

# Python for scientific research

## Advanced topics

John Joseph Valletta

University of Exeter, Penryn Campus, UK

June 2017



Researcher  
Development



`statsmodels` is a package for the estimation of different statistical models

```
import statsmodels.api as sm
import statsmodels.formula.api as smf

# Read Boston housing data set (a Pandas data frame)
df = sm.datasets.get_rdataset("Boston", "MASS").data
df.head()
```

|   | crim    | zn   | indus | chas | nox   | rm    | age  | dis    | rad | tax | ptratio | \ |
|---|---------|------|-------|------|-------|-------|------|--------|-----|-----|---------|---|
| 0 | 0.00632 | 18.0 | 2.31  | 0    | 0.538 | 6.575 | 65.2 | 4.0900 | 1   | 296 | 15.3    |   |
| 1 | 0.02731 | 0.0  | 7.07  | 0    | 0.469 | 6.421 | 78.9 | 4.9671 | 2   | 242 | 17.8    |   |
| 2 | 0.02729 | 0.0  | 7.07  | 0    | 0.469 | 7.185 | 61.1 | 4.9671 | 2   | 242 | 17.8    |   |
| 3 | 0.03237 | 0.0  | 2.18  | 0    | 0.458 | 6.998 | 45.8 | 6.0622 | 3   | 222 | 18.7    |   |
| 4 | 0.06905 | 0.0  | 2.18  | 0    | 0.458 | 7.147 | 54.2 | 6.0622 | 3   | 222 | 18.7    |   |

|   | black  | lstat | medv |
|---|--------|-------|------|
| 0 | 396.90 | 4.98  | 24.0 |
| 1 | 396.90 | 9.14  | 21.6 |
| 2 | 392.83 | 4.03  | 34.7 |
| 3 | 394.63 | 2.94  | 33.4 |
| 4 | 396.90 | 5.33  | 36.2 |

# Statsmodels: Generalised linear model

```
# Dependent variable
# medv - median value of owner-occupied homes in $1000's

# Covariates
# crim - per capita crime rate by town
# nox - nitric oxides concentration (parts per 10 million)
# rm - average number of rooms per dwelling
# indus - proportion of non-retail business acres per town.
# rad - index of accessibility to radial highways

# Set up model
model = smf.glm(formula="medv ~ crim + nox + rm + indus + rad",
                 family=sm.families.Gaussian(),
                 data=df)

# Fit model
model = model.fit()
```

# Statsmodels: Generalised linear model

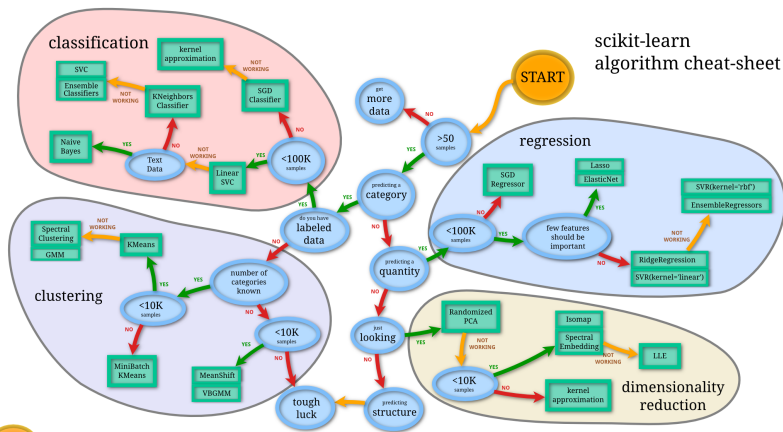
```
# Show summary
model.summary()
```

## Generalized Linear Model Regression Results

```
=====
Dep. Variable:          medv    No. Observations:          506
Model:                  GLM      Df Residuals:              500
Model Family:           Gaussian Df Model:                  5
Link Function:           identity Scale:                36.7202989747
Method:                  IRLS    Log-Likelihood:         -1626.6
Date:                   Tue, 30 May 2017 Deviance:             18360.
Time:                   15:00:23    Pearson chi2:           1.84e+04
No. Iterations:          2
=====
```

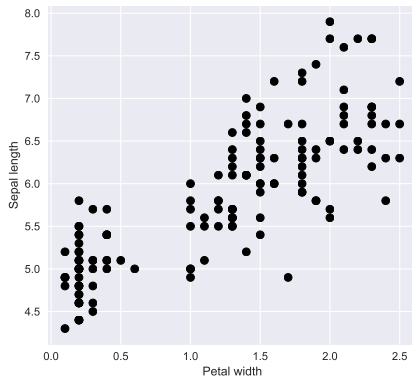
```
=====
              coef      std err          z      P>|z|      [0.025      0.975]
-----
Intercept    -19.9794      3.267      -6.115      0.000     -26.383     -13.576
crim          -0.1608      0.040      -3.973      0.000      -0.240      -0.081
nox           -5.7432      3.784      -1.518      0.129     -13.160       1.674
rm             7.7004      0.420      18.353      0.000       6.878      8.523
indus         -0.1361      0.065      -2.089      0.037      -0.264      -0.008
rad           -0.0628      0.047      -1.342      0.179      -0.154       0.029
=====
```

**sklearn** is a package for machine learning algorithms



```
from sklearn import datasets

# Load popular iris data set
iris = datasets.load_iris()
xTrain = iris.data # petal/sepal width/length
yTrain = iris.target
```

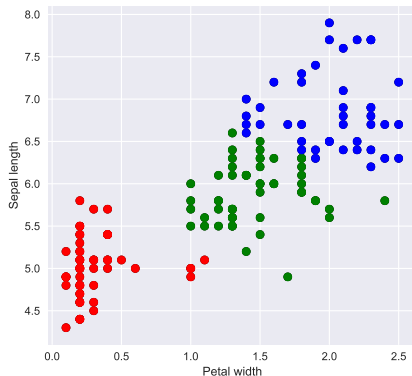


# Scikit-learn: k-means clustering

```
from sklearn.cluster import KMeans

# Set up k-means clustering model
model = KMeans(n_clusters=3)

# Fit model with supplied data (unsupervised)
model.fit(xTrain)
```



# Scikit-learn: Random forests

```
from sklearn.ensemble import RandomForestClassifier

# Set up Random Forest model
model = RandomForestClassifier(n_estimators=500, oob_score=True)

# Fit model with supplied data (supervised)
model.fit(xTrain, yTrain)
```

| Confusion Matrix |        |            |           |
|------------------|--------|------------|-----------|
| Actual label     | Setosa | Versicolor | Virginica |
|                  | 50     | 0          | 0         |
|                  | 0      | 47         | 3         |
|                  | 0      | 6          | 44        |
|                  | Setosa | Versicolor | Virginica |
| Predicted label  |        |            |           |



# Networkx

`networkx` is a package for the creation, manipulation, and study of the structure, dynamics, and functions of complex networks

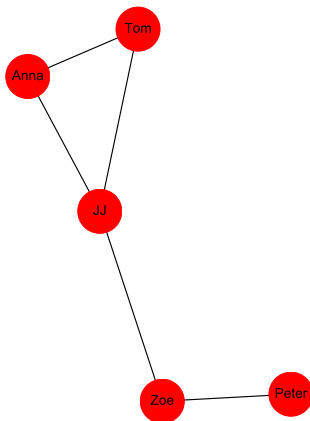
```
import networkx as nx

# Creating a new empty Graph object
g = nx.Graph()

# Adding nodes
g.add_nodes_from(["Tom", "Zoe",
                  "JJ", "Anna", "Peter"])

# Adding an edge
g.add_edge("JJ", "Zoe")
g.add_edge("JJ", "Anna")
g.add_edge("JJ", "Tom")
g.add_edge("Peter", "Zoe")
g.add_edge("Tom", "Anna")

# Draw network
nx.draw(g, node_size=1500,
        with_labels=True)
```

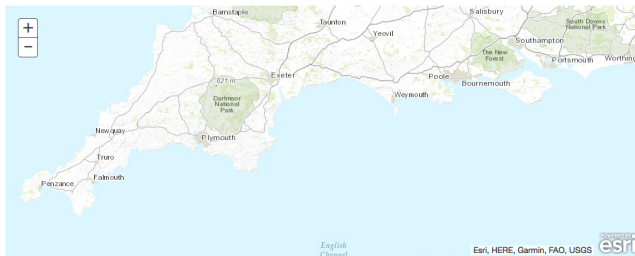


`arcgis` is a package for GIS visualisation and analysis, spatial data management and GIS system administration tasks

```
from arcgis.gis import GIS

# Create a GIS object (anonymous user)
gis = GIS()

# Get map of Cornwall
myMap = gis.map("Cornwall, UK")
myMap
```



**mygene** provides web services to query/retrieve gene annotation data from **MyGene.info**

```
import mygene

# Instantiate MyGeneInfo class
mg = mygene.MyGeneInfo()

# Query for the name and EnsemblID of genes Ifng and Ccl3
mg.querymany(qterms=["Ifng", "Ccl3"], scopes="symbol",
             fields=["name", "ensembl"], species="human")

[{'_id': '3458',
  '_score': 98.66912,
  'ensembl': {'gene': 'ENSG00000111537',
             'protein': 'ENSP00000229135',
             'transcript': 'ENST00000229135',
             'translation': [{'protein': 'ENSP00000229135', 'rna': 'ENST00000229135'}]},
  'name': 'interferon gamma',
  'query': 'Ifng'},
....
....
....]
```

`tweepy` provides access to Twitter for posting/reading tweets

How about analysing tweets from **Mr President**?

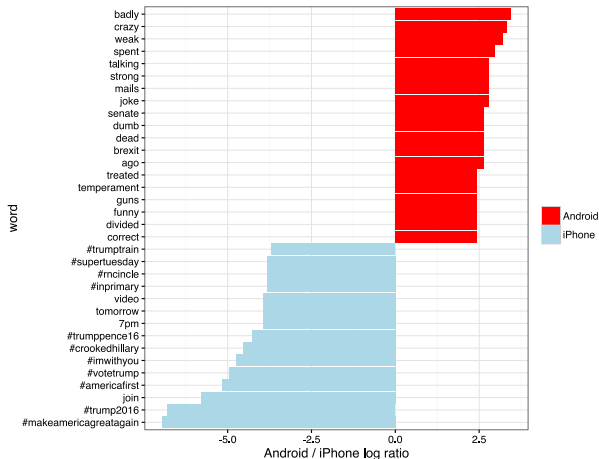


Image taken from [here](#) (analysis done in R)