Introduction to Data Science

JP-Morgan workshop

CAMBRIDGE SPARK

@cambridgespark

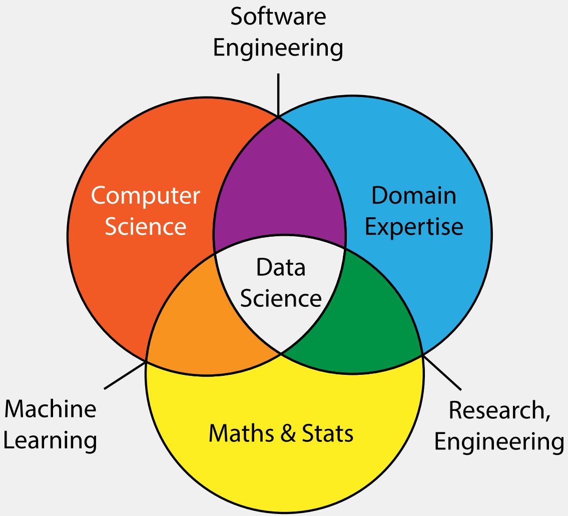
Schedule

- Exploratory Data Analysis (EDA) in Jupyter with Pandas
- Classification methods and the Decision Tree
- Ensemble methods and the Random Forest
- Competition!

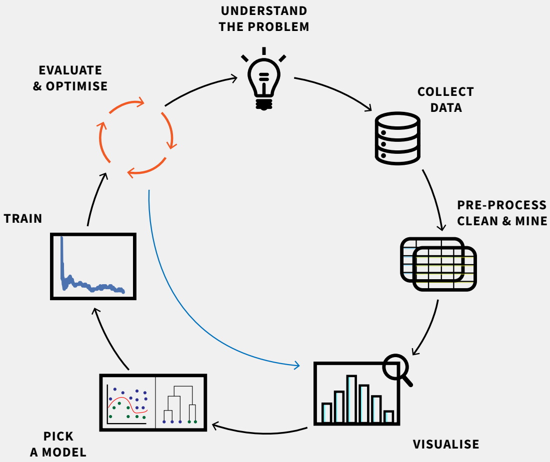
Organisation

- work in pairs on the notebooks
- if you get stuck, ask us and look at the solutions (but try first!)
- if you're ahead, look things up, ask for pointers

Data Science: bridging fields



Data analysis wheel



Jupyter

Starting Jupyter

In the Terminal or Anaconda Prompt:

```
$> jupyter notebook
```

(demo)

⚠️ Get the initial path right…

Jupyter is awesome : doc and tab completion

Most important tools:

- Execute a cell: `SHIFT+ENTER`
- Get documentation about `command`: `?command`
- `TAB` completion

(demo)

Other useful commands

Command mode is triggered by pressing `ESC`. Then:

- `A` or `B`, add new cell before or after current cell
- `M` or `Y`, interpret current cell as a markdown cell or as a code cell (default)
- `D` $\times$2, delete current cell

(demo)

Pandas

Pandas , the “excel” of Python

- huge userbase, someone else has asked your question before

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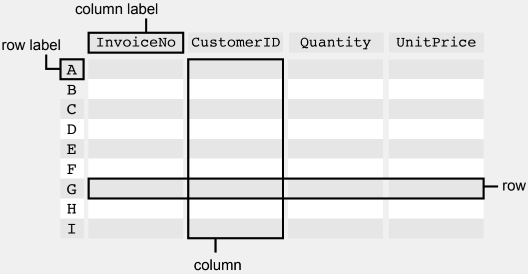
- today, the basics: loading data, basic manipulations, …
- central class: `DataFrame`

Anatomy of a pandas dataframe



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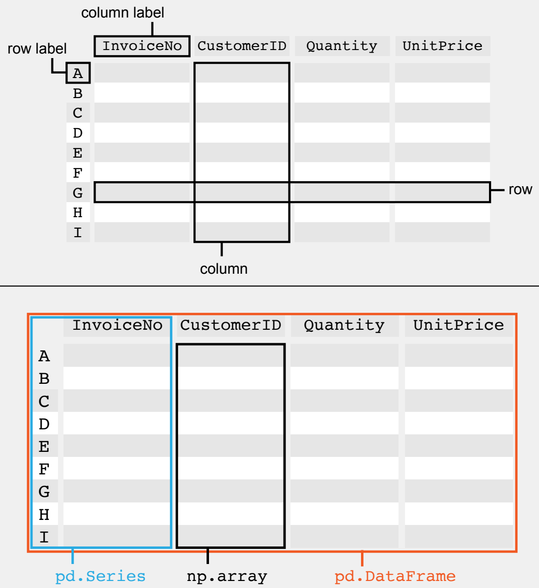

Loading a data file

```python
import pandas as pd
df = pd.read_csv(fpath, ...)
df.head()
```

Many options:

- `sep`, `header`, `index_col`,...
- remember to use `?`, Pandas documentation is excellent

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Writing a `DataFrame` is easy too

```
df.to_csv(fpath)
```

Accessing elements in a `DataFrame`

Accessing one of the column by name:

```
series = df[colname]    # returns a pd.Series object
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```

Accessing elements using row/column names `loc()` :

```
val = df.loc[10, [c for c in df.columns if 'le' in c]]
```

`pandas.Series`: `np.array` with a plus

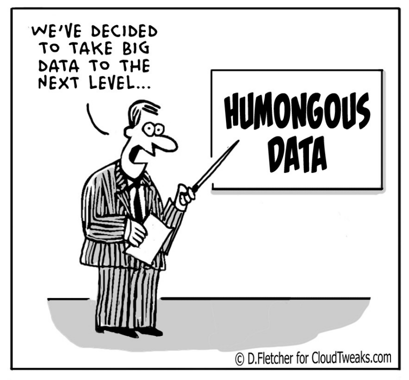
- “Wrapped around” a numpy vector
- Useful methods attached: `unique()`, `max()`, `median()`, ...
- Useful attributes: `hasnans`, `index`, `shape`, ...

Hands-on session

>>> Accessing elements in a `DataFrame`

Feature Engineering

Garbage in, garbage out, ...



"Humongous data" is no substitute for good pre-processing and feature engineering .

Feature engineering is essential

*Coming up with features is difficult, time consuming, requires **expert knowledge**. "Applied machine learning" is basically feature engineering*

– Andrew Ng

Data comes in many shapes and sizes

Features can be

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- categorical (may or may not be ordinal)

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Encoding categorical data: one-hot-encoding

	Gender
0	Male
1	Female
2	Not Specified
3	Not Specified
4	Female

	Female	Male	Not Specified
0	0	1	0
1	1	0	0
2	0	0	1
3	0	0	1
4	1	0	0

A few more useful tricks with Pandas

- `pd.describe()` summary statistics
- `drop` to remove row(s) or column(s)
- `groupby`, `apply`, (next slide)

`groupby` followed by `apply`

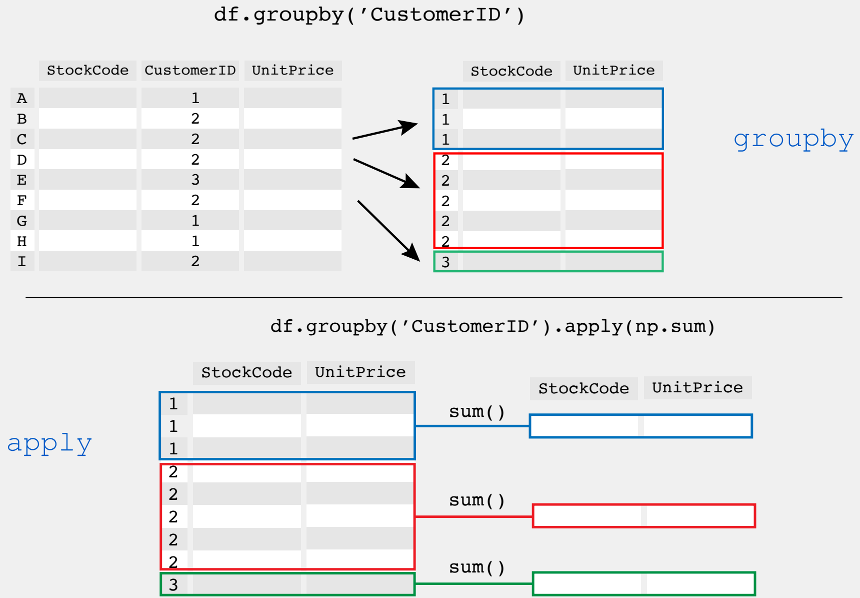
```
df.groupby('CustomerID')
```

	StockCode	CustomerID	UnitPrice
A		1	
B		2	
C		2	
D		2	
E		3	
F		2	
G		1	
H		1	
I		2	

	StockCode	UnitPrice
1		
1		
1		
2		
2		
2		
2		
2		
3		

`groupby`

groupby followed by apply



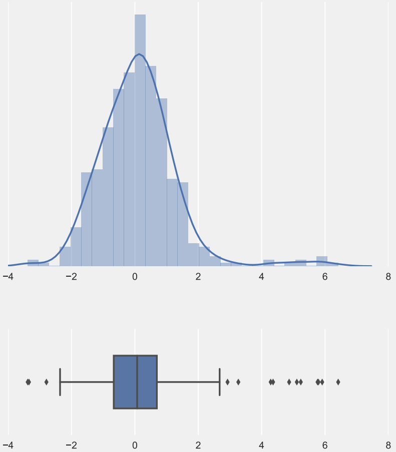
Hands-on session

>>> Load the retail data set, explore the features.

Preprocessing the data: the important steps

- Selection and Encoding : get rid of nonsensical variables, encode ordinal variables (e.g.: OHE)
- Outliers and Imputation : what to do with rows with extreme values? and with missing values?
- Scaling : weigh features equally (*if your model is sensitive to scaling*)

Dealing with outliers , no silver bullet



- get rid of them?
- focus on them?
- how to decide which are *really* “outliers”?

Dealing with missing values, no silver bullet

What are the pros/cons of the following approaches?

- remove observations (rows) with missing values

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Dealing with missing values, no silver bullet

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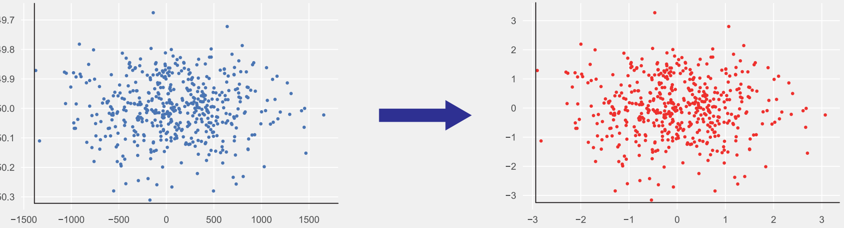
- remove observations (rows) with missing values
- remove features (columns) with missing values
- replace missing values with
  - column mean, median or mode
  - something else

Scaling : putting features on a comparable scale



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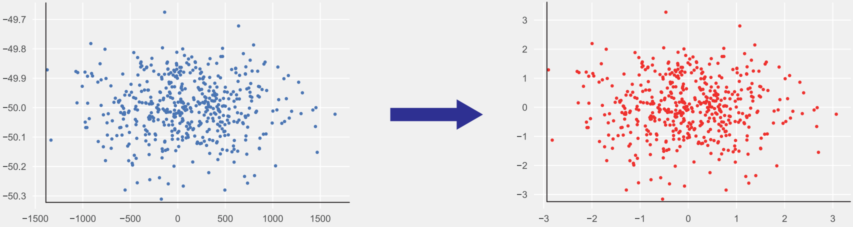
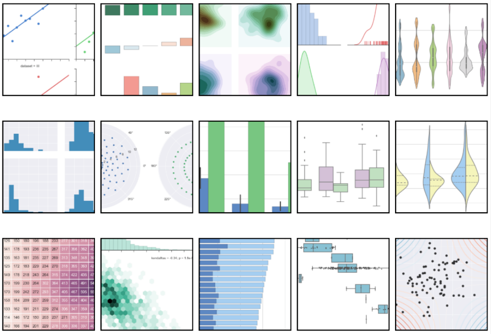


Typically, we use the standard scaler but you could also use the `MinMax` scaler (all values on [0, 1]).

Visualising data



- What data do I want to plot?
- What type of plot is suitable?
- How to convey a message with a plot?

Hands-on session

>>> Check for missing values, impute if necessary, remove outliers, visualise and scale

Machine Learning

Unsupervised vs. Supervised learning

Unsupervised Learning

- Data points x_i in feature space with p dimensions
- Aim = visualise points or group points based on similarity

Supervised Learning

- Data points x_i **and** response y_i (usually a single value)
- Eg: a transaction and whether it’s fraud or not
- Aim = model how $x_i \mapsto y_i$

Building a supervised model

You can represent the data you have as coming from a hidden function *f* (“nature”)

$$\text{x} \quad \rightarrow \quad f(x) = y$$

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$$\mathrm{x} \quad \rightarrow \quad f(x) = y$$

The aim is to build a model $\widehat{f}$ which approximates f:

$$\mathrm{x} \quad \rightarrow \quad \widehat{f}(x) \approx f(x)$$

Training and testing a model

Workflow:

TRAINING Consider some of the data (= training data):
build a model $\widehat{f}$ which works well on it

TESTING Consider the **rest** of the data (= test data):
check how $\widehat{f}$ is doing on that

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⚠ The test data **must be distinct** from the training data in order to assess how the model generalises

Training and testing: the cases

- good on training, poor on testing $\rightarrow$ **overfitting**
- poor on training, poor on testing $\rightarrow$ **underfitting**
- good on training, good on testing $\rightarrow$ good sign

more about this later, now how do we build a model!?

Classification vs Regression

Classification (what you will learn):

- Training data : $(\texttt{point}, \texttt{class})_i$
- **ex**. *Fraud detection*: $(\texttt{email}, \texttt{0/1})_i$

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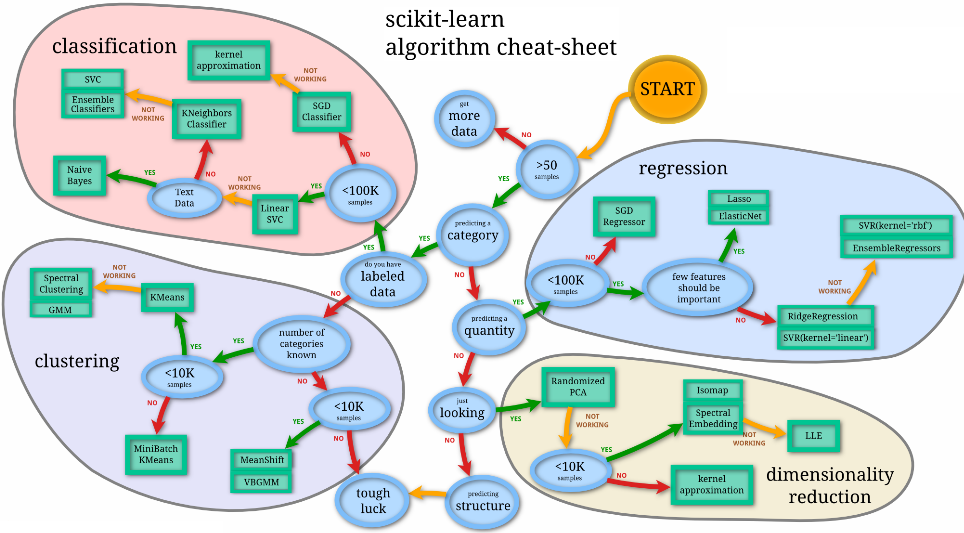
Regression:

- Training data : $(\texttt{point}, \texttt{value})_i$
- **ex**. *Salary prediction*: $(\texttt{characteristics}, \texttt{salary})_i$


scikit-learn
algorithm cheat-sheet
START
classification
kernel approximation
SVC
Ensemble Classifiers
KNeighbors Classifier
SGD Classifier
Naive Bayes
Text Data
Linear SVC
<100K samples
NOT WORKING
YES
NO
get more data
>50 samples
predicting a category
do you have labeled data
regression
SGD Regressor
Lasso
ElasticNet
SVR(kernel='rbf')
EnsembleRegressors
<100K samples
few features should be important
RidgeRegression
SVR(kernel='linear')
predicting a quantity
clustering
Spectral Clustering
GMM
KMeans
number of categories known
<10K samples
MiniBatch KMeans
MeanShift
VBGMM
just looking
predicting structure
tough luck
dimensionality reduction
Randomized PCA
Isomap
Spectral Embedding
LLE
kernel approximation

Testing a binary classifier

On the test data, compare the predicted responses $\hat{y}_i = \widehat{f}(x_i)$ to the actual response y_i:

		PREDICTED	
		Positive	Negative
ACTUAL	Positive	TP	FN
	Negative	FP	TN

- jargon from clinical trials, positive/negative defined by context
- this is the confusion matrix

Testing a binary classifier 2

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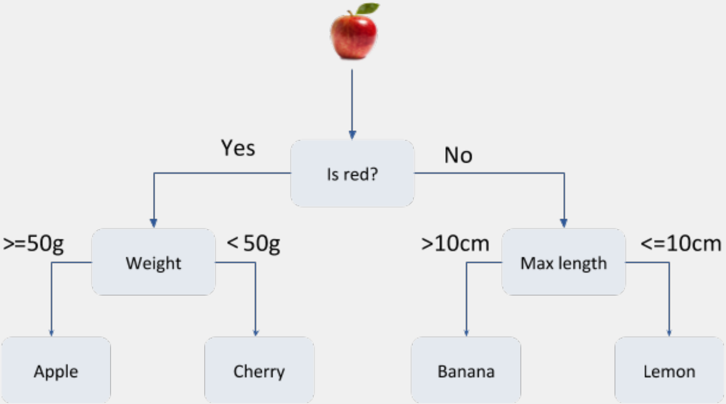
- Accuracy : $\frac{TP+TN}{N}$, sensitivity/recall : $\frac{TP}{TP+FN}, \ldots$
- metric of importance usually dictated by *context*. In fraud:
  - + flagging a clean transaction as fraudulent (ok)
  - - not flagging a fraudulent transaction (bad)

Decision Trees

Decision trees



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Once a DTC is adjusted, classification is trivial: just follow the tree!

When to stop splitting?

- Pick a maximum depth
- Otherwise, get one sample per “leaf node” $\rightarrow$ overfitting (one decision path for every single sample)

Hands-on session

>>> Decision trees

Decision trees, recap

+ Very easy model to interpret
+ No need to normalise data and it handles ordinal/boolean data
- Propensity to overfit

Ensemble models

Getting the intuition

Say you have a set of symptoms and you go see two doctors…

- Doctor A has 60% chance of providing an accurate diagnostic
- Doctor B has 75% chance of providing an accurate diagnostic

Both say you have X. *How confident are you about the diagnostic and why?*

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Both say you have X. *How confident are you about the diagnostic and why?*

How about if you added 5 other doctors to the mix?

Key elements of ensembles

For ensembles to work, the following properties must be met:

- weak learner : any single expert need to be more right than wrong on average ($>$ 50% accurate)

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Multiple ways of *aggregating*, simplest: majority voting .

How about doing that with decision trees?

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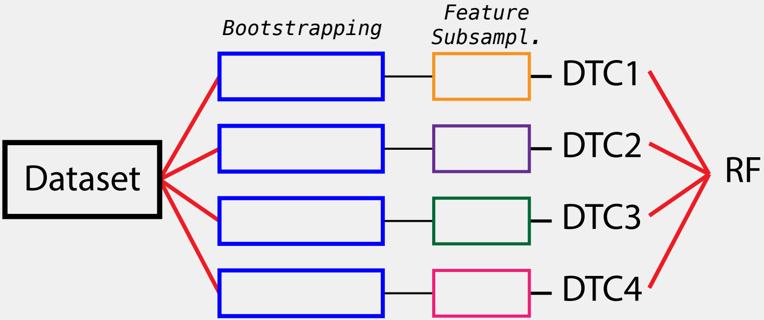
You know that fitting a DTC is easy. How can you come up with a lot of diverse trees?

1. create statistically similar datasets, train a DTC on each
2. only consider a random subset of the features when training


Bootstrapping
Feature
Subsampl.
Dataset
DTC1
DTC2
DTC3
DTC4
RF

Creating statistically similar datasets

- a sample drawn uniformly at random from the dataset will have similar statistical properties (mean, variance, …)

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- this can be done in parallel

Feature subsampling

- If there is a dominant feature, it will likely be selected every time as root on most bootstrapped datasets $\rightarrow$ correlation .

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- If there is a dominant feature, it will likely be selected every time as root on most bootstrapped datasets $\rightarrow$ correlation .
- Randomly selecting a smaller set of features helps avoiding this $\rightarrow$ diversity while reducing correlation.

Ensemble models recap

- aggregate output of multiple weak learners that are diverse will increase the accuracy

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- random forest = many decision trees. Diversity by bootstrapping the data and random subsampling of the features.

The Competition

Tips for the competition

- groups of 2 or 3
- start simple, make it work
- tune it, try more things, repeat
- you can ask us for *technical help* but not for *advice*

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⚠ Make sure to **test** your model (`tester.py`) before submission.