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`

Introduction

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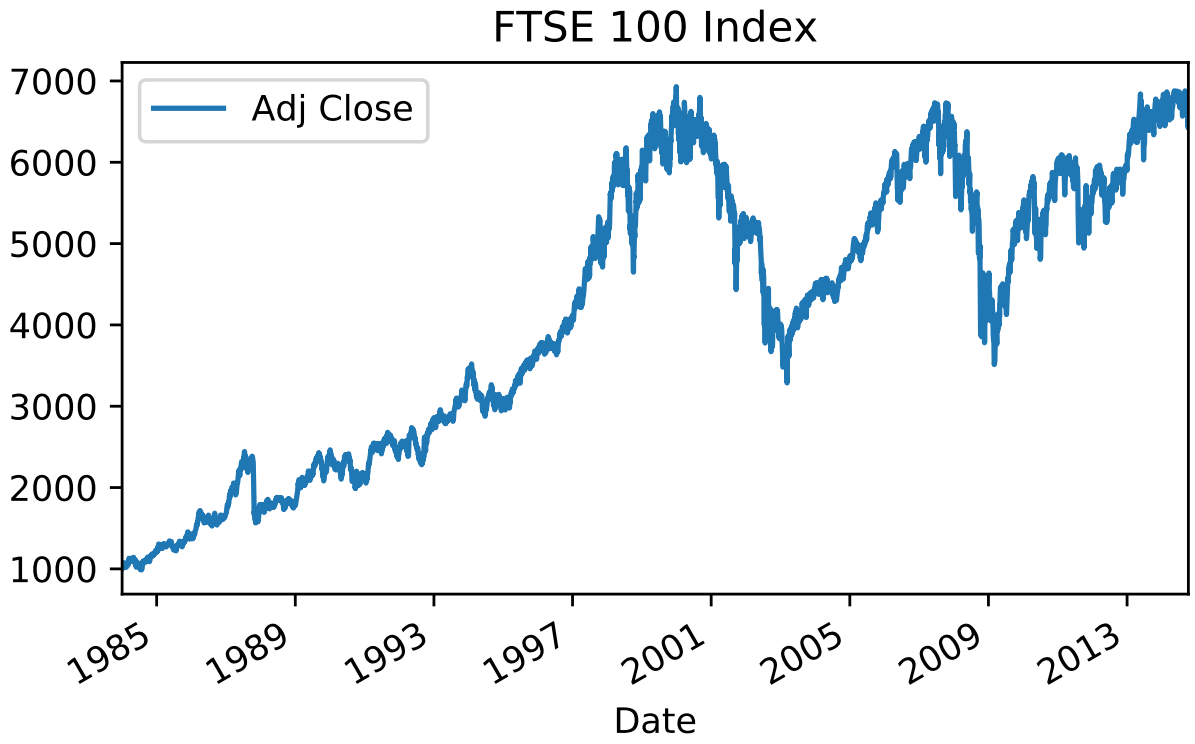
- ...

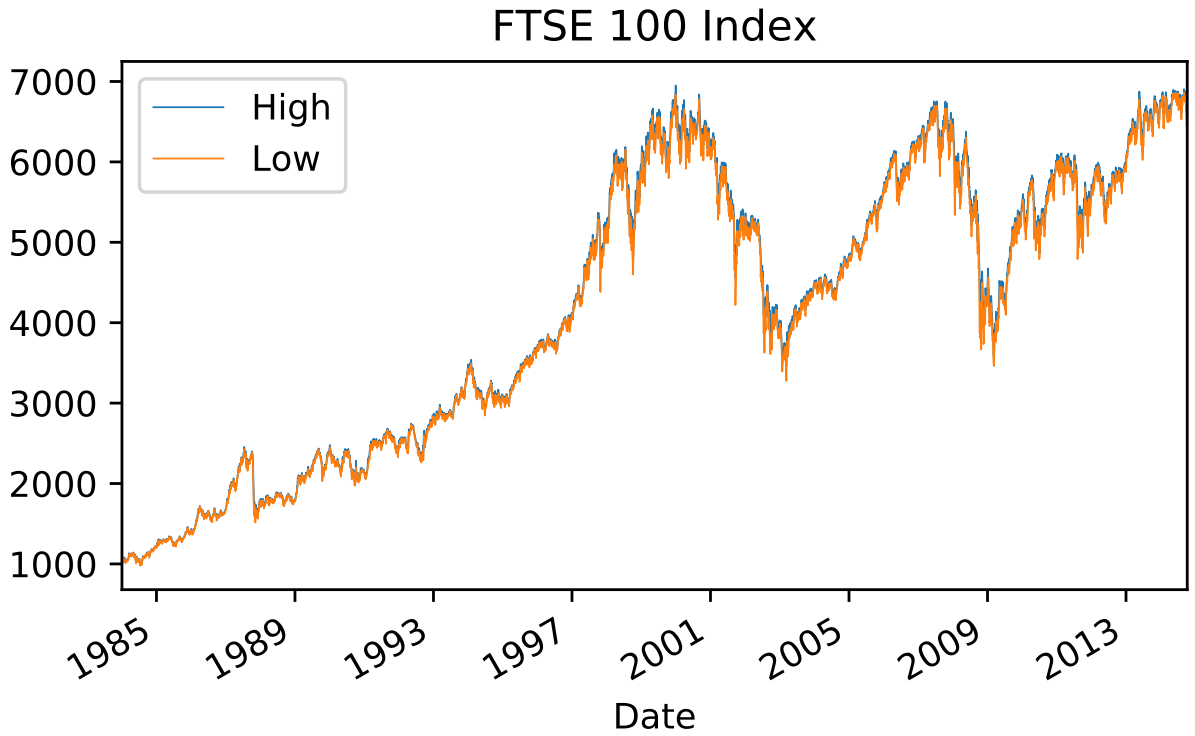
Pandas data structures

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

```
1  import pandas as pd
2
3  df = pd.DataFrame(
4          {"Sample" : ["R100" , "R201", "R203", "R340", "R453"
               ],
5           "t0" : [0.2, 0.1, 0.3, 0.25, 0.13],
6           "t1" : [1.3, 1.8, 0.8, 1.5, 0.6],
7           "t2" : [2.8, 3.1, 1.9, 2.3, 1.8],
8           "t3" : [3.2, 3.7, 2.3, 3.5, 2.5],
9           "t4" : [1.2, 1.8, 3.9, 1.3, 3.7],
10          "t5" : [0.7, 0.4, 3.4, 0.3, 3.6]})
11
12 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

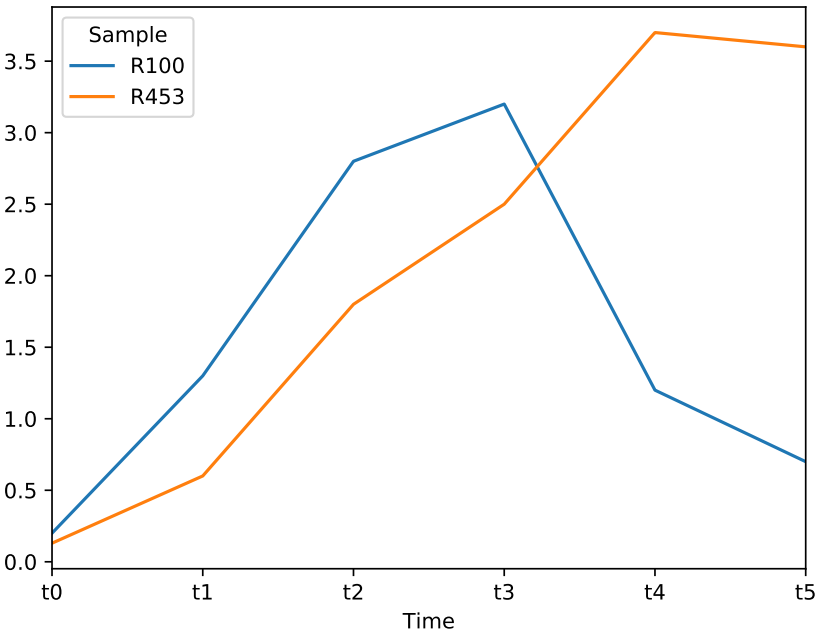
Reshaping data

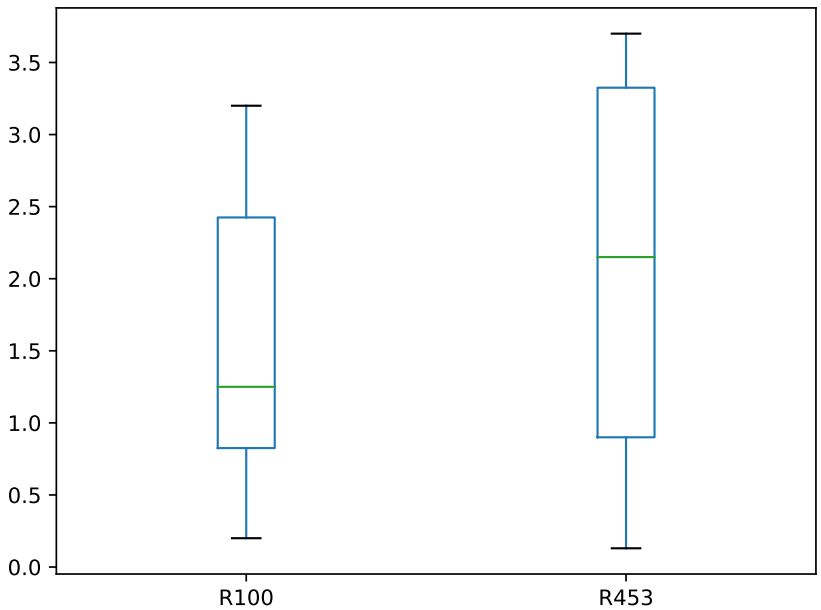
```
# Spread rows into columns [by time]
df = pd.pivot_table(df,
                    values="Exprs",
                    columns="Sample",
                    index="Time")
```

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

```
1 # Time-plot
2 df.plot(y=["R100", "R453"])
3
4 # Box-plot
5 df.plot(y=["R100", "R453"], kind="box")
```





Reading data files: Births per women

```
1 # Read data file
2 data = pd.read_csv("births_per_woman.csv", header=0)
3
4 # Explore what's in the data
5 data.head() # show first 5 rows of data
6 data.tail() # show last 5 rows of data
```

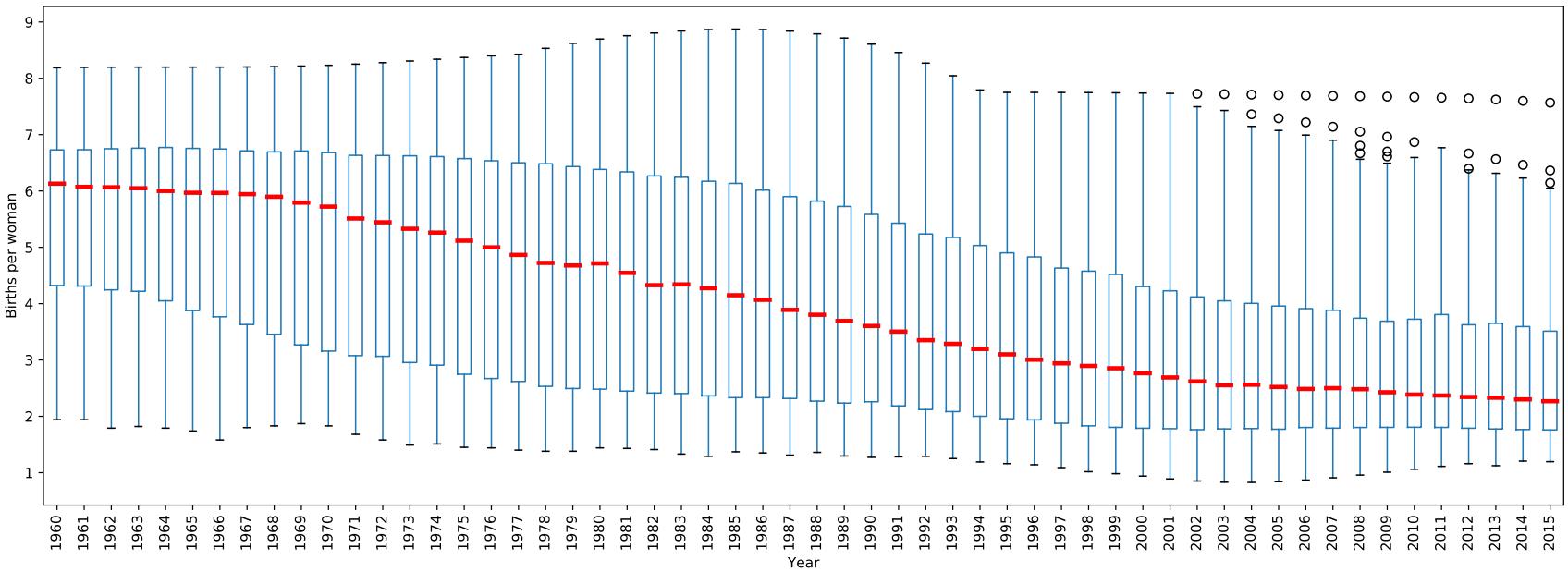
```
   CountryName                     Region          IncomeGroup   1960   1961  \
0        Aruba  Latin America & Caribbean          High income  4.820  4.655
1  Afghanistan                 South Asia           Low income  7.450  7.450
2       Angola        Sub-Saharan Africa  Upper middle income  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

```
1 # Median births per woman 1970 vs 1990 vs 2010
2 data["1970"].median() # 5.7 births per woman
3 data["1990"].median() # 3.6 births per woman
4 data["2010"].median() # 2.4 births per woman
5
6 # Box plot
7 data.plot(kind="box", rot=90, color={"medians": "red"},
8            medianprops={"linewidth": 3})
```



Reshaping data

```
# 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

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

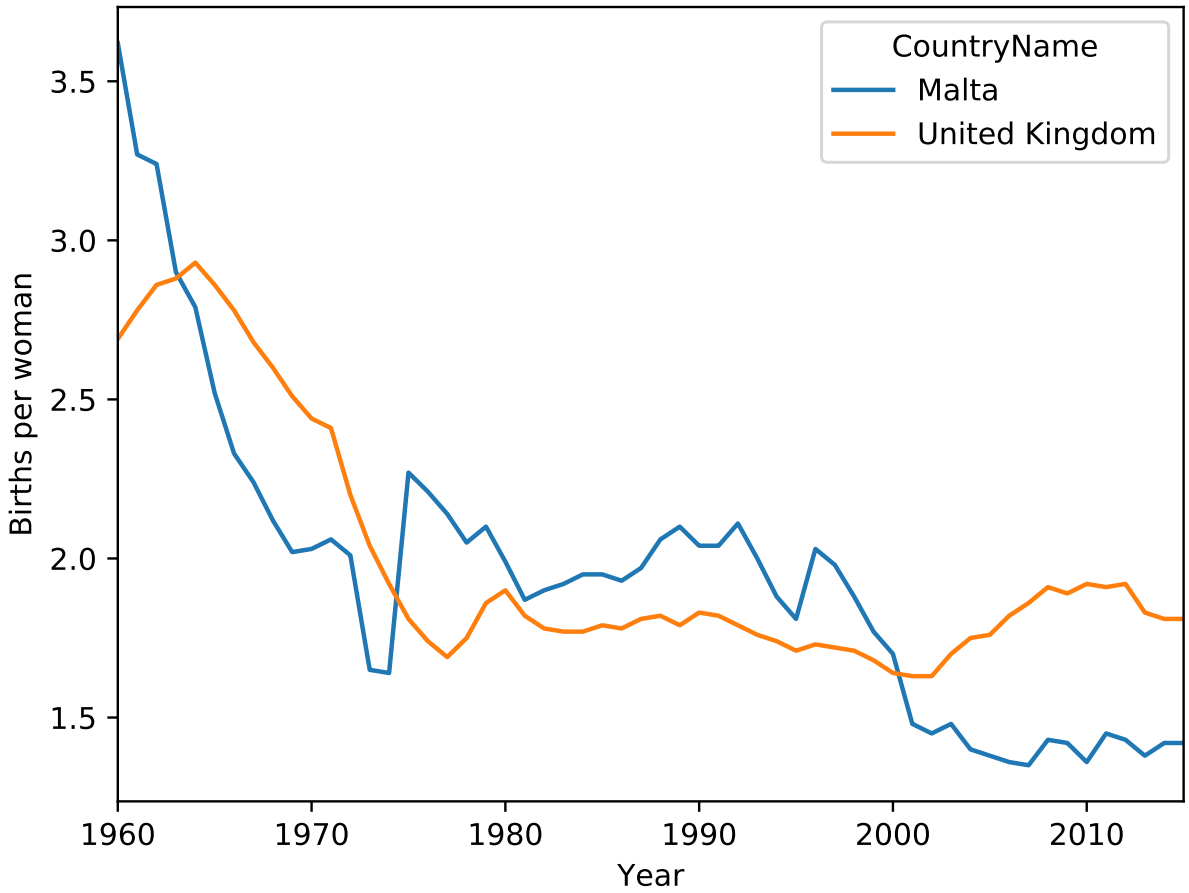
```
CountryName  Afghanistan  Albania  Algeria  American Samoa  Andorra  Angola  \
Year
1960                7.45    6.489    7.524             NaN      NaN   7.379
1961                7.45    6.401    7.573             NaN      NaN   7.388
1962                7.45    6.282    7.614             NaN      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

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



Try yourself with `pandas`

- Change data with `pandas.apply()`