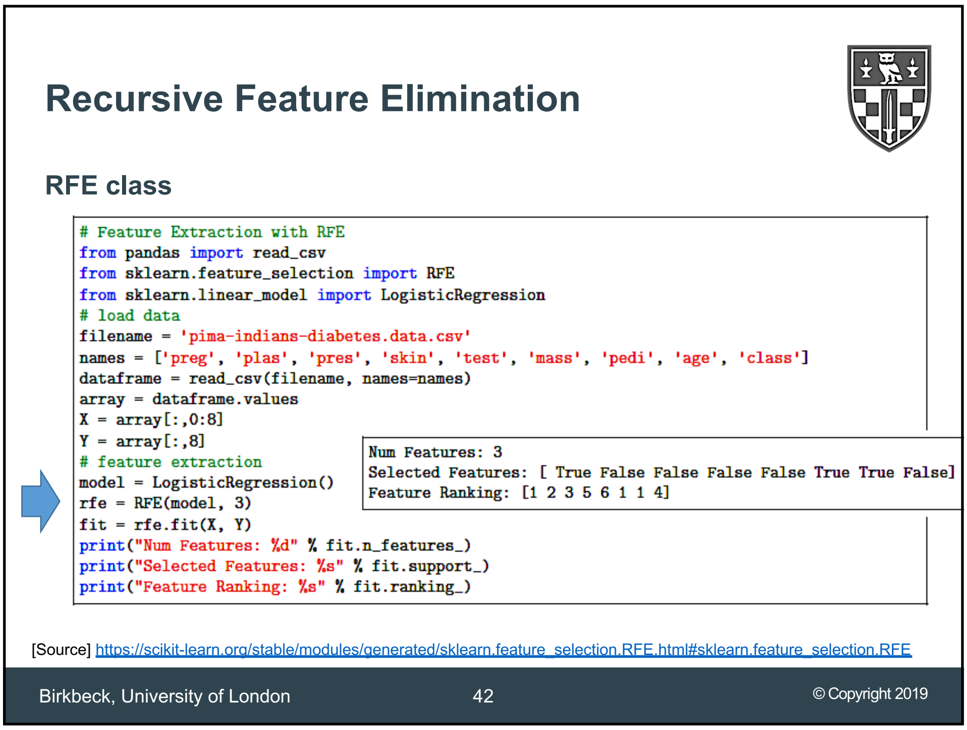
`SelectFpr`
Select features based on a false positive rate test.

`SelectFdr`
Select features based on an estimated false discovery rate.

`SelectFwe`
Select features based on family-wise error rate.

`GenericUnivariateSelect`
Univariate feature selector with configurable mode.

[Source]
https://scikit-learn.org/stable/modules/generated/sklearn.feature_selection.SelectKBest.html#sklearn.feature_selection.SelectKBest



Recursive Feature Elimination

RFE class

```
# Feature Extraction with RFE
from pandas import read_csv
from sklearn.feature_selection import RFE
from sklearn.linear_model import LogisticRegression
# load data
filename = 'pima-indians-diabetes.data.csv'
names = ['preg', 'plas', 'pres', 'skin', 'test', 'mass', 'pedi', 'age', 'class']
dataframe = read_csv(filename, names=names)
array = dataframe.values
X = array[:,0:8]
Y = array[:,8]
# feature extraction
model = LogisticRegression()
rfe = RFE(model, 3)
fit = rfe.fit(X, Y)
print("Num Features: %d" % fit.n_features_)
print("Selected Features: %s" % fit.support_)
print("Feature Ranking: %s" % fit.ranking_)
```

```
Num Features: 3
Selected Features: [ True False False False False True True False]
Feature Ranking: [1 2 3 5 6 1 1 4]
```

[Source] https://scikit-learn.org/stable/modules/generated/sklearn.feature_selection.RFE.html#sklearn.feature_selection.RFE

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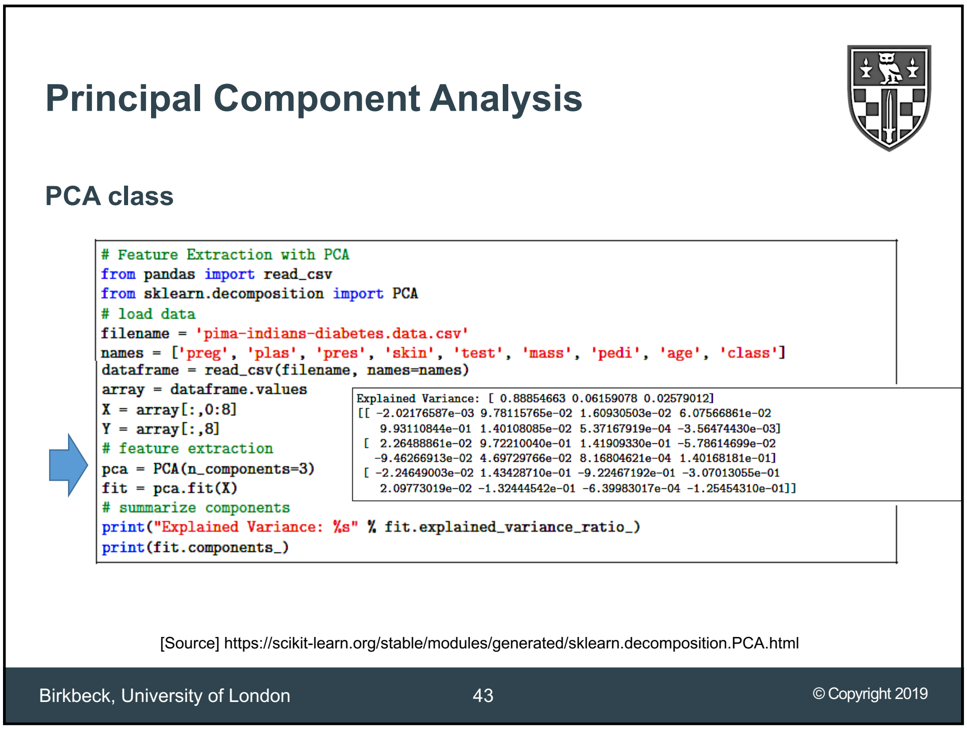

Principal Component Analysis

PCA class

```
# Feature Extraction with PCA
from pandas import read_csv
from sklearn.decomposition import PCA
# load data
filename = 'pima-indians-diabetes.data.csv'
names = ['preg', 'plas', 'pres', 'skin', 'test', 'mass', 'pedi', 'age', 'class']
dataframe = read_csv(filename, names=names)
array = dataframe.values
X = array[:,0:8]
Y = array[:,8]
# feature extraction
pca = PCA(n_components=3)
fit = pca.fit(X)
# summarize components
print("Explained Variance: %s" % fit.explained_variance_ratio_)
print(fit.components_)
```

```
Explained Variance: [ 0.88854663 0.06159078 0.02579012]
[[ -2.02176587e-03 9.78115765e-02 1.60930503e-02 6.07566861e-02
    9.93110844e-01 1.40108085e-02 5.37167919e-04 -3.56474430e-03]
 [  2.26488861e-02 9.72210040e-01 1.41909330e-01 -5.78614699e-02
   -9.46266913e-02 4.69729766e-02 8.16804621e-04 1.40168181e-01]
 [ -2.24649003e-02 1.43428710e-01 -9.22467192e-01 -3.07013055e-01
    2.09773019e-02 -1.32444542e-01 -6.39983017e-04 -1.25454310e-01]]
```

[Source] https://scikit-learn.org/stable/modules/generated/sklearn.decomposition.PCA.html

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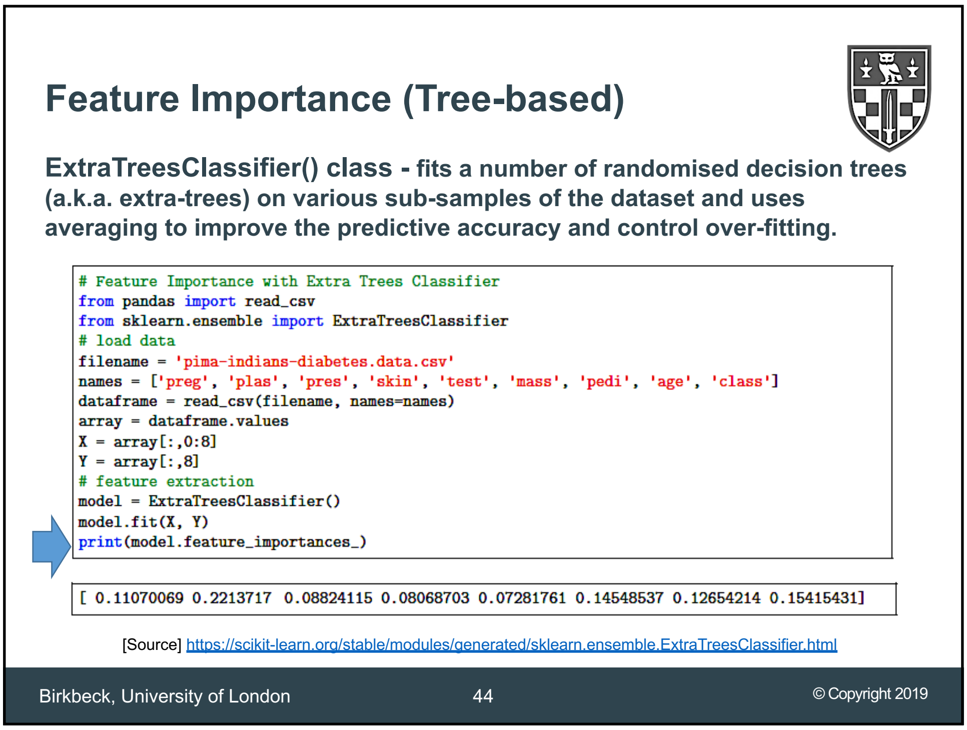

Feature Importance (Tree-based)

ExtraTreesClassifier() class - fits a number of randomised decision trees (a.k.a. extra-trees) on various sub-samples of the dataset and uses averaging to improve the predictive accuracy and control over-fitting.

```
# Feature Importance with Extra Trees Classifier
from pandas import read_csv
from sklearn.ensemble import ExtraTreesClassifier
# load data
filename = 'pima-indians-diabetes.data.csv'
names = ['preg', 'plas', 'pres', 'skin', 'test', 'mass', 'pedi', 'age', 'class']
dataframe = read_csv(filename, names=names)
array = dataframe.values
X = array[:,0:8]
Y = array[:,8]
# feature extraction
model = ExtraTreesClassifier()
model.fit(X, Y)
print(model.feature_importances_)
```

```
[ 0.11070069 0.2213717  0.08824115 0.08068703 0.07281761 0.14548537 0.12654214 0.15415431]
```

[Source] https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.ExtraTreesClassifier.html

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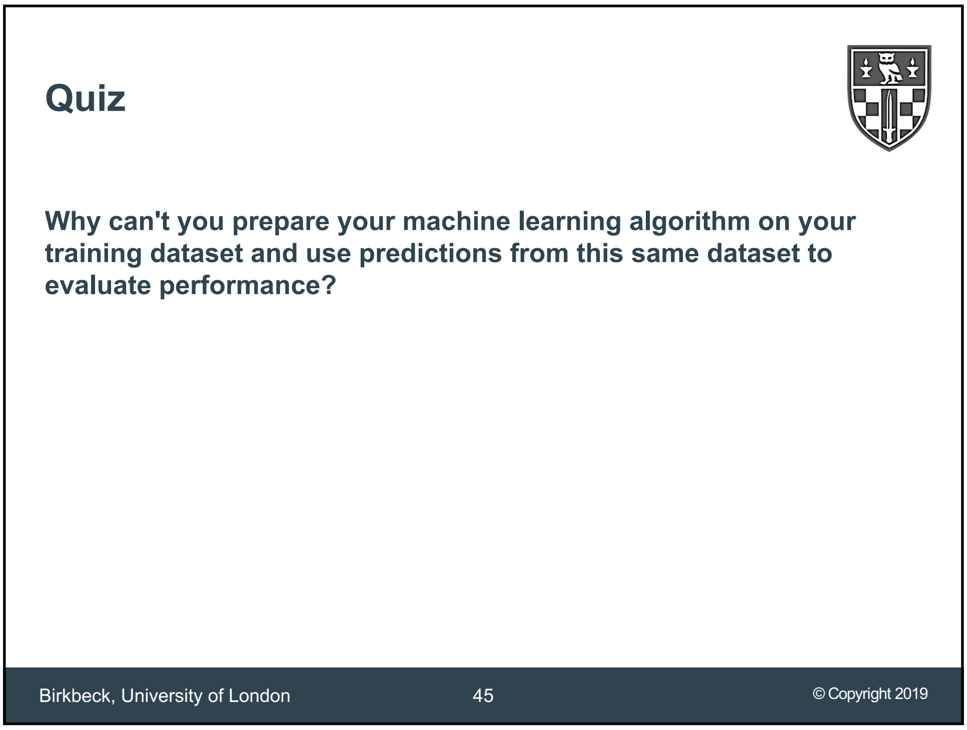

Quiz

Why can't you prepare your machine learning algorithm on your training dataset and use predictions from this same dataset to evaluate performance?

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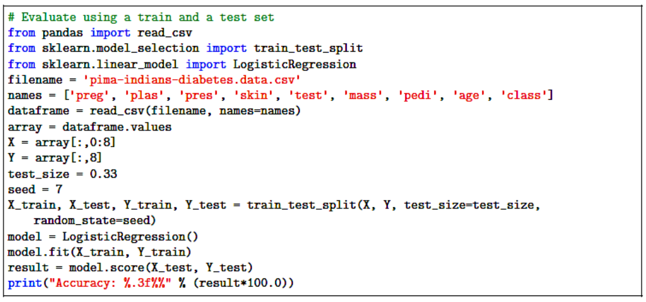
Re-sampling

- Train and Test Sets
- *k*-fold Cross Validation
- Leave One Out Cross Validation
- Repeated Random Test-Train Splits

Train and Test Sets - train_test_split class

The simplest method - train the algorithm on the first part, make predictions on the second part and evaluate the predictions against the expected results.

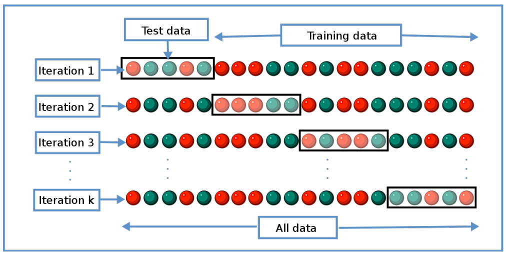
- The size of the split varies - common to use 67%/33% splits

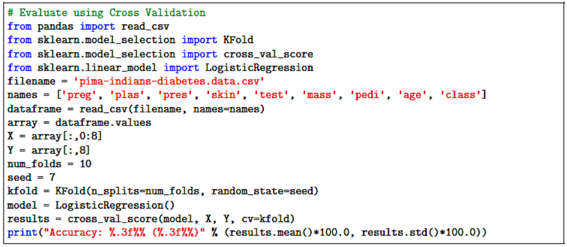


```
# Evaluate using a train and a test set
from pandas import read_csv
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LogisticRegression
filename = 'pima-indians-diabetes.data.csv'
names = ['preg', 'plas', 'pres', 'skin', 'test', 'mass', 'pedi', 'age', 'class']
dataframe = read_csv(filename, names=names)
array = dataframe.values
X = array[:,0:8]
Y = array[:,8]
test_size = 0.33
seed = 7
X_train, X_test, Y_train, Y_test = train_test_split(X, Y, test_size=test_size,
    random_state=seed)
model = LogisticRegression()
model.fit(X_train, Y_train)
result = model.score(X_test, Y_test)
print("Accuracy: %.3f%%" % (result*100.0))
```

k-Fold Cross Validation

Kfold class - Cross-validation is an approach that you can use to estimate the performance of a ML algorithm with less variance than a single train-test set split.





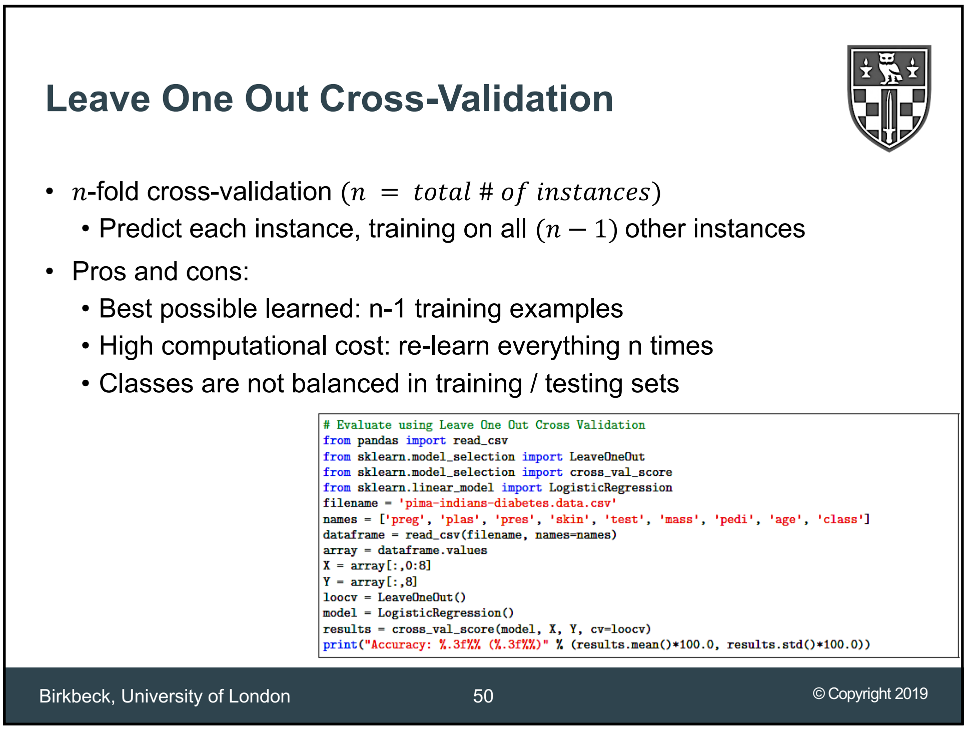
```
# Evaluate using Cross Validation
from pandas import read_csv
from sklearn.model_selection import KFold
from sklearn.model_selection import cross_val_score
from sklearn.linear_model import LogisticRegression
filename = 'pima-indians-diabetes.data.csv'
names = ['preg', 'plas', 'pres', 'skin', 'test', 'mass', 'pedi', 'age', 'class']
dataframe = read_csv(filename, names=names)
array = dataframe.values
X = array[:,0:8]
Y = array[:,8]
num_folds = 10
seed = 7
kfold = KFold(n_splits=num_folds, random_state=seed)
model = LogisticRegression()
results = cross_val_score(model, X, Y, cv=kfold)
print("Accuracy: %.3f%% (%.3f%%)" % (results.mean()*100.0, results.std()*100.0))
```

Sample mean $\overline{x} = \dfrac{\Sigma\, x_i}{n}$

Variance $\sigma^2 = \dfrac{\Sigma\,(x_i - \overline{x})^2}{n-1}$

Standard deviation σ

holdout (10%)	cross-validation (10-fold)
75.3	73.8
77.9	75.0
80.5	75.5
74.0	75.5
71.4	74.4
70.1	75.6
79.2	73.6
71.4	74.0
80.5	74.5
67.5	73.0
$\overline{x}$ = 74.8	$\overline{x}$ = 74.5
σ = 4.6	σ = 0.9



Leave One Out Cross-Validation

- n-fold cross-validation ($n = total\ \#\ of\ instances$)
  - Predict each instance, training on all $(n-1)$ other instances
- Pros and cons:
  - Best possible learned: n-1 training examples
  - High computational cost: re-learn everything n times
  - Classes are not balanced in training / testing sets

```
# Evaluate using Leave One Out Cross Validation
from pandas import read_csv
from sklearn.model_selection import LeaveOneOut
from sklearn.model_selection import cross_val_score
from sklearn.linear_model import LogisticRegression
filename = 'pima-indians-diabetes.data.csv'
names = ['preg', 'plas', 'pres', 'skin', 'test', 'mass', 'pedi', 'age', 'class']
dataframe = read_csv(filename, names=names)
array = dataframe.values
X = array[:,0:8]
Y = array[:,8]
loocv = LeaveOneOut()
model = LogisticRegression()
results = cross_val_score(model, X, Y, cv=loocv)
print("Accuracy: %.3f%% (%.3f%%)" % (results.mean()*100.0, results.std()*100.0))
```

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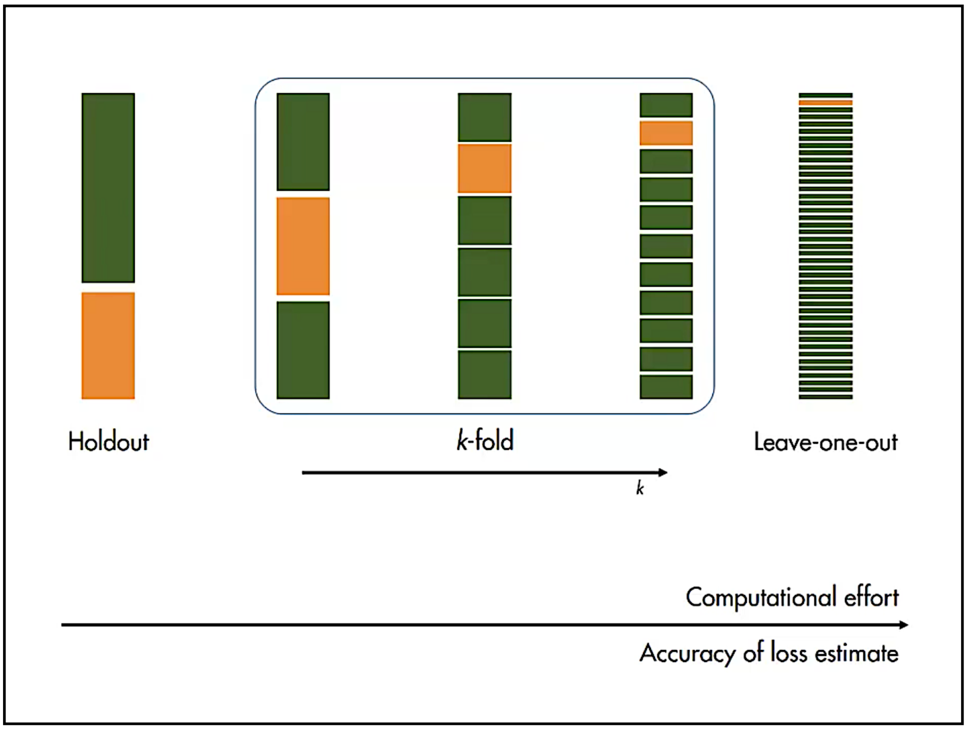

Holdout

k-fold

k

Leave-one-out

Computational effort

Accuracy of loss estimate

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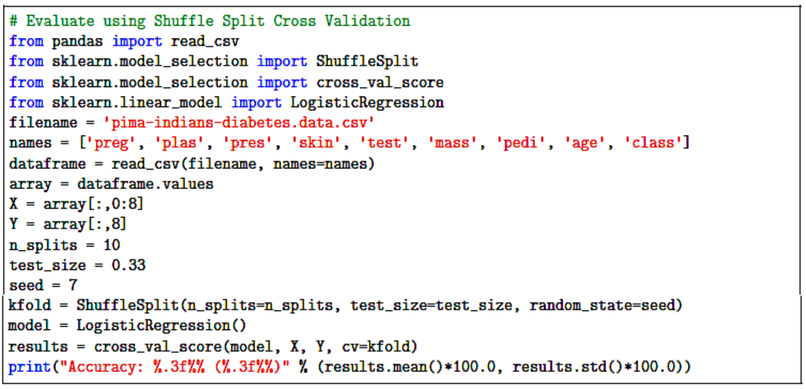
Repeated Random Test-Train Splits

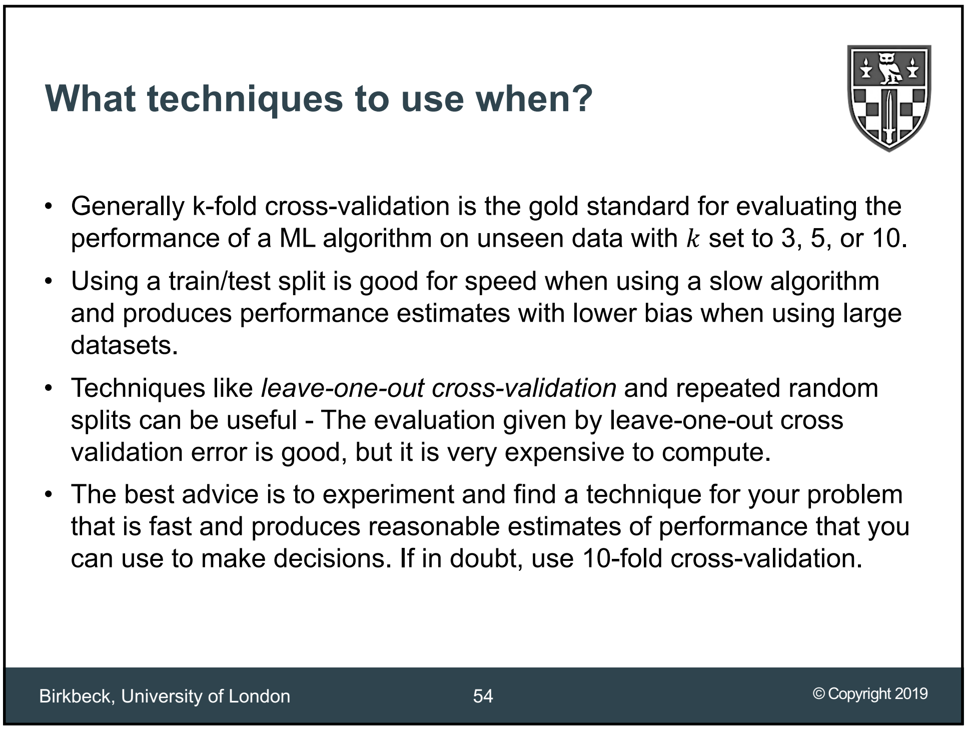
Create a random split of the data like the train/test split, but repeat the process of splitting and evaluation of the algorithm multiple times, like CV.

- Pros and cons:
  - the reduction in variance in the estimated performance of k-fold cross-validation.
  - repeat the process many more times as needed to improve the accuracy.
  - repetitions may include much of the same data in the train or the test split from run to run - introducing redundancy into the evaluation.

Repeated Random Test-Train Splits



```
# Evaluate using Shuffle Split Cross Validation
from pandas import read_csv
from sklearn.model_selection import ShuffleSplit
from sklearn.model_selection import cross_val_score
from sklearn.linear_model import LogisticRegression
filename = 'pima-indians-diabetes.data.csv'
names = ['preg', 'plas', 'pres', 'skin', 'test', 'mass', 'pedi', 'age', 'class']
dataframe = read_csv(filename, names=names)
array = dataframe.values
X = array[:,0:8]
Y = array[:,8]
n_splits = 10
test_size = 0.33
seed = 7
kfold = ShuffleSplit(n_splits=n_splits, test_size=test_size, random_state=seed)
model = LogisticRegression()
results = cross_val_score(model, X, Y, cv=kfold)
print("Accuracy: %.3f%% (%.3f%%)" % (results.mean()*100.0, results.std()*100.0))
```



What techniques to use when?

- Generally k-fold cross-validation is the gold standard for evaluating the performance of a ML algorithm on unseen data with k set to 3, 5, or 10.
- Using a train/test split is good for speed when using a slow algorithm and produces performance estimates with lower bias when using large datasets.
- Techniques like *leave-one-out cross-validation* and repeated random splits can be useful - The evaluation given by leave-one-out cross validation error is good, but it is very expensive to compute.
- The best advice is to experiment and find a technique for your problem that is fast and produces reasonable estimates of performance that you can use to make decisions. If in doubt, use 10-fold cross-validation.

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Questions?

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