Python for scientific research

Data analysis with `pandas`

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What we’ve done so far

1. Declare variables using built-in data types and execute operations on them
2. Use flow control commands to dictate the order in which commands are run and when
3. Encapsulate programs into reusable functions, modules and packages
4. Use string manipulation and regex to work with textual data
5. Interact with the file system
6. Number crunching using `NumPy/SciPy`
7. Publication-ready graphs with `Matplotlib`
8. **Next:** working with data using `pandas`

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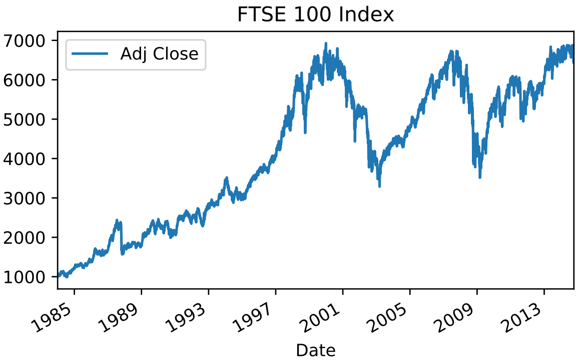
- . . .

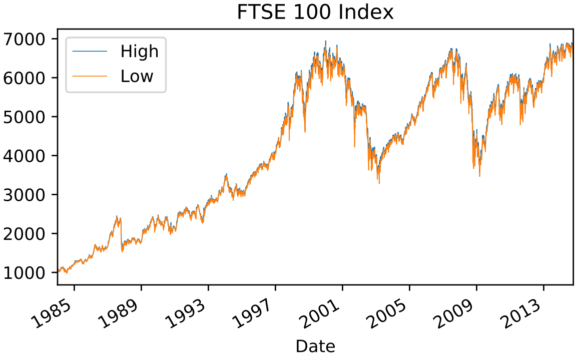
Pandas data structures

1. Series
   - A one dimensional object
   - Similar to a list or array
   - Each entry has a unique index
   - Useful for time-series analysis



Pandas data structures

2. DataFrame
   - A two dimensional object to store data
   - Like a spreadsheet with rows and columns (akin to R's data.frame)
   - Each column is a Pandas Series
   - Each row has a unique index
   - Useful for any kind of data wrangling and analysis



Create a DataFrame

```python
import pandas as pd

df = pd.DataFrame(
        {"Sample" : ["R100" , "R201", "R203", "R340", "R453"],
         "t0" : [0.2, 0.1, 0.3, 0.25, 0.13],
         "t1" : [1.3, 1.8, 0.8, 1.5, 0.6],
         "t2" : [2.8, 3.1, 1.9, 2.3, 1.8],
         "t3" : [3.2, 3.7, 2.3, 3.5, 2.5],
         "t4" : [1.2, 1.8, 3.9, 1.3, 3.7],
         "t5" : [0.7, 0.4, 3.4, 0.3, 3.6]})

df.shape # return size of data set (5, 7)
```

```
  Sample    t0   t1   t2   t3   t4   t5
0   R100  0.20  1.3  2.8  3.2  1.2  0.7
1   R201  0.10  1.8  3.1  3.7  1.8  0.4
2   R203  0.30  0.8  1.9  2.3  3.9  3.4
3   R340  0.25  1.5  2.3  3.5  1.3  0.3
4   R453  0.13  0.6  1.8  2.5  3.7  3.6
```

Reshaping data

```
# Gather time columns [t0,...,t5] into rows
df = pd.melt(df,
             id_vars="Sample",
             var_name="Time",
             value_name="Exprs")
```

```
   Sample Time  Exprs
0    R100   t0   0.20
1    R201   t0   0.10
2    R203   t0   0.30
3    R340   t0   0.25
4    R453   t0   0.13
5    R100   t1   1.30
6    R201   t1   1.80
7    R203   t1   0.80
8    R340   t1   1.50
9    R453   t1   0.60
10   R100   t2   2.80
11   R201   t2   3.10
12   R203   t2   1.90
13   R340   t2   2.30
14   R453   t2   1.80
15   R100   t3   3.20
16   R201   t3   3.70
17   R203   t3   2.30
18   R340   t3   3.50
19   R453   t3   2.50
20   R100   t4   1.20
21   R201   t4   1.80
22   R203   t4   3.90
23   R340   t4   1.30
24   R453   t4   3.70
25   R100   t5   0.70
26   R201   t5   0.40
27   R203   t5   3.40
28   R340   t5   0.30
29   R453   t5   3.60
```

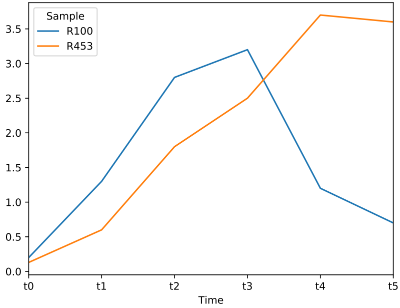
Reshaping data

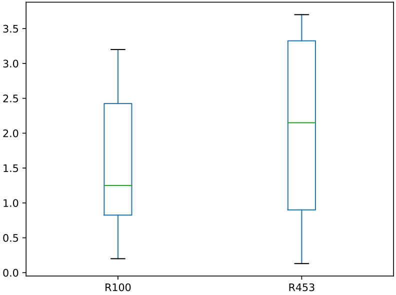
```python
# Spread rows into columns [by time]
df = pd.pivot_table(df,
                    values="Exprs",
                    columns="Sample",
                    index="Time")
```

```
Sample  R100  R201  R203  R340  R453
Time
t0       0.2   0.1   0.3  0.25  0.13
t1       1.3   1.8   0.8  1.50  0.60
t2       2.8   3.1   1.9  2.30  1.80
t3       3.2   3.7   2.3  3.50  2.50
t4       1.2   1.8   3.9  1.30  3.70
t5       0.7   0.4   3.4  0.30  3.60
```

Plot samples R100 and R453

```python
# Time-plot
df.plot(y=["R100", "R453"])

# Box-plot
df.plot(y=["R100", "R453"], kind="box")
```





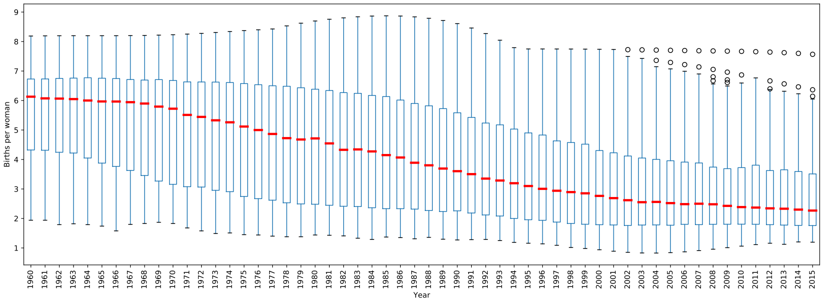
Reading data files: Births per women

```python
# Read data file
data = pd.read_csv("births_per_woman.csv", header=0)

# Explore what's in the data
data.head() # show first 5 rows of data
data.tail() # show last 5 rows of data
```

```
   CountryName                     Region          IncomeGroup   1960   1961  \
0        Aruba  Latin America & Caribbean          High income  4.820  4.655
1  Afghanistan                 South Asia           Low income  7.450  7.450
2       Angola         Sub-Saharan Africa  Upper middle income  7.379  7.388
3      Albania      Europe & Central Asia  Upper middle income  6.489  6.401
4      Andorra      Europe & Central Asia          High income    NaN    NaN

    1962   1963   1964   1965   1966  ...     2006   2007   2008   2009  \
0  4.471  4.271  4.059  3.842  3.625  ...    1.754  1.741  1.728  1.716
1  7.450  7.450  7.450  7.450  7.450  ...    6.639  6.437  6.218  5.985
2  7.396  7.402  7.406  7.408  7.406  ...    6.671  6.619  6.559  6.492
3  6.282  6.133  5.960  5.773  5.581  ...    1.668  1.635  1.625  1.636
4    NaN    NaN    NaN    NaN    NaN  ...    1.240  1.180  1.250  1.190

    2010   2011   2012   2013   2014   2015
0  1.704  1.692  1.680  1.669  1.657  1.647
1  5.746  5.506  5.272  5.050  4.843  4.653
2  6.416  6.335  6.251  6.165  6.080  5.996
3  1.663  1.699  1.735  1.765  1.784  1.793
4  1.270    NaN    NaN    NaN    NaN    NaN
```

Descriptive statistics

```python
# Median births per woman 1970 vs 1990 vs 2010
data["1970"].median() # 5.7 births per woman
data["1990"].median() # 3.6 births per woman
data["2010"].median() # 2.4 births per woman

# Box plot
data.plot(kind="box", rot=90, color={"medians": "red"},
          medianprops={"linewidth": 3})
```



Reshaping data

```python
# Gather year columns into rows
df = pd.melt(data,
             id_vars = ["CountryName", "Region", "IncomeGroup"],
             var_name="Year",
             value_name="Birth")
```

```
  CountryName                     Region           IncomeGroup  Year  Birth
0       Aruba  Latin America & Caribbean           High income  1960  4.820
1 Afghanistan                 South Asia            Low income  1960  7.450
2      Angola         Sub-Saharan Africa  Upper middle income  1960  7.379
3     Albania      Europe & Central Asia  Upper middle income  1960  6.489
4     Andorra      Europe & Central Asia           High income  1960    NaN
```

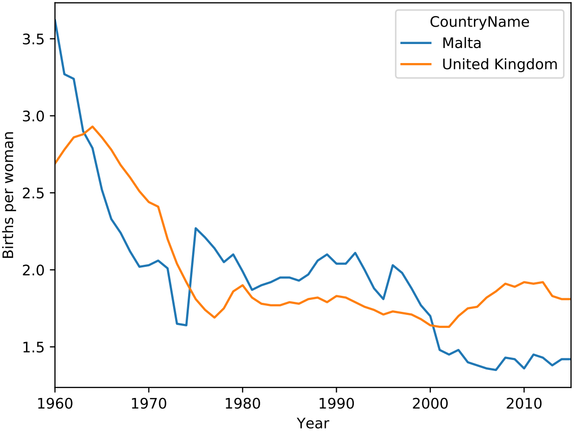
Reshaping data

```python
# Spread rows into columns
df = pd.pivot_table(df, values="Birth", columns="CountryName", index="Year")
```

```
CountryName  Afghanistan  Albania  Algeria  American Samoa  Andorra  Angola  \
Year
1960                7.45    6.489    7.524             NaN      NaN   7.379
1961                7.45    6.401    7.573             NaN      NaN   7.388
1962                7.45    6.282    7.614             NaN      NaN   7.396
1963                7.45    6.133    7.646             NaN      NaN   7.402
1964                7.45    5.960    7.665             NaN      NaN   7.406

CountryName  Antigua and Barbuda  Arab World  Argentina  Armenia    ...      \
Year                                                                ...
1960                       4.425    6.919764      3.109    4.550    ...
1961                       4.386    6.941085      3.100    4.512    ...
1962                       4.344    6.958855      3.089    4.435    ...
1963                       4.299    6.970768      3.078    4.317    ...
1964                       4.250    6.974893      3.068    4.161    ...

CountryName  Zambia  Zimbabwe
Year
1960          7.018     7.158
1961          7.071     7.215
1962          7.127     7.267
1963          7.184     7.311
1964          7.240     7.347
```

Compare birth rates

```
# Compare Malta vs United Kingdom
df.plot(y=["Malta", "United Kingdom"])
```



Try yourself with `pandas`

- Change data with `pandas.apply()`