Python for Numerical Computations and Data Analysis

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Contents

Preface

This document is intended as an introduction to the Python programming language and was compiled for a course given at the University of Glasgow as part of the MSc program *Data Analytics for Economics and Finance*. The focus is on language elements and libraries that are useful for data analysis, statistics and numerical computations in general.

The course consists of a collection of interactive notebooks hosted in a Github repository. While the content in this document and in the interactive notebooks is the same, the notebooks have the added benefit that they can be run directly in a browser, allowing you to immediately experiment with the provided code examples.

We omit numerous features of Python which are not of first-order importance to master the topics mentioned above. This includes manipulation of text data, advanced input/output, generators, decorators and object-oriented programming, among others.

The material does not assume any existing knowledge of Python or programming, but moves at a brisk pace compared to other introductory general-purpose Python programming textbooks. It is therefore important to work through the exercises provided for most chapters to practice applying the concepts covered. Suggested solutions are available for all exericses.

Special thanks go to Jonna Olsson for reading through all units and suggesting various improvements.

1 Crash course for the impatient

This crash course is intended to illustrate the main concepts involved when using Python for data analysis in less than 30 minutes.

1.1 Language syntax

Python has a very straightforward syntax:

1. Everything following a `#` is a comment.
2. Names are case sensitive.
3. Variables are dynamically typed and are created by assignment:

   `varname = value`
4. There is no need to terminate a statement with `;`
5. Indentation matters and is used to group blocks of code such as functions.

1.1.1 Built-in data types

For data analysis, the most important built-in data types are integers, floats, strings and lists.

[1]:
```
x = 1            # integer
x = 1.0          # floating-point number (float)
x = 'abc'        # string
x = [1, 2, 3]    # list
```

1.1.2 Indexing

Lists and other containers are indexed using brackets `[]`. Python indices start at 0:

[2]:
```
x = [1, 2, 3]          # list containing 3 integers
x[0]                   # returns first item
```

[2]: 1

Negative integer values index items from the *end* of the list:

[3]:
```
x[-1]                  # returns last item
```

[3]: 3

Ranges of items can be selected using slices, which are triples of the form `start:stop:step`. Any of the three tokens can be omitted. `stop` is not included in the selection:

[4]:
```
x = [1,2,3]            # create list of three integers

x[:]                   # all items; equivalent to x[::], or just x
x[::2]                 # every second item, returns [1, 3]
x[1:3]                 # second and third items, returns [2, 3]
x[::-1]                # all items in reverse order, returns [3, 2, 1]
```

[4]: [3, 2, 1]

1.2 NumPy arrays

We store numerical data in NumPy arrays. NumPy is not part of the standard library and has to be imported before usage:

```
import numpy as np
```

1.2.1 Creating arrays

NumPy arrays can be created using a number of ways:

[5]:
```
import numpy as np
x = np.array([1, 2, 3])          # integer array from list
x = np.array([1.0, 2.0, 3.0])    # floating-point array from list

x = np.arange(10)                # range of integers 0,...,9
x = np.linspace(0.0, 1.0, 11)    # 11 floats uniformly spaced on [0, 1]

x = np.zeros((3,3))              # 3x3 matrix of zeros
x = np.ones(10)                  # 10-element vector of ones
```

1.2.2 Element-wise operations

With NumPy, the default is to apply operators element-by-element (unlike in Matlab, where you would use `.*` for element-wise multiplication):

[6]:
```
import numpy as np
x = np.arange(5)                 # vector [0,1,2,3,4]
y = np.arange(5,10)              # vector [5,6,7,8,9]

# resulting vector is of the same size
x + y                            # vector [5,7,9,11,13]
x * y
x - y
x / y
```

[6]:
```
array([0.        , 0.16666667, 0.28571429, 0.375     , 0.44444444])
```

1.2.3 Matrix operations

Matrix-matrix and matrix-vector multiplication is performed using the `np.dot()` function, or alternatively, the `@` operator:

[7]:
```
import numpy as np

# create 2x3 matrix
mat = np.array([[1, 2, 3],
                [4, 5, 6]])
mat                              # print matrix
```

[7]:
```
array([[1, 2, 3],
       [4, 5, 6]])
```

[8]:
```
# create length-2 vector
vec = np.array([1, 2])
```

```
vec                                 # print vector
```

[8]:
```
array([1, 2])
```

[9]:
```
# vector-matrix multiplication
np.dot(vec, mat)                    # or vec @ mat
```

[9]:
```
array([ 9, 12, 15])
```

[10]:
```
# matrix-matrix multiplication
np.dot(mat, mat.T)                  # or mat @ mat
```

[10]:
```
array([[14, 32],
       [32, 77]])
```

We use `.T` to transpose a matrix.

1.2.4 NumPy functions

NumPy implements the usual gamut of mathematical functions you'd expect, such as:

[11]:
```
import numpy as np
x = np.arange(1,5)                  # integers 1,...,5

np.sqrt(x)                          # square root
np.exp(x)                           # exponential function
np.log(x)                           # natural logarithm
np.sin(x)                           # sine function
```

[11]:
```
array([ 0.84147098,  0.90929743,  0.14112001, -0.7568025 ])
```

1.3 Plotting

The most common plotting library used in Python is *matplotlib*. To use it, we need to import it as follows:

`import matplotlib.pyplot as plt`

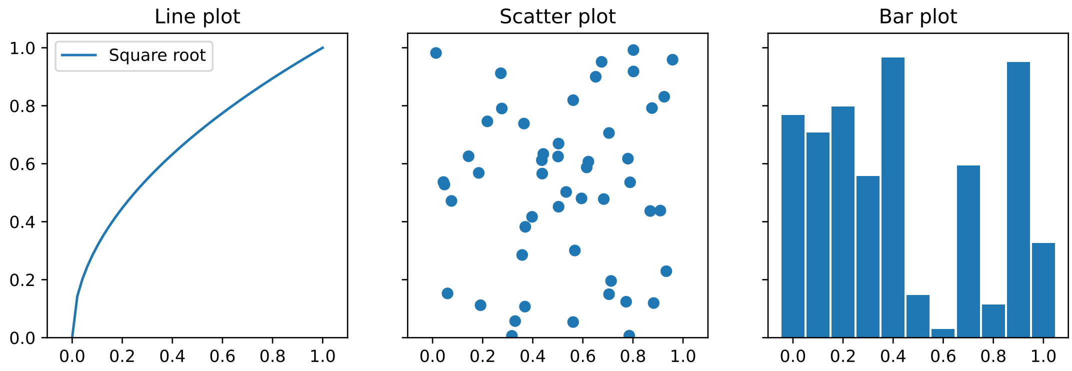
The main plotting routine is `plot()` which displays lines; other useful routines are `scatter()` and `bar()`.

The following code demonstrates how to plot some randomly generated data:

[12]:
```
import matplotlib.pyplot as plt
import numpy as np

# Create figure with three panels (axes) arranged in three columns
fig, ax = plt.subplots(1,3, sharex=True, sharey=True, figsize=(11,3.3))

# plot square-root function
xvalues = np.linspace(0.0, 1.0, 50)
ax[0].plot(xvalues, np.sqrt(xvalues), label='Square root')
ax[0].legend()
ax[0].set_title('Line plot')

# scatter plot of random uniformly distributed data
np.random.seed(1234)
xvalues = np.random.rand(50)
yvalues = np.random.rand(50)
ax[1].scatter(xvalues, yvalues)
ax[1].set_title('Scatter plot')
```

```
xvalues = np.linspace(0.0, 1.0, 11)
yvalues = np.random.rand(len(xvalues))
ax[2].bar(xvalues, yvalues, 0.09)
ax[2].set_title('Bar plot')
```

[12]: Text(0.5, 1.0, 'Bar plot')



1.4 Functions

Functions are the most important way to reuse and encapsulate code. They are defined using the `def` keyword. The function body is written as an indented block:

```
def func(x):
    # perform computations on x
    return y
```

For example, assume that we have a 3rd-order polynomial given by

$$p(x;\alpha) = \alpha x^3 + b_2 x^2 + b_1 x + b_0$$

where α is a parameter and b_2, b_1 and b_0 are fixed. A function to evaluate this polynomial could be implemented as follows:

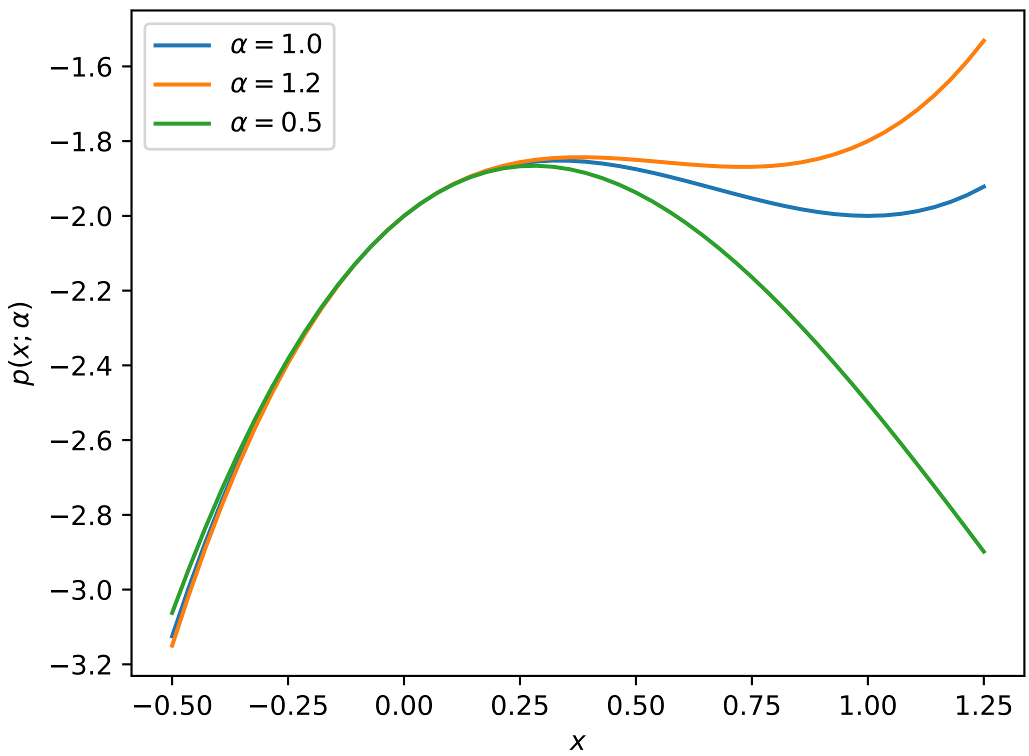
[13]:
```
def poly(x, alpha=1.0):
    b2 = - 2.0
    b1 = 1.0
    b0 = -2.0
    p = alpha * x**3.0 + b2 * x**2.0 + b1 * x + b0
    return p
```

We can use this definition to evaluate and plot the polynomial for various values of α.

[14]:
```
import matplotlib.pyplot as plt
import numpy as np

xvalues = np.linspace(-0.5, 1.25, 50)

fig, ax = plt.subplots(1,1, figsize=(6, 4.5))

# Evaluate polynomial with alpha = 1.0
yvalues = poly(xvalues, alpha=1.0)
ax.plot(xvalues, yvalues, label=r'$\alpha=1.0$')

# Evaluate polynomial with alpha = 1.2
```

```
yvalues = poly(xvalues, alpha=1.2)
ax.plot(xvalues, yvalues, label=r'$\alpha=1.2$')

# Evaluate polynomial with alpha = 0.5
yvalues = poly(xvalues, alpha=0.5)
ax.plot(xvalues, yvalues, label=r'$\alpha=0.5$')

ax.set_xlabel('$x$')
ax.set_ylabel(r'$p(x; \alpha)$')
ax.legend()
```

[14]: `<matplotlib.legend.Legend at 0x7f9e1a89e6e0>`



Note that *matplotlib* allows us to use LaTeX symbols in labels and legends.

1.5 Working with data

1.5.1 Loading data

The `data/` directory contains the text file `FRED.csv` of comma-separated annual U.S. data for the following variables:

- real GDP (in billions of chained 2012 dollars);
- the consumer price index (CPI); and
- the unemployment rate (UNRATE, in percent).

The data was downloaded from the FRED database, a standard source for macroeconomic time series.

The first two rows of this data are

Year	GDP	CPI	UNRATE
1948	2118.5	24.0	3.8
1949	2106.6	23.8	6.0

We use the `loadtxt` function to read the CSV file into a NumPy array as follows:

[15]:
```
import numpy as np

filename = '../data/FRED.csv'
# Load data into NumPy array
data = np.loadtxt(filename, delimiter=',', skiprows=1)
# Print first 5 rows of data
data[:5]
```

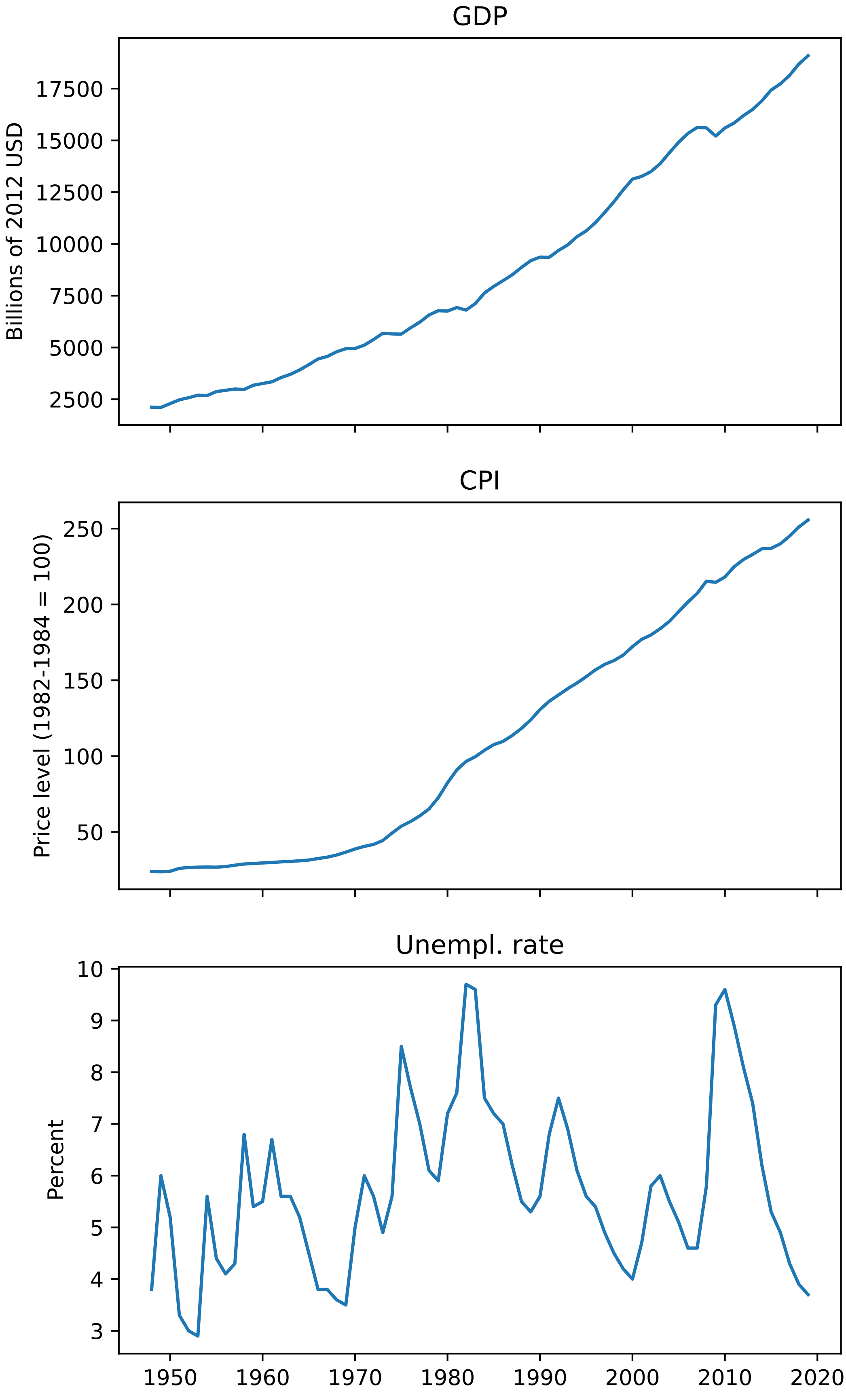
[15]:
```
array([[1948. , 2118.5,   24. ,    3.8],
       [1949. , 2106.6,   23.8,    6. ],
       [1950. , 2289.5,   24.1,    5.2],
       [1951. , 2473.8,   26. ,    3.3],
       [1952. , 2574.9,   26.6,    3. ]])
```

1.5.2 Visualising data

We can now proceed to analyse the data. First, we plot all three time series in separate graphs (since their scales are vastly different).

[16]:
```
import matplotlib.pyplot as plt

# Split array into separate time series
# Years are in the first column; convert them to integer values
years = np.array(data[:, 0], dtype=int)

gdp = data[:, 1]     # GDP in column 2
cpi = data[:, 2]     # CPI in column 3
unr = data[:, 3]     # unemployment rate in column 4

# create figure and 3 sub-plots, each in a new row
fig, ax = plt.subplots(3, 1, sharex=True, figsize=(6, 11))

# Plot GDP in first panel
ax[0].plot(years, gdp)
ax[0].set_title('GDP')
ax[0].set_ylabel('Billions of 2012 USD')

# Plot CPI in second panel
ax[1].plot(years, cpi)
ax[1].set_ylabel('Price level (1982-1984 = 100)')
ax[1].set_title('CPI')

# Plot unemployment rate in third panel
ax[2].plot(years, unr)
ax[2].set_title('Unempl. rate')
ax[2].set_ylabel('Percent')
```

[16]:
```
Text(0, 0.5, 'Percent')
```


GDP
Billions of 2012 USD
17500
15000
12500
10000
7500
5000
2500
CPI
Price level (1982-1984 = 100)
250
200
150
100
50
Unempl. rate
Percent
10
9
8
7
6
5
4
3
1950
1960
1970
1980
1990
2000
2010
2020

1.5.3 Transforming data

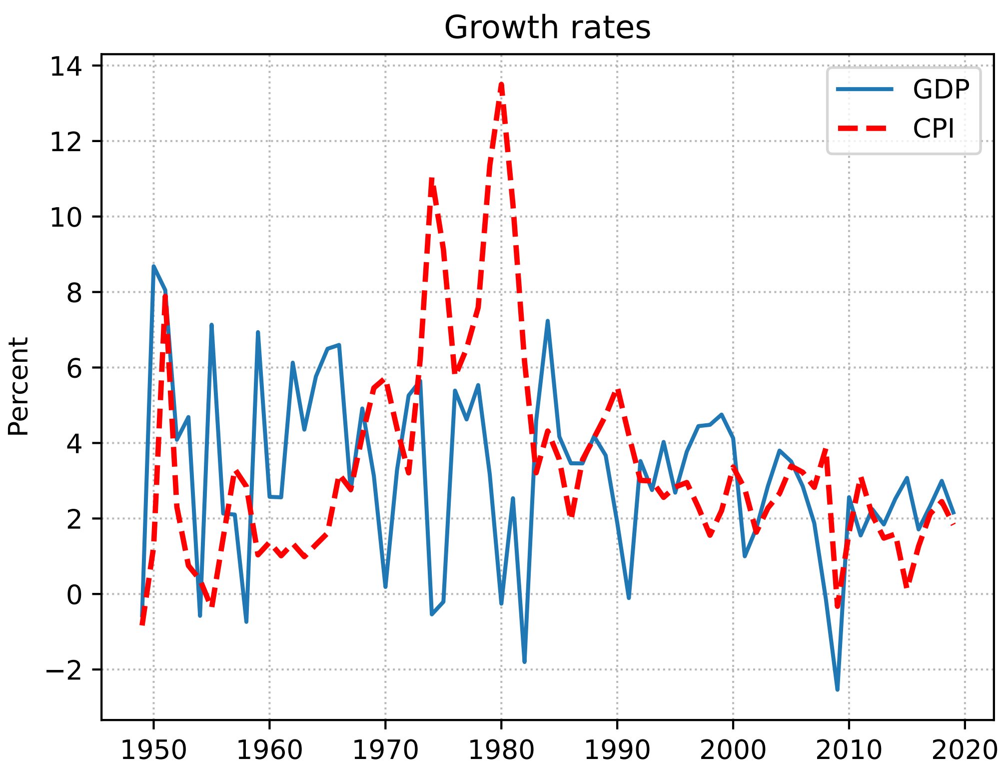
GDP and CPI levels are not that informative, so let's transform them to annual growth rates.

- We do this by defining a function that accepts a vector as input and computes the percentage changes.
- The output vector has one fewer element as we need two observations to compute a growth rate.

[17]:
```
# Define function to compute growth rates
def growth_rate(x):
    # Compute absolute difference: subtract lagged observations
    diff = x[1:] - x[:-1]
    # Growth rate = relative difference
    # Return growth rates in percent!
    reldiff = (diff / x[:-1]) * 100.0
    return reldiff

# Apply function to GDP and CPI
gdp_growth = growth_rate(gdp)
cpi_growth = growth_rate(cpi)        # CPI growth rate, a.k.a. inflation
```

We can now plot the growth rates. Since they will be of similar magnitude, we use a single graph.

[18]:
```
fig, ax = plt.subplots(1, 1, figsize=(6,4.5))
ax.plot(years[1:], gdp_growth, label='GDP')
ax.plot(years[1:], cpi_growth, label='CPI', color='red', linestyle='--',␣
↪linewidth=2.0)
ax.set_ylabel('Percent')
ax.set_title('Growth rates')
ax.legend()
ax.grid(linestyle=':', alpha=0.9, linewidth=0.75, zorder=-100)
```



1.5.4 Summary statistics

We can compute some summary statistics for all three time series using functions such as `np.mean()` and `np.std()`, where the latter returns the standard deviation:

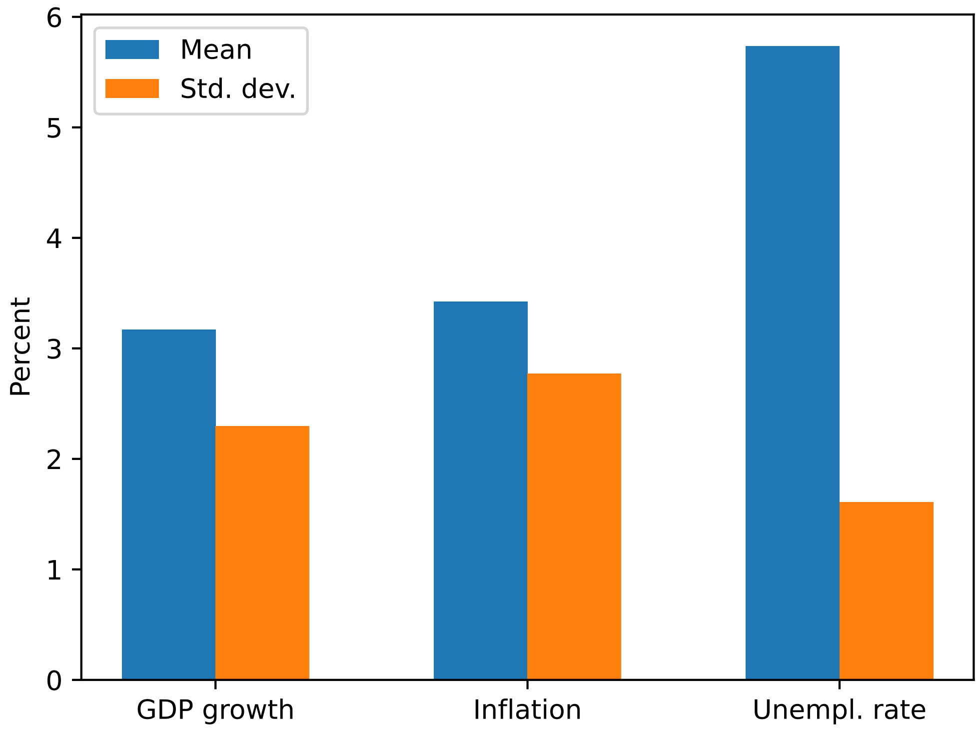
[19]:
```
def print_stats(name, x):
    # Define formatting string to print results
    fmt = '{:12s}: mean = {:.2f}, std. dev. = {:.2f}'
    mean = np.mean(x)
    std = np.std(x)
    print(fmt.format(name, mean, std))

# GDP growth rate
print_stats('GDP growth', gdp_growth)
# CPI growth rate = inflation
print_stats('Inflation', cpi_growth)
# Unempl. rate
print_stats('Unempl. rate', unr)
```

```
GDP growth  : mean = 3.17, std. dev. = 2.30
Inflation   : mean = 3.42, std. dev. = 2.77
Unempl. rate: mean = 5.73, std. dev. = 1.61
```

We can of course also plot these moments, for example using a bar graph:

[20]:
```
labels = ['GDP growth', 'Inflation', 'Unempl. rate']
means = [np.mean(x) for x in (gdp_growth, cpi_growth, unr)]
stds = [np.std(x) for x in (gdp_growth, cpi_growth, unr)]
fig, ax = plt.subplots(1, 1, figsize=(6, 4.5))
width = 0.3
xticks = np.arange(3)
ax.bar(xticks - width/2.0, means, width, label='Mean')
ax.bar(xticks + width/2.0, stds, width, label='Std. dev.')
ax.set_xticks(xticks)
ax.set_xticklabels(labels)
ax.set_ylabel('Percent')
ax.legend(loc='upper left')
```

[20]:
```
<matplotlib.legend.Legend at 0x7f9de4ae1360>
```



1.6 Next steps

This truly was a crash course, conveying the minimum information necessary to get you started with data analysis using Python.

We will flesh out these concepts in much more detail in the next few units.

2 Language and NumPy basics

In this unit we start exploring the Python language, covering the following topics:

1. Basic syntax
2. Built-in data types
3. NumPy arrays

2.1 Basic syntax

- Everything after a # character (until the end of the line) is a comment and will be ignored.
- Variable names are case sensitive.
- Whitespace characters matter (unlike in most languages)!
- Python uses indentation (usually 4 spaces) to group statements, for example loop bodies, functions, etc.
- You don't need to add a character to terminate a line, unlike in some languages.
- You can use the `print()` function to inspect almost any object.

[21]:
```
# First example

# create a variable named 'text' that stores the string 'Hello, world!'
text = 'Hello, world!'

# print contents of 'text'
print(text)
```

```
Hello, world!
```

In Jupyter notebooks and interactive command-line environments, we can also display a value by simply writing the variable name.

[22]:
```
text
```

[22]:
```
'Hello, world!'
```

Alternatively, we don't even need to create a variable but can instead directly evaluate expressions and print the result:

[23]:
```
2*3
```

[23]:
```
6
```

This does not print anything in *proper* Python script files that are run through the interpreter, though.

Calling `print()` is also useful if we want to display multiple expressions from a single notebook cell, as otherwise only the last value is shown:

[24]:
```
text = 'Hello world!'
var = 1
text        # does NOT print contents of text
var         # prints only value of var
```

[24]:
```
1
```

[25]:
```
print(text) # print text explicitly
var         # var is shown automatically
```

```
Hello world!
```

[25]:
```
1
```

2.2 Built-in data types

Pythons is a dynamically-typed language:

- Unlike in C or Fortran, you don't need to declare a variable or its type.
- You can inspect a variable's type using the built-in `type()` function, but you rarely need to do this.

We now look at the most useful built-in data types:

Basic types

- integers (`int`)
- floating-point numbers (`float`)
- boolean (`bool`)
- strings (`str`)

Containers (or collections)

- tuples (`tuple`)
- lists (`list`)
- dictionaries (`dict`)

2.2.1 Integers and floats

Integers and floats (floating-point numbers) are the two main built-in data types to store numerical data (we ignore complex numbers in this tutorial). Floating-point is the standard way to represent real numbers on computers since these cannot store real numbers with arbitrary precision.

[26]:
```
# Integer variables
i = 1
type(i)
```

[26]:
```
int
```

[27]:
```
# Floating-point variables
x = 1.0
type(x)
```

[27]:
```
float
```

[28]:
```
# A name can reference any data type:
# Previously, x was a float, now it's an integer!
x = 1
type(x)
```

[28]:
```
int
```

It is good programming practice to specify floating-point literals using a decimal point. It makes a difference in a few cases (especially when using NumPy arrays, or Python extensions such as Numba or Cython):

[29]:
```
x = 1.0         # instead of x = 1
```

A boolean (`bool`) is a special integer type that can only store two values, `True` and `False`. We create booleans by assigning one of these values to a variable:

[30]:
```
x = True
x = False
```

Boolean values are most frequently used for conditional execution, i.e., a block of code is run only when some variable is `True`. We study conditional execution in the next unit.

2.2.2 Strings

The string data type stores sequences of characters:

[31]:
```
# Strings need to be surrounded by single (') or double (") quotes!
institution = 'University of Glasgow'
institution = "University of Glasgow"
```

Strings support various operations some of which we explore in the exercises at the end of this section. For example, we can use the addition operation + to concatenate strings:

[32]:
```
# Define two strings
str1 = 'Python'
str2 = 'course'

# Concatenate strings using +
str1 + ' ' + str2
```

[32]: 'Python course'

An extremely useful variant of strings are the so-called *f-strings*. These allow us to dynamically insert a variable value into a string, a feature we'll use throughout this course.

[33]:
```
# Approximate value of pi
pi = 3.1415

# Use f-strings to embed the value of the variable version inside the string
s = f'Pi is approximately equal to {pi}'
s
```

[33]: 'Pi is approximately equal to 3.1415'

2.2.3 Tuples

Tuples represent a collection of several items which can have different data types. They are created whenever several items are separated by commas. The parentheses are optional:

```
(item1, item2, ...)
```

[34]:
```
# A tuple containing a string, an integer and a float
items = ('foo', 1, 1.0)
items
```

[34]: ('foo', 1, 1.0)

The parenthesis are optional, but improve readability:

[35]:
```
items = 'foo', 1, 1.0        # equivalent way to create a tuple
items
```

[35]: ('foo', 1, 1.0)

We use brackets `[]` to access an element in a tuple (or any other container object)

[36]:
```
first = items[0]            # variable first now contains 'foo'
first
```

[36]:
```
'foo'
```

Python indices are 0-based, so 0 references the first element, 1 the second element, etc.

[37]:
```
second = items[1]           # second element
second
```

[37]:
```
1
```

Tuples are immutable, which means that the items stored in the tuple cannot be changed!

[38]:
```
# This raises an error!
items = 'foo', 1, 1.0
items[0] = 123
```

```
TypeError: 'tuple' object does not support item assignment
```

2.2.4 Lists

Lists are like tuples, except that they can be modified. We create lists using brackets,

```
[item1, item2, ...]
```

[39]:
```
# Create list which contains a string, an integer and a float
lst = ['foo', 1, 1.0]
lst
```

[39]:
```
['foo', 1, 1.0]
```

Accessing list items works the same way as with tuples

[40]:
```
lst[0]                  # print first item
```

[40]:
```
'foo'
```

Lists items can be modified:

[41]:
```
lst[0] = 'bar'          # first element is now 'bar'
lst
```

[41]:
```
['bar', 1, 1.0]
```

Lists are full-fledged objects that support various operations, for example

[42]:
```
lst.insert(0, 'abc')    # insert element at position 0
lst.append(2.0)         # append element at the end
del lst[3]              # delete the 4th element
lst
```

[42]:
```
['abc', 'bar', 1, 2.0]
```

The built-in function `len()` returns the number of elements in a list (and any other container object)

[43]:
```
len(lst)
```

[43]: 4

2.2.5 Dictionaries

Dictionaries are container objects that map keys to values.

- Both keys and values can be (almost any) Python objects, even though usually we use strings as keys.
- Dictionaries are created using curly braces: `{key1: value1, key2: value2, ...}`.

For example, to create a dictionary with three items we write

[44]:
```
dct = {
    'institution': 'University of Glasgow',
    'course': 'Python course',
    'year': 2021
}
dct
```

[44]:
```
{'institution': 'University of Glasgow',
 'course': 'Python course',
 'year': 2021}
```

Specific values are accessed using the syntax `dict[key]`:

[45]:
```
dct['institution']
```

[45]:
```
'University of Glasgow'
```

We can use the same syntax to either modify an existing key or add a new key-value pair:

[46]:
```
dct['course'] = 'Introduction to Python'        # modify value of existing key
dct['city'] = 'Glasgow'                         # add new key-value pair
dct
```

[46]:
```
{'institution': 'University of Glasgow',
 'course': 'Introduction to Python',
 'year': 2021,
 'city': 'Glasgow'}
```

Moreover, we can use the methods `keys()` and `values()` to get the collection of a dictionary's keys and values:

[47]:
```
dct.keys()
```

[47]:
```
dict_keys(['institution', 'course', 'year', 'city'])
```

[48]:
```
dct.values()
```

[48]:
```
dict_values(['University of Glasgow', 'Introduction to Python', 2021,
'Glasgow'])
```

When we try to retrieve a key that is not in the dictionary, this will produce an error:

[49]:
```
dct['country']
```

```
KeyError: 'country'
```

One way to get around this is to use the `get()` method which accepts a default value that will be returned whenever a key is not present:

```
[50]: dct.get('country', 'Scotland')      # return 'Scotland' if 'country' is
                                         # not a valid key
```

```
[50]: 'Scotland'
```

2.3 NumPy arrays

NumPy is a library that allows us to efficiently store and access (mainly) numerical data and apply numerical operations similar to those available in Matlab.

- NumPy is not part of the core Python project.
- Python itself has an array type, but there is really no reason to use it. Use NumPy!
- NumPy types and functions are not built-in, we must first import them to make them visible. We do this using the `import` statement.

The convention is to make NumPy functionality available using the `np` namespace:

```
[51]: import numpy as np
```

2.3.1 Creating arrays

NumPy offers a multitude of functions to create arrays.

```
[52]: # Create a 1-dimensional array with 10 elements, initialise values to 0.
      # We need to prefix the NumPy function zeros() with 'np'
      arr = np.zeros(10)
      arr
```

```
[52]: array([0., 0., 0., 0., 0., 0., 0., 0., 0., 0.])
```

```
[53]: arr1 = np.ones(5)         # vector of five ones
      arr1
```

```
[53]: array([1., 1., 1., 1., 1.])
```

We can also create sequences of integers using the `np.arange()` function:

```
[54]: arr2 = np.arange(5)       # vector [0,1,2,3,4]
      arr2
```

```
[54]: array([0, 1, 2, 3, 4])
```

`np.arange()` accepts initial values and increments as optional arguments. The end value is *not* included.

```
[55]: start = 2
      end = 10
      step = 2
      arr3 = np.arange(start, end, step)
      arr3
```

```
[55]: array([2, 4, 6, 8])
```

As in Matlab, there is a `np.linspace()` function that creates a vector of uniformly-spaced real values.

[56]:
```python
# Create 11 elements, equally spaced on the interval [0.0, 1.0]
arr5 = np.linspace(0.0, 1.0, 11)
arr5
```

[56]:
```
array([0. , 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1. ])
```

We create arrays of higher dimension by specifying the desired shape. Shapes are specified as `tuple` arguments; for example, the shape of an $m \times n$ matrix is `(m,n)`.

[57]:
```python
mat = np.ones((2,2))     # Create 2x2 matrix of ones
mat
```

[57]:
```
array([[1., 1.],
       [1., 1.]])
```

Creating arrays from other Python objects

Arrays can be created from other objects such as lists and tuples by calling `np.array()`

[58]:
```python
# Create array from list [1,2,3]
arr = np.array([1, 2, 3])
arr
```

[58]:
```
array([1, 2, 3])
```

[59]:
```python
# Create array from tuple
arr = np.array((1.0, 2.0, 3.0))
arr
```

[59]:
```
array([1., 2., 3.])
```

[60]:
```python
# Create two-dimensional array from nested list
arr = np.array([[1, 2, 3], [4, 5, 6]])
arr
```

[60]:
```
array([[1, 2, 3],
       [4, 5, 6]])
```

2.3.2 Reshaping arrays

The `reshape()` method of an array object can be used to reshape it to some other (conformable) shape.

[61]:
```python
# Create vector of 4 elements and reshape it to a 2x2 matrix
mat = np.arange(4).reshape((2,2))
mat
```

[61]:
```
array([[0, 1],
       [2, 3]])
```

[62]:
```python
# reshape back to vector of 4 elements
vec = mat.reshape(4)
vec
```

[62]:
```
array([0, 1, 2, 3])
```

We use `-1` to let NumPy automatically compute the size of *one* remaining dimension.

[63]:
```python
# with 2 dimensions, second dimension must have size 2
mat = np.arange(4).reshape((2, -1))
mat
```

```
[63]: array([[0, 1],
             [2, 3]])
```

If we want to convert an arbitrary array to a vector, we can alternatively use the `flatten()` method.

```
[64]: mat.flatten()
```

```
[64]: array([0, 1, 2, 3])
```

Important: the reshaped array must have the same number of elements!

```
[65]: import numpy as np
      mat = np.arange(6).reshape((2,-1))
      mat.reshape((2,2))        # Cannot reshape 6 into 4 elements!
```

```
ValueError: cannot reshape array of size 6 into shape (2,2)
```

2.3.3 Indexing

Single element indexing

To retrieve a single element, we specify the element's index on each axis (axis is the NumPy terminology for an array dimension).

- Remember that just like Python in general, NumPy arrays use 0-based indices.
- Unlike lists or tuples, NumPy arrays support multi-dimensional indexing.

```
[66]: import numpy as np

      mat = np.arange(6).reshape((3,2))
      mat
```

```
[66]: array([[0, 1],
             [2, 3],
             [4, 5]])
```

```
[67]: mat[0,1]     # returns element in row 1, column 2
```

```
[67]: 1
```

It is important to pass multi-dimensional indices as a tuple within brackets, i.e., `[0,1]` in the above example. We could alternatively write `mat[0][1]`, which would give the same result:

```
[68]: mat[0][1] == mat[0,1]        # don't do this!
```

```
[68]: True
```

This is substantially less efficient, though, as it first creates a sub-dimensional array `mat[0]`, and then applies the second index to this array.

Index slices

There are numerous ways to retrieve a subset of elements from an array. The most common way is to specify a triplet of values `start:stop:step` called `slice` for some axis:

```
[69]: # Create a 3x2 matrix
      mat = np.arange(6).reshape((2,3))
      mat
```

[69]: array([[0, 1, 2],
       [3, 4, 5]])

[70]:
```
# Retrieve only the first and third columns:
mat[0:2,0:3:2]
```

[70]: array([[0, 2],
       [3, 5]])

Indexing with slices can get quite intricate. Some basic rules:

- all tokens in `start:stop:step` are optional, with the obvious default values. We could therefore write `::` to include all indices, which is the same as `:`
- The end value is *not* included. Writing `vec[0:n]` does not include element with index n!
- Any of the elements of `start:stop:step` can be negative.
  - If `start` or `stop` are negative, elements are counted from the end of the array: `vec[:-1]` retrieves the whole vector except for the last element.
  - If `step` is negative, the order of elements is reversed.

[71]:
```
vec = np.arange(5)
# These are equivalent ways to return the WHOLE vector
vec[0:5:1]      # all three tokens present
vec[::]         # omit all tokens
vec[:]          # omit all tokens
vec[:5]         # end value only
vec[-5:]        # start value only, using negative index
```

[71]: array([0, 1, 2, 3, 4])

You can reverse the order like this:

[72]:
```
vec[::-1]
```

[72]: array([4, 3, 2, 1, 0])

With multi-dimensional arrays, the above rules apply for each dimension.

- We can, however, omit explicit indices for higher-order dimensions if all elements should be included.

[73]:
```
mat[1]      # includes all columns of row 2; same as mat[1,:]
```

[73]: array([3, 4, 5])

We cannot omit the indices for leading axes, though! If an entire leading axis is to be included, we specify this using `:`

[74]:
```
mat[:, 1]   # includes all rows of column 2
```

[74]: array([1, 4])

Indexing lists and tuples

The basic indexing rules we have covered so far also apply to the built-in `tuple` and `list` types. However, `list` and `tuple` do not support advanced indexing available for NumPy arrays which we study in later units.

[75]:
```
# Apply start:stop:step indexing to tuple
tpl = (1,2,3)
tpl[:3:2]
```

[75]: (1, 3)

2.3.4 Numerical data types (advanced)

We can explicitly specify the numerical data type when creating NumPy arrays.

So far we haven't done so, and then NumPy does the following:

- Functions such as `zeros()` and `ones()` default to using `np.float64`, a 64-bit floating-point data type (this is also called *double precision*)
- Other functions such as `arange()` and `array()` inspect the input data and return a corresponding array.
- Most array creation routines accept a `dtype` argument which allows you to explicitly set the data type.

Examples:

[76]:
```
import numpy as np

# Floating-point arguments return array of type np.float64
arr = np.arange(1.0, 5.0, 1.0)
arr.dtype
```

[76]:
```
dtype('float64')
```

[77]:
```
# Integer arguments return array of type np.int64
arr = np.arange(1,5,1)
arr.dtype
```

[77]:
```
dtype('int64')
```

Often we don't care about the data type too much, but keep in mind that

- Floating-point has limited precision, even for integers if these are larger than (approximately) 10^{16}
- Integer values cannot represent fractional numbers and (often) have a more limited range.

This might lead to surprising consequences:

[78]:
```
# Create integer array
arr = np.ones(5, dtype=np.int64)
# Store floating-point in second element
arr[1] = 1.234
arr
```

[78]:
```
array([1, 1, 1, 1, 1])
```

The array is unchanged because it's impossible to represent 1.234 as an integer value!

The take-away is to explicitly write floating-point literal values and specify a floating-point `dtype` argument when we want data to be interpreted as floating-point values. For example, always write 1.0 instead of 1, unless you *really* want an integer!

2.4 Exercises

2.4.1 Exercise 1: string operations

Experiment with operators applied to strings and integers.

1. Define two string variables and concatenate them using +
2. Define a string variable and multiply it by 2 using `*`. What happens?
3. Define two strings and compare whether they are equal using the == and `!=` relational operators.
4. Define a string. Use the operators `in` and `not in` to test whether a character is contained in the string.

5. Define two string variables and assign them the same value. Use the `is` operator to test whether these are identical objects.

6. Define a string variable and use the += assignment operator to append another string.

   The += operator is one of several operators in Python that combine assignment with another operation, such as addition. In this particular case, these statements are equivalent:

   ```
   a += b
   a = a + b
   ```

2.4.2 Exercise 2: string formatting

We frequently want to create strings that incorporate integer and floating-point data, possibly formatted in a particular way.

Python offers quite powerful formatting capabilities which can become so complex that they are called the *Format Specification Mini-Language* (see the docs). In this exercise, we explore a small but useful subset of formatting instructions.

A format specification is a string that contains one or several `{}`, for example:

```
s = 'The current version of Python is {}'
```

The token `{}` will be replaced with data converted to a string when we apply the `format()` method:

```
s = 'The current version of Python is {}'.format(3.10)
```

The string `s` now contains the value

```
'The current version of Python is 3.10'
```

What if we want to format the float `3.10` in a particular way? We can augment the `{}` to achieve that goal. For example, if the data to be formatted is of type integer, we can specify

- `{:wd}` where `w` denotes the total field width and `d` indicates that the data type is an integer.

  To print an integer into a field that is 3 characters wide, we would thus write `{:3d}`.

For floats we have additional options:

- `{:w.df}` specifies that a float should be formatted using a field width `w` and `d` decimal digits.

  To print a float into a field of 10 characters using 5 decimal digits, we would thus specify `{:10.5f}`
- `{:w.de}` is similar, but instead uses scientific notation with exponents.

  This is particularly useful for very large or very small numbers.
- `{:w.dg}`, where `g` stands for *general* format, is a superset of `f` and `e` formatting. Either fixed or exponential notation is used depending on a number's magnitude.

In all these cases the field width `w` is optional and can be omitted. Python then uses however many characters are required.

Now what we have introduced the formatting language, you are asked to perform the following exercises:

1. Define two strings and concatenate them using the `format()` function. Add a space between them.

2. Use the above example format string, but truncate the Python version to its major version number. Do you get the expected result?

3. Print π using a precision of 10 decimal digits. *Hint:* the value of π is available as

   ```
   from math import pi
   ```

4. Print `exp(10.0)` using exponential notation and three decimal digits. *Hint:* To use the exponential function, you need to import it using

   ```
   from math import exp
   ```

2.4.3 Exercise 3: string formatting with f-strings

Since Python 3.6 there is an additional, more convenient way to format strings, the so-called *formatted string literals* or *f-strings* (official documentation). Instead of calling the `format()` method as in the previous example, one can instead define a string which contain expressions that will be evaluated at runtime.

The simplest example is to print the value of a variable using default formatting:

[79]:
```
name = 'Python'
s = f'{name} programming is fun!'
print(s)
```

```
Python programming is fun!
```

Note that the string needs to be prefixed by an `f` to indicate that it contains expressions which need to be evaluated. These expressions are again wrapped in braces. Within braces, a syntax similar to the one shown in the previous exercise can be used to specify detailed formatting instructions. For example, you can specify the number of decimal digits as follows:

[80]:
```
value = 1.2345
s = f'Value with 2 significant digits: {value:.2f}'
print(s)
```

```
Value with 2 significant digits: 1.23
```

Note that in the above examples, the variables `name` and `value` need to be known when the f-string is being defined. Otherwise, you'll get the following error:

[81]:
```
# cannot create f-string using unknown names
s = f'{unknown} is not defined'
```

```
NameError: name 'unknown' is not defined
```

Now that you have seen the basic usage, repeat Exercise 2 using f-strings instead of the `format()` method!

2.4.4 Exercise 4: operations on tuples and lists

Perform the following tasks and examine their results:

1. Create two lists and add them using +.
2. Multiply a list by the integer 2.
3. Create a list `list1` and inspect the result of

   ```
   list1 += ['x', 'y', 'z']
   ```

4. Create a list `list1` and inspect the result of

   ```
   list1 *= 2
   ```

Repeat steps 1-4 using tuples instead of lists.

Finally, create a list and a tuple and try to add them using +. Does this work?

2.5 Solutions

2.5.1 Solution for exercise 1

[82]:
```
# 1. string concatenation using addition
str1 = 'abc'
str2 = 'xyz'

# Concatenate two strings using +
str1 + str2
```

[82]: 'abcxyz'

[83]:
```
# 2. string multiplication by integers
str1 = 'abc'
# Repeat string using multiplication!
str1 * 2
```

[83]: 'abcabc'

[84]:
```
# 3. Test for string equality
str1 = 'abc'
str2 = 'xyz'
str1 == str2
```

[84]: False

[85]:
```
# 3. Test for string inequality
str1 = 'abc'
str2 = 'xyz'
str1 != str2
```

[85]: True

[86]:
```
# 4. Test whether individual character is included in string
str1 = 'abc'
'b' in str1
```

[86]: True

[87]:
```
# 4. Test whether individual character is NOT included in string
str1 = 'abc'
'x' not in str1
```

[87]: True

The last two examples illustrate that in Python strings will be interpreted as collections (of characters), just like lists or tuples, if the context requires it. We can therefore apply the `in` operator to test for membership.

[88]:
```
# 5. Test for identity
str1 = 'abc'
str2 = 'abc'
str1 is str2
```

[88]: True

This result should be surprising and is somewhat specific to Python. We would not expect two objects that were created completely independently from each other to be *identical*, i.e., point to the same memory. Python, however, caches string literals for reasons of efficiency, so it actually does keep only *one* copy of `'abc'` around, irrespective of how many variables containing `abc` are created.

[89]:
```
# 6. Append using +=
str1 = 'abc'
str1 += 'xyx'        # Append 'xyz' to value in str1, assign result to str1
str1
```

[89]:
```
'abcxyx'
```

2.5.2 Solution for exercise 2

[90]:
```
# 1. String concatenation
str1 = 'abc'
str2 = 'xyz'

# format specification to concatenate two string with a space in between
fmt = '{} {}'
fmt.format(str1, str2)
```

[90]:
```
'abc xyz'
```

[91]:
```
# 2. Truncate Python version to major version number
# To do this, we specify 0 decimal digits!
fmt = 'The current major version of Python is {:.0f}'
fmt.format(3.10)      # Now this didn't work out as intended :)
```

[91]:
```
'The current major version of Python is 3'
```

This does not work as intended because formatting with zero decimal digits rounds the floating-point number, instead of just truncating the decimal part. We could instead convert the `float` to `int` before applying formatting, since the function `int()` will truncate the fractional part:

[92]:
```
version = 3.10
fmt = 'The current major version of Python is {:d}'
print(fmt.format(int(version)))
```

```
The current major version of Python is 3
```

[93]:
```
# 3. Print pi using 10 decimal digits
from math import pi
fmt = 'The first 10 digits of pi: {:.10f}'
fmt.format(pi)
```

[93]:
```
'The first 10 digits of pi: 3.1415926536'
```

[94]:
```
# 4. Print exp(10.0) using three decimal digits and exponential notation
from math import exp
fmt = 'exp(10.0) = {:.3e}'
fmt.format(exp(10.0))
```

[94]:
```
'exp(10.0) = 2.203e+04'
```

2.5.3 Solution for exercise 3

We now repeat exercise 2 using f-strings instead of the `format()` method.

[95]:
```
# 1. String concatenation
str1 = 'abc'
str2 = 'xyz'

# format specification to concatenate two string with a space inbetween
```

```
s = f'{str1} {str1}'
print(s)
```

```
abc abc
```

[96]:
```
# 2. Truncate Python version to major version number
# To do this, we specify 0 decimal digits!
version = 3.10
s = f'The current major version of Python is {version:.0f}'
print(s)         # does not work as intended!
```

```
The current major version of Python is 3
```

This does not work as intended because formatting with zero decimal digits rounds the floating-point number, instead of just truncating the decimal part. See the previous exercise for one possible solution.

[97]:
```
# 3. Print pi using 10 decimal digits
from math import pi
s = f'The first 10 digits of pi: {pi:.10f}'
print(s)
```

```
The first 10 digits of pi: 3.1415926536
```

[98]:
```
# 4. Print exp(10.0) using three decimal digits and exponential notation
from math import exp
s = f'exp(10.0) = {exp(10.0):.3e}'
print(s)
```

```
exp(10.0) = 2.203e+04
```

The last example illustrates that f-string expressions can also be function calls, not just variable names!

2.5.4 Solution for exercise 4

List operators

[99]:
```
list1 = [1, 2, 3]
list2 = ['a', 'b', 'c']

# 1. Adding two lists concatenates the second list to the first
# and returns a new list object
list1 + list2
```

[99]:
```
[1, 2, 3, 'a', 'b', 'c']
```

[100]:
```
# 2. multiplication of list and integer replicates the list!
list1 * 2
```

[100]:
```
[1, 2, 3, 1, 2, 3]
```

[101]:
```
# 3. Extending list in place using +=
list1 += ['x', 'y', 'z']
list1
```

[101]:
```
[1, 2, 3, 'x', 'y', 'z']
```

Note that we cannot append an element to the list that is not a list:

[102]:
```
list1 += 10
```

```
TypeError: 'int' object is not iterable
```

Instead, we need to wrap a singular element to create a list like this:

[103]:
```
list1 += [10]
list1
```

[103]: [1, 2, 3, 'x', 'y', 'z', 10]

[104]:
```
# 4. Replicating list in place using *=
list1 *= 2
list1
```

[104]: [1, 2, 3, 'x', 'y', 'z', 10, 1, 2, 3, 'x', 'y', 'z', 10]

Tuple operators

[105]:
```
tpl1 = 1, 2, 3
tpl2 = 'a', 'b', 'c'

# 1. Adding two tuples concatenates the second tuple to the first
# and returns a new tuple object
tpl1 + tpl2
```

[105]: (1, 2, 3, 'a', 'b', 'c')

[106]:
```
# 2. multiplication of tuple and integer replicates the tuple!
tpl1 * 2
```

[106]: (1, 2, 3, 1, 2, 3)

[107]:
```
# 3. Extending tuple in place
tpl1 += ('x', 'y', 'z')
tpl1
```

[107]: (1, 2, 3, 'x', 'y', 'z')

It might be surprising that this works since a `tuple` is an immutable object. However, what happens is that the original `tuple` is discarded and the reference `tpl1` now points to a newly created `tuple`.

The same happens when we replicate a `tuple` with `*=`:

[108]:
```
# 4. Replicate tuple in place using *=
tpl1 *= 2
tpl1
```

[108]: (1, 2, 3, 'x', 'y', 'z', 1, 2, 3, 'x', 'y', 'z')

Tuple and list operators

We cannot mix tuples and lists as operands!

[109]:
```
lst = [1, 2, 3]
tpl = 'a', 'b', 'c'

# Cannot concatenate list and tuple!
lst + tpl
```

```
TypeError: can only concatenate list (not "tuple") to list
```

3 Control flow and list comprehensions

In this lecture, we continue to explore basic concepts of the Python programming language such as conditional execution and loops.

3.1 Conditional execution

Frequently, we want to execute a code block only if some condition holds. We can do this using the `if` statement:

[110]:
```
if 2*2 == 4:
    print('Python knows arithmetic!')
```

```
Python knows arithmetic!
```

A few observations:

- Conditional blocks are grouped using indentation (leading spaces). Remember from the previous unit that whitespace matters in Python!
- We write the equality operator using *two* equal signs, ==. This is to distinguish it from the assignment operator =.

We can also add an `else` block that will be executed whenever a condition is false:

[111]:
```
if 2*2 == 3:
    # this branch will never be executed
    print('Something is fishy here')
else:
    print('Python knows arithmetic!')
```

```
Python knows arithmetic!
```

Finally, we can add more than one conditional branch using the `elif` clause:

[112]:
```
var = 1
if var == 0:
    print('var is 0')
elif var == 1:
    print('var is 1')
else:
    print('var is neither 0 nor 1')
```

```
var is 1
```

3.1.1 Truth value testing

We already encountered == to test whether two values are equal. Python offers many more operators that return either `True` or `False` and can be used to control conditional execution.

Expression	Description
==	Equal. Works for numerical values, strings, etc.
!=	Not equal. Works on numerical values, strings, etc.

Expression	Description
`>, >=, <,<=`	Usual comparison of numerical values
`a is b, a is not b`	Test identity. `a is b` is `True` if `a` and `b` are the same object
`a in b, a not in b`	Test whether `a` is or is not included in `b` where `b` is a collection
`if obj, if not obj`	Any Python object evaluates to `True` or `False` in an intuitive fashion (see below)

Additionally, there are logical operators that allow us to combine two logical values:

Expression	Description
`a and b`	`True` if both `a` and `b` are `True`
`a or b`	`True` if at least one of `a` or `b` is `True`

Examples:

[113]:
```
# list1 and list2 reference the same object
list1 = [1,2]
list2 = list1
list1 is list2      # objects are identical, returns True
```

[113]: True

[114]:
```
# list1 and list2 do NOT reference the same object, but contain
# identical elements.
list2 = list1.copy()
list1 is list2      # returns False
```

[114]: False

[115]:
```
# Check if collections contain the same elements
list1 == list2      # returns True
```

[115]: True

[116]:
```
# Check whether element is in collection
1 in list1          # returns True
```

[116]: True

[117]:
```
# Combine logical expressions using 'and'
1 in list1 and 2 in list1    # returns True
```

[117]: True

We can also use the `in` operator to determine whether a key is contained in a dictionary:

[118]:
```
dct = {'institution': 'University of Glasgow'}
'institution' in dct         # prints True
```

[118]: True

[119]:
```
# check whether a key is NOT in the dictionary
'course' not in dct          # prints True
```

[119]: True

As mentioned above, any object evaluates to `True` or `False` in an `if` statement:

```
if obj:
    # do something if obj evaluates to True
```

The rules are quite intuitive: an object evaluates to `False` if

- it has a numerical type and is `0` (or `0.0`, or complex `0+0j`)
- it is an empty collection (tuple, list, dictionary, array, etc.)
- it is of logical (boolean) type and has value `False`
- it is `None`, a special built-in value used to denote that a variable does not reference anything.

In most other cases, an expression evaluates to `True`.

Examples:

[120]:
```
# evaluate numerical variable
x = 0.0
if x:
    print('Value is non-zero')
else:
    print('Value is zero')
```

```
Value is zero
```

[121]:
```
# Evaluate boolean variable
flag = True
if flag:
    print('Flag is True')
else:
    print('Flag is False')
```

```
Flag is True
```

The most important exception to the rule that objects intuitively evaluate to `True` or `False` if needed are NumPy arrays:

[122]:
```
import numpy as np

# Create array with 5 zeros
arr = np.zeros(5)
if arr:
    print('true!')
```

```
ValueError: The truth value of an array with more than one element is ambiguous.␣
↪Use a.any() or a.all()
```

As the error message indicates, Python requires you to be more specific about what exactly should be tested.

3.1.2 Conditional expressions

Conditional expression are more compact than conditional statements and can be used to return a value depending on some condition. A conditional expression takes three arguments using the syntax

```
<value if true> if <condition> else <value if false>
```

The value of this expression can be assigned to a variable, passed to a function, etc.

To illustrate, imagine we have the following code:

[123]:
```python
x = 1

# Test whether x is divisible by 2 without remainder using
# the modulo operator %
if (x % 2) == 0:
    var = 'even'
else:
    var = 'odd'
```

This code sets the value of `var` to either `'even'` or `'odd'`, depending on whether `x` is an even or odd integer. We can formulate this more concisely using a conditional expression:

[124]:
```python
var = 'even' if (x % 2) == 0 else 'odd'
```

We can even directly print the value of this expression!

[125]:
```python
x = 1
print('even' if (x % 2) == 0 else 'odd')
```

```
odd
```

3.2 Loops

Whenever we want to iterate over several items, we use the `for` loop. The `for` loop in Python is particularly powerful because it can "magically" iterate over all sorts of data, not just integer ranges.

The standard use-case is to iterate over a set of integers:

[126]:
```python
# iterate over 0,...,3 and print each element
for i in range(4):
    print(i)
```

```
0
1
2
3
```

We use the built-in `range` function to define the sequence of integers over which to loop. As usual in Python, the last element is *not* included. We can explicitly specify the start value and increment using the more advanced syntax `range(start, stop, step)`:

[127]:
```python
# iterate over 1,3
for i in range(1, 4, 2):
    print(i)
```

```
1
3
```

Unlike with some other languages, we can directly iterate over elements of a collection:

[128]:
```python
cities = ('Glasgow', 'Edinburgh', 'St. Andrews')
for city in cities:
    print(city)
```

```
Glasgow
Edinburgh
St. Andrews
```

We could of course alternatively iterate over indices and extract the corresponding element, but there is no need to:

[129]:
```
# Needlessly complicated and non-Pythonic
for i in range(len(cities)):
    # print city at index i
    print(cities[i])
```

```
Glasgow
Edinburgh
St. Andrews
```

Note that when looping over dictionaries, the default is to iterate over *keys*:

[130]:
```
dct = {'key1': 'value1', 'key2': 'value2'}
for key in dct:
    print(key)
```

```
key1
key2
```

We can explicitly choose whether to iterate over keys, values, or both:

[131]:
```
# iterate over keys, same as example above.
for key in dct.keys():
    print(key)
```

```
key1
key2
```

[132]:
```
# iterate over values
for value in dct.values():
    print(value)
```

```
value1
value2
```

[133]:
```
# iterate over keys and values at the same time
# using the items() method
for key, value in dct.items():
    # use format string to print key: value
    print(f'{key}: {value}')
```

```
key1: value1
key2: value2
```

Note that `items()` returns the key-value pairs as `tuples`, so we need to unpack each tuple by writing `key, value` as the running variables of the `for` loop.

Sometimes the set of items over which to iterate is not known ex ante, and then we can instead use the `while` loop with a terminal condition:

[134]:
```
z = 1.001
i = 0

# How many iterations will be performed? Not obvious ex ante.
while z < 100.0:
    z = z*z + 0.234
    i = i + 1

# print number of iterations
print(f'loop terminated after {i} iterations')
```

```
loop terminated after 5 iterations
```

3.2.1 Advanced looping

Oftentimes, we want to iterate over a list of items and at the same time keep track of an item's index. We can do this elegantly using the `enumerate()` function:

[135]:
```
cities = ('Glasgow', 'Edinburgh', 'St. Andrews')

# Iterate over cities, keep track of index in variable i
for i, city in enumerate(cities):
    print(f'City {i}: {city}')
```

```
City 0: Glasgow
City 1: Edinburgh
City 2: St. Andrews
```

We can skip an iteration or terminate the loop using the `continue` and `break` statements, respectively:

[136]:
```
for city in cities:
    if city == 'Edinburgh':
        # skip to next iteration in case of Edinburgh
        continue
    print(city)
```

```
Glasgow
St. Andrews
```

[137]:
```
for city in cities:
    if city == 'Glasgow':
        # Terminate iteration as soon as we find Glasgow
        print('Found Glasgow')
        break
```

```
Found Glasgow
```

3.3 List comprehensions

Python implements a powerful feature called *list comprehensions* that can be used to create collections such as tuples and lists without writing loop statements.

For example, imagine we want to create a list of squares of the integers $0, \ldots, 4$. We can do this using a loop and a list's `append()` method:

[138]:
```
# Initialise empty list
squares = []

# Loop over integers 0,...,4
for i in range(5):
    # The power operator in Python is **
    squares.append(i**2)
squares
```

[138]:
```
[0, 1, 4, 9, 16]
```

This is quite bloated and can be collapsed into a single expression using a list comprehension:

[139]:
```
squares = [i**2 for i in range(5)]
squares
```

[139]:
```
[0, 1, 4, 9, 16]
```

If the desired result should be a `tuple`, we can instead write

```
[140]: squares = tuple(i**2 for i in range(5))
       squares
```

```
[140]: (0, 1, 4, 9, 16)
```

Alternatively, we can also create a dictionary using curly braces and the syntax `{key: <expression> for ...}`:

```
[141]: squares = {i: i**2 for i in range(5)}
       squares
```

```
[141]: {0: 0, 1: 1, 2: 4, 3: 9, 4: 16}
```

List comprehensions can be nested and combined with conditions to create almost arbitrarily complex expressions (this doesn't mean that you should, though!)

```
[142]: # Create incomprehensible list comprehension.
       # The modulo operator in Python is %
       items = [i*j for i in range(5) if i % 2 == 0 for j in range(i)]
       items
```

```
[142]: [0, 2, 0, 4, 8, 12]
```

Written out as two nested loops, this code is equivalent to

```
[143]: items = []
       for i in range(5):
           if i % 2 == 0:
               for j in range(i):
                   items.append(i*j)
       items
```

```
[143]: [0, 2, 0, 4, 8, 12]
```

3.4 Exercises

These exercises are not meant to demonstrate the most efficient use of Python, but to help you practice the material we have studied above. In fact, you'd most likely *not* want to use the solutions presented here in real code!

3.4.1 Exercise 1: Approximate Euler's number

Euler's number is defined as

$$e = \lim_{n \to \infty} \left(1 + \frac{1}{n}\right)^n$$

1. Create a sequence of the approximations to e for $n = 10, 20, 30, \ldots, 100$ using a list comprehension.
2. Compute the approximation error for each of the elements. *Hint:* To get the built-in value for e, use the import statement

   ```
   from math import e
   ```

3.4.2 Exercise 2: Approximate the sum of a geometric series

Let $\alpha \in (0, 1)$. The sum of the geometric series $(1, \alpha, \alpha^2, \ldots)$ is given by

$$\sigma = \sum_{i=0}^{\infty} \alpha^i = \frac{1}{1 - \alpha}$$

Assume that $\alpha = 0.1$. Write a loop that accumulates the values of the sequence $(1, \alpha, \alpha^2, \dots)$ until the difference to the true value is smaller than 1×10^{-8}. How many elements does it take?

Hint: In Python (and many other languages) the floating-point value 1×10^{-8} is written as `1e-8`.

3.4.3 Exercise 3: Binary search (advanced)

The bisection method can be used to find to root of a function $f(x)$, i.e., the point x_0 such that $f(x_0) = 0$. In this exercise, we will use the same algorithm to find the interval of a strictly monotonic sequence of numbers that brackets the value zero (this is a binary search algorithm with approximate matching).

Assume that we have an array `x` of 11 increasing real numbers given by

[144]:
```
import numpy as np
x = np.linspace(-0.5, 1.0, 11)
x
```

[144]:
```
array([-0.5 , -0.35, -0.2 , -0.05,  0.1 ,  0.25,  0.4 ,  0.55,  0.7 ,
        0.85,  1.  ])
```

Write code that identifies the bracketing interval (in this case [-0.05,0.1]) using the following algorithm:

1. Initialize the index of the bracket lower bound to `lbound=0` and the index of the bracket upper bound to `ubound=len(x)-1`.
2. Compute the midpoint between these two indices (rounded to the nearest integer), `mid = (ubound + lbound) // 2`.

   Hint: The operator `//` truncates the result of a division to the nearest integer.
3. Inspect `x[mid]`, the value at index `mid`. If `x[mid]` has the same sign as `x[ubound]`, update the upper bound, `ubound=mid`. Otherwise, update the lower bound.
4. Continue until `ubound = lbound + 1`, i.e., until you have found the bracket `x[lbound] <= 0 < x[ubound]`.

3.4.4 Exercise 4: Diagonal and band matrices

Let `a` be a matrix of zeros with shape `(m,n)` with an integer data type:

```
a = np.zeros((m,n), dtype=int)
```

1. Set `m = n = 4`. Fill up the diagonal of `a` with ones so that it becomes an identity matrix. Verify that `np.identity()` gives the same result.
2. Recreate `a` to have dimensions `m = 4` and `n = 5`. Modify the main, first lower and first upper diagonals so that the resulting matrix looks like this, where omitted elements are zeros:

$$\begin{bmatrix} 1 & 2 & & & \\ 3 & 1 & 2 & & \\ & 3 & 1 & 2 & \\ & & 3 & 1 & 2 \end{bmatrix}$$

   Hint: Use nested `for` loops to set the diagonal elements.

3.4.5 Exercise 5: Triangular matrices

Let `a` be a matrix of zeroes with shape `(m,n)` and integer data type:

```
a = np.zeros((m,n), dtype=int)
```

Assume that `m = n = 4`. Using loops and `if` statements, modify the elements of `a` to obtain the following upper-triangular matrix, where omitted elements are set to zero:

$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ & 5 & 6 & 7 \\ & & 8 & 9 \\ & & & 10 \end{bmatrix}$$

3.5 Solutions

3.5.1 Solution for exercise 1

[145]:
```
# Compute approximation for n = 10, 20,..., 100
euler_approx = [(1.0+1.0/i)**i for i in range(10,101,10)]
print('Approximate values')
print(euler_approx)

# import 'correct' value
from math import e

# We need to subtract e from each element to get the approximation error
euler_error = [approx - e for approx in euler_approx]
print('Approximation error')
print(euler_error)
```

```
Approximate values
[2.5937424601000023, 2.653297705144422, 2.6743187758703026, 2.685063838389963,
2.691588029073608, 2.6959701393302162, 2.6991163709761854, 2.7014849407533275,
2.703332461058186, 2.7048138294215285]
Approximation error
[-0.12453936835904278, -0.06498412331462289, -0.043963052588742446,
-0.03321799006908188, -0.026693799385437256, -0.02231168912882886,
-0.019165457482859694, -0.016796887705717634, -0.01494936740085917,
-0.01346799903751661]
```

3.5.2 Solution for exercise 2

We don't know now many iterations we will need to get to the required tolerance of 1×10^{-8}, so this is a good opportunity to use a `while` loop.

[146]:
```
# Convergence tolerance
tol = 1e-8
alpha = 0.1
# The correct value
sigma_exact = 1.0/(1.0 - alpha)

# keep track of number of iterations
n = 0

# Initialise approximated sum
sigma = 0.0

# Iterate until absolute difference is smaller than tolerance level.
# The built-in function abs() returns the absolute value.

while abs(sigma - sigma_exact) > tol:
    # We can combine addition and assignment into a single operator +=
    # This is equivalent to
    #   sigma = sigma + alpha**n
    sigma += alpha**n
    # Increment exponent
```

```
    n += 1

print(f'Number of iterations: {n}, approx. sum: {sigma:.8f}')
```

```
Number of iterations: 9, approx. sum: 1.11111111
```

3.5.3 Solution for exercise 3

To complete the exercise, all you have to do is to translate the algorithm given in the exercise into code.

Since we don't know how many iterations it takes to find the bracket, we use a `while` loop that continues as long as `lbound` and `ubound` are more than 1 apart.

[147]:
```
import numpy as np

# Given array of increasing numbers
x = np.linspace(-0.5, 1.0, 11)


lbound = 0
ubound = len(x) - 1

while ubound > (lbound + 1):
    # Index of mid point. Indices have to be integers, so
    # we need to truncate the division result to an integer.
    mid = (ubound + lbound) // 2

    if (x[mid] * x[ubound]) > 0.0:
        # x[mid] and x[ubound] have same sign!
        ubound = mid
        print(f'Setting upper bound index to {ubound}')
    else:
        # x[mid] and x[lbound] have the same sign
        # or at least one of them is zero
        lbound = mid
        print(f'Setting lower bound index to {lbound}')

print(f'Value at lower bound: {x[lbound]:.4g}')
print(f'Value at upper bound: {x[ubound]:.4g}')
```

```
Setting upper bound index to 5
Setting lower bound index to 2
Setting lower bound index to 3
Setting upper bound index to 4
Value at lower bound: -0.05
Value at upper bound: 0.1
```

In this implementation, we use the fact that two non-zero real numbers a and b have the same sign whenever $a \cdot b > 0$.

3.5.4 Solution for exercise 4

For the first part, we need to loop over the diagonal elements and overwrite the zeros with ones:

[148]:
```
# Part 1: create identity matrix

import numpy as np

n = 4
a = np.zeros((n,n), dtype=int)

# loop over diagonal elements, set them to 1
```

```
for i in range(n):
    a[i,i] = 1

# print identity matrix
a
```

[148]:
```
array([[1, 0, 0, 0],
       [0, 1, 0, 0],
       [0, 0, 1, 0],
       [0, 0, 0, 1]])
```

You can get the same result using NumPy's `np.identity()` function:

[149]:
```
n = 4
np.identity(n, dtype=int)
```

[149]:
```
array([[1, 0, 0, 0],
       [0, 1, 0, 0],
       [0, 0, 1, 0],
       [0, 0, 0, 1]])
```

For the second part, we need nested loops over rows and columns and we check at each position (i, j) whether it is on the main diagonal, or on the first upper or lower diagonal.

[150]:
```
# Part 2: create band matrix

import numpy as np

m = 4
n = 5

a = np.zeros((m,n), dtype=int)

# loop over rows
for i in range(m):
    # loop over columns
    for j in range(n):
        if i == j:
            # main diagonal element
            a[i,j] = 1
        elif i == (j - 1):
            # upper diagonal element
            a[i,j] = 2
        elif i == (j + 1):
            # lower diagonal element
            a[i,j] = 3

# print final matrix
a
```

[150]:
```
array([[1, 2, 0, 0, 0],
       [3, 1, 2, 0, 0],
       [0, 3, 1, 2, 0],
       [0, 0, 3, 1, 2]])
```

3.5.5 Solution for exercise 5

We solve this exercise using two nested `for` loops, the first over rows, the second over columns:

[151]:
```
import numpy as np
```

```
m = 4
n = 4

a = np.zeros((m,n), dtype=int)

# keep track of value to be inserted
value = 1

# loop over rows
for i in range(m):
    # loop over columns
    for j in range(i, n):
        a[i,j] = value
        # increment value for next matching element
        value += 1

# print final matrix
a
```

```
[151]: array([[ 1,  2,  3,  4],
              [ 0,  5,  6,  7],
              [ 0,  0,  8,  9],
              [ 0,  0,  0, 10]])
```

Note that the loop over columns uses the current row index as the lower bound, since we never need to insert anything at element (i, j) if $j < i$.

4 Reusing code: Functions, modules and packages

In this unit, we learn how to build reusable code with functions. We will also briefly discuss modules and packages.

4.1 Functions

Functions are used to implement code that performs a narrowly defined task. We use functions for two reasons:

1. A function can be called repeatedly without having to write code again and again.
2. Even if a function is not called frequently, functions allow us to write code that is "shielded" from other code we write and is called via a clean interface. This helps to write more robust and error-free code.

Functions are defined using the `def` keyword, and the function body needs to be an indented block:

[152]:
```
def func():
    print('func called')

# invoke func without arguments
func()
```

```
func called
```

4.1.1 Arguments

Functions can have an arbitrary number of positional arguments (also called parameters).

[153]:
```
# Define func to accept argument x
def func(x):
    print(f'func called with argument {x}')

# call function with various arguments.
func(1)
func('foo')
```

```
func called with argument 1
func called with argument foo
```

4.1.2 Return values

Functions can also return values to their caller using the `return` statement.

[154]:
```
def func(x):
    return x * 2.0

result = func(1.0)
print(result)        # prints 2.0
```

```
2.0
```

A `return` statement without any argument immediately exits the functions. The default return value is the special type `None`.

A function can return multiple values which are then automatically collected into a tuple:

[155]:
```
def func():
    return 1, 2, 3

values = func()          # call func(), get tuple of values
type(values)
```

[155]:
```
tuple
```

Python supports "unpacking" of tuples, lists, etc. We can use this to directly assign names to multiple return values:

[156]:
```
def func():
    return 'a', 'b', 'c'

value1, value2, value3 = func()      # call func(), unpack return values
print(f'Value 1: {value1}, Value 2: {value2}, Value 3: {value3}')
```

```
Value 1: a, Value 2: b, Value 3: c
```

4.1.3 Accessing data from the outer scope

A function need not have arguments or a return value, but that limits its usefulness somewhat. However, a function can access outside data which is defined in the so-called outer scope:

[157]:
```
x = 1.0
def func():
    # Read x from outer scope
    print(f'func accessing x from outer scope: x = {x}')

# prints value of x from within func()
func()
```

```
func accessing x from outer scope: x = 1.0
```

We can write functions without any arguments that only operate on outside data. However, this is terrible programming practice and should be avoided in most cases.

Because functions can operate on external data, they are not analogous to mathematical functions. If we write $f(x)$, we usually mean that f is a function of x only (and possibly some constant parameters). By definition we must have

$$x_1 = x_2 \Longrightarrow f(x_1) = f(x_2),$$

i.e., a function always returns the same value when called with the same parameters. However, this is not the case in Python or most other programming languages:

[158]:
```
a = 1.0
def func(x):
    return a*x

x = 1.0
print(func(x))       # prints 1.0

a = 2.0
print(func(x))       # x unchanged, but prints 2.0
```

```
1.0
2.0
```

4.1.4 More on arguments

Default arguments

Python offers an extremely convenient way to specify default values for arguments, so these need not be passed when the function is called:

[159]:
```
# define function with a default value for argument alpha
def func(x, alpha=1.0):
    return x * alpha

print(func(2.0))         # uses default value for alpha
print(func(2.0, 1.0))    # explicitly specified optional argument
print(func(2.0, 3.0))    # use some other value for alpha
```

```
2.0
2.0
6.0
```

Keyword (or named) arguments

Arguments don't need to be provided in the same order as specified in the function signature. We can use argument names to explicitly assign values to the corresponding argument.

[160]:
```
def func(arg1, arg2):
    print(f'arg1: {arg1}, arg2: {arg2}')

func(1, 2)              # Call using purely positional arguments
func(arg1=1, arg2=2)    # Use argument names to explicitly assign values
func(arg2=2, arg1=1)    # With keyword arguments, the order does not matter!
```

```
arg1: 1, arg2: 2
arg1: 1, arg2: 2
arg1: 1, arg2: 2
```

Arbitrary number of optional arguments

Python supports functions which accept an arbitrary number of positional and keyword arguments. This is accomplished via two special tokens:

- `*args`: collects any number of "excess" *positional arguments* and packs them into a tuple.
- `**kwargs`: collects any number of "excess" *keyword arguments* and packs them into a dictionary. Needs to be placed at the end of the argument list!

Examples:

[161]:
```
# Define function with mandatory, optional, optional positional
# and optional keyword arguments

def func(x, opt='default', *args, **kwargs):
    print(f'Required argument x: {x}')
    print(f'Optional argument opt: {opt}')
    if args:
        # if the tuple 'args' is non-empty, print its contents
        print('Optional positional arguments:')
        for arg in args:
            print(f'  {arg}')
    if kwargs:
        # if the dictionary 'kwargs' is non-empty, print its contents
        print('Optional keyword arguments:')
        for key, value in kwargs.items():
```

```
            print(f'  {key}: {value}')
```

[162]:
```
# Call only with required argument
func(0)
```

```
Required argument x: 0
Optional argument opt: default
```

[163]:
```
# Call with required and optional arguments
func(0, 'optional')
```

```
Required argument x: 0
Optional argument opt: optional
```

[164]:
```
# Call with required and optional arguments, and
# optional positional arguments
func(0, 'optional', 1, 2, 3)
```

```
Required argument x: 0
Optional argument opt: optional
Optional positional arguments:
  1
  2
  3
```

[165]:
```
# Call with required and optional arguments, and
# optional positional and keyword arguments
func(0, 'optional', 1, 2, 3, arg1='value1', arg2='value2')
```

```
Required argument x: 0
Optional argument opt: optional
Optional positional arguments:
  1
  2
  3
Optional keyword arguments:
  arg1: value1
  arg2: value2
```

We don't even need to specify arguments in the order they are defined in the function, except for optional positional arguments, since these have no argument names. We can just use the `name=value` syntax:

[166]:
```
# call func() with interchanged argument order
func(opt='optional value', x=1)
```

```
Required argument x: 1
Optional argument opt: optional value
```

Note, however, that in a function call any positional arguments must come first and those passed as `name=value` pairs last:

[167]:
```
x = 1

# this will not work, cannot specify positional arguments last
func(opt='optional value', x)
```

```
  Input In [167]
    func(opt='optional value', x)
                                ^
SyntaxError: positional argument follows keyword argument
```

The same applies for optional arguments passed in via `*args` and `**kwargs`:

[168]:
```
# fails because arguments collected in *args must
# be specified before arguments collected in **kwargs!
func(1.0, 'opt', arg1='value1', arg2='value2', 1, 2, 3)
```

```
  Input In [168]
    func(1.0, 'opt', arg1='value1', arg2='value2', 1, 2, 3)
                                                          ^
SyntaxError: positional argument follows keyword argument
```

4.1.5 Modifying data in the outer scope

So far, we covered read-only access to data defined outside of a function and relied on return values to pass results back to the caller. However, it is possible to directly *modify* data in the outer scope, even though this should usually be avoided:

- Using arguments and return values clearly defines a function's interface, there are no unpleasant surprises.
- Conversely, if a function starts modifying values in the caller's environment, there is no way to be sure what the function is changing in the outer scope
  other than examining its source code.

Consider first the following attempt to modify a value defined outside of the function:

[169]:
```
var = 'outer scope'

# Create function, assign value to var
def modify_var():
    var = 'inner scope'

print(var)
modify_var()
print(var)
```

```
outer scope
outer scope
```

This code prints `'outer scope'` twice. What happened? Without any further instructions, the assignment inside the function creates a *local* variable `var` that is completely disconnected from `var` in the outer scope!

We need to use the `global` statement to tell Python to instead assign to a variable in the global (outer) scope:

[170]:
```
var  = 'outer scope'

def modify_var():
    global var
    var = 'inner scope'

print(var)
modify_var()
print(var)
```

```
outer scope
inner scope
```

The second output now reads `'inner scope'`.

Note that `global` in Python actually means global to a module, i.e., a symbol that is defined at the top level within a module (we discuss modules below). There are no truly global variables in Python unlike in languages such as C.

The requirement that the name in the `global` statement refers to a global variable has subtle implications. Consider the following example of two *nested* functions:

[171]:
```
def outer():
    var = 'outer function'

    def inner():
        # Bind var to global name var
        global var
        var = 'inner function'

    print(var)
    inner()
    print(var)

outer()
```

```
outer function
outer function
```

Surprisingly, the code above prints `'outer function'` twice. The reason is that `var` defined in `outer()` is *not* a global variable as it was not defined at the top level within a module. Instead, it is a *local* variable in `outer()`.

For such scenarios, Python has the `nonlocal` statement which works similarly to `global` except that it operates on a name in the immediate outer scope, irrespective of whether this outer scope is another function or the module itself.

We can use `nonlocal` to get the desired behaviour:

[172]:
```
def outer():
    # var is in outer's local scope
    var = 'outer function'

    def inner():
        # bind var to name in immediate outer scope,
        # which is the local scope of outer()
        nonlocal var
        var = 'inner function'

    print(var)
    inner()
    print(var)

outer()
```

```
outer function
inner function
```

4.1.6 Pass by value or pass by reference?

Can functions modify their arguments? This questions usually comes down to whether a function call uses *pass by value* or *pass by reference*:

- *pass by value* means that a copy of every argument is created before it is passed into the function. A function therefore cannot modify a value in the caller's environment.
- *pass by reference* means that only a reference to a value is passed to the function, so the function can directly modify values at the call site.

This programming model is used in languages such as C (pass by value) or Fortran (pass by reference), but not in Python. Sloppily speaking, we can say that in Python a reference ("variable name") is passed by value. This means assigning a different value to an argument ("the reference") within a function has no effect outside of the function:

[173]:
```
def func(x):
    # x now points to something else
    x = 1.0

x = 123
func(x)

x       # prints 123, x in the outer scope is unchanged
```

[173]:
```
123
```

However, if a variable is a mutable object (such as a `list` or a `dict`), the function can use its own copy of the reference to that object to modify the object even in the outer scope:

[174]:
```
def func(x):
    # uses reference x to modify list object outside of func()
    x.append(4)

lst = [1,2,3]
func(lst)
lst     # prints [1,2,3,4]
```

[174]:
```
[1, 2, 3, 4]
```

Nevertheless, even for mutable objects the rule from above applies: when a new value is *assigned* to a named argument, that name then references a different object, leaving the original object unmodified:

[175]:
```
def func(x):
    # this does not modify object in outer scope,
    # x now references a new (local) object.
    x = ['a', 'b', 'c']

lst = [1,2,3]
# pass list, which is mutable and can thus be changed in func()
func(x)

lst     # prints [1,2,3]
```

[175]:
```
[1, 2, 3]
```

For immutable objects such as tuples, the reference passed to the function of course cannot be used to modify the object inside the function:

[176]:
```
def func(x):
    x[0] = 'modified in func'

items = (1, 2, 3)           # create tuple of integers
func(items)
```

```
TypeError: 'tuple' object does not support item assignment
```

Passing in a mutable collection such as a list, however, works as expected:

[177]:
```
items = [1, 2, 3]
```

```
func(items)

items
```

[177]: ['modified in func', 2, 3]

4.1.7 Methods

Methods are simply functions that perform an action on a particular object which they are bound to. We will not write methods in this course ourselves (they are part of what's called object-oriented programming), but we frequently use them when we invoke actions on objects such as lists:

[178]:
```python
# Create a list
lst = [1,2,3]

# append() is a method of the list class and can be invoked
# on list objects.
lst.append(4)
lst
```

[178]: [1, 2, 3, 4]

4.1.8 Functions as objects

Functions are objects in their own right, which means that you can perform various operations with them:

- Assign a function to a variable.
- Store functions in collections.
- Pass function as an argument to other functions.

Examples:

[179]:
```python
def func1(x):
    print(f'func1 called with argument {x}')

def func2(x):
    print(f'func2 called with argument {x}')


# List of functions
funcs = [func1, func2]

# Assign functions to variable f
for f in funcs:
    # call function referenced by f
    f('foo')
```

```
func1 called with argument foo
func2 called with argument foo
```

[180]:
```python
# Pass one function as argument to another function
func1(func2)
```

```
func1 called with argument <function func2 at 0x7f9de4b45360>
```

4.1.9 lambda expressions

You can think of lambda expressions as light-weight functions. The syntax is

```
lambda x: <do something with x>
```

The return value of a lambda expression is whatever its body evaluates to. There is no need (or possibility) to explicitly add a `return` statement.

One big difference to regular functions is that lambda expressions are *expressions*, not statements.

- At this point we gain little from a technical discussion on *statements* vs *expressions*. Loosely speaking, statements are one level above expressions in the Python syntax hierarchy, and the language puts restrictions on where statements can appear. Function definitions, `for` and `while` loops, and `if/elif/else` blocks are statements, among others.
- Conversely, *expressions* are more flexible and can appear basically anywhere. They usually evaluate to some object that can be assigned, passed to a function, etc., whereas statements usually can't.

The take-away is that we can fiddle in lambda expressions almost anywhere, even as arguments in function calls!

For example, we might have a function that applies some algebraic operation to its arguments, and the operation can be flexibly defined by the caller.

[181]:
```
def func(items, operation=lambda z: z + 1):
    # default operation: increment value by 1
    result = [operation(i) for i in items]
    return result

numbers = [1.0, 2.0, 3.0]
# call with default operation
func(numbers)                    # prints [2.0, 3.0, 4.0]
```

[181]:
```
[2.0, 3.0, 4.0]
```

[182]:
```
# We can also use lambda expressions to specify
# an alternative operation directly in the call!

func(numbers, lambda x: x**2.0)      # prints [1.0, 4.0, 9.0]
```

[182]:
```
[1.0, 4.0, 9.0]
```

While we could have defined the operation using a "regular" function statement, this is shorter.

4.2 Modules and packages

4.2.1 Modules

Modules allow us to further encapsulate code that implements some particular functionality.

- Each Python file (with the extension `.py`) automatically corresponds to a module of the same name.
- Objects defined within such a module are by default not visible outside of the module, thus helping to avoid naming conflicts.

To actually demonstrate the usage of modules, we need to use files outside of this notebook. To this end, there is an additional Python file in the current directory:

```
lectures/
    unit04_mod.py
```

The module `unit04_mod.py` contains the following definitions:

```
# Contents of unit04_mod.py

# global variable in this module
var = 'Variable defined in unit04_mod'
```

```
# global function in this module
def func():
    print(f'func in module unit04_mod called')
```

Module search path

Before getting into the details, we first need to verify that we can import the module `unit04_mod` using the `import` statement:

[183]:
```
import unit04_mod
```

Depending on where exactly you are running this code, the above import statement might fail with a `ModuleNotFoundError` (if no error was raised you can skip the rest of this section). This happens whenever the directory in which the module resides is not in the *module search path* used by Python.

To fix this, check the module search path as follows:

[184]:
```
import sys
sys.path
```

[184]:
```
['/home/richard/repos/python-statistics/lectures',
 '/home/richard/.conda/envs/py3-default/lib/python310.zip',
 '/home/richard/.conda/envs/py3-default/lib/python3.10',
 '/home/richard/.conda/envs/py3-default/lib/python3.10/lib-dynload',
 '',
 '/home/richard/.conda/envs/py3-default/lib/python3.10/site-packages',
 '/home/richard/.conda/envs/py3-default/lib/python3.10/site-
packages/PyQt5_sip-12.11.0-py3.10-linux-x86_64.egg']
```

If the `lectures/` directory is not included in this list, you can add it manually. For example, this notebook is executed in the git repository's root directory, you need to exectute

[185]:
```
import sys
# add lectures/ directory using a relative path
sys.path.append('./lectures/')
```

Importing symbols

We now want to use `func` and `var` in our notebook. However, by default these symbols are not visible and first need to be imported. We can do this in several ways:

1. We can import the module and use fully qualified names to reference objects from `unit04_mod`.
2. We can select which names from `unit04_mod` should be directly accessible.

The first variant looks like this:

[186]:
```
import unit04_mod

# Access variable defined in unit04_mod
print(unit04_mod.var)

# Call function defined in unit04_mod
unit04_mod.func()
```

```
Variable defined in unit04_mod
func in module unit04_mod called
```

If a symbol from `unit04_mod` is used frequently, we might want to make it accessible without the `unit04_mod` prefix. This is the second variant:

[187]:
```
from unit04_mod import var, func

# Access variable defined in unit04_mod
print(var)
```

```
# Call function defined in unit04_mod
func()
```

```
Variable defined in unit04_mod
func in module unit04_mod called
```

What if our notebook itself defines a function `func()` which would overwrite the reference to the one imported from `unit04_mod`, as in the following example?

[188]:
```python
from unit04_mod import func

# Calls func() defined in unit04_mod
func()

# overwrites definition from unit04_mod with local version
def func():
    print('func in notebook called')

# Calls func() defined in notebook
func()
```

```
func in module unit04_mod called
func in notebook called
```

In such a scenario, we can assign aliases to imported symbols using `as`:

[189]:
```python
from unit04_mod import func as imported_func     # The function formerly known
                                                 # as func is now imported_func

def func():
    print('func in notebook called')

# call our own func
func()

# call func from module unit04_mod
imported_func()
```

```
func in notebook called
func in module unit04_mod called
```

We can even alias the module name itself, as we frequently do with widely used modules such as `numpy`:

[190]:
```python
import unit04_mod as u4m

u4m.func()    # call function from module unit04_mod
```

```
func in module unit04_mod called
```

[191]:
```python
# universal convention to import numpy like this
import numpy as np
```

4.2.2 Packages

Packages are roughly speaking collections of modules and a little magic on top. We will not be creating packages, but we have already been using them: basically everything besides the built-in functions is defined in some package. For example, the NumPy library is a collection of packages.

4.3 Exercises

4.3.1 Exercise 1: Sign function

Implement a function `sign` which returns the following values:

$$sign(x) = \begin{cases} -1 & \text{if } x < 0 \\ 0 & \text{if } x = 0 \\ 1 & \text{if } x > 0 \end{cases}$$

Test your function on a negative, zero and positive argument.

4.3.2 Exercise 2: Sum of arbitrary number of elements

Create a function called `my_sum` which accepts an arbitrary number of arguments (possibly zero) and returns their sum. Assume that all arguments are numeric.

Test your function with the following arguments:

```
my_sum(10.0)     # one argument
my_sum(1,2,3)    # multiple arguments
my_sum()         # no arguments
```

Make sure that in the last case your function returns zero, which is the sum over an empty set.

4.3.3 Exercise 3: Fibonacci sequence

A classical introductory exercise to programming is to write a function that returns the first n terms of the Fibonacci sequence. The i-th element of this sequence is the integer x_i defined as

$$x_i = \begin{cases} 0 & \text{if } i = 0 \\ 1 & \text{if } i = 1 \\ x_{i-1} + x_{i-2} & \text{else} \end{cases}$$

Write a function `fibonacci(i)`,

```
def fibonacci(i):
    ...
```

which returns the i-th item in the sequence using recursion. A recursive function is a function that calls itself to perform (part of) its task, i.e., you should compute x_i like this:

```
xi = fibonacci(i-1) + fibonacci(i-2)
```

Use this function to compute the first 10 elements of this sequence with a list comprehension.

4.3.4 Exercise 4: Factorials

1. Implement a function that computes the factorial of a non-negative integer n defined as $n! = \prod_{i=1}^{n} i$. Keep in mind that this definition implies that $0! = 1$. Use the list comprehension syntax to create a tuple that contains the factorials for the integers $n = 1, \dots, 10$.

   Hint: The factorial can be written as a recurrence relation $n! = n \cdot (n-1)!$, which you can use to implement the recursive function.

2. Provide an alternative implementation that does not rely on recursion, but instead uses NumPy's `prod()` function to compute the product of a sequence of numbers. Again, create a `tuple` that contains the factorials for the integers $n = 1, \dots, 10$ using a list comprehension.

   Hint 1: To compute the product of the integers $i, i+1, \dots, j$, you can use `np.prod(range(i, j+1))`.

   Hint 2: The product of an empty set is 1, which is what `np.prod()` returns.

4.3.5 Exercise 5: Bisection root-finding algorithm (advanced)

We revisit the binary search algorithm from unit 3, this time applied to finding the root of a continuous function. This is called the bisection method.

Implement a function `bisection(f, a, b, tol, xtol)` which finds the root of the function $f(x)$, i.e., the value x_0 where $f(x_0) = 0$, on the interval $[a, b]$. Assume that $a < b$ and that the function values $f(a)$ and $f(b)$ have opposite signs.

Test your implementation using the function $f(x) = x^2 - 4$ on the interval $[-3, 0]$, which has a (unique) root at $x_0 = -2$.

Hint: The bisection algorithm proceeds as follows:

1. Define tolerance levels $\epsilon > 0$ and $\epsilon_x > 0$. The algorithm completes successfully whenever we have either $|f(x_0)| < \epsilon$ or $|b - a| < \epsilon_x$.
2. Main loop of the algorithm:
   1. Compute the midpoint $x_m = (a + b)/2$
   2. Compute function value $f_m = f(x_m)$
   3. If either $|f_m| < \epsilon$ or $|b - a| < \epsilon_x$, accept x_m as the solution and exit.
   4. Otherwise, update either a or b:
      1. If $sign(f(b)) = sign(f_m)$, set $b = x_m$
         Hint: One way to check whether two non-zero values have the same sign is to check if $f(b) \cdot f_m > 0$.
      2. Otherwise, $a = x_m$
   5. Proceed to next iteration of main loop.

4.4 Solutions

4.4.1 Solution for exercise 1

[192]:
```python
import numpy as np

def sign(x):
    if x < 0.0:
        return -1.0
    elif x == 0.0:
        return 0.0
    elif x > 0.0:
        return 1.0
    else:
        # Argument is not a proper numerical value, return NaN
        # (NaN = Not a Number)
        return np.nan

# Test on a few values
print(sign(-123))
print(sign(0))
print(sign(12345))
```

```
-1.0
0.0
1.0
```

Note that NumPy has a "proper" sign function, `np.sign()`, which implements the same logic but is more robust, accepts array arguments, etc.

4.4.2 Solution for exercise 2

For a function to accept an arbitrary number of elements, we need to declare an `*args` argument.

One possible implementation of `my_sum()` looks as follows:

```
[193]: def my_sum(*args):
           # Initialise sum to 0
           s = 0
           for x in args:
               s += x
           return s


       # Test with built-in range() object
       print(my_sum(10.0))
       print(my_sum(1, 2, 3))
       print(my_sum())
```

```
10.0
6
0
```

Of course in real code we would use the built-in function `sum()`, or preferably the NumPy variant `np.sum()`:

```
[194]: import numpy as np

       print(np.sum(10.0))

       # Need to pass argument as collection
       print(np.sum((1, 2, 3)))

       # np.sum() cannot be invoked without arguments, but we can
       # call it with an empty tuple ()
       np.sum(())
```

```
10.0
6

[194]: 0.0
```

4.4.3 Solution for exercise 3

The recursive definition of `fibonacci(i)` could look like this:

```
[195]: def fibonacci(i):
           if i == 0:
               # No recursion needed
               xi = 0
           elif i == 1:
               # No recursion needed
               xi = 1
           else:
               # Assume that i > 1. We will learn later how to
               # return an error if this is not the case.
               # Use recursion to compute the two preceding values
               # of the sequence.
               xi = fibonacci(i-1) + fibonacci(i-2)
           return xi

       # Compute the first 10 elements of the sequence using a list comprehension
       first10 = [fibonacci(i) for i in range(10)]
       first10
```

```
[195]: [0, 1, 1, 2, 3, 5, 8, 13, 21, 34]
```

Note that this is a terribly inefficient way to compute things, as the same elements of the sequence will needlessly be calculated over and over again.

Also, Python has a built-in recursion limit, so you cannot call a function recursively arbitrarily many times. You can find out what this limit is as follows:

[196]:
```
import sys
print(sys.getrecursionlimit())
```

```
3000
```

4.4.4 Solution for exercise 4

The following code shows a function computing the factorial $n!$ using recursion:

[197]:
```
def factorial(n):
    if n == 0:
        return 1
    else:
        # Use recursion to compute factorial
        return n * factorial(n-1)

fact10 = tuple(factorial(n) for n in range(10))
fact10
```

[197]:
```
(1, 1, 2, 6, 24, 120, 720, 5040, 40320, 362880)
```

An implementation without recursion can be created using NumPy's `prod()` function which computes the product of a sequence of numbers:

[198]:
```
import numpy as np
fact10 =  tuple(np.prod(range(1,n+1)) for n in range(10))
fact10
```

[198]:
```
(1.0, 1, 2, 6, 24, 120, 720, 5040, 40320, 362880)
```

Notice that the first element of this sequence is a floating-point value 1.0, while the remaining elements are integers. Why is that? Examine the argument passed to `np.prod()` for `n=0`:

[199]:
```
n = 0
# We have to embed range() in an expression that forces the Python
# interpreter to actually expand the range object, such as a tuple().
tuple(range(1,n+1))
```

[199]:
```
()
```

As you see, for `n=0` this is an empty container without elements. The mathematical convention is that the product over an empty set is $\prod_{i\in\emptyset} = 1$, and this is exactly what `np.prod()` returns. However, by default NumPy creates floating-point values, and so the return value is 1.0, not 1.

You can get around this by explicitly specifying the data type using the `dtype` argument, which is accepted by many NumPy functions.

[200]:
```
import numpy as np
# Force result to be of integer type
fact10 =  tuple(np.prod(range(1,n+1), dtype=int) for n in range(10))
fact10
```

[200]:
```
(1, 1, 2, 6, 24, 120, 720, 5040, 40320, 362880)
```

Alternatively, we can use `np.arange()` instead of `range()` as the former by default returns integer arrays, even if they are empty:

[201]:
```python
import numpy as np
# Force result to be of integer type
fact10 =  tuple(np.prod(np.arange(1,n+1)) for n in range(10))
fact10
```

[201]:
```
(1, 1, 2, 6, 24, 120, 720, 5040, 40320, 362880)
```

Finally, you of course would not need to implement the factorial function yourself, as there is one in the `math` module shipped with Python:

[202]:
```python
import math
fact10 = tuple(math.factorial(n) for n in range(10))
fact10
```

[202]:
```
(1, 1, 2, 6, 24, 120, 720, 5040, 40320, 362880)
```

4.4.5 Solution for exercise 5

Below you find a simple implementation of a bisection algorithm. This function does not perform any error checking and assumes that the initial bracket $[a, b]$ actually contains a root, and that the values $f(a)$ and $f(b)$ have opposite signs.

Note that we impose two termination criteria, and the algorithm will end successfully whenever one of them is satisfied:

1. The function value is sufficiently close to zero, i.e., $|f(x_0)| < \epsilon$ for some small $\epsilon > 0$.
2. The bracket is sufficiently small, i.e., $|b - a| < \epsilon_x$, again for some small $\epsilon_x > 0$

This is standard practice in numerical optimisation since we don't want the algorithm to continue unnecessarily if the desired degree of precision was achieved.

We specify the termination tolerance as optional arguments `tol` and `xtol` with sensible defaults. We also add the maximum permissible number of iterations as an optional argument `maxiter`.

[203]:
```python
def bisect(f, a, b, tol=1.0e-6, xtol=1.0e-6, maxiter=100):

    for iteration in range(maxiter):
        # Compute candidate value as midpoint between a and b
        mid = (a + b) / 2.0
        if abs(b-a) < xtol:
            # Remaining interval is too small
            break

        fmid = f(mid)

        if abs(fmid) < tol:
            # function value is close enough to zero
            break

        print(f'Iteration {iteration}: f(mid) = {fmid:.4e}')
        if fmid*f(b) > 0.0:
            # f(mid) and f(b) have the same sign, update upper bound b
            print(f'  Updating upper bound to {mid:.8f}')
            b = mid
        else:
            # f(mid) and f(a) have the same sign, or at least one of
            # them is zero.
            print(f'  Updating lower bound to {mid:.8f}')
            a = mid

    return mid
```

```python
# Compute root of f(x) = x^2 - 4 on the interval [-3, 0]
# We pass the function f as the first argument, and use a lambda expression
# to define the function directly in the call.
x0 = bisect(lambda x: x**2.0 - 4.0, -3.0, 0.0)

# Print root. The true value is -2.0
x0
```

```
Iteration 0: f(mid) = -1.7500e+00
  Updating upper bound to -1.50000000
Iteration 1: f(mid) = 1.0625e+00
  Updating lower bound to -2.25000000
Iteration 2: f(mid) = -4.8438e-01
  Updating upper bound to -1.87500000
Iteration 3: f(mid) = 2.5391e-01
  Updating lower bound to -2.06250000
Iteration 4: f(mid) = -1.2402e-01
  Updating upper bound to -1.96875000
Iteration 5: f(mid) = 6.2744e-02
  Updating lower bound to -2.01562500
Iteration 6: f(mid) = -3.1189e-02
  Updating upper bound to -1.99218750
Iteration 7: f(mid) = 1.5640e-02
  Updating lower bound to -2.00390625
Iteration 8: f(mid) = -7.8087e-03
  Updating upper bound to -1.99804688
Iteration 9: f(mid) = 3.9072e-03
  Updating lower bound to -2.00097656
Iteration 10: f(mid) = -1.9529e-03
  Updating upper bound to -1.99951172
Iteration 11: f(mid) = 9.7662e-04
  Updating lower bound to -2.00024414
Iteration 12: f(mid) = -4.8827e-04
  Updating upper bound to -1.99987793
Iteration 13: f(mid) = 2.4414e-04
  Updating lower bound to -2.00006104
Iteration 14: f(mid) = -1.2207e-04
  Updating upper bound to -1.99996948
Iteration 15: f(mid) = 6.1035e-05
  Updating lower bound to -2.00001526
Iteration 16: f(mid) = -3.0518e-05
  Updating upper bound to -1.99999237
Iteration 17: f(mid) = 1.5259e-05
  Updating lower bound to -2.00000381
Iteration 18: f(mid) = -7.6294e-06
  Updating upper bound to -1.99999809
Iteration 19: f(mid) = 3.8147e-06
  Updating lower bound to -2.00000095
Iteration 20: f(mid) = -1.9073e-06
  Updating upper bound to -1.99999952
```

```
[203]: -2.000000238418579
```

5 Plotting

In this unit, we take a first look at plotting numerical data. Python itself does not have any built-in plotting capabilities, so we will be using *matplotlib (MPL)*, the most popular graphics library for Python.

- For details on a particular plotting function, see the official documentation.
- There is an official introductory tutorial which you can use along-side this unit.

When using matplotlib in interactive Jupyter notebooks (such as this one), we can enable a more fancy plotting backend that allows us to dynamically adjust the zoom, etc. This is done by adding the line

```
%matplotlib widget
```

For this to work, the `ipympl` package needs to be installed, see here for details. Note that this is not supported (and in fact produces a syntax error) in regular `*.py` Python script files.

In order to access the functions and objects from matplotlib, we first need to import them. The general convention is to use the namespace `plt` for this purpose:

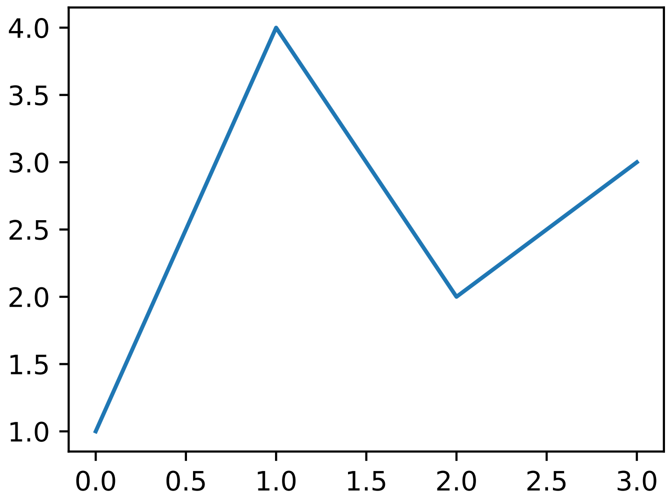
[204]:
```
import matplotlib.pyplot as plt
```

5.1 Line plots

One of the simplest plots we can generate is a line defined by a list of points.

[205]:
```
# import matplotlib library
import matplotlib.pyplot as plt

# Plot list of integers
yvalues = [1, 4, 2, 3]
plt.plot(yvalues)
```

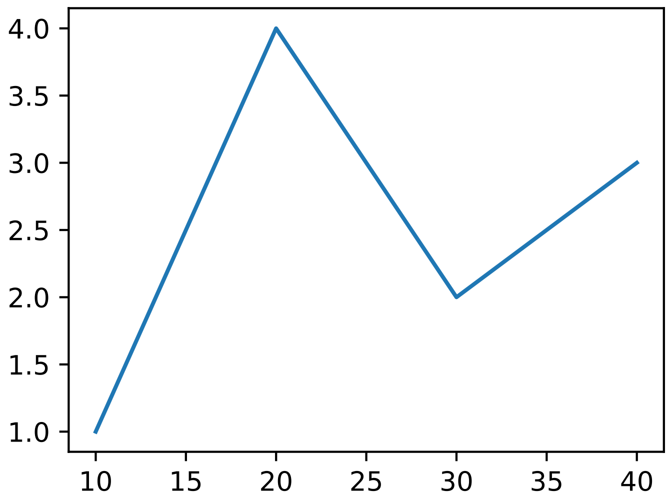
[205]:
```
[<matplotlib.lines.Line2D at 0x7f9de49ad6c0>]
```



We didn't even have to specify the corresponding x-values, as MPL automatically assumes them to be [0, 1, 2, ...]. Usually, we want to plot for a given set of x-values like this:

[206]:
```
# explicitly specify x-values
xvalues = [10, 20, 30, 40]
plt.plot(xvalues, yvalues)
```

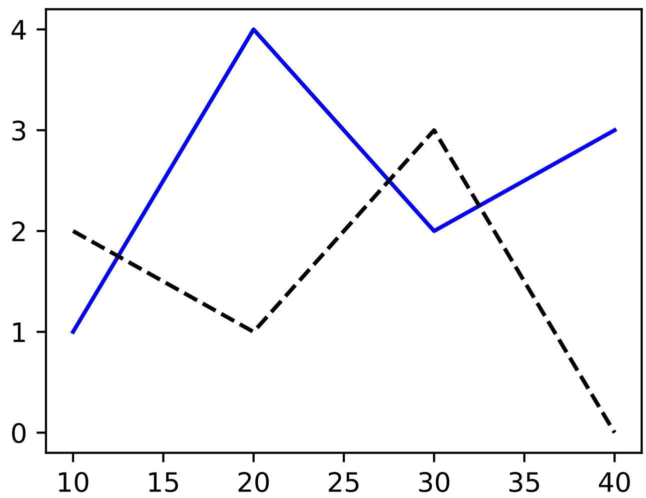
[206]:
```
[<matplotlib.lines.Line2D at 0x7f9de4c59f00>]
```



Similar to Matlab, we can also specify multiple lines to be plotted in a single graph:

[207]:
```
yvalues2 = [2.0, 1.0, 3.0, 0.0]
plt.plot(xvalues, yvalues, 'b-', xvalues, yvalues2, 'k--')
```

[207]:
```
[<matplotlib.lines.Line2D at 0x7f9de4c8eb30>,
 <matplotlib.lines.Line2D at 0x7f9de4c8e2c0>]
```



The characters following each set of y-values are style specifications that are very similar to the ones used in Matlab. More specifically, the letters are short-hand notations for colours (see here for details):

- `b`: blue

- `g`: green
- `r`: red
- `c`: cyan
- `m`: magenta
- `y`: yellow
- `k`: black
- `w`: white

The remaining characters set the line styles. Valid values are

- `-` solid line
- `--` dashed line
- `-.` dash-dotted line
- `:` dotted line

Additionally, we can append marker symbols to the style specification. The most frequently used ones are

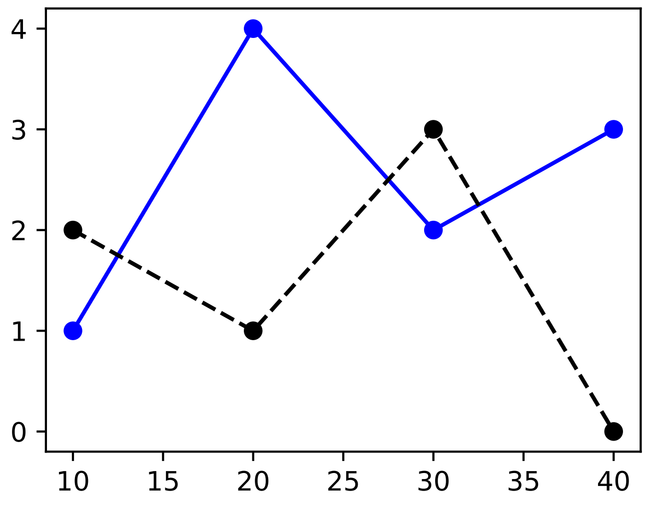
- `o`: circle
- `s`: square
- `*`: star
- `x`: x
- `d`: (thin) diamond

The whole list of supported symbols can be found here.

Instead of passing multiple values to be plotted at once, we can also repeatedly call `plot()` to add additional elements to a graph. This is more flexible since we can pass additional arguments which are specific to one particular set of data, such as labels displayed in legends

[208]:
```
# Plot two lines by calling plot() twice
plt.plot(xvalues, yvalues, 'b-o')
plt.plot(xvalues, yvalues2, 'k--o')
```

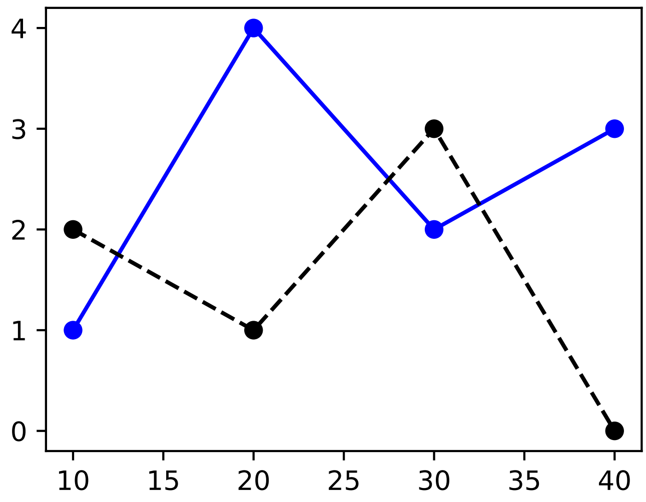
[208]: `[<matplotlib.lines.Line2D at 0x7f9de49fa920>]`



Individual calls to `plot()` also allow us to specify styles more explicitly using keyword arguments:

[209]:
```
# pass plot styles as explicit keyword arguments
plt.plot(xvalues, yvalues, color='blue', linestyle='-', marker='o')
plt.plot(xvalues, yvalues2, color='black', linestyle='--', marker='o')
```

[209]: [<matplotlib.lines.Line2D at 0x7f9de4a8aa40>]



Note that in the example above, we use named colours such as `red` or `blue`. Alternatively, we can use RGB color codes of the form `#dddddd` where `d` are hexadecimal digits.

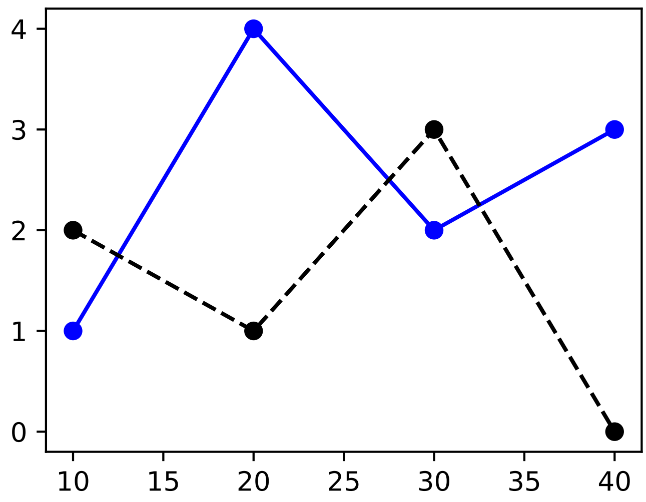
Matplotlib accepts abbreviations for the most common style definitions using the following shortcuts:

- `c` or `color`
- `ls` or `linestyle`
- `lw` or `linewidth`

We can write thus rewrite the above code as follows:

[210]:
```
# abbreviate plot style keywords
plt.plot(xvalues, yvalues, c='blue', ls='-', marker='o')
plt.plot(xvalues, yvalues2, c='black', ls='--', marker='o')
```

[210]: [<matplotlib.lines.Line2D at 0x7f9de2e767a0>]



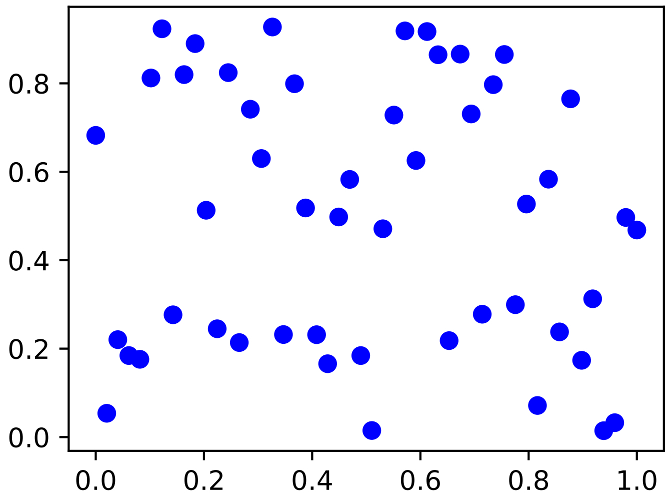
There is a third way to plot multiple lines in the same plot by passing the y-values as a 2-dimensional array. We explore this alternative in the exercises.

5.2 Scatter plots

We use the `scatter()` function to create scatter plots in a similar fashion to line plots:

[211]:
```
import matplotlib.pyplot as plt
import numpy as np

# Create 50 uniformly-spaced values on unit interval
xvalues = np.linspace(0.0, 1.0, 50)
# Draw random numbers (we learn how to do this in a later unit)
yvalues = np.random.default_rng(123).random(50)

plt.scatter(xvalues, yvalues, color='blue')
```

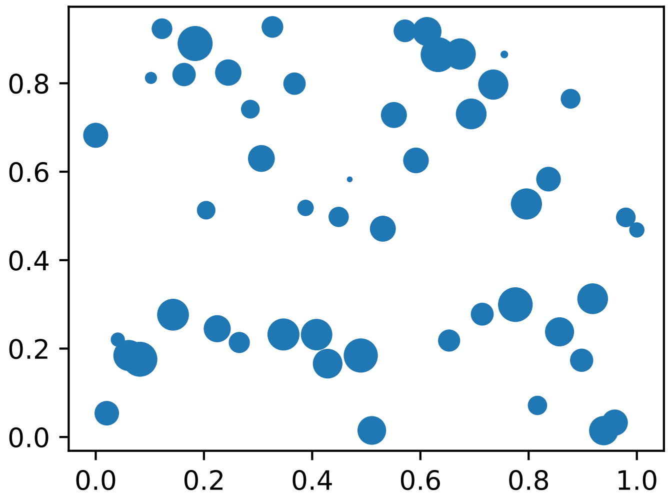
[211]: <matplotlib.collections.PathCollection at 0x7f9de2ebe4a0>



We could in principle create scatter plots using `plot()` by turning off the connecting lines. However, `scatter()` allows us to specify the color and marker size as collections, so we can vary these for every point. `plot()`, on the other hand, imposes the same style on all points plotted in that particular function call.

[212]:
```
# Draw random marker sizes
size = np.random.default_rng(456).random(len(yvalues)) * 150.0

# plot with point-specific marker sizes
plt.scatter(xvalues, yvalues, s=size)
```

[212]: <matplotlib.collections.PathCollection at 0x7f9de2f0d5d0>



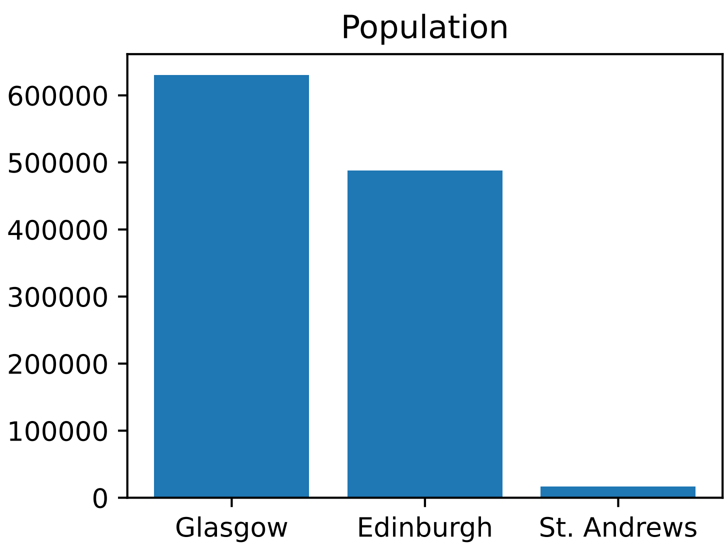
5.3 Plotting categorical data

Instead of numerical values on the x-axis, we can also plot categorical variables by passing them directly to the plotting function.

For example, assume we have three categories and each has an associated numerical value:

[213]:
```
import matplotlib.pyplot as plt

cities = ['Glasgow', 'Edinburgh', 'St. Andrews']
population = [630000, 488000,  16800]
plt.bar(cities, population)
plt.title('Population')
```

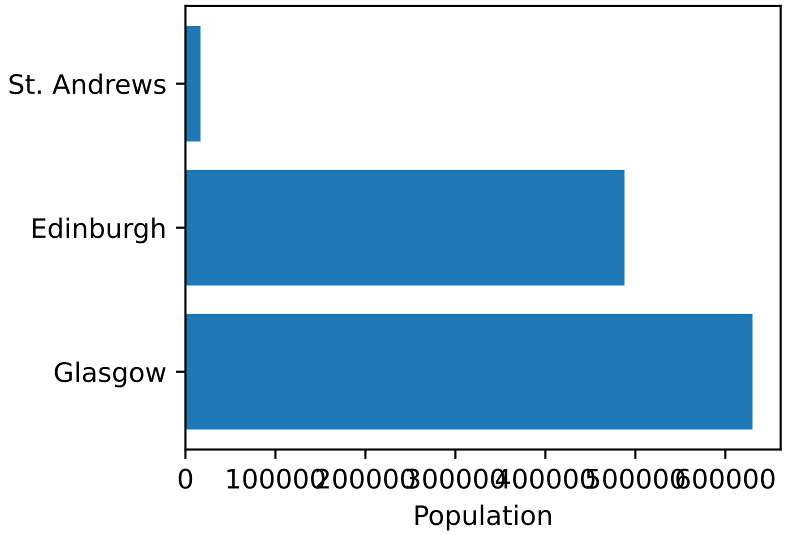
[213]:
```
Text(0.5, 1.0, 'Population')
```



We use `barh()` to create *horizontal* bars:

[214]:
```
plt.barh(cities, population)
plt.xlabel('Population')
```

[214]: Text(0.5, 0, 'Population')



5.4 Adding labels and annotations

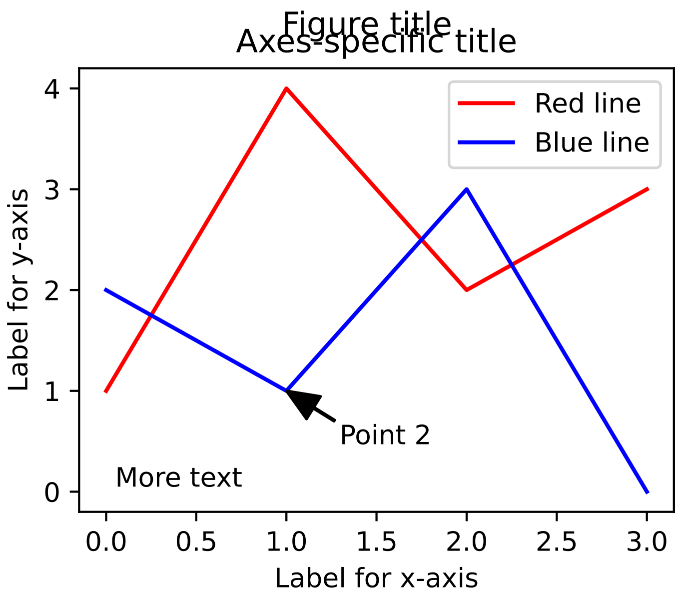
Matplotlib has numerous functions to add labels and annotations:

- Use `title()` and `suptitle()` to add titles to your graphs. The latter adds a title for the whole figure, which might span multiple plots (axes).
- We can add axis labels by calling `xlabel()` and `ylabel()`.
- To add a legend, call `legend()`, which in its most simple form takes a list of labels which are in the same order as the plotted data. [documentation]
- Use `text()` to add additional text at arbitrary locations. [documentation]
- Use `annotate()` to display text next to some data point; it's easier to position correctly than `text()` and you can add arrows! [documentation]

[215]:
```
import matplotlib.pyplot as plt

xvalues = [0, 1, 2, 3]
yvalues = [1, 4, 2, 3]
yvalues2 = [2.0, 1.0, 3.0, 0.0]

plt.plot(xvalues, yvalues, 'r', xvalues, yvalues2, 'b')
plt.suptitle('Figure title')
plt.title('Axes-specific title')
plt.xlabel('Label for x-axis')
plt.ylabel('Label for y-axis')
plt.legend(['Red line', 'Blue line'])

# Adds text at data coordinates (0.05, 0.05)
plt.text(0.05, 0.05, 'More text')

# Annotate second point
plt.annotate('Point 2', (xvalues[1], yvalues2[1]), (20, -20),
             textcoords='offset points',
             arrowprops={
```

```
                'facecolor': 'black', 'width': 0.5, 'headwidth': 10.0
                })
```

[215]: Text(20, -20, 'Point 2')



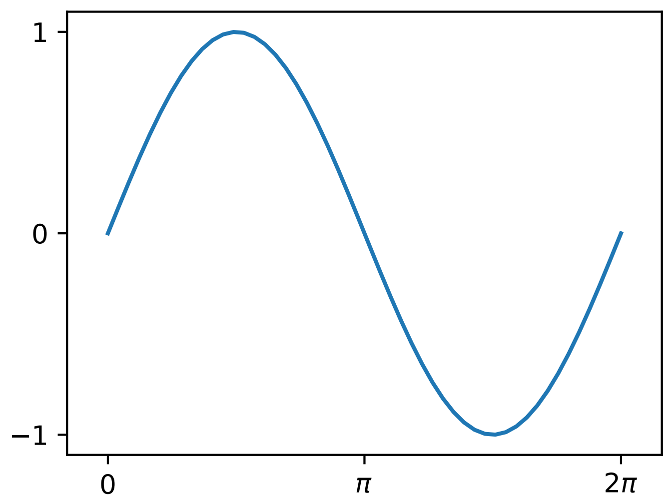
5.5 Plot limits, ticks and tick labels

We adjust the plot limits, ticks and tick labels as follows:

- Plotting limits are set using the `xlim()` and `ylim()` functions. Each accepts a tuple `(min,max)` to set the desired range.
- Ticks and tick labels can be set by calling `xticks()` or `yticks()`.

[216]:
```
import matplotlib.pyplot as plt
import numpy as np

xvalues = np.linspace(0.0, 2*np.pi, 50)
plt.plot(xvalues, np.sin(xvalues))

# Set major ticks for x and y axes, and xtick labels.
# We can use LaTeX code in labels!
plt.xticks([0.0, np.pi, 2*np.pi], ['0', r'$\pi$', r'$2\pi$'])
plt.yticks([-1.0, 0.0, 1.0])

# Adjust plot limits in x and y direction
plt.xlim((-0.5, 2*np.pi + 0.5))
plt.ylim((-1.1, 1.1))
```

[216]: (-1.1, 1.1)



5.6 Object-oriented interface

So far, we have only used the so-called `pyplot` interface which involves calling *global* plotting functions from `matplotlib.pyplot`. This interface is intended to be similar to Matlab, but is also somewhat limited and less clean.

We can instead use the object-oriented interface (called this way because we call methods of the `Figure` and `Axes` objects). While there is not much point in using the object-oriented interface in a Jupyter notebook when we want to create a single graph, it should be the preferred method when writing re-usable code in Python files.

To use the object-oriented interface, we need to get figure and axes objects. The easiest way to accomplish this is using the `subplots()` function, like this:

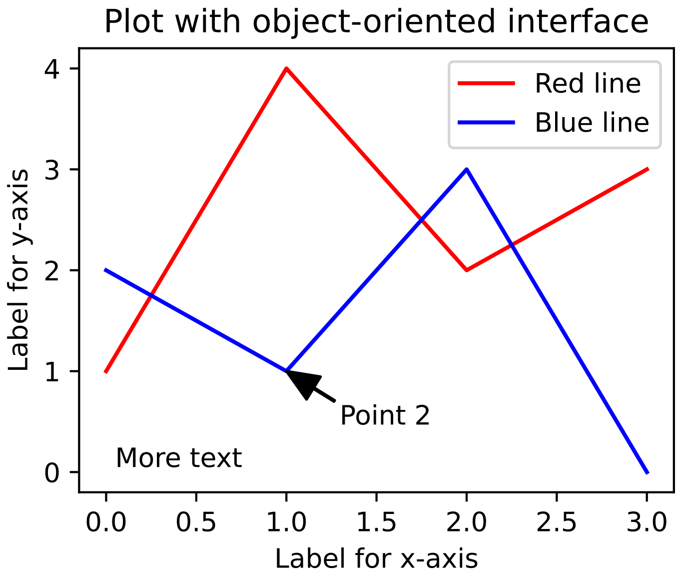
```
fig, ax = plt.subplots()
```

As an example, we recreate the graph from the section on labels and annotations using the object-oriented interface:

[217]:

```
import matplotlib.pyplot as plt

xvalues = [0, 1, 2, 3]
yvalues = [1, 4, 2, 3]
yvalues2 = [2.0, 1.0, 3.0, 0.0]

fig, ax = plt.subplots()
ax.plot(xvalues, yvalues, color='red', label='Red line')
ax.plot(xvalues, yvalues2, color='blue', label='Blue line')
ax.set_xlabel('Label for x-axis')
ax.set_ylabel('Label for y-axis')
ax.legend()
ax.set_title('Plot with object-oriented interface')
ax.text(0.05, 0.05, 'More text')

# Annotate second point
plt.annotate('Point 2', (xvalues[1], yvalues2[1]), (20, -20),
             textcoords='offset points',
             arrowprops={'facecolor': 'black', 'width': 0.5,
                         'headwidth': 10.0})
```

```
[217]: Text(20, -20, 'Point 2')
```



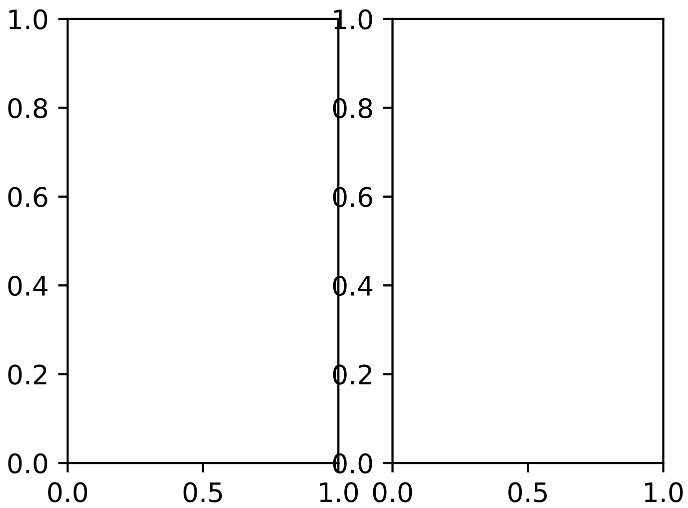
The code is quite similar, except that attributes are set using the `set_xxx()` methods of the `ax` object. For example, instead of calling `xlim()`, we use `ax.set_xlim()`.

5.7 Working with multiple plots (axes)

The object-oriented interface becomes particularly useful if we want to create multiple axes (or figures). This can also be achieved using with the `pyplot` programming model but is somewhat more obscure.

For example, to create a row with two plots, we use:

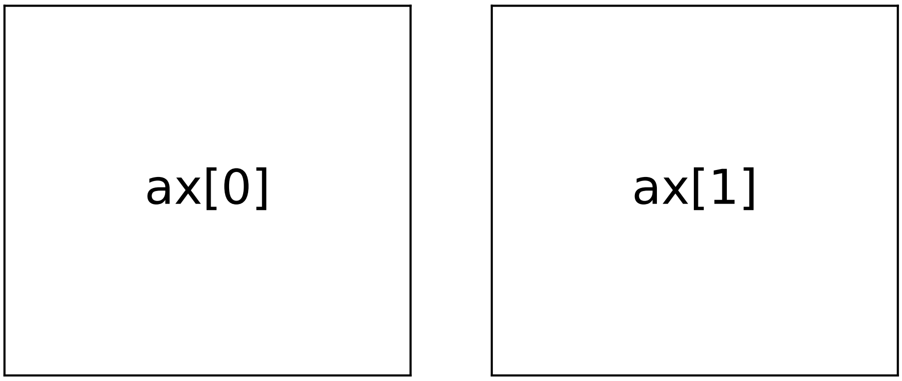
```
[218]: import matplotlib.pyplot as plt

       # Create one figure with 2 axes objects, arranged as two columns in a single row
       fig, ax = plt.subplots(1, 2)
```



With multiple axes objects in a single figure (as in the above example), the `ax` returned by `subplots()` is a NumPy array. Its elements map to the individual panels within the figure in a natural way.

We can visualise this mapping for the case of a single row and two columns as follows:

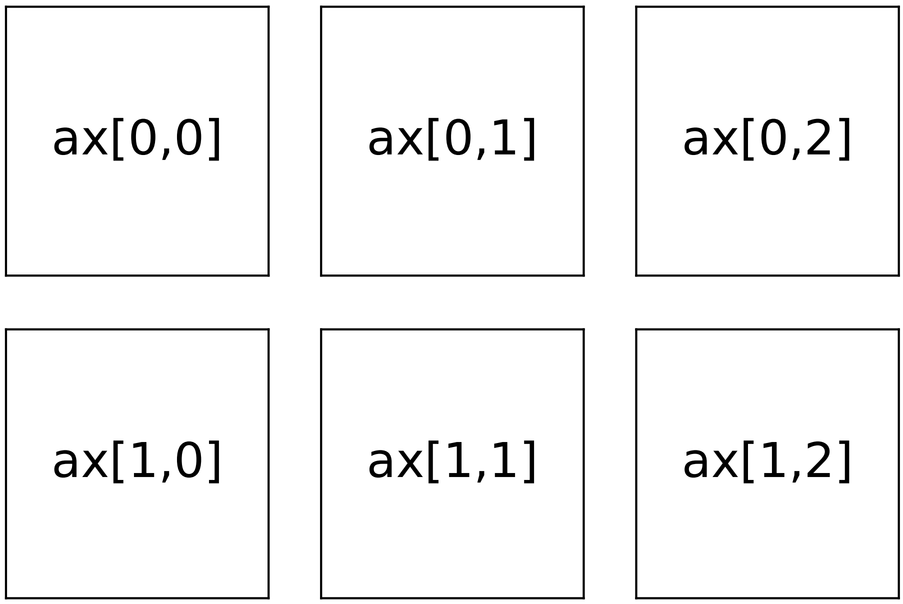
[219]:
```
fig, ax = plt.subplots(1, 2, figsize=(6,2.5))
for i, axes in enumerate(ax):
    # Turn off ticks of both axes
    axes.set_xticks(())
    axes.set_yticks(())
    # Label axes object
    text = f'ax[{i}]'
    axes.text(0.5, 0.5, text, transform=axes.transAxes, va='center', ha='center',␣
↪fontsize=18)
```



Don't worry about the details of how this graph is generated, the only take-away here is how axes objects are mapped to the panels in the figure.

If we request panels in two dimensions, the `ax` object will be a 2-dimensional array, and the mapping of axes objects to panels will look like this instead:

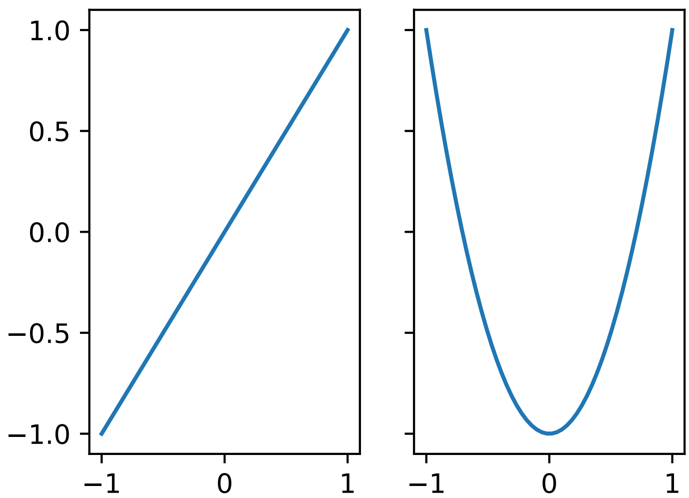
[220]:
```
# Request figure with 2 rows, 3 columns
fig, ax = plt.subplots(2, 3, figsize=(6,4))
for i, axrow in enumerate(ax):
    for j, axes in enumerate(axrow):
        # Turn off ticks of both axes
        axes.set_xticks(())
        axes.set_yticks(())
        # Label axes object
        text = f'ax[{i},{j}]'
        axes.text(0.5, 0.5, text, transform=axes.transAxes, va='center',␣
↪ha='center', fontsize=18)
```



Returning to our initial example, we can use the elements of `ax` to plot into individual panels:

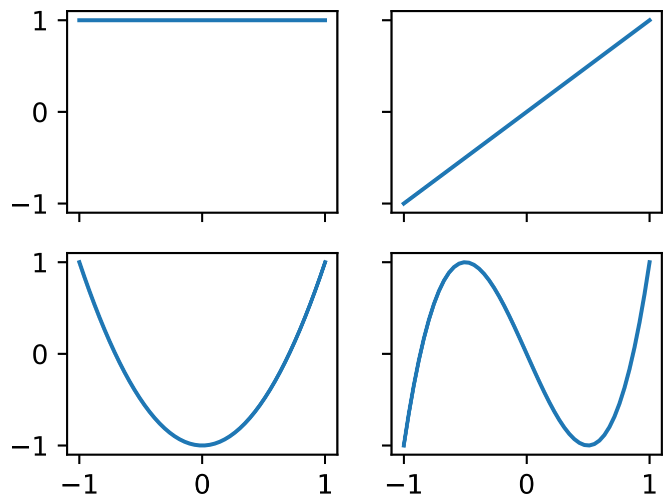
[221]:
```
import matplotlib.pyplot as plt
import numpy as np

fig, ax = plt.subplots(1, 2, sharex=True, sharey=True)
xvalues = np.linspace(-1.0, 1.0, 50)

# Plot into first column
ax[0].plot(xvalues, xvalues)

# Plot into second column
ax[1].plot(xvalues, 2*xvalues**2.0 - 1)
```

[221]:
```
[<matplotlib.lines.Line2D at 0x7f9de29dcb50>]
```



The next example illustrates how to create a figure with four panels:

[222]:
```python
# create figure with 2 rows, 2 columns
fig, ax = plt.subplots(2, 2, sharex=True, sharey=True)

xvalues = np.linspace(-1.0, 1.0, 50)

# Plot the first four Chebyshev polynomials on the interval [-1,1]
for i in range(2):
    for j in range(2):
        yvalues = np.cos((j + i*2) * np.arccos(xvalues))
        ax[i,j].plot(xvalues, yvalues)
```



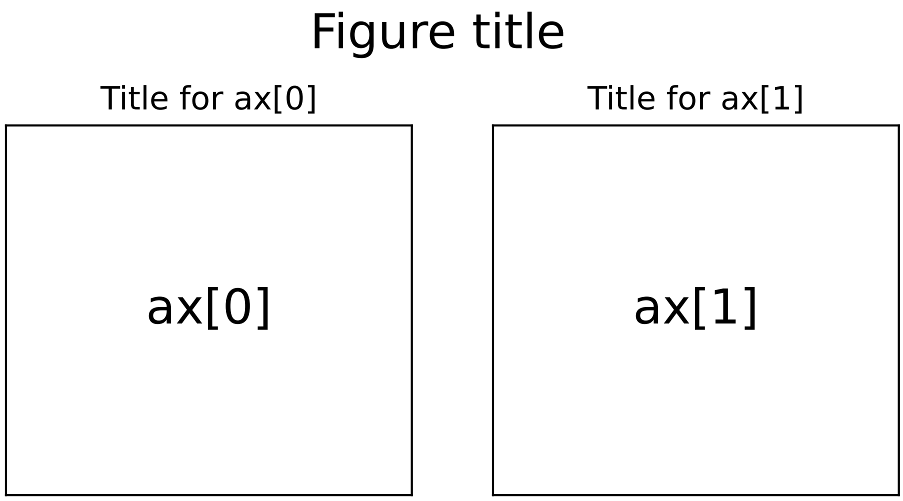
Note the use of `sharex=True` and `sharey=True`. This tells matplotlib that all axes share the same plot limits, so the tick labels can be omitted in the figure's interior to preserve space.

With multiple axes per figure, we can also see the difference between the labels generated by `set_title()` and `suptitle()`.

To illustrate, we re-use the previous example with two panels in a single row:

[223]:
```python
fig, ax = plt.subplots(1, 2, figsize=(6,2.5))
for i, axes in enumerate(ax):
    axes.set_xticks(())
    axes.set_yticks(())
    text = f'ax[{i}]'
    axes.text(0.5, 0.5, text, transform=axes.transAxes, va='center', ha='center',␣
↪fontsize=18)

    # Add axes-specific title
    axes.set_title(f'Title for ax[{i}]')

# set overall figure title:
# this is an attribute of the Figure object!
fig.suptitle('Figure title', fontsize=18, va='bottom', y=1.02)
```

[223]:
```
Text(0.5, 1.02, 'Figure title')
```



5.8 Exercises

5.8.1 Exercise 1: Trigonometric functions

Plot the functions $\sin(x)$ and $\cos(x)$ on the interval $[-\pi, \pi]$, each in a separate graph. Include a legend for each plot, and add pretty tick labels at $[-\pi, 0, \pi]$ which use the LaTeX symbol for π. Add an overall title "Trigonometric functions".

Hint: NumPy defines the functions `np.sin()` and `np.cos()` as well as the value `np.pi`.

5.8.2 Exercise 2: Logarithmic scaling

In economics and finance, we often plot using the $\log_{10}$ scale if the plotted data are of very different orders of magnitude.

Create a figure with two sub-plots, each plotting the function $f(x) = 10^x$ on a uniformly-spaced interval $[-5, 5]$ with 100 points. Use the (default) linear scale in the first plot, but apply the $\log_{10}$ scale in the second.

Hint: You can set the axis scale to log by calling `yscale('log')`, or `set_yscale('log')` when using the object-oriented interface.

5.8.3 Exercise 3: Multiple lines in single plot

In this exercise, we explore yet another alternative to plot multiple lines in a single graph.

The `plot()` function accepts y-values specified as a matrix in which each column corresponds to a different line. The number of rows must correspond to the length of the vector of x-values, which are assumed to be identical for all columns of y-values.

1. Consider the following family of polynomials in x parametrised by a:

$$p(x; a) = a(x - 0.5)^2$$

   Assume there are 5 such polynomials with a's given by the values

```
a = np.linspace(0.4, 4.0, 5)
```

   - Create a common set of x-values using an equidistant grid of 50 points on the interval $[0, 1]$.

- Construct the matrix of y-values with shape `(50, 5)` and plot all polynomials with a single call to `plot()`.
- Add a legend that maps a value of a to the corresponding line in the plot.

2. Plot each polynomial separately using a loop. Use the `i`-th elements of the following arrays as plot styles for the `i`-th polynomial:

```
colors = ['red', 'blue', 'black', 'green', 'purple']
linewidths = [1.0, 1.5, 2.0, 1.5, 1.0]
linestyles = ['-', '--', '-.', ':', '-']
```

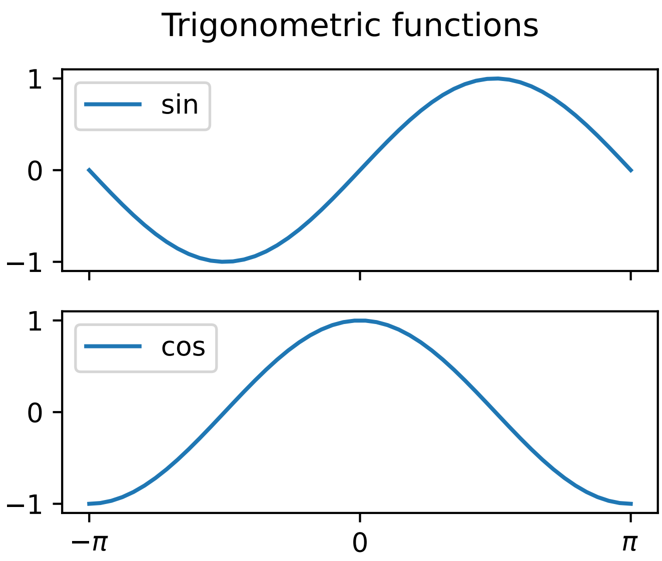
Add a legend that maps a value of a to the corresponding line in the plot.

5.9 Solutions

5.9.1 Solution for exercise 1

[224]:
```python
import matplotlib.pyplot as plt
import numpy as np

xvalues = np.linspace(-np.pi, np.pi, 50)
# Create figure with two rows, one column
fig, ax = plt.subplots(2, 1, sharey=True, sharex=True)

xticks = [-np.pi, 0.0, np.pi]
# Tick labels use LaTeX notation for pi, which is \pi and has to be
# surrounded by $$.
xticklabels = [r'$-\pi$', '0', r'$\pi$']
yticks = [-1.0, 0.0, 1.0]

# Create sin() plot using first axes object
ax[0].plot(xvalues, np.sin(xvalues), label='sin')
ax[0].set_xticks(xticks)
ax[0].set_xticklabels(xticklabels)
ax[0].set_yticks(yticks)
ax[0].legend(loc='upper left')

# Create cos() plot using second axes object
ax[1].plot(xvalues, np.cos(xvalues), label='cos')
ax[1].set_xticks(xticks)
ax[1].set_xticklabels(xticklabels)
ax[1].set_yticks(yticks)
ax[1].legend(loc='upper left')

# Add overall figure title (this is not axes-specific)
fig.suptitle('Trigonometric functions')
```

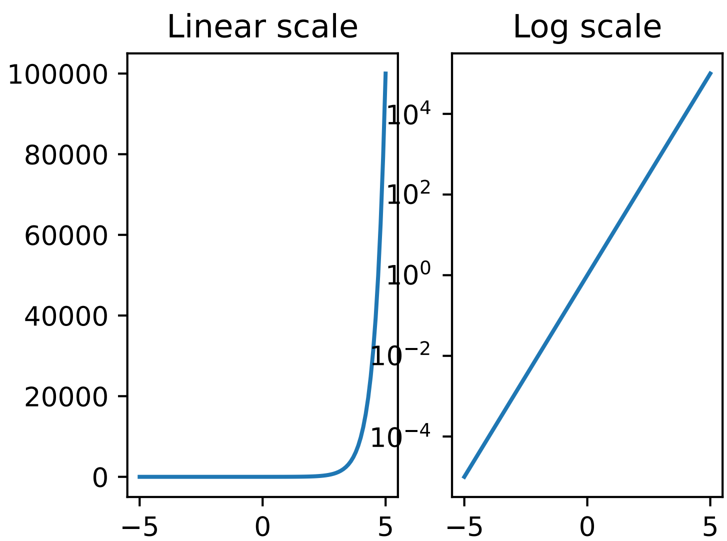
[224]:
```
Text(0.5, 0.98, 'Trigonometric functions')
```



5.9.2 Solution for exercise 2

[225]:
```
import matplotlib.pyplot as plt
import numpy as np

xvalues = np.linspace(-5.0, 5.0, 100)
fig, ax = plt.subplots(1, 2, sharex=True)
ax[0].plot(xvalues, 10.0**xvalues)
ax[0].set_title('Linear scale')

ax[1].plot(xvalues, 10.0**xvalues)
# Set y-axis to log scale (assumes base-10 log)
ax[1].set_yscale('log')
ax[1].set_title('Log scale')
```

[225]:
```
Text(0.5, 1.0, 'Log scale')
```

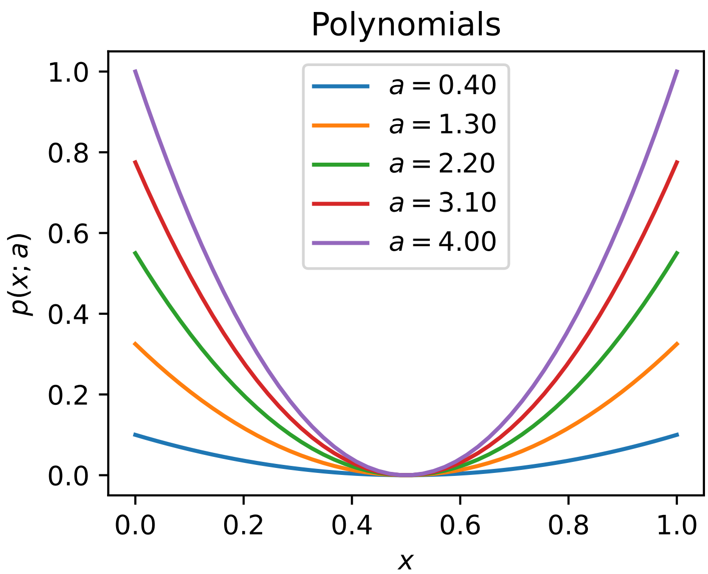


5.9.3 Solution for exercise 3

First we plot all polynomials in a single call to `plot()`. For this to work, we need to pass the y-values as a matrix where each column corresponds to a different line.

[226]:
```
import numpy as np
import matplotlib.pyplot as plt

# Create common x-values
xvalues = np.linspace(0.0, 1.0, 50)

# Create parameters
a = np.linspace(0.4, 4.0, 5)

# Evaluate polynomials on common x-values:
# each column corresponds to a different parametrisation
poly = np.zeros((len(xvalues), len(a)))
# Iterate over parameters and create each set of corresponding y-values
for i, ai in enumerate(a):
    poly[:,i] = ai * (xvalues - 0.5)**2.0

plt.plot(xvalues, poly)
plt.xlabel('$x$')
plt.ylabel(r'$p(x;a)$')
plt.title('Polynomials')

# Create legend:
# we need to pass labels in same order as the corresponding columns
labels = [r'$a={:.2f}$'.format(ai) for ai in a]
plt.legend(labels)
```

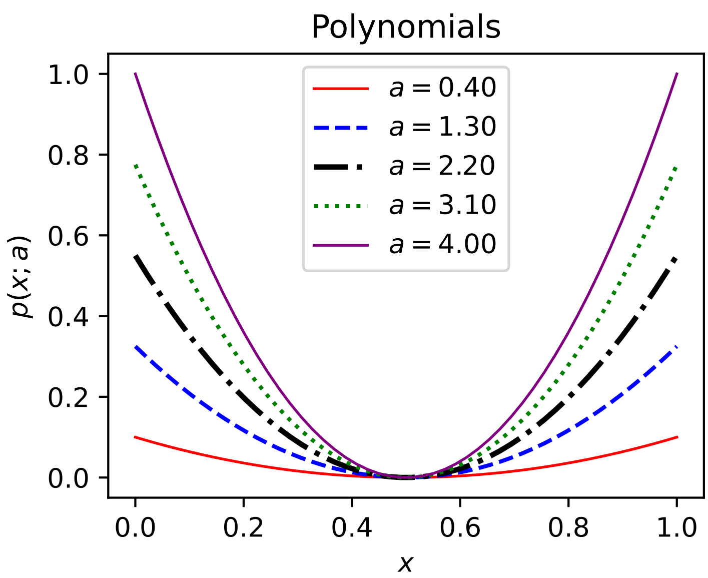
[226]:
```
<matplotlib.legend.Legend at 0x7f9de289e1d0>
```



We now call `plot()` for each polynomial separately. This allows us to specify detailed style settings for each line.

[227]:
```python
fig, ax = plt.subplots(1,1)

# Different styles for each parametrisation
colors = ['red', 'blue', 'black', 'green', 'purple']
linewidths = [1.0, 1.5, 2.0, 1.5, 1.0]
linestyles = ['-', '--', '-.', ':', '-']

n = poly.shape[1]
for i in range(n):
    label = r'$a={:.2f}$'.format(a[i])
    ax.plot(xvalues, poly[:,i], c=colors[i], lw=linewidths[i],
            ls=linestyles[i], label=label)

# calling legend without arguments will use the
# text provided as label argument to each plot()
ax.legend()
ax.set_xlabel('$x$')
ax.set_ylabel(r'$p(x;a)$')
ax.set_title('Polynomials')
```

[227]:
```
Text(0.5, 1.0, 'Polynomials')
```



6 Advanced NumPy

We already encountered NumPy arrays and their basic usage throughout this course. In this unit, we will take a more in-depth look at NumPy.

6.1 Why NumPy arrays?

Why don't we just stick with built-in types such as Python lists to store and process data? It turns out that while the built-in objects are quite flexible, this flexibility comes at the cost of decreased performance:

- `list` objects can store arbitrary data types, and the data type of any item can change:

  ```
  items = ['foo']
  items[0] = 1.0      # item was a string, now it's a float!
  ```

- There is no guarantee where in memory the data will be stored. In fact, two consecutive items could be very "far" from each other in memory, which imposes a performance penalty.
- Even primitive data types such as `int` and `float` are not "raw" data, but full-fledged objects. That, again, is bad for performance.

On the other hand, the approach taken by NumPy is to store and process data in a way very similar to low-level languages such as C and Fortran. This means that

- arrays contain a *homogenous* data type. *All* elements are either 64-bit integers (`np.int64`), 64-bit floating-point numbers (`np.float64`), or some other of the many data types supported by NumPy.

  It is technically possible to get around this by specifying an array's data type (`dtype`) to be `object`, which is the most generic Python data type. However, we would never want to do this for numerical computations.

- NumPy arrays are usually *contiguous* in memory. This means that adjacent array elements are actually guaranteed to be stored next to each other, which allows for much more efficient computations.
- NumPy arrays support numerous operations used in scientific computing. For example, with a NumPy array we can write

  ```
  x = np.array([1, 2, 3])
  y = x + 1        # We would expect this to work
  ```

  With lists, however, we cannot:

  ```
  x = [1, 2, 3]
  y = x + 1        # Does not work!
  ```

  Lists don't implement an addition operator that accepts integer arguments, so this code triggers an error.

You can see the performance uplift provided by NumPy arrays in this simple example:

[228]:
```
# Create list 0, 1, 2, ..., 999
lst = list(range(1000))

# Compute squares, time how long it takes
%timeit [i**2 for i in lst]
```

```
168 µs ± 1.97 µs per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
```

[229]:
```
# Repeat using NumPy arrays
import numpy as np
arr = np.arange(1000)

%timeit arr**2
```

```
943 ns ± 2.88 ns per loop (mean ± std. dev. of 7 runs, 1,000,000 loops each)
```

- On my machine, squaring 1000 elements of a `list` takes approximately 200 times longer than the computation using NumPy arrays!
- Also, as mentioned above, NumPy supports squaring an array directly, while we have to manually loop through the `list` and square each element individually.

Note: `%timeit` is a so-called magic command that only works in notebooks, but not in regular Python files. [See documentation]

6.2 Creating arrays

We have already encountered some of the most frequently used array creation routines:

- `np.array()` creates an array from a given argument, which can be
  - a scalar;
  - a collection such as a list or tuple;
  - some other iterable object, e.g., something created by `range()`.
- `np.empty()` allocates memory for a given array shape, but does not overwrite it with initial values.
- `np.zeros()` creates an array of a given shape and initializes it to zeros.
- `np.ones()` creates an array of a given shape and initializes it to ones.
- `np.arange(start, stop, step)` creates an array with evenly spaced elements over the range $[start, stop)$.
  - `start` and `step` can be omitted and then default to `start=0` and `step=1`.
  - Note that the number `stop` is never included in the resulting array!
- `np.linspace(start, stop, num)` returns a vector of `num` elements which are evenly spaced over the interval $[start, stop]$.
- `np.identity(n)` returns the identity matrix of a size $n \times n$.
- `np.eye()` is a more flexible variant of `identity()` that can, for example, also create non-squared matrices.

There are many more array creation functions for more exotic use-cases, see the NumPy documentation for details.

Examples:

[230]:
```
import numpy as np

# Create array from list
lst = [1, 2, 3]
np.array(lst)
```

[230]:
```
array([1, 2, 3])
```

[231]:
```
# Create array from tuple
tpl = 1.0, 2.0, 3.0
np.array(tpl)
```

[231]:
```
array([1., 2., 3.])
```

[232]:
```
# arange: end point is not included!
np.arange(5)
```

[232]: array([0, 1, 2, 3, 4])

```
[233]: # arange: increments can be negative too!
np.arange(5, 1, -1)
```

[233]: array([5, 4, 3, 2])

```
[234]: # arange also works on floats
np.arange(1.0, 3.0, 0.5678)
```

[234]: array([1.   , 1.5678, 2.1356, 2.7034])

```
[235]: # linspace DOES include the end point
np.linspace(0.0, 1.0, 11)
```

[235]: array([0. , 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.])

6.3 Array shape

Many of the array creation routines take the desired shape of the array as their first argument. Array shapes are usually specified as tuples:

- A vector with 5 elements has shape `(5, )`.

  Note the comma `,`: we need to specify a tuple with a single element using this comma, since `(5)` is just the integer 5, not a tuple.

  It is worth pointing out that this is not the same as a 2-dimensional array with shape `(1, 5)` or `(5, 1)`, even though they have the same number of elements.
- A 2×2 matrix has shape `(2, 2)`.
- A higher-dimensional array has shape `(k, l, m, n, ...)`.
- A *scalar* NumPy array has shape `()`, an empty tuple.

  While "scalar array" sounds like an oxymoron, it does exist.

We can query the shape of an array using the `shape` attribute, and the number of dimensions is stored in the `ndim` attribute.

Examples:

```
[236]: import numpy as np

# Scalar array
x = np.array(0.0)
print(f'Scalar array with shape={x.shape} and ndim={x.ndim}')
```

```
Scalar array with shape=() and ndim=0
```

Note that a scalar NumPy array is not the same as a Python scalar. The built-in type `float` has neither a `shape`, nor an `ndim`, nor any other of the NumPy array attributes.

```
[237]: scalar = 1.0
scalar.shape
```

```
AttributeError: 'float' object has no attribute 'shape'
```

We create an empty array as follows:

[238]:
```
# 1-dimensional array (vector), values not initialised
x = np.empty((5,))
x       # could contain arbitrary garbage
```

[238]:
```
array([  0.       , -14.671875, -29.34375 , -44.015625, -58.6875  ])
```

An array created with `empty()` will contain arbitrary garbage since the memory block assigned to the array is not initialised. The result will most likely differ on each invocation and across computers.

Most functions accept an integer value instead of a `tuple` when creating 1-dimensional arrays, which is interpreted as the number of elements:

[239]:
```
# 1-dimensional array
x = np.empty(5)          # equivalent to np.empty((5,))
```

Higher-dimensional arrays are creating by passing in tuples with more than one element:

[240]:
```
np.ones((1, 2, 3))       # 3d-array
```

[240]:
```
array([[[1., 1., 1.],
        [1., 1., 1.]]])
```

Recall from unit 2 that we can use the `reshape()` method to convert arrays to a different shape:

- The resulting number of elements must remain unchanged!
- *One* dimension can be specified using `-1`, which will prompt NumPy to compute the implied dimension size itself.

[241]:
```
x = np.zeros((2, 1, 3))
x = x.reshape((3, -1))       # Infer number of columns
x
```

[241]:
```
array([[0., 0.],
       [0., 0.],
       [0., 0.]])
```

We can reshape any array to a 1-dimensional vector using any of the following expressions:

[242]:
```
x.reshape((-1, ))            # pass shape as tuple
x.reshape(-1)                # pass shape as integer
x.flatten()
```

[242]:
```
array([0., 0., 0., 0., 0., 0.])
```

This even works on scalar (0-dimensional) arrays:

[243]:
```
np.array(0.0).flatten()
```

[243]:
```
array([0.])
```

6.4 Advanced indexing

We previously discussed single element indexing and slicing, which works the same way for both Python `list` and `tuple` objects as well as NumPy arrays.

NumPy additionally implements more sophisticated indexing mechanisms which we cover now.

- You might also want to consult the NumPy indexing tutorial and the detailed indexing reference.

6.4.1 Boolean or "mask" indexing

We can pass logical arrays as indices:

- Logical (or boolean) arrays consist of elements that can only take on values `True` and `False`
- We usually don't create logical arrays manually, but apply an operation that results in `True/False` values, such as a comparison.
- The boolean index array usually has the *same* shape as the indexed array.

Examples:

[244]:
```
import numpy as np

vec = np.arange(5)
mask = (vec > 1)          # apply comparison to create boolean array
mask
```

[244]:
```
array([False, False,  True,  True,  True])
```

[245]:
```
vec[mask]                 # use mask to retrieve only elements greater than 1
```

[245]:
```
array([2, 3, 4])
```

We can even apply boolean indexing to multi-dimensional arrays. The result will be flatted to a 1-dimensional array, though.

[246]:
```
mat = np.arange(6).reshape((2,3))
mat
```

[246]:
```
array([[0, 1, 2],
       [3, 4, 5]])
```

[247]:
```
mask = (mat > 1)          # create boolean array
mask
```

[247]:
```
array([[False, False,  True],
       [ True,  True,  True]])
```

[248]:
```
mat[mask]              # collapses result to 1-d array
```

[248]:
```
array([2, 3, 4, 5])
```

Note that logical indexing does *not* work with `tuple` and `list`

[249]:
```
tpl = (1, 2, 3)
mask = (True, False, True)
tpl[mask]                 # error
```

```
TypeError: tuple indices must be integers or slices, not tuple
```

6.4.2 Integer index arrays

We can also use index arrays of *integer* type to select specific elements on each axis. These are straightforward to use for 1-dimensional arrays, but can get fairly complex with multiple dimensions.

[250]:
```
import numpy as np

data = np.arange(10)
index = [1, 2, 9]         # select second, third and 10th element
data[index]
```

[250]: array([1, 2, 9])

As you see, the index array does not have to be a NumPy array, but can also be a list (not a tuple, though!).

In general, if we are using an index array to select elements along an axis of length n, then

- the index must only contain integers between 0 and $n-1$, or negative integers from $-n$ to -1 (which, as usual, count from the end of the axis).
- the index can be of arbitrary length. We can therefore select the same element multiple times.

[251]:
```
data = np.arange(5, 10)      # array with 5 elements, [5,...,9]
data
```

[251]: array([5, 6, 7, 8, 9])

[252]:
```
index = [0, 1, 1, 2, 2, 3, 3, 4, 4]          # select elements multiple times
data[index]
```

[252]: array([5, 6, 6, 7, 7, 8, 8, 9, 9])

The same restrictions apply when indexing multi-dimensional arrays. Moreover,

- if more than one axis is indexed using index arrays, the index arrays have to be of equal length.
- we can combine integer array indexing on one axis with other types of indices on the remaining axes.

Examples:

[253]:
```
data = np.arange(12).reshape((3, 4))
data
```

[253]:
```
array([[ 0,  1,  2,  3],
       [ 4,  5,  6,  7],
       [ 8,  9, 10, 11]])
```

[254]:
```
index1 = [0, 2]      # row indices
index2 = [1, 3]      # column indices
data[index1, index2]
```

[254]: array([1, 11])

The code above selects two elements, the first at position `(0,1)`, the second at position `(2,3)`.

We can combine index arrays on one axis with another indexing method on a different axis:

[255]:
```
data[index1, 2]      # return elements in 3rd column from rows given
                     # in index1
```

[255]: array([2, 10])

Using different indexing methods, in particular index arrays, on higher-dimensional data can quickly become a mess, and you should be extra careful to see if the results make sense.

6.5 Numerical operations

6.5.1 Element-wise operations

Element-wise operations are performed on each element individually and leave the resulting array's shape unchanged.

There are three types of such operations:

1. One operand is an array and one is a scalar.
2. Both operands are arrays, either of identical shape, or broadcastable to an identical shape (we discuss broadcasting below)
3. A function is applied to each array element.

Case 1: Array-scalar operations. These intuitively behave as you would expect:

[256]:
```
import numpy as np

x = np.arange(10)
scalar = 1

# The resulting array y has the same shape as x:
y = x + scalar      # addition
y = x - scalar      # subtraction
y = x * scalar      # multiplication
y = x / scalar      # division
y = x // scalar     # division with integer truncation
y = x % scalar      # modulo operator
y = x ** scalar     # power function
y = x == scalar     # comparison: also >, >=, <=, <
```

Note that unlike in Matlab, the "standard" operators work element-wise, so `x * y` is *not* matrix multiplication!

Case 2: Both operands are arrays of equal shape:

[257]:
```
x = np.arange(10)
y = np.arange(10, 20)       # has same shape as x

# Resulting array z has the same shape as x and y:
z = x + y           # addition
z = x - y           # subtraction
z = x * y           # multiplication
z = x / y           # division
z = x // y          # division with integer truncation
z = x % y           # modulo operator
z = x ** y          # power function
z = x == y          # comparison: also >, >=, <=, <
```

Case 3: Applying element-wise functions. This case covers numerous functions defined in NumPy, such as

- `np.sqrt`: square root
- `np.exp`, `np.log`, `np.log10`: exponential and logarithmic functions
- `np.sin`, `np.cos`, etc.: trigonometric functions

You can find a complete list of mathematical functions in the NumPy documentation (not all functions listed there operate element-wise, though!).

[258]:
```
# element-wise functions
x = np.arange(1, 11)
y = np.exp(x)       # apply exponential function
y = np.log(x)       # apply natural logarithm
```

6.5.2 Matrix operations

Transpose

You can transpose a matrix using the `T` attribute:

[259]:
```
mat = np.arange(6).reshape((2,3))
mat
```

[259]:
```
array([[0, 1, 2],
       [3, 4, 5]])
```

[260]:
```
mat.T
```

[260]:
```
array([[0, 3],
       [1, 4],
       [2, 5]])
```

For higher-dimensional arrays, the `np.transpose()` function can be used to permute the axes of an array. For two-dimensional arrays, `np.transpose(mat)` and `mat.T` are equivalent.

Matrix multiplication

Matrix multiplication is performed using the `np.dot()` function ("dot product"). The operands need not be matrices but can be vectors as well, or even high-dimensional arrays (the result is then not entirely obvious and one should check the documentation).

Every newer version of Python and NumPy additionally interprets `@` as the matrix multiplication operator.

[261]:
```
import numpy as np

mat = np.arange(9).reshape((3, 3))       # 3x3 matrix
vec = np.arange(3)                        # vector of length 3

# matrix-matrix multiplication
np.dot(mat, mat)     # or: mat @ mat
```

[261]:
```
array([[ 15,  18,  21],
       [ 42,  54,  66],
       [ 69,  90, 111]])
```

[262]:
```
# vector dot product (returns a scalar)
np.dot(vec, vec)     # or: vec @ vec
```

[262]:
```
5
```

[263]:
```
# matrix-vector product (returns vector)
np.dot(mat, vec)     # or: mat @ vec
```

[263]:
```
array([ 5, 14, 23])
```

We must of course make sure that matrices and vector have conformable dimensions!

[264]:
```
mat = np.arange(6).reshape((2, 3))
mat
```

[264]:
```
array([[0, 1, 2],
       [3, 4, 5]])
```

[265]:
```
np.dot(mat, mat)         # raises error, cannot multiply 2x3 matrix with
                         # 2x3 matrix
```

```
ValueError: shapes (2,3) and (2,3) not aligned: 3 (dim 1) != 2 (dim 0)
```

[266]:
```
np.dot(mat, mat.T)       # transpose second operand, then it works!
```

[266]:
```
array([[ 5, 14],
       [14, 50]])
```

6.5.3 Reductions

Reductions are operations that reduce the dimensionality of the data. For example, computing the mean of an array reduces a collection of data points to a single scalar, its mean.

Basic reduction operations include:

- `np.sum()`: sum of array elements
- `np.prod()`: product of array elements
- `np.amin(),np.amax()`: minimum and maximum element
- `np.argmin(),np.argmax()`: location of minimum and maximum element
- `np.mean(),np.average()`: mean of array elements
- `np.median()`: median of array elements
- `np.std(),np.var()`: standard deviation and variance of array elements
- `np.percentile()`: percentiles of array elements

Most if not all reductions accept an `axis` argument which restricts the operation to a specific axis.

- If an axis is specified, the resulting array will have one dimension less than the input.
- If no axis is specified, the operation is applied to the whole (flattened) array.

Examples:

[267]:
```
import numpy as np

# 1-dimensional input data
data = np.linspace(0.0, 1.0, 11)

# Compute mean and std. of input data
m = np.mean(data)
s = np.std(data)
print(f'Mean: {m:.2f}, std. dev.: {s:.2f}')
```

```
Mean: 0.50, std. dev.: 0.32
```

[268]:
```
# 2-dimensional input data
data = np.linspace(0.0, 1.0, 21).reshape((3, 7))
data
```

[268]:
```
array([[0.  , 0.05, 0.1 , 0.15, 0.2 , 0.25, 0.3 ],
       [0.35, 0.4 , 0.45, 0.5 , 0.55, 0.6 , 0.65],
       [0.7 , 0.75, 0.8 , 0.85, 0.9 , 0.95, 1.  ]])
```

[269]:
```
# Compute mean of each row, ie along the column axis
m = np.mean(data, axis=1)
m            # Result is a vector of 3 elements, one for each row
```

[269]:
```
array([0.15, 0.5 , 0.85])
```

6.5.4 Broadcasting

Element-wise operations in most programming languages require input arrays to have identical shapes. NumPy relaxes this constraint and allows us to use arrays with different shapes that can be "broadcast" to identical shapes.

Simple example

What do we mean by "broadcasting"? We introduce the concept using a specific example, and will discuss the technical details below.

- Imagine we want to add a 2×3 matrix to a length-2 vector.
- This operation does not make sense, unless we interpret the (column) vector as a 2×1 matrix, and replicate it 3 times to obtain a 2×3 matrix. This is exactly what NumPy does.

Examples:

[270]:
```python
import numpy as np

# Create 3x2 matrix
mat = np.arange(6).reshape((2, 3))
mat
```

[270]:
```
array([[0, 1, 2],
       [3, 4, 5]])
```

[271]:
```python
# Create 2-element vector
vec = np.arange(2)
vec
```

[271]:
```
array([0, 1])
```

[272]:
```python
# Trying to add matrix to vector fails
mat + vec
```

```
ValueError: operands could not be broadcast together with shapes (2,3) (2,)
```

[273]:
```python
# However, we can explicitly reshape the vector to a 2x1 column vector
colvec = vec.reshape((-1, 1))
colvec
```

[273]:
```
array([[0],
       [1]])
```

[274]:
```python
# Now, broadcasting replicates column vector to match matrix columns
mat + colvec
```

[274]:
```
array([[0, 1, 2],
       [4, 5, 6]])
```

We do not need to `reshape()` data, but can instead use a feature of NumPy that allows us to increase the number of dimensions on the spot:

[275]:
```python
# use vec[:, None] to append an additional dimension to vec
mat + vec[:, None]
```

[275]:
```
array([[0, 1, 2],
       [4, 5, 6]])
```

Specifying `None` as an array index inserts a new axis of length 1 at that position (since it's of length 1, this new axis does not change the overall size of the array!).

For more examples, see the official NumPy tutorial on broadcasting.

Technical details

We are now ready to look at the technical details underlying broadcasting. The NumPy documentation on broadcasting is quite comprehensive, so we will just summarise the points made there.

Broadcasting is applied in four steps:

1. Determine the largest dimension (`ndim` attribute) among all arrays involved in an operation. Any array of smaller dimension will have 1's *prepended* to its shape until its dimension corresponds to the largest one.

   Example: given array `a` with shape `(m,n)` and array `b` with shape `(n,)`, the maximum dimension is 2, and `b` will be implicitly reshaped to `(1,n)`.

2. The size of the output array is determined as the maximum size of all arrays along each dimension.

   Example: Continuing with our example from above, the maximum size along dimension 1 is `m`, and the maximum size along dimension 2 is `n`, so the output array has shape `(m, n)`.

3. An input array can be used in the computation if for every dimension its size either matches the output size or is equal to 1. If this is not the case, broadcasting cannot be applied and the operation fails.

   Example: In the above example, the shape of `a` matches the output shape exactly. The implied shape of `b` is `(1, n)`, so it matches exactly along the second dimension, and is 1 along the first, and thus can be used.

4. For any input array with size 1 along some dimension, the (unique) element in this dimension will be used for all calculations along that dimension.

   Example: Any element `a[i, j]` will be matched with the element `b[0, j]` to the calculate the output value at `(i, j)`.

Because additional dimensions are added *at the beginning* to create the desired output shape, broadcasting will not work automatically if we want to multiply arrays of shape `a.shape = (m,n)` and `b.shape = (m,)`.

- Following the above steps, `b` will implicitly be reshaped to `(1,m)` and the operation will fail at step 3:

[276]:
```
m = 3
n = 2
a = np.arange(m*n).reshape((m, n))       # matrix of shape (m,n)
b = np.arange(1, m+1)                    # vector of shape (m,)

a * b            # will not work!
```

```
ValueError: operands could not be broadcast together with shapes (3,2) (3,)
```

We therefore have to explicitly *append* a degenerate axis to `b` such that both arrays have the same dimension:

[277]:
```
b = b[:,None]
a * b
```

[277]:
```
array([[ 0,  1],
       [ 4,  6],
       [12, 15]])
```

Because `a` has shape `(m,n)` and `b` now has shape `(m,1)`, `b[:,0]` will be replicated across all columns of `a` to perform the operation.

It is worthwhile to take some time to master broadcasting as it's essential to using NumPy efficiently. You might think that one can simply replicate array operands along some dimension to get the same effect, which is what we do in languages that do not support broadcasting.

- This included Matlab until release R2016b, where implicit expansion for some arithmetic and logical operations was introduced.

  Prior to that, users had to manually expand input arrays using `repmat()`, or use the rather inelegant `bsxfun()` function.

  Note that even today, NumPy broadcasting goes beyond Matlab's capabilities.

To illustrate the difference between broadcasting and manual replication of data, we perform the element-wise multiplication of a 3-dimensional array with a (1-dimensional) vector:

[278]:
```
# Dimensions of 3d array
k = 10
m = 11
n = 12

a = np.arange(k*m*n).reshape((k, m, n))      # create 3d array
b = np.arange(n)                             # create 1d vector
```

We can manually expand the vector to have the same shape as the array `a` using `np.tile()` which creates `k * m` copies of the `n` elements in `b`:

[279]:
```
b_exp = np.tile(b, reps=(k, m, 1))
b_exp.shape
```

[279]:
```
(10, 11, 12)
```

The following code compares the execution time of computing `a * b` using broadcasting to the case where we first explicitly expand `b`:

[280]:
```
# Multiplication with broadcasting
%timeit a * b
```

```
2.02 µs ± 12 ns per loop (mean ± std. dev. of 7 runs, 100,000 loops each)
```

[281]:
```
# Multiplication with explicitly expanded operands
%timeit a * np.tile(b, reps=(k, m, 1))
```

```
5.81 µs ± 50.2 ns per loop (mean ± std. dev. of 7 runs, 100,000 loops each)
```

As you see, not only is the second operation more complex and difficult to read, it also takes approximately three times as long to execute! The reason is that `np.tile()` replicates the data in memory, which is expensive. No copying is done when using broadcasting.

6.6 Vectorisation

Vectorisation is the concept of applying operations to whole arrays of data instead of every singular element (note that the term also has other meanings in computer science). In Python, as well as languages such as Matlab and R, we use this programming technique to increase performance for two reasons:

1. Looping over elements is slow.
2. Calling a function on every single element is also slow.

These performance penalties are less pronounced for compiled languages such as C or Fortran, so we try to move the looping to code written in one of these languages. In particular, since NumPy's core parts are implemented in C, we always want to do looping "within" NumPy.

For example, consider element-wise addition of two arrays, `a` and `b`:

[282]:
```
import numpy as np

# array size
N = 100

# input arrays
a = np.linspace(0.0, 1.0, N)
b = np.linspace(1.0, 2.0, N)
```

Benchmarking a non-vectorised loop in pure Python against NumPy's vectorised implementation reveals some striking differences:

[283]:
```
%%timeit
# Compute c = a + b using Python loops
c = np.empty(N)          # allocate output array
for i in range(N):
    c[i] = a[i] + b[i]
```

```
20.9 µs ± 724 ns per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
```

[284]:
```
# Compute c = a + b using vectorised addition
%timeit c = a + b
```

```
388 ns ± 1.33 ns per loop (mean ± std. dev. of 7 runs, 1,000,000 loops each)
```

We see that the vectorised variant is about 100 times faster! What is going on?

- NumPy implements a vectorised operator + which accepts arrays as operands.
- NumPy performs looping over individual elements in C which is compiled to high-performance machine code.

Of course this example is somewhat artificial: you would not have implemented a loop in Python in the first place, you probably just assumed that + works with array operands.

However, we can easily construct more complex computations which may not be implemented in NumPy but which can use vectorised building blocks to speed up computations.

As an example, consider the following function which computes the sum of finite of elements of an array, ignoring infinity and NaNs.

[285]:
```
# Compute sum of finite elements in x
def finite_sum(x):
    # initialise sum
    s = 0.0
    # loop over array elements
    for xi in x:
        # Check whether a value is finite
        if np.isfinite(xi):
            # Add to running sum
            s += xi
    return s
```

Next, we create a sample array with a few NaNs and infinite values and to test `finite_sum()`. `NaN` stands for "not a number" as is used as a special value to flag results of invalid operations such as `0/0`:

[286]:
```
arr = np.linspace(0.0, 1.0, 100)
arr[::3] = np.inf        # assign infinity to every 3rd element
arr[::5] = np.nan        # assign NaN to every 5th element
```

Comparing our `finite_sum()` to a vectorised version again shows the performance advantage of vectorised code:

[287]:
```
%timeit finite_sum(arr)
```

```
130 µs ± 860 ns per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
```

[288]:
```
%timeit np.sum(arr[np.isfinite(arr)])
```

```
4.27 µs ± 36.4 ns per loop (mean ± std. dev. of 7 runs, 100,000 loops each)
```

The vectorised version is approximately 25 times faster, despite the fact that

- NumPy does not implement this specific function; and
- the vectorised implementation creates two temporary arrays:
    - one when calling `np.isfinite()`; and

- one when indexing `arr` with the boolean array returned by `np.isfinite()`. As we discuss below, indexing with boolean arrays always creates a copy!

This illustrates that creating vectorised code by combining several vectorised functions also yields considerable speed-ups.

As an aside, note that NumPy actually implements `np.nansum()` which drops NaNs, but it does not discard infinite values.

6.7 Copies and views (advanced)

Recall that assignment in Python does *not* create a copy (unlike in C, Fortran or Matlab):

[289]:
```
a = [0, 0, 0]
b = a           # b references the same object as a
b[1] = 1        # modify second element of b (and a!)
a == b          # a and b are still the same
```

[289]:
```
True
```

NumPy adds another layer to this type of data sharing: whenever you perform an assignment or indexing operation, NumPy tries hard *not* to copy the underlying data but instead creates a so-called view which points to the same block of memory. It does so for performance reasons (copying is expensive).

We can illustrate this using array slicing:

[290]:
```
import numpy as np

x = np.arange(10)
x
```

[290]:
```
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

[291]:
```
y = x[3:8]          # Create array that points to elements 4-8 of x
y
```

[291]:
```
array([3, 4, 5, 6, 7])
```

The arrays `x` and `y` are two different Python objects, which we can verify using the built-in `id()` function:

[292]:
```
print(id(x))
print(id(y))
```

```
140316087064528
140316087070960
```

[293]:
```
id(x) == id(y)
```

[293]:
```
False
```

And yet, the NumPy implementation makes sure that they reference the same block of memory!

We can see this easily by modifying `y`:

[294]:
```
y[:] = 0        # overwrite all elements of y with zeros
y
```

[294]:
```
array([0, 0, 0, 0, 0])
```

[295]:
```
x               # elements of x that are also referenced by y
                # are now also zero!
```

[295]: array([0, 1, 2, 0, 0, 0, 0, 0, 8, 9])

This behaviour is even triggered when `y` references non-adjacent elements in `x`. For example, we can let `y` be a view onto every *second* element in `x`:

[296]:
```
x = np.arange(10)
y = x[::2]       # y now points to every second element of x
y[:] = 0         # overwrite all elements of y with zeros
x                # every second element in x is now zero!
```

[296]: array([0, 1, 0, 3, 0, 5, 0, 7, 0, 9])

As a rule of thumb, NumPy will create a view as opposed to copying data if

- An array is created from another array via slicing (i.e., indexing using the `start:stop:step` triplet)

Conversely, a *copy* is created whenever

- An array is created from another array via boolean (mask) indexing.
- An array is created from another array via integer array indexing.

Moreover, you can always force NumPy to create a copy by calling `np.copy()`!

Examples:

[297]:
```
# Copies are created with boolean indexing
x = np.arange(10)
mask = (x > 4)       # boolean mask
y = x[mask]          # create y using boolean indexing
y[:] = 0
x                    # x is unmodified
```

[297]: array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])

[298]:
```
# Copies are created with integer array indexing
x = np.arange(10)
index = [3, 4, 5]    # List of indices to include in y
y = x[index]
y[:] = 0
x                    # x is unmodified
```

[298]: array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])

[299]:
```
# Forced copy with slicing
x = np.arange(10)
y = np.copy(x[3:8]) # force copy with np.copy()
y[:] = 0
x                    # x is unmodified
```

[299]: array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])

As an alternative to `np.copy()`, we can directly call the `copy()` method of an array:

[300]:
```
y = x[3:8].copy()
```

6.8 NumPy data types (advanced)

6.8.1 Default data types

We have already touched upon the numerical data types used by NumPy. If we do not explicitly request a data type using the `dtype` keyword argument, NumPy by default behaves as follows:

1. The default data type for most array creation routines which create arrays of a given shape or size, such as `np.empty()`, `np.ones()` and `np.zeros()`, is a 64-bit floating-point number (`np.float64`).
2. Array creation routines that accept numerical input data will use the data type of this input data to determine the array data type.

   Examples of such functions are `np.arange()` and `np.array()`.
3. Arrays that are implicitly created as a result of an operation (addition, etc.) are assigned the most suitable type to represent the result.

   For example, when adding a floating-point and an integer array, the result will be a floating-point array.

Examples:

Case 1: default data type is `np.float64`:

[301]:
```
import numpy as np

x = np.ones(1)        # length-1 vector of ones
x.dtype               # default type: float64
```

[301]:
```
dtype('float64')
```

Case 2: data type depends on input data:

[302]:
```
# Argument is an integer
x = np.arange(5)
x.dtype               # data type is np.int64
```

[302]:
```
dtype('int64')
```

[303]:
```
# Argument is a float
x = np.arange(5.0)
x.dtype               # data type is np.float64
```

[303]:
```
dtype('float64')
```

Case 3: data type determined to accommodate result

[304]:
```
# Add two integer arrays
arr1 = np.arange(3)
arr2 = np.arange(3, 0, -1)      # creates [3, 2, 1]
result = arr1 + arr2
print(result)
result.dtype                    # data type is np.int64
```

```
[3 3 3]
```

[304]:
```
dtype('int64')
```

[305]:
```
# Add integer to floating-point array
arr1 = np.arange(3)
arr2 = np.arange(3.0, 0.0, -1.0)    # creates [3.0, 2.0, 1.0]
result = arr1 + arr2
print(result)
result.dtype                        # data type is np.float64
```

```
[3. 3. 3.]
```

[305]:
```
dtype('float64')
```

Even though the resulting array is `[3.0, 3.0, 3.0]` and can thus be represented as integers without loss of data, NumPy only takes into account that one of the operands is floating-point, and thus the result has to be of floating-point type!

6.8.2 Explicit data types

We can almost always explicitly request an array to be of a particular data type by passing the `dtype` keyword argument. The most common types are:

- `np.float64`: a 64-bit floating-point number, also called *double precision* in other languages.

  This is the most commonly used floating-point data type. It can represent numbers with up to 16 decimal digits, and covers a range of approximately $\pm 10^{308}$.

  Note that `dtype=float` is a synonym for `dtype=np.float64` on most platforms you are likely to encounter, and we'll be using the shorter variant.

- `np.int64`: a 64-bit integer which can represent integer values on the interval of (approximately) $\pm 10^{19}$.

  Unlike floating-point, the integer representation is *exact*, but covers a much smaller range (and, obviously, no fractional numbers)

  Note that `dtype=int` is a synonym for `dtype=np.int64` on most platforms you are likely to encounter, and we'll be using the shorter variant.

- `np.float32`, `np.float16`: single-precision and half-precision floating-point numbers. These occupy only 32 and 16 bits of memory, respectively.

  They thus trade off storage requirements for a loss of precision and range.

- `np.int32`, `np.int16`, `np.int8` represent integers using 32, 16 and 8 bits, respectively.

  They require less memory, but can represent only a smaller range of integers. For example, `np.int8` can only store integer values from -128 to 127.

- NumPy also supports complex numerical types to represent imaginary numbers. We will not be using those in this tutorial.

You can find a complete list of NumPy data types here and here.

Would we ever want to use anything other than the default data types, which in most cases are either `np.float64` and `np.int64`? These, after all, support the largest range and highest precision. This is true in general, but there are special cases where other data types need to be used:

1. *Storage requirements:* if you work with large amounts of data, for example arrays with many dimensions, you can run out of memory or storage space (when saving results to files).

   In this case, you can store data as `np.float32` instead of `np.float64`, which halves the storage requirement.

   Similarly, if you know that your integer data only takes on values between -128 and 127, you can store them as `np.int8` which consumes only 1/8 of the space compared to `np.int64`!

2. *Performance:* Some tasks simply don't require high precision or range. For example, some machine learning tasks can be performed using only 8-bit integers, and companies like Google have developed dedicated processors to considerably speed up workloads using 8-bit integers.

   Even if you are not using any specialised CPUs or GPUs, data has to be transferred from memory to the processor and this is a major performance bottleneck. The less data needs to be transferred, the better!

   In general, this is nothing you need to worry about at this point, but might become relevant once you start writing complex high-performance code.

Examples:

[306]:
```python
import numpy as np

# Explicitly specify data type
x = np.ones(1, dtype=np.float16)
x       # prints np.float16
```

[306]:
```
array([1.], dtype=float16)
```

We can use `dtype` to override the data type inferred from input data:

[307]:
```python
lst = [1, 2, 3]
x = np.array(lst)        # given list of integers, creates integer array
x.dtype                  # prints np.int64
```

[307]:
```
dtype('int64')
```

[308]:
```python
# override inferred data type:
# created floating-point array even if integers were given
x = np.array(lst, dtype=np.float64)
x.dtype                  # prints np.float64
```

[308]:
```
dtype('float64')
```

[309]:
```python
# override inferred data type:
# created integer array even if floats were given,
# thus truncating input data!
lst = [1.234, 4.567, 6.789]
x = np.array(lst, dtype=int)
print(x)                 # prints [1, 4, 6]
x.dtype                  # prints np.int64
```

```
[1 4 6]
```

[309]:
```
dtype('int64')
```

6.9 Array storage order (advanced)

Computer memory is linear, so a multi-dimensional array is mapped to a one-dimensional block in memory. This can be done in two ways:

1. NumPy uses the so-called *row-major order* (also called *C order*, because its the same as in C programming language)
2. This is exactly the opposite of Matlab, which uses *column-major order* (also called *F order*, because its the same as in the Fortran programming language)

[310]:
```python
import numpy as np

mat = np.arange(6).reshape((2,3))
mat
```

[310]:
```
array([[0, 1, 2],
       [3, 4, 5]])
```

[311]:
```python
# The matrix mat is stored in memory like this
mat.reshape(-1, order='C')
```

[311]:
```
array([0, 1, 2, 3, 4, 5])
```

[312]:
```python
# ... and NOT like this
```

```
mat.reshape(-1, order='F')      # use order='F' to convert to column-major␣
↪storage order
```

[312]:
```
array([0, 3, 1, 4, 2, 5])
```

While this is not particularly important initially, as an advanced user you should remember that you usually want to avoid performing operations on non-contiguous blocks of memory. This can have devastating effects on performance!

[313]:
```
# Avoid operations on non-contiguous array sections such as
mat[:, 1]

# Contiguous array sections are fine
mat[1]
```

[313]:
```
array([3, 4, 5])
```

6.10 Exercises

6.10.1 Exercise 1: Broadcasting

Let `m = 2`, `n = 3` and `k = 4`. Create an array `a` with shape `(m, n)` like this:

`a = np.arange(m*n).reshape((m,n))`

Perform the following tasks:

1. Define the vector `b = np.arange(n) * 10` and use broadcasting to compute `c = a * b` such that `c` has shape `(m,n)`.
2. Define the vector `b = np.arange(m) * 10` and use broadcasting to compute `c = a * b` such that `c` has shape `(m,n)`.
3. Define the 3-dimensional array `b`,

   `b = np.arange(m*n*k).reshape((m,k,n)) * 10`

   and use broadcasting to compute `c = a * b` such that `c` has shape `(m,k,n)`.

6.10.2 Exercise 2: Boolean indexing

Let `m = 8` and `n = 9`. Create an array `a` with shape `(m,n)` as follows:

`a = np.arange(m*n).reshape((m,n)) % 7`

The `%` is the modulo operator which returns the remainder of a division of one number by another (in this case the division by 7). The resulting array `a` will therefore contain integers between 0 and 6.

1. Create a boolean array called `mask` which has the same shape as `a` and is `True` whenever an element in `a` is between 1 and 4 (inclusive).

   Hint: The character `&` works as a logical `and` operator for NumPy arrays. Alternatively, you can use the function `np.logical_and()`.
2. Compute the number of elements in `a` that satisfy this criterion.
3. Compute the average of these elements.

6.10.3 Exercise 3: Diagonal matrices

In this exercise, we'll create diagonal matrices using integer array indexing.

1. Create a square matrix of zeros with shape `(n,n)` for `n = 5` and `dtype = int` as its data type:

```
a = np.zeros((n,n), dtype=int)
```

Use integer array indexing to modify its diagonal to construct the following matrix, where omitted elements are zero:

$$\begin{bmatrix} 1 & & & & \\ & 2 & & & \\ & & 3 & & \\ & & & 4 & \\ & & & & 5 \end{bmatrix}$$

2. Repeat the exercise, but now use a non-squared matrix with shape `(4,5)`, and insert `1,2,...` as the values of the first diagonal above the main diagonal:

$$\begin{bmatrix} 0 & 1 & & & \\ & & 2 & & \\ & & & 3 & \\ & & & & 4 \end{bmatrix}$$

3. Repeat the exercise, but now use a matrix with shape `(6,5)`. Adapt your code so that it can handle matrix shapes `(m,n)` for cases `n > m`, `n = m` and `n < m`:

$$\begin{bmatrix} 0 & 1 & & & \\ & & 2 & & \\ & & & 3 & \\ & & & & 4 \\ & & & & \\ & & & & \end{bmatrix}$$

6.10.4 Exercise 4: Triangular matrices

Create a matrix of zeros with shape `(m,n)`, with `m = 4`, `n = 5`, and `dtype = int`:

```
a = np.zeros((m,n), dtype=int)
```

Transform it to an upper-triangular matrix so that it looks like this:

$$\begin{bmatrix} 1 & 2 & 3 & 4 & 5 \\ & 6 & 7 & 8 & 9 \\ & & 10 & 11 & 12 \\ & & & 13 & 14 \end{bmatrix}$$

where the omitted elements are zeros. Do this without using loops.

Hint: For any upper-diagonal element at position (i,j) it holds that $j \geq i$. Create arrays of row and column indices and use these to build a mask with shape `(m,n)` which selects all upper-triangular elements. Exploit the fact that logical array operations support broadcasting!

Challenge: Modify your code to construct the following upper-triangular matrix instead:

$$\begin{bmatrix} 1 & 2 & 4 & 7 & 11 \\ & 3 & 5 & 8 & 12 \\ & & 6 & 9 & 13 \\ & & & 10 & 14 \end{bmatrix}$$

Hint: One solution is to build a lower-triangular matrix and transpose it!

6.10.5 Exercise 5: Row averages (ignoring NaNs)

Construct a matrix with shape `(m,n)` where `m = 5` and `n = 8` as follows:

```
a = np.arange(m*n, dtype=float).reshape((m, n))
mask = (a % 5) == 0
a[mask] = np.nan
```

Lines two and three set all elements of `a` which are divisible by 5 without remainder to `np.nan`, the floating-point value signalling that something is "not a number" (NaN).

Write code to perform the following tasks:

1. Define a function `rowmeans(x)` which takes a matrix `x` as an argument and returns a vector of row averages of elements in `x` which are not NaN. The return vector should therefore have the same length as the number of rows in `x`.

   Hint: Use `np.isnan()` to check whether something is NaN.

2. Compare your results to the output of `np.nanmean()` with argument `axis = 1`.
3. Use the `%timeit` magic to benchmark the run time of your routine against the (vectorised) `np.nanmean()`.

6.10.6 Exercise 6: Locating maxima (advanced)

Consider the following quadratic polynomial in x which is parametrised by the positive real numbers a, b and c:

$$p(x; a, b, c) = -a(x-b)^2 + c$$

Imagine that we have a set of `m = 10` such functions, each with different values for a, b and c. These parameters take on the following values:

```
m = 10

a = np.linspace(0.4, 2.0, m)
b = np.linspace(-1.0, 0.0, m)
c = np.linspace(0.0, 3.0, m)
```

The parameters for the first polynomial are thus `a[0]`, `b[0]` and `c[0]`, and similarly for the remaining polynomials.

Perform the following tasks:

1. Evaluate each polynomial on an equidistant grid of `n = 50` points on the interval `[-2.0, 2.0]`. Store the results as an $m \times n$ matrix called `pvalues`.
2. Create a (single) graph which plots all `m` polynomials.
3. Write a function `find_max(pvalues)` which accepts this matrix as an argument and returns an integer array of length `m`. Each element `i` should contain the location of the maximum for the `i`-th row of `pvalues`.
4. Add the maxima you found to the graph you created: each maximum should be marked as a black dot at the correct (x, y) coordinates.
5. Use vectorised code to perform the same task as the function `find_max()`:
   1. You actually don't have to do anything here since NumPy implements the function `np.argmax()` which does what you need (just correctly specify the `axis` argument.)
   2. Use the `%timeit` magic to compare the runtime of your `find_max()` to NumPy's `np.argmax()`.

6.11 Solutions

6.11.1 Solution for exercise 1

To solve this exercise, we need to make sure that the broadcasting rules can be applied by inserting an additional axis in either `a` or `b` as needed.

[314]:
```python
# Define problem dimensions
m = 2
n = 3
k = 4

# Create array a
a = np.arange(m*n).reshape((m, n))
a
```

[314]:
```
array([[0, 1, 2],
       [3, 4, 5]])
```

[315]:
```python
# Task 1
b = np.arange(n) * 10
# Broadcasting works as is, axis will be prepended to b
c = a * b

# If we really want, we can prepend new axis manually:
c = a * b[None]
c
```

[315]:
```
array([[  0,  10,  40],
       [  0,  40, 100]])
```

[316]:
```python
# Task 2
b = np.arange(m) * 10
# Manually append new axis to b to make broadcasting work
c = a * b[:,None]
c
```

[316]:
```
array([[ 0,  0,  0],
       [30, 40, 50]])
```

[317]:
```python
# Task 3
b = np.arange(n*m*k).reshape((m, k, n)) * 10
b
```

[317]:
```
array([[[  0,  10,  20],
        [ 30,  40,  50],
        [ 60,  70,  80],
        [ 90, 100, 110]],

       [[120, 130, 140],
        [150, 160, 170],
        [180, 190, 200],
        [210, 220, 230]]])
```

[318]:
```python
# Need to insert new axis in between existing axes in a
c = a[:,None] * b
c
```

[318]:
```
array([[[   0,   10,   40],
        [   0,   40,  100],
        [   0,   70,  160],
        [   0,  100,  220]],

       [[ 360,  520,  700],
        [ 450,  640,  850],
        [ 540,  760, 1000],
        [ 630,  880, 1150]]])
```

6.11.2 Solution for exercise 2

[319]:
```
import numpy as np

# Array dimensions
m = 8
n = 9

# Create array a
a = np.arange(m*n).reshape((m,n)) % 7

# Create mask that selects all elements
# between 1 and 4
mask = (a > 0) & (a < 5)     # same as np.logical_and(a > 0, a < 5)
mask
```

[319]:
```
array([[False,  True,  True,  True,  True, False, False, False,  True],
       [ True,  True,  True, False, False, False,  True,  True,  True],
       [ True, False, False, False,  True,  True,  True,  True, False],
       [False, False,  True,  True,  True,  True, False, False, False],
       [ True,  True,  True,  True, False, False, False,  True,  True],
       [ True,  True, False, False, False,  True,  True,  True,  True],
       [False, False, False,  True,  True,  True,  True, False, False],
       [False,  True,  True,  True,  True, False, False, False,  True]])
```

We use `&` to obtain the set of elements for which the conditions `a > 0` and `a < 5` are `True` at the same time.

Boolean arrays only contain values `False` and `True`. However, arithmetic operations automatically interpret `False` as 0 and `True` as 1, so we can simply sum over the array to obtain the number of elements that are `True`:

[320]:
```
# Count number of elements
nmask = np.sum(mask)
nmask
```

[320]:
```
41
```

Finally, we compute the average as follows:

[321]:
```
# Compute average of elements selected by mask
# We do this by summing over selected elements and
# dividing by the number of such elements.
mean = np.sum(a[mask]) / nmask
mean
```

[321]:
```
2.4634146341463414
```

6.11.3 Solution for exercise 3

[322]:
```
import numpy as np

# Square matrix with 1,2,...n diagonal

n = 5
# Create matrix of zeros
mat = np.zeros((n,n), dtype=int)

# Create row and column indices for the diagonal elements
irow = np.arange(n)
icol = irow               # column indices are the same since
                          # this is the diagonal of a square matrix
```

```
# Vector to insert as diagonal
diag = np.arange(1, n+1)

# Set new diagonal
mat[irow, icol] = diag

mat          # print result
```

[322]:
```
array([[1, 0, 0, 0, 0],
       [0, 2, 0, 0, 0],
       [0, 0, 3, 0, 0],
       [0, 0, 0, 4, 0],
       [0, 0, 0, 0, 5]])
```

You can achieve the same result with NumPy's `np.diag()` function:

[323]:
```
np.diag(np.arange(n) + 1)
```

[323]:
```
array([[1, 0, 0, 0, 0],
       [0, 2, 0, 0, 0],
       [0, 0, 3, 0, 0],
       [0, 0, 0, 4, 0],
       [0, 0, 0, 0, 5]])
```

For task 2, we need to specify row and column index arrays that are no longer identical:

[324]:
```
# Task 2: set upper diagonal elements of non-square matrix
import numpy as np

m = 4
n = 5

# Create matrix of zeros
mat = np.zeros((m, n), dtype=int)

# Row and column indices
irow = np.arange(m)
icol = np.arange(n-1) + 1

diag = np.arange(m) + 1

# Set new diagonal
mat[irow, icol] = diag

mat                  # print result
```

[324]:
```
array([[0, 1, 0, 0, 0],
       [0, 0, 2, 0, 0],
       [0, 0, 0, 3, 0],
       [0, 0, 0, 0, 4]])
```

We now create a more generic version of the code above that can handle the cases `m < n`, `m = n` and `m > n`. The above code will fail for `m > n`.

[325]:
```
import numpy as np

m = 6
n = 5

# Create matrix of zeros
mat = np.zeros((m, n), dtype=int)
```

```
# Row indices: this is the minimum of the number of rows,
#       and the number of cols-1, since the first col
#       is newer included.
irow = np.arange(min(m,n-1))

# Column indices: array needs to have same length as
# row indices. First column is omitted so we
# need to shift all indices by 1.
icol = np.arange(len(irow)) + 1

# Number of elements to insert needs to be identical
# to length of array index.
diag = np.arange(len(irow)) + 1

# Set new diagonal
mat[irow, icol] = diag

mat                    # print result
```

[325]:
```
array([[0, 1, 0, 0, 0],
       [0, 0, 2, 0, 0],
       [0, 0, 0, 3, 0],
       [0, 0, 0, 0, 4],
       [0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0]])
```

For the special case of `m = n`, NumPy's `np.diag()` can also insert values at diagonals other than the main diagonal. For example, for `m = n = 5`, we can create a similar matrix as follows:

[326]:
```
n = 5
# the k argument tells diag() which diagonal to manipulate.
# k = 1 corresponds to first diagonal above
# the main diagonal.
np.diag(np.arange(n-1)+1, k=1)
```

[326]:
```
array([[0, 1, 0, 0, 0],
       [0, 0, 2, 0, 0],
       [0, 0, 0, 3, 0],
       [0, 0, 0, 0, 4],
       [0, 0, 0, 0, 0]])
```

6.11.4 Solution for exercise 4

[327]:
```
m = 4
n = 5

# Create arrays of valid row and column indices.
irow = np.arange(m)
icol = np.arange(n)

# Use broadcasting to identify all upper-triangular elements
mask = icol[None] >= irow[:,None]
mask
```

[327]:
```
array([[ True,  True,  True,  True,  True],
       [False,  True,  True,  True,  True],
       [False, False,  True,  True,  True],
       [False, False, False,  True,  True]])
```

[328]:
```python
# Create matrix of zeros
mat = np.zeros((m, n), dtype=int)

# count number of True values in mask
ntrue = np.sum(mask)

# Values to insert into upper-triangular part:
# 1, 2, ...
values = np.arange(ntrue) + 1

mat[mask] = values
mat
```

[328]:
```
array([[ 1,  2,  3,  4,  5],
       [ 0,  6,  7,  8,  9],
       [ 0,  0, 10, 11, 12],
       [ 0,  0,  0, 13, 14]])
```

To create the second matrix, we need to make sure that the sequence of integers is arranged column-wise instead of by row, as in the code above.

This is most likely not possible to achieve with masked indexing and C-ordered arrays. If we want to use masked indexing, we instead create the transposed matrix using the same approach as above, and then transpose it to get the final matrix.

[329]:
```python
# dimensions of TRANSPOSED matrix
m = 5
n = 4

# row and column indices of TRANSPOSED matrix
irow = np.arange(m)
icol = np.arange(n)

# mask to select lower-triangular elements
# of transposed matrix
mask = irow[:, None] >= icol[None]
mask
```

[329]:
```
array([[ True, False, False, False],
       [ True,  True, False, False],
       [ True,  True,  True, False],
       [ True,  True,  True,  True],
       [ True,  True,  True,  True]])
```

[330]:
```python
# Create matrix of zeros
mat = np.zeros((m, n), dtype=int)

# Number of True elements in mask
ntrue = np.sum(mask)

# Values to insert into lower-triangular part:
# 1, 2, ...
values = np.arange(ntrue) + 1
mat[mask] = values

# Transpose to get final matrix
mat = mat.T
mat
```

[330]:
```
array([[ 1,  2,  4,  7, 11],
       [ 0,  3,  5,  8, 12],
       [ 0,  0,  6,  9, 13],
       [ 0,  0,  0, 10, 14]])
```

Of course, you can also solve this using the brute-force way with loops, but that does not help us practice using NumPy:

[331]:
```
m = 4
n = 5

mat = np.zeros((m, n), dtype=int)

# keep track of current value to be inserted
# into matrix
value = 1

# loop over columns
for j in range(n):
    # loop over rows
    for i in range(m):
        if j >= i:
            mat[i,j] = value
            # increment value for next applicable
            # element
            value += 1

mat
```

[331]:
```
array([[ 1,  2,  4,  7, 11],
       [ 0,  3,  5,  8, 12],
       [ 0,  0,  6,  9, 13],
       [ 0,  0,  0, 10, 14]])
```

6.11.5 Solution for exercise 5

One implementation of `rowmeans()` could look as follows:

[332]:
```
import numpy as np

def rowmeans(x):
    # Number of rows and columns in x
    m, n = x.shape

    # Array to store results
    means = np.zeros(m)

    # Loop over rows
    for i in range(m):
        # number of non-NaN elements in current row
        count = 0
        # sum of non-Nan elements in current row
        s = 0.0
        for j in range(n):
            value = x[i,j]
            if not np.isnan(value):
                s += value
                # increments number of non-NaN elements
                count += 1

        # compute mean, store in output vector
        means[i] = s / count

    return means
```

We create the array given in the exercise to test our function:

[333]:
```
m = 5
n = 8
a = np.arange(m*n, dtype=float).reshape((m, n))
mask = (a % 5) == 0
a[mask] = np.nan
a
```

[333]:
```
array([[nan,  1.,  2.,  3.,  4., nan,  6.,  7.],
       [ 8.,  9., nan, 11., 12., 13., 14., nan],
       [16., 17., 18., 19., nan, 21., 22., 23.],
       [24., nan, 26., 27., 28., 29., nan, 31.],
       [32., 33., 34., nan, 36., 37., 38., 39.]])
```

As you see, NumPy indicates elements that are NaN using the string 'nan'.

[334]:
```
# call rowmeans() using test data
means = rowmeans(a)
means
```

[334]:
```
array([ 3.83333333, 11.16666667, 19.42857143, 27.5       , 35.57142857])
```

We verify our results using the NumPy routine `np.nanmean()` which implements the same functionality. Since we are computing row averages (and thus compute averages *across* columns), we need to pass in the argument `axis = 1`: axes are numbered starting at 0, so `axis = 1` refers to the second axis, i.e., the columns.

[335]:
```
means2 = np.nanmean(a, axis=1)
means2
```

[335]:
```
array([ 3.83333333, 11.16666667, 19.42857143, 27.5       , 35.57142857])
```

To test whether the results are the same, we check whether their absolute difference is below some tolerance level, in this case 10^{-8}. The routine `np.all()` evaluates to `True` if this is the case for *all* elements.

[336]:
```
np.all(np.abs(means - means2) < 1.0e-8)
```

[336]:
```
True
```

Note that we rarely want to compare floating-point numbers resulting from computations for exact equality using ==. Floating-point has limited precision, and different operations can potentially produce different rounding errors. It is therefore unlikely that two floating-point results will be *exactly* identical.

Finally, we use the %timeit magic to benchmark our implementation against NumPy's.

[337]:
```
%timeit rowmeans(a)
```

```
59.1 µs ± 431 ns per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
```

[338]:
```
%timeit np.nanmean(a, axis=1)
```

```
22.8 µs ± 1.04 µs per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
```

You may be surprised that `np.nanmean()` is only twice as fast as our implementation, but this is purely due to the small array size, as then there are only a few iterations performed in our Python loop.

Try increasing the array dimensions to `(500,800)` instead of `(5,8)` and you will see that then NumPy is about 500 times faster!

6.11.6 Solution for exercise 6

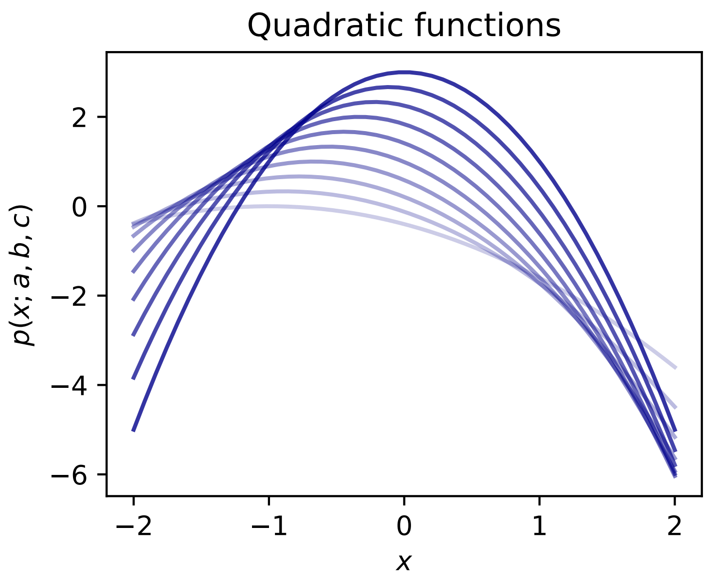
We first create the matrix `pvalues` which contains the all polynomials (for all `m = 10`) parametrisations evaluated on a common grid of x-values. Each row of this matrix represents a different polynomial parametrisation.

[339]:
```
import numpy as np
import matplotlib.pyplot as plt

m = 10
n = 50

# Parameters for each polynomial
a = np.linspace(0.4, 2.0, m)
b = np.linspace(-1.0, 0.0, m)
c = np.linspace(0.0, 3.0, m)

# grid of x values on which to evaluate polynomials
xgrid = np.linspace(-2.0, 2.0, n)

# polynomials on x, for each parameter tuple (a,b,c)
pvalues = - a[:,None] * (xgrid[None] - b[:,None])**2.0 + c[:,None]
```

Next, we create a function to plot all polynomials. We will be reusing this code, so it is convenient to encapsulate it in a function instead of copy-pasting it again and again!

[340]:
```
# function to plot quadratic polynomials
def plot_quad(xvalues, pvalues):
    # Number of different polynomials in pvalues
    m = pvalues.shape[0]

    # Use different transparency (alpha) level for each polynomial
    alphas = np.linspace(0.2, 0.8, m)

    # Plot each row against the common x-values
    for i in range(m):
        plt.plot(xvalues, pvalues[i], color='darkblue', alpha=alphas[i])

    # Label axes, figure
    plt.xlabel(r'$x$')
    plt.ylabel(r'$p(x;a,b,c)$')
    plt.title('Quadratic functions')
```

[341]:
```
# Call plotting routine, passing x-values and y-values
# as arguments
plot_quad(xgrid, pvalues)
```



6.11.7 Locating maxima using loops

Below is one possible way to implement a function that returns a vector of indices, each index storing the location of the maximum element in the corresponding row.

[342]:
```
# Function to locate the maximum value in each row
def find_max(pvalues):
    # unpack rows and columns from shape attribute
    nrow, ncol = pvalues.shape
    # Create array to store location of maximum for each row.
    # Location is an index, so choose integer array type!
    imax = np.zeros(nrow, dtype=int)

    # iterate over all row
    for i in range(nrow):
        # initial guess for location of row maximum
        jmax = 0
        # iterate over all columns, locate index of maximum
        for j in range(1, ncol):
            if pvalues[i,j] > pvalues[i,jmax]:
                # value at (i,j) is larger than
                # value at current max:
                # update jmax
                jmax = j
        # store index of maximum for current row
        imax[i] = jmax

    return imax
```

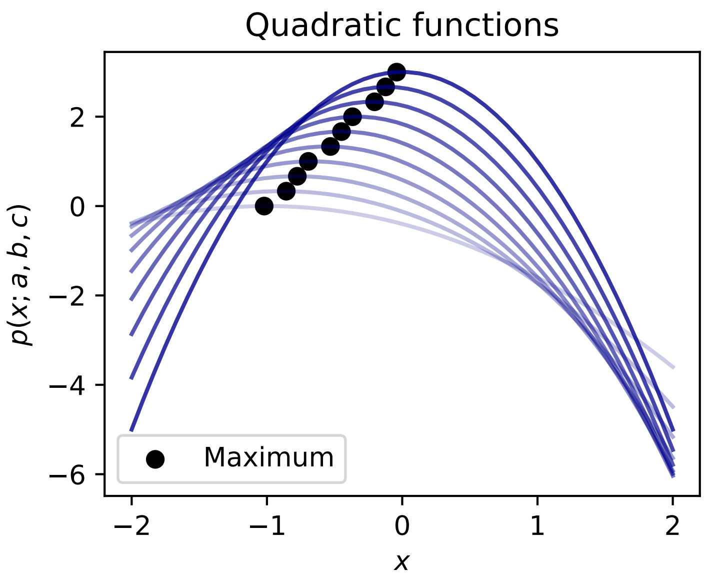
[343]:
```
# use find_max() to locale indices of each row maximum
ipmax = find_max(pvalues)
ipmax
```

[343]:
```
array([12, 14, 15, 16, 18, 19, 20, 22, 23, 24])
```

We plot the polynomials using the function we defined above. We then add the maxima to the *same* plot.

[344]:
```python
# Recreate original plot from above
plot_quad(xgrid, pvalues)

# Plot maxima on top of previous graph
ix = np.arange(m)
plt.scatter(xgrid[ipmax], pvalues[ix,ipmax], c='black', label='Maximum')
plt.legend()
```

[344]:
```
<matplotlib.legend.Legend at 0x7f9de2dd1120>
```



6.11.8 Vectorised version

The vectorised version simply uses NumPy's `np.argmax()` function. We need to pass the argument `axis = 1` as the maximum should be computed across all columns for any given row.

[345]:
```python
# Find row maxima using np.argmax()

ipmax2 = np.argmax(pvalues, axis=1)
ipmax2
```

[345]:
```
array([12, 14, 15, 16, 18, 19, 20, 22, 23, 24])
```

We verify that the results of our and NumPy's implementation are identical. Since the values here are integers, we can directly compare them using ==.

[346]:
```python
# Check that these are the same as what we computed above
np.all(ipmax == ipmax2)
```

[346]:
```
True
```

Finally, we benchmark both implementations using `%timeit`. The NumPy version is approximately 100 times faster!

[347]:
```python
# Time our manual implementation
%timeit find_max(pvalues)
```

```
96.9 µs ± 307 ns per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
```

[348]:

```
# Time NumPy's implementation
%timeit np.argmax(pvalues, axis=1)
```

```
1.38 µs ± 13.6 ns per loop (mean ± std. dev. of 7 runs, 1,000,000 loops each)
```

7 Random number generation and statistics

In this unit, we examine how to generate random numbers for various probability distributions in NumPy. Additionally, we take a look at SciPy's `stats` package which implements PDFs and other functions for numerous probability distributions.

7.1 Random number generators

Currently, there are several ways to draw random numbers in Python:

1. The *new* programming interface implemented in NumPy, introduced in version 1.17 (the current version as of this writing is 1.23) [official documentation].
2. The *legacy* programming interface implemented in NumPy [official documentation].

   While these functions have been superseded by the new implementation, they continue to work. If you are familiar with the legacy interface, you can read about what has changed in the new interface here.
3. The Python standard library itself also includes random number generators in the `random` module [official documentation].

   We won't be using this implementation at all, since for our purposes `numpy.random` is preferable as it supports NumPy arrays.

The programming interface for generating random numbers in NumPy changed substantially in release 1.17. We discuss the new interface in this unit since it offers several advantages, including faster algorithms for some distributions. Moreover, one would expect the legacy interface to be removed at some point in the future. However, most examples you will find in textbooks and on the internet are likely to use the old variant.

A note on random-number generation

Computers usually cannot draw truly random numbers, so we often talk about *pseudo-random number generators* (PRNG). Given an initial seed, these PRNGs will always produce the same sequence of "random" numbers, at least if run on the same machine, using the same underlying algorithm, etc. For scientific purposes this is actually desirable as it allows us to create reproducible results. For simplicity, we will nevertheless be using the terms "random number" and "random number generator" (RNG), omitting the "pseudo" prefix.

7.1.1 Simple random data generation

Before we can generate any random numbers using the new interface, we need to obtain an RNG instance. We can get the default RNG by calling `default_rng()` as follows:

[349]:
```
# import function that returns the default RNG
from numpy.random import default_rng

# get an instance of the default RNG
rng = default_rng()
```

Let's begin with the most simple case, which uses the `random()` function to draw numbers that are uniformly distributed on the half-open interval $[0.0, 1.0)$.

[350]:
```
from numpy.random import default_rng
rng = default_rng()          # obtain default RNG implementation

rng.random(5)                # return array of 5 random numbers
```

[350]: `array([0.12809314, 0.33179404, 0.82173284, 0.90343088, 0.44394492])`

Calling `random()` this way will return a different set of numbers each time (this might, for example, depend on the system time). To obtain the same draw each time, we can pass an initial *seed* when creating an instance of the RNG like this:

[351]:
```
seed = 123
rng = default_rng(seed)      # obtain default RNG implementation,
                             # initialise seed

rng.random(5)                # return array of 5 random numbers
```

[351]: `array([0.68235186, 0.05382102, 0.22035987, 0.18437181, 0.1759059 ])`

The `seed` argument needs to be an integer or an array of integers. This way, each call gives the same numbers, as can easily be illustrated with a loop:

[352]:
```
seed = 123
for i in range(5):
    rng = default_rng(seed)
    print(rng.random(5))
```

```
[0.68235186 0.05382102 0.22035987 0.18437181 0.1759059 ]
[0.68235186 0.05382102 0.22035987 0.18437181 0.1759059 ]
[0.68235186 0.05382102 0.22035987 0.18437181 0.1759059 ]
[0.68235186 0.05382102 0.22035987 0.18437181 0.1759059 ]
[0.68235186 0.05382102 0.22035987 0.18437181 0.1759059 ]
```

You can remove the `seed` to verify that the set of number will then differ in each iteration.

Alternatively, we might want to draw random integers by calling `integers()`, which returns numbers from a "discrete uniform" distribution on a given interval:

[353]:
```
rng.integers(2, size=5)         # vector of 5 integers from set {0, 1}
                                # here we specify only the (non-inclusive)
                                # upper bound 2
```

[353]: `array([0, 1, 0, 1, 0])`

Alternatively, we can specify the lower and upper bounds like this:

[354]:
```
rng.integers(1, 10, size=5)     # specify lower and upper bound
```

[354]: `array([3, 8, 8, 8, 9])`

Following the usual convention in Python, the upper bound is not included by default. We can change this by additionally passing `endpoint=True`:

[355]:
```
rng.integers(1, 10, size=5, endpoint=True)       # include upper bound
```

[355]: `array([1, 6, 3, 3, 3])`

We can create higher-order arrays by passing a list or tuple as the `size` argument:

[356]:
```
rng.random(size=[2, 5])             # Create 2x5 array of floats
                                    # on [0.0, 1.0)
```

[356]: array([[0.21376296, 0.74146705, 0.6299402 , 0.92740726, 0.23190819],
       [0.79912513, 0.51816504, 0.23155562, 0.16590399, 0.49778897]])

[357]:
```
rng.integers(2, size=[2,3,4])        # Create 2x3x4 array of integers {0,1}
```

[357]:
```
array([[[1, 0, 1, 0],
        [0, 0, 0, 0],
        [0, 0, 1, 0]],

       [[1, 0, 1, 1],
        [1, 1, 1, 0],
        [0, 0, 1, 0]]])
```

Legacy interface

For completeness, let's look how you would accomplish the same using the *legacy* NumPy interface.

To draw floats on the unit interval, we use `random_sample()`:

[358]:
```
from numpy.random import random_sample, randint, seed
seed(123)
random_sample(5)
```

[358]:
```
array([0.69646919, 0.28613933, 0.22685145, 0.55131477, 0.71946897])
```

Random integers can be generated using `randint()`:

[359]:
```
randint(2, size=5)       # draw random integers from {0,1}
```

[359]:
```
array([1, 1, 0, 1, 0])
```

The legacy interface defines global functions `seed`, `random_sample`, etc. within the `numpy.random` module, which are implicitly associated with a global RNG object. This implicit association has been removed in the new programming model and you now have to obtain an RNG instance explicitly, for example by using the `default_rng()` function, as demonstrated above.

7.1.2 Drawing random numbers from distributions

Often we want to draw random numbers from a specific distribution, such as the normal or log-normal distributions. The RNGs in `numpy.random` support a multitude of distributions, including:

- `binomial()`
- `exponential()`
- `normal()`
- `lognormal()`
- `multivariate_normal()`
- `uniform()`

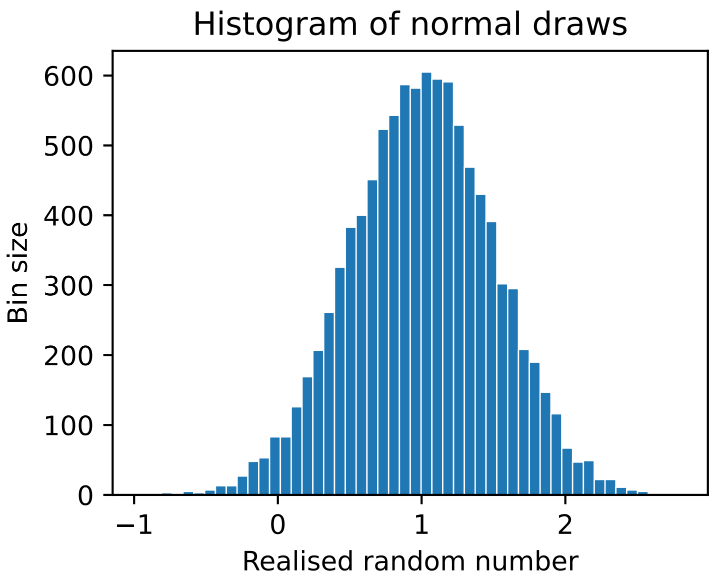
and many others. For a complete list, see the official documentation.

We will illustrate the use of these functions for the normal and multivariate normal distributions. For example, you can draw from the normal distribution with mean $\mu = 1.0$ and standard deviation $\sigma = 0.5$ using `normal()` as follows:

[360]:
```
from numpy.random import default_rng
rng = default_rng(123)

# location and scale parameters of normal distribution
mu = 1.0
sigma = 0.5

# Draw 10000 normal numbers;
# mean and std. are passed as loc and scale arguments
```

```
x = rng.normal(loc=mu, scale=sigma, size=10000)

# plot the results
import matplotlib.pyplot as plt
plt.hist(x, bins=50, linewidth=0.5, edgecolor='white')
plt.xlabel('Realised random number')
plt.ylabel('Bin size')
plt.title('Histogram of normal draws')
```

[360]: Text(0.5, 1.0, 'Histogram of normal draws')



To draw from the multivariate normal, we need to specify a vector of means μ and the variance-covariance matrix Σ, which we set to

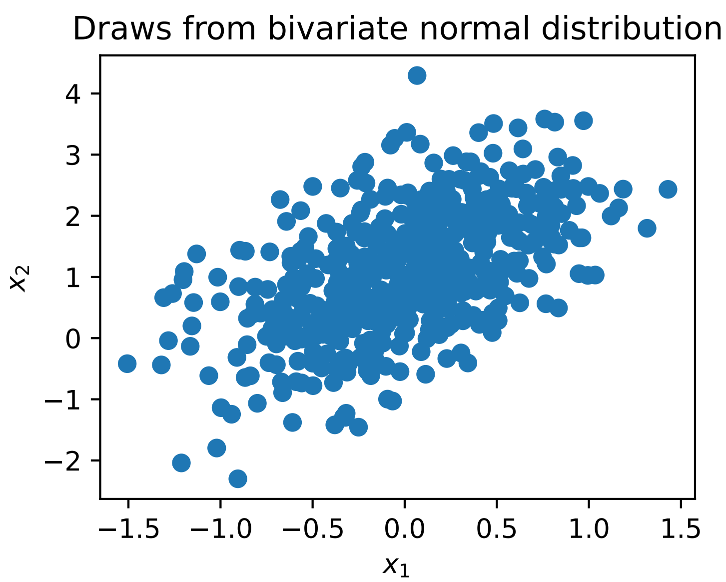
$$\mu = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \qquad \Sigma = \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix}$$

with $\sigma_1 = 0.5$, $\sigma_2 = 1.0$ and $\rho = 0.5$. We call `multivariate_normal()` to draw a sample:

[361]:
```
import numpy as np
from numpy.random import default_rng
import matplotlib.pyplot as plt

rng = default_rng(123)

mu = np.array((0.0, 1.0))        # vector of means
sigma1 = 0.5                     # Std. dev. of first dimension
sigma2 = 1.0                     # Std. dev. of second dimension
rho = 0.5                        # Correlation coefficient

# Compute covariance
cov = rho * sigma1 * sigma2

# Create variance-covariance matrix
vcv = np.array([[sigma1**2.0, cov],
                [cov, sigma2**2.0]])

# Draw MVN random numbers:
```

```
# each row represents one sample draw.
x = rng.multivariate_normal(mean=mu, cov=vcv, size=500)

# Scatter plot of sample
plt.scatter(x[:, 0], x[:, 1])
plt.xlabel(r'$x_1$')
plt.ylabel(r'$x_2$')
plt.title('Draws from bivariate normal distribution')
```

[361]: Text(0.5, 1.0, 'Draws from bivariate normal distribution')



7.2 More functions for probability distributions

NumPy itself only implements distribution-specific RNGs. Frequently, we want to evaluate probability density functions (PDFs), cumulative distribution functions (CDFs) or compute some moments such as the mean of a random variable following some distribution. The SciPy project implements these functions for a wide range of discrete and continuous univariate distributions as well as for a few multivariate ones in the `scipy.stats` package.

The most useful functions include:

- `pdf()`: probability density function
- `cdf()`: cumulative distribution function
- `ppf()`: percent point function (inverse of `cdf`)
- `moment()`: non-central moment of some order n
- `expect()`: expected value of a function (of one argument) with respect to the distribution

The parameters that need to be passed to these functions are distribution dependent. See the official documentation for details.

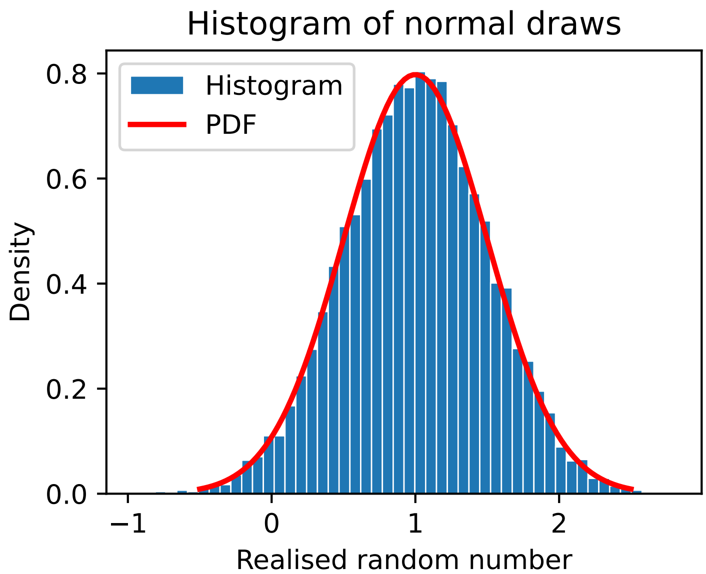
Examples:

We can overlay the histogram of normal draws with the actual normal PDF using SciPy's `norm` distribution as follows:

[362]:
```
from numpy.random import default_rng
from scipy.stats import norm                    # import normal distribution
import matplotlib.pyplot as plt
```

```
rng = default_rng(123)

# location and scale parameters of normal distribution
mu = 1.0
sigma = 0.5

# Draw 10000 normal numbers
x = rng.normal(loc=mu, scale=sigma, size=10000)    # mean and std. are passed as
                                                   # loc and scale arguments

# plot histogram
plt.hist(x, bins=50, density=True, linewidth=0.5, edgecolor='white',
         label='Histogram')

# Create x-values for PDF plot, using mean +/- 3 std.
xvalues = np.linspace(mu - 3*sigma, mu + 3*sigma, 100)
# Compute PDF of normal distr. at given x-values
pdf = norm.pdf(xvalues, loc=mu, scale=sigma)
# Plot PDF
plt.plot(xvalues, pdf, linewidth=2.0, color='red', label='PDF')
plt.xlabel('Realised random number')
plt.ylabel('Density')
plt.title('Histogram of normal draws')
plt.legend()
```

```
[362]: <matplotlib.legend.Legend at 0x7f9de232ff40>
```



In the above example we pass `density=True` to Matplotlib's `hist()` plotting function so that the result is rescaled to be comparable to the actual PDF.

Sometimes we need to compute the expectation of a function $g(x)$ with respect to a given distribution with PDF $f(x)$ on some interval (a, b):

$$E[g(x)] = \int_a^b g(x) f(x) dx$$

For example, we might want to know the mean of a *truncated* normal with parameters $\mu = 0, \sigma = 1.0$ with support on $(-\infty, 0)$, i.e.,

$$E[x|x \leq 0] = \int_{-\infty}^{0} x \frac{f(x)}{F(0)} dx$$

where $f(x)$ and $F(x)$ are the PDF and CDF of the standard normal. We can compute it as follows:

[363]:
```
from scipy.stats import norm
import numpy as np

lb = -np.inf                # integration lower bound
ub = 0.0                    # integration upper bound

mu = 0.0                    # mean of the (untruncated) normal
sigma = 1.0                 # std. dev. of the (untruncated) normal

cdf0 = norm.cdf(0.0, loc=mu, scale=sigma)        # CDF at 0

# Compute conditional expected value
Ex = norm.expect(lambda x: x/cdf0, loc=mu, scale=sigma, lb=lb, ub=ub)
Ex                          # print conditional expectation
```

[363]: `-0.7978845608028651`

Here we define the function to be integrated as $g(x) = \frac{x}{F(0)}$, and we pass it to `expect()` as a lambda expression.

We can alternatively let `expect()` do the conditioning automatically by specifying `conditional=True`, and then we don't even need to apply the scaling factor $\frac{1}{F(0)}$:

[364]:
```
norm.expect(lambda x: x, loc=mu, scale=sigma, lb=lb, ub=ub,
            conditional=True)
```

[364]: `-0.7978845608028643`

7.3 Statistics functions

In the previous section we examined functions associated with specific distributions. Additionally, there are numerous routines to process *sample* data which are spread across NumPy and SciPy.

In NumPy, the most useful routines include:

- `np.mean()`, `np.average()`: sample mean; the latter variant can also compute weighted means.
- `np.std()`, `np.var()`: sample standard deviation and variance
- `np.percentile()`, `np.quantile()`: percentiles or quantiles of a given array
- `np.corrcoef()`: Pearson correlation coefficient
- `np.cov()`: sample variance-covariance matrix
- `np.histogram()`: histogram of data. This only bins the data, as opposed to Matplotlib's `hist()` which plots it.

In addition, there are the variants `np.nanmean()`, `np.nanstd()`, `np.nanvar()` `np.nanpercentile()` and `np.nanquantile()` which ignore `NaN` values. You can find the full list of routines in the official documentation.

On top of that, the `scipy.stats` package contains functions to compute all sorts of descriptive statistics and statistical hypothesis tests. Many of these routines are too specific to be listed here, so have a look at the official documentation if you need to perform statistical analysis of your sample data.

Examples:

To compute the pairwise correlations of a sample drawn from a multivariate normal distribution we proceed as follows:

[365]:
```
import numpy as np
from numpy.random import default_rng

rng = default_rng(123)

# vector of multivariate normal means
mu = np.array([-1.0, 1.0])

sigma1 = 0.5                    # Std. dev. of first dimension
sigma2 = 1.0                    # Std. dev. of second dimension
rho = 0.5                       # Correlation coefficient

# Compute covariance
cov = rho * sigma1 * sigma2

# variance-covariance matrix
vcv = np.array([[sigma1**2.0, cov],
                [cov, sigma2**2.0]])

# Draw some multivariate normal random numbers
x = rng.multivariate_normal(mean=mu, cov=vcv, size=1000)

# Compute correlation coefficient
np.corrcoef(x.T)         # expects each row to contain one variable
```

[365]:
```
array([[1.        , 0.51768322],
       [0.51768322, 1.        ]])
```

Depending on the sample size, the correlation coefficient reported in the off-diagonal elements might or might not be close to the ρ used to draw the random data.

In the next example, we demonstrate how to compute some descriptive statistics using SciPy's `describe()` for a sample drawn from a 3-dimensional multivariate normal distribution:

[366]:
```
import scipy.stats
import numpy as np
from numpy.random import default_rng

rng = default_rng(123)

# vector of multivariate normal means
mu = np.array([-1.0, 0.0, 1.0])

# variance-covariance matrix
vcv = np.array([[1.0, 0.5, 0.2],
                [0.5, 2.0, 0.7],
                [0.2, 0.7, 0.5]])

# Draw some multivariate normal random numbers
x = rng.multivariate_normal(mean=mu, cov=vcv, size=100)

# Compute some descriptive statistics
nobs, minmax, mean, variance, skewness, kurtosis = scipy.stats.describe(x)
mean        # array of means
```

[366]:
```
array([-0.98486214, -0.0719401 ,  0.99084898])
```

[367]:
```
variance    # array of variances
```

[367]:
```
array([0.80017787, 1.96834418, 0.37118602])
```

To illustrate how to use one of the many tests implemented in `scipy.stats`, we compute the Jarque-Bera test statistic using `jarque_bera()`. This is a goodness-of-fit test to assess whether a sample has zero skewness and excess kurtosis and could thus be normally distributed.

[368]:
```
from scipy.stats import jarque_bera
from numpy.random import default_rng

rng = default_rng(123)

# Draw from univariate normal
x = rng.normal(loc=1.0, scale=2.0, size=10000)

# Compute Jarque-Bera test statistic
jb_stat, pvalue = jarque_bera(x)
print(f'Test statistic: {jb_stat:.3f}, p-value: {pvalue:.3f}')
```

```
Test statistic: 3.472, p-value: 0.176
```

With a p-value of about 0.18 we cannot reject the null hypothesis of zero skewness and zero excess kurtosis.

7.4 Exercises

The following exercises are considerably longer than those in previous units. The reason is that they incorporate everything we have covered so far, and we are finally able to use larger data sets (albeit only randomly generated ones) instead of just calling `np.arange(5)` all the time. In this sense, the exercises are starting to resemble (simplified) real-world applications.

7.4.1 Exercise 1: Histograms for increasing sample sizes

In this exercise, we plot histograms against the actual PDF of a standard-t distributed random variable for increasing sample sizes.

Consider the standard-t distribution with 20 degrees of freedom (this is the only parameter of this distribution):

- To draw samples from this distribution, use NumPy RNG's `standard_t()` method.
- To plot the PDF of this distribution, use the `t` distribution from `scipy.stats`. You can import it as follows

  ```
  from scipy.stats import t as standard_t
  ```

  It is a good idea to assign more descriptive names to imported symbols than a `t`.

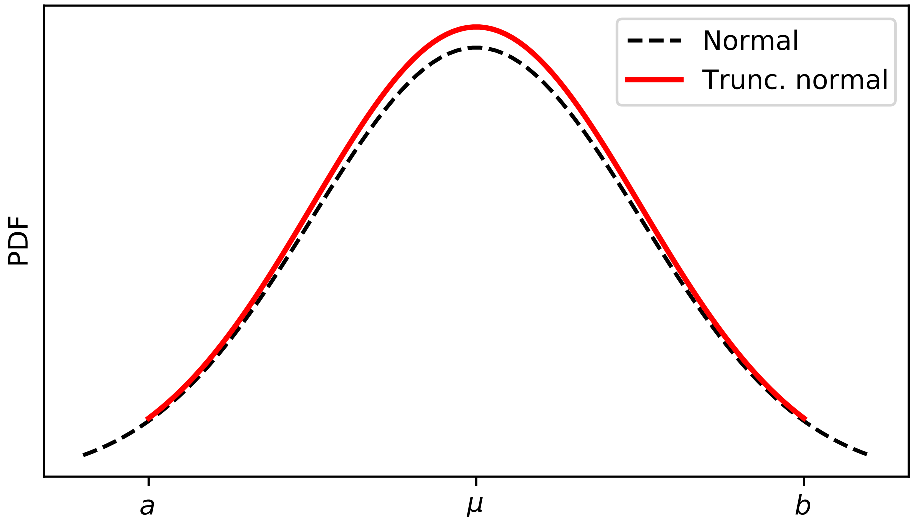
Perform the following tasks:

1. Draw random samples from the standard-t distribution for a sequence of increasing sample sizes of 50, 100, 500, 1000, 5000 and 10000.
2. Create a single figure with 6 panels in which you plot a histogram of the samples you have drawn. Use matplotlib's `hist()` function to do this, and pass the argument `bins = 50` so that each panel uses the same number of bins.
3. Add the actual PDF of the standard-t distribution to each panel. To evaluate the PDF, use the `pdf()` method of the `t` distribution you imported from `scipy.stats`.

7.4.2 Exercise 2: Moments of truncated normal

In this exercise, you are asked to compute the second non-central moment of a truncated normal distribution.

Consider a truncated normal distribution with support on the interval $[a, b]$ with $a = \mu - 2\sigma$ and $b = \mu + 2\sigma$. Assume the underlying (untruncated) normal distribution has mean $\mu = 0$ and variance $\sigma^2 = 1$. Compared to the untruncated normal PDF, the truncated PDF is rescaled upwards so that it integrates to 1, as illustrated in the following figure:



Compute the second non-central moment $E[X^2]$ in four different ways:

1. Use the fact that $Var(X) = E[X^2] - E[X]^2$. Call the methods `mean()` and `var()` of the truncated normal implemented in SciPy to compute the (squared) mean and variance.

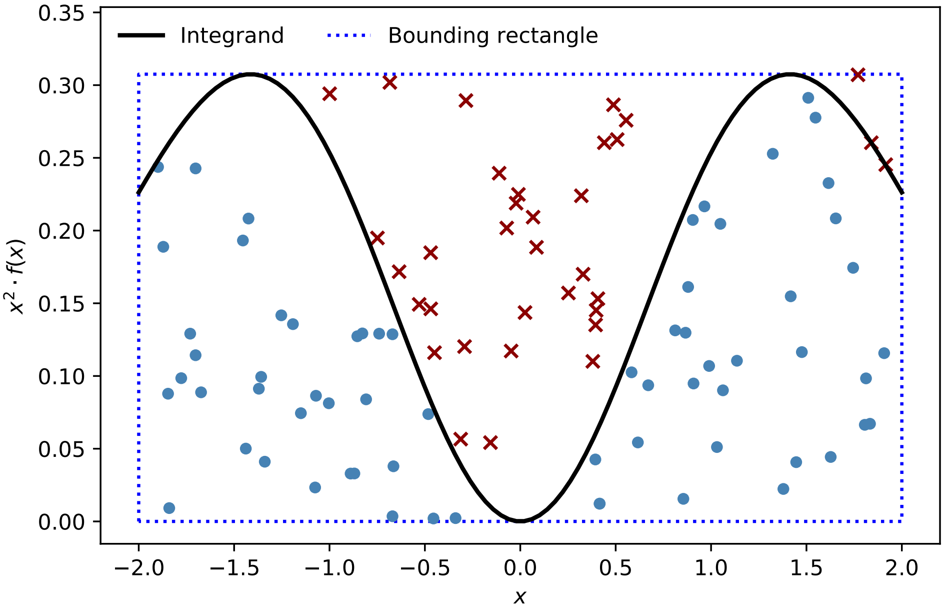
   Hint: Import the truncated normal as follows:

   ```
   from scipy.stats import truncnorm
   ```

2. Use the `moment()` method of SciPy's truncated normal to directly compute the desired moment.
3. Use the `expect()` method of SciPy's truncated normal to compute the expectation $E[X^2]$.
4. Use Monte Carlo integration to compute the expectation $E[X^2]$. There are numerous ways to do MC integration. In this exercise, we use a variant which draws random samples from a 2-dimensional uniform distribution to compute an area under the integrand:

   - To do this, define the integrand as $x^2 \cdot f_t(x; a, b, \mu, \sigma)$ where f_t is the PDF of the truncated normal with parameters a, b, μ and σ.
   - Draw random numbers in the rectangle which has length $b - a$ and a height which is the maximum of the integrand on the integration interval $[a, b]$.
   - Determine the fraction of sampled points that are below the integral, and use this to compute the area under the integrand.

   The following figure illustrates this approach to integration. The blue dots are included in the integral whereas the red crosses are not:



This may not be the most practical way to do MC integration, and we will examine a more common approach in the next exercise.

Note: SciPy's truncated normal expects *normalised* boundaries a and b. Whenever the underlying distribution is *not* standard normal, you have to pass $z_a = (a - \mu)/\sigma$ and $z_b = (b - \mu)/\sigma$ instead of a and b to all of `truncnorm`'s methods.

7.4.3 Exercise 3: Multi-period asset returns

Consider an investor with initial assets a and a 2-period investment horizon (we assume the investor does not change the asset position after the first period).

Denote by R the total gross return over two periods, so that the terminal wealth is given by $W = a \cdot R$. The total gross return is the product of the period-1 and period-2 gross returns, $R = R_1 \cdot R_2$. We impose that per-period log returns $r_t = \log R_t$ are jointly normally distributed with mean $E[r_t] = \mu$, variance $Var(r_t) = \sigma^2$ for $t \in \{1, 2\}$ with a correlation coefficient $Corr(r_1, r_2) = \rho$. Let $a = 1$, $\mu = 0.04$, $\sigma = 0.16$ and $\rho = 0.5$.

1. Derive the analytical expression for the expected total gross return after 2 periods.

   Hint:

   - Remember that since (r_1, r_2) are jointly normally distributed, so is their sum, $\log R = r_1 + r_2$.
   - Moreover, if $\log R$ is normally distributed with mean μ_R and variance σ_R^2, then R is log-normally distributed and has the expected value

   $$E[R] = \exp\left(\mu_R + \frac{1}{2}\sigma_R^2\right)$$

2. Compute the expected terminal wealth after 2 periods using Monte Carlo simulation. To do this,
   1. Draw N samples of multivariate normally distributed vectors (r_{1i}, r_{2i}) using NumPy's multivariate_normal().
   2. Compute the terminal wealth for each draw i: $W_i = a \exp(r_{1i}) \exp(r_{2i})$.

3. Compute the expected wealth as the sample average:

$$E[W] \approx \overline{W} = \frac{1}{N} \sum_{i=1}^{N} W_i$$

Make sure you get approximately the same result as in part 1 (you may need to increase the sample size if this is not the case).

3. Plot a histogram of the simulated total gross returns, and overlay it with the PDF of the log-normal distribution you derived in the first part.

7.4.4 Exercise 4: Standard error and increasing sample size

Consider a setting in which we draw multiple samples indexed by k such that these samples are increasing in the sample size N_k, given by N_k = 10, 50, 100, 500, 1000, 5000, 10000, 50000 and 100000.

The data for the k-th sample are $(x_{ik})_{i=1}^{N_k}$ where i indexes some draw within the k-th sample. Assume that the data are log-normally distributed such that the underlying normal distribution has mean $\mu = 0.5$ and variance $\sigma^2 = 1.5^2$.

1. For each sample size N_k, use NumPy's `lognormal()` to draw a log-normally distributed sample.
2. For each sample, compute the sample mean and its standard error. As a reminder, the standard error of the k-th sample mean $\overline{x}_k$ is defined as

$$se(\overline{x}_k) = \sqrt{\frac{\widehat{\sigma}_k^2}{N_k}}$$

where $\widehat{\sigma}_k^2$ is the variance of residuals $u_{ik} = x_{ik} - \overline{x}_k$ for each sample k,

$$\widehat{\sigma}_k^2 = \frac{1}{N_k - 1} \sum_{i=1}^{N_k} u_{ik}^2$$

3. Plot the sample means for all samples, using the sample size on the x-axis and the estimated mean on the y-axis. Use the $\log_{10}$ scale on the x-axis.

   Hint: You can activate log scaling by calling `xscale('log')`, or `set_xscale('log')` when using the object-oriented plotting interface.
4. Add a horizontal line showing the true mean (which is the same for all sample sizes).
5. Add confidence intervals (CI) for each sample size: use the interval $\overline{x}_k \pm 2 \times se(\overline{x}_k)$ to get a CI of approximately 95%.

7.4.5 Exercise 5: The jackknife

We continue with the setting from exercise 4, but instead of computing the standard error as above, we now use a resampling technique known as the jackknife to get the sample mean and its standard error.

1. For each sample k, compute N_k sample means $\overline{x}_{-i,k}$ which are obtained by leaving out the i-th observation:

$$\overline{x}_{-i,k} = \frac{1}{N_k - 1} \sum_{j=1, j \neq i}^{N_k} x_{jk} \qquad i = 1, \dots, N_k$$

where x_{jk} is the j-th draw in the k-th sample.

2. Compute the jackknife estimate of the sample mean as the average of these sub-sample means:

$$\overline{x}_{k,jack} = \frac{1}{N_k} \sum_{i=1}^{N_k} \overline{x}_{-i,k}$$

For the special case of a sample mean, it is straightforward to show that this is just the regular sample mean computed on the whole sample, $\overline{x}_{k,jack} = \overline{x}_k$, where

$$\overline{x}_k = \frac{1}{N_k} \sum_{i=1}^{N_k} x_{ik}$$

3. The jackknife estimate of the error variance for sample size N_k is then given by

$$\begin{aligned} \widehat{var}(\overline{x}_k) &= \frac{N_k - 1}{N_k} \sum_{i=1}^{N_k} \left(\overline{x}_{-i,k} - \overline{x}_{jack,k} \right)^2 \\ &= \frac{1}{N_k(N_k - 1)} \sum_{i=1}^{N_k} (x_{ik} - \overline{x}_k)^2 \end{aligned}$$

where the second line again follows as a special case if we are estimating the sample mean. The standard error of the sample mean is thus

$$se(\overline{x}_k) = \sqrt{\widehat{var}(\overline{x}_k)}$$

4. Recreate the plot from exercise 4, but now use the jackknife estimate of the standard error instead.

7.4.6 Exercise 6: The bootstrap

We continue with the setting from exercises 4 and 5, but now we use the bootstrap to estimate the confidence intervals of the mean estimate.

1. For each sample size N_k proceed as follows:
   1. Draw an initial sample of size N_k as before and compute the sample mean.
   2. Resample N_k observations by drawing from this initial sample *with replacement* using NumPy's `choice()` function.
   3. For each "resample", compute the sample mean. Say we have the j-th resample which consists of the draws $(x_{ik}^j)_{i=1}^{N_k}$, so we compute the j-th mean

   $$\overline{x}_k^j = \frac{1}{N_k} \sum_{i=1}^{N_k} x_{ik}^j$$

   4. Repeat steps 2 and 3 $N_{bs} = 999$ times.
   5. Use these N_{bs} means to find the 2.5% and 97.5% percentiles of the mean estimate distribution, $\overline{x}_k^{p2.5}$ and $\overline{x}_k^{p97.5}$.
   6. The bootstrapped 95% confidence interval is then given by $\left[\overline{x}_k^{p2.5}, \overline{x}_k^{p97.5}\right]$.
2. Recreate the same plot as in exercises 4 and 5, but this time use the bootstrapped 95% confidence interval you computed for each sample size.
3. For each sample size, store all bootstrapped means and use these to create a histogram of sample means. You will thus have to create 9 histograms. Use vertical lines to indicate the 95% confidence interval.

7.5 Solutions

The solutions are also provided as Python scripts in the lectures/solutions/unit7/ folder.

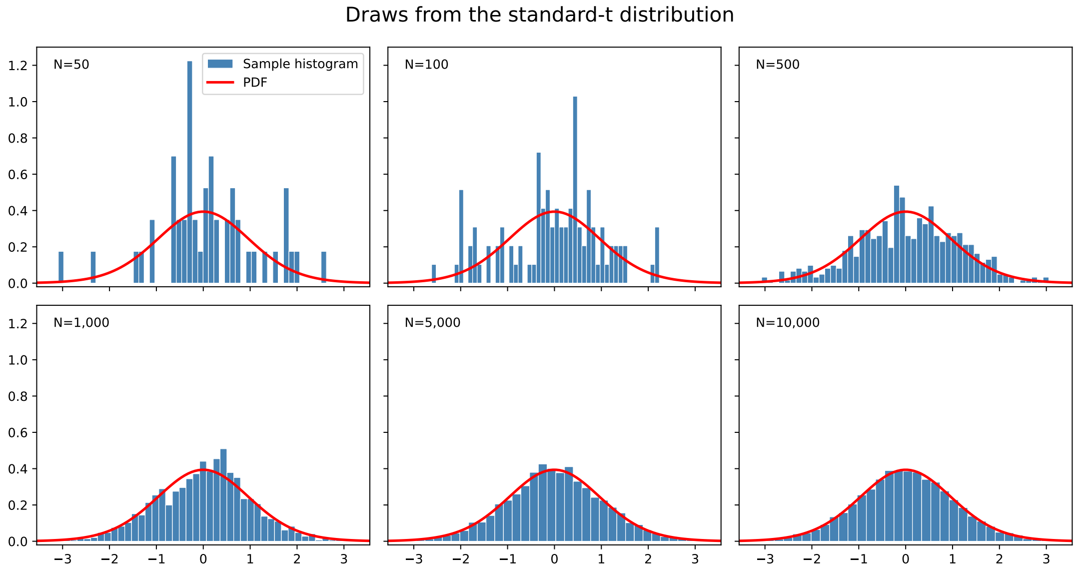
7.5.1 Solution for exercise 1

In the following solution, we create a figure with six panels (axes) and iterate over these axes. In each iteration, we

1. draw a random sample for the given (increasing) size;
2. plot the histogram using the current axes object; and
3. overlay the actual PDF.

[369]:
```
import matplotlib.pyplot as plt
import numpy as np
from numpy.random import default_rng
from scipy.stats import t as standard_t

# Sample sizes
Nobs = np.array((50, 100, 500, 1000, 5000, 10000))

# degrees of freedom
df = 20

# Determine xlims such that we cover the (0.1, 99.9) percentiles
# of the distribution.
xmin, xmax = standard_t.ppf((0.001, 0.999), df=df)

xvalues = np.linspace(xmin, xmax, 100)
pdf = standard_t.pdf(xvalues, df=df)

fig, ax = plt.subplots(2, 3, sharex=True, sharey=True, figsize=(12, 6))

# initialize default RNG
rng = default_rng(123)

for i, axes in enumerate(ax.flatten()):
    # Sample size to be plotted in current panel
    N = Nobs[i]
    # Draw sample of size N
    data = rng.standard_t(df=df, size=N)

    # plot histogram of given sample
    axes.hist(data, bins=50, linewidth=0.5, edgecolor='white',
              color='steelblue', density=True, label='Sample histogram')

    # overlay actual PDF
    axes.plot(xvalues, pdf, color='red', lw=2.0, label='PDF')

    # create text with current sample size
    axes.text(0.05, 0.95, f'N={N:,d}', transform=axes.transAxes, va='top')

    axes.set_xlim((xmin, xmax))
    axes.set_ylim((-0.02, 1.3))

    # plot legend only for the first panel
    if i == 0:
        axes.legend(loc='upper right')

# compress space between individual panels
fig.tight_layout()
# Add overall title
fig.suptitle('Draws from the standard-t distribution', fontsize=16, y=1.05)
```

[369]:
```
Text(0.5, 1.05, 'Draws from the standard-t distribution')
```



A few comments on how we create the x-values and the plot range for these graphs:

1. In principle, we could draw arbitrarily large or small realised values, but we want to restrict the plot limits to a reasonable interval.
2. To find such an interval, we compute the percentiles corresponding to 0.1% and 99.9%, which will cover almost any point we'd want to plot.
3. Moreover, we need to compute the x-values and evaluate the PDF at these points only once since these will remain unchanged for all sample sizes.

Note also that the `subplots()` function returns a 2-dimensional array (since we requested a 2×3 layout). We iterate over the *flattened* array of axes objects instead of writing two nested loops over rows and columns.

7.5.2 Solution for exercise 2

Computing the second non-central moment using the first three methods is straightforward. All you need to do is to make sure that you pass the correct parameters to SciPy's `truncnorm` methods:

[370]:
```
import numpy as np
from scipy.stats import truncnorm

# Parameters
mu = 0.0
sigma = 1.0
a = mu - 2*sigma
b = mu + 2*sigma

# Standardised boundaries if underlying non-truncated distr. is
# NOT standard normal
za = (a-mu)/sigma
zb = (b-mu)/sigma

# Method 1: Compute from E[X^2] = Var(X) + E[X]^2
var = truncnorm.var(za, zb, loc=mu, scale=sigma)
mean = truncnorm.mean(za, zb, loc=mu, scale=sigma)
m2_var_mean = var + mean ** 2.0

# Method 2: Compute using moment()
m2 = truncnorm.moment(2, za, zb, loc=mu, scale=sigma)
```

```
# Method 3: Compute moment using expect() function
m2_expect = truncnorm.expect(lambda x: x**2.0, args=(za, zb),
                             loc=mu, scale=sigma)

print(f'Second non-central moment, var + mean^2: {m2_var_mean:.5e}')
print(f'Second non-central moment, moment(): {m2:.5e}')
print(f'Second non-central moment, expect(): {m2_expect:.5e}')
```

```
Second non-central moment, var + mean^2: 7.73741e-01
Second non-central moment, moment(): 7.73741e-01
Second non-central moment, expect(): 7.73741e-01
```

The fourth method is more involved. We first define the integrand as follows:

[371]:
```
# Function to compute integrand
def f_integrand(x, a, b, mu, sigma):
    # Transform to boundaries required by SciPy's truncnorm
    za = (a - mu) / sigma
    zb = (b - mu) / sigma
    # Evaluate truncated normal PDF
    pdf = truncnorm.pdf(x, za, zb, loc=mu, scale=sigma)
    # Compute integrand x^2 * f(x)
    result = x ** 2.0 * pdf
    return result
```

The remainder of the Monte Carlo code look as follows:

[372]:
```
from numpy.random import default_rng

# Initialise RNG
rng = default_rng(123)
# Sample size for Monte Carlo integration
Nsample = 50000

# x-values should be uniformly distributed on [a, b]
xsample = rng.uniform(a, b, size=Nsample)
# Alternatively we can also just use equidistant x-values, in
# low-dimensional problems it makes no difference.
# xsample = np.linspace(a, b, Nsamples)

# Evaluate integrand at sampled x-values
integrand = f_integrand(xsample, a, b, mu, sigma)

# Compute size of bounding rectangle:
# the height is taken as the largest realisation of the integrand.
length = b - a
height = np.amax(integrand)
area = height * length
# draw y-values from uniform distribution on [0, height]
ysample = rng.uniform(0, height, size=Nsample)
# Compute fraction of points that are underneath the PDF
frac = np.mean(ysample <= integrand)
integral_MC = frac * area

print(f'Second non-central moment, MC integration: {integral_MC:.5e}')
```

```
Second non-central moment, MC integration: 7.72828e-01
```

You might have noticed that MC integration is not the fastest to converge, but using 50000 draws is sufficient to get somewhat close to the other three methods.

In this case we do not actually need Monte Carlo methods, because the dimensionality of the problem is so low. We could just as well have used a dense deterministic rectangular grid instead of randomly-drawn points.

The entire Python script which also generates the graphs displayed in the exercise can be found in the solutions folder

7.5.3 Solution for exercise 3

Part 1

The first part is purely analytical. We use it to verify that the code in part 2 yields the correct result.

Since (r_1, r_2) are jointly normal, a standard result is that their sum $r_1 + r_2$ is normally distributed with mean and variance given by

$$\mu_{rr} = E[r_1 + r_2] = 2\mu$$

$$\sigma_{rr}^2 = Var(r_1 + r_2) = Var(r_1) + Var(r_2) + 2 \cdot Cov(r_1, r_2) = 2\sigma^2 + 2\rho\sigma^2$$

This is even simpler than the usual formulas since both per-period log returns have the same mean and variance.

Moreover, since $\log R = r_1 + r_2$ is normally distributed, R is log-normally distributed and has the expected value

$$E[R] = \exp\left(\mu_{rr} + \frac{1}{2}\sigma_{rr}^2\right) = \exp\left(2\mu + (1+\rho)\sigma^2\right)$$

Since $a = 1$, this is also the expected value of terminal wealth W.

We can plug in the parameter values to compute the numerical value:

[373]:
```
import numpy as np

# Parameters
a = 1.0                             # Initial assets
mu = np.array((0.04, 0.04))         # average log returns
sigma = 0.16                        # std. dev. of log returns
rho = 0.5                           # serial correlation

# Exact expectation
var_rr = 2.0 * sigma ** 2.0 + 2.0 * rho * sigma ** 2.0
sigma_rr = np.sqrt(var_rr)
mu_rr = np.sum(mu)

exp_exact = a * np.exp(mu_rr + sigma_rr ** 2.0 / 2.0)

print(f'Expected portfolio value (exact): {exp_exact:.4f}')
```

```
Expected portfolio value (exact): 1.1257
```

Parts 2 and 3

To perform the Monte Carlo simulation, we need to define the vector of means and the variance-covariance matrix which we can pass to NumPy's `multivariate_normal()` to sample returns (r_1, r_2):

[374]:
```
import numpy as np
from numpy.random import default_rng
from scipy.stats import lognorm

# Parameters
a = 1.0                             # Initial assets
mu = np.array((0.04, 0.04))         # average log returns
sigma = 0.16                        # std. dev. of log returns
rho = 0.5                           # serial correlation
```

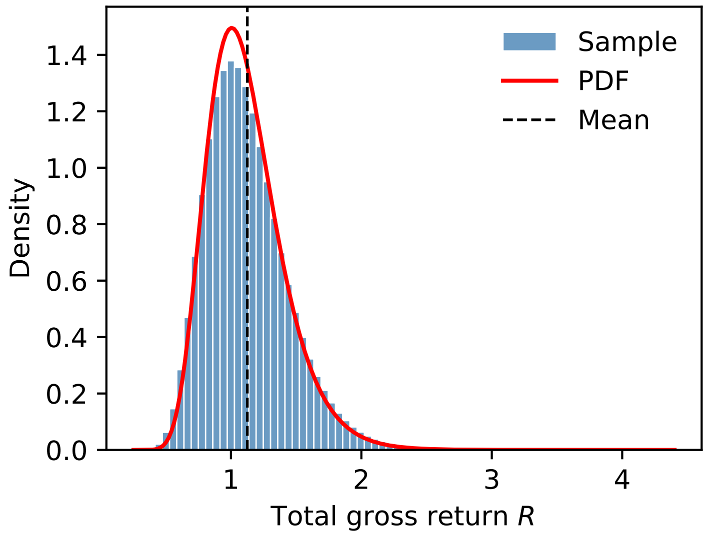
```python
# Covariance
cov = rho*sigma**2.0
# variance-covariance matrix
vcv = np.array([[sigma**2.0, cov],
                [cov, sigma**2.0]])

Nsample = 5000000
rng = default_rng(123)
# Draw MV normal samples: each row corresponds to one draw
samples = rng.multivariate_normal(mean=mu, cov=vcv, size=Nsample)

# Evaluate total gross return at sampled points:
#   R = exp(r_1) * exp(r_2)
returns = np.prod(np.exp(samples), axis=1)
# Sampled terminal wealth after 2 periods
wealth = a * returns
# Expected terminal wealth
exp_MC = np.mean(wealth)

print(f'Expected portfolio value (MC): {exp_MC:.4f}')
```

```
Expected portfolio value (MC): 1.1256
```

Finally, we use the sampled points and the `pdf()` method of SciPy's lognorm to plot the histogram and the true PDF.

[375]:
```python
import matplotlib.pyplot as plt

fig, ax = plt.subplots(1, 1)

ax.hist(returns, bins=75, density=True, color='steelblue', lw=0.5,
        edgecolor='white', alpha=.8, label='Sample')

# Plot log-normal PDF of total gross return
xmin, xmax = np.amin(returns), np.amax(returns)
xvalues = np.linspace(xmin, xmax, 200)
pdf = lognorm.pdf(xvalues, s=sigma_rr, loc=mu_rr)
ax.plot(xvalues, pdf, c='red', lw=1.5, label='PDF')

# Add line with true expected value
ax.axvline(exp_exact, lw=1.0, color='black', ls='--', label='Mean')

ax.set_xlabel('Total gross return $R$')
ax.set_ylabel('Density')
ax.legend(loc='upper right', frameon=False)
```

[375]:
```
<matplotlib.legend.Legend at 0x7f9ddb2dd030>
```



The dashed black line shows the analytically derived expected total gross return.

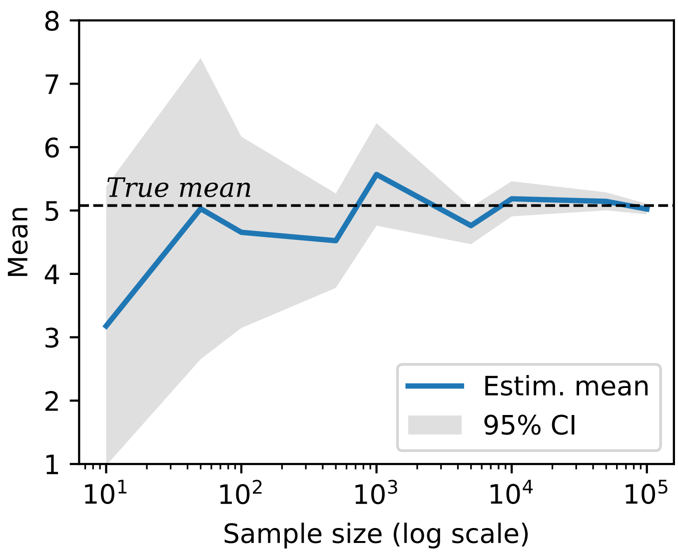
7.5.4 Solution for exercise 4

We solve the exercise by iterating over all sample sizes, drawing a new log-normal sample and computing the sample mean and standard error. These are stored in the arrays `mean_hat` and `std_err`, which we then use the generate the plot.

[376]:
```
import numpy as np
from numpy.random import default_rng
import matplotlib.pyplot as plt

sample_sizes = np.array([10, 50, 100, 500, 1000, 5000, 10000, 50000, 100000])
# initialize default RNG
rng = default_rng(123)

# Parameters of underlying normal distribution
mu = 0.5
sigma = 1.5

# Array to store estimated mean for each sample size
mean_hat = np.zeros(len(sample_sizes))
# Array to store std. error for each sample size
std_err = np.zeros_like(mean_hat)

for k, N in enumerate(sample_sizes):
    data = rng.lognormal(mean=mu, sigma=sigma, size=N)
    # sample mean
    x_k = np.mean(data)
    # residuals around mean
    resid = data - x_k
    # Residual variance
    var_resid = np.sum(resid**2.0) / (N-1)
    # std. error of mean estimate
    se_k = np.sqrt(var_resid / N)

    # store sample estimates in array
    mean_hat[k] = x_k
    std_err[k] = se_k
```

```
# Plot results
plt.plot(sample_sizes, mean_hat, lw=2.0, label='Estim. mean')

# Add line indicating true mean of log-normal
mean = np.exp(mu + sigma**2.0 / 2.0)
plt.axhline(mean, lw=1.0, color='black', ls='--')
plt.text(sample_sizes[0], mean + 0.05, 'True mean', va='bottom',
         fontstyle='italic', fontfamily='serif')

plt.fill_between(sample_sizes, mean_hat - 2*std_err, mean_hat + 2*std_err,
                 color='grey', alpha=0.25, zorder=-1, lw=0.0,
                 label='95% CI')

plt.xscale('log')
plt.legend(loc='lower right')
plt.xlabel('Sample size (log scale)')
plt.ylabel('Mean')
# Use identical y-lims across ex. 4-6
plt.ylim((1.0, 8.0))
```

```
[376]: (1.0, 8.0)
```



7.5.5 Solution for exercise 5

Much of this solution proceeds in the very same way as in exercise 4. Additionally,

- For each sample, we now have to loop over all observations, create a sub-sample which omits a particular observation and calculate the mean of this sub-sample.
- We compute the estimate of the sample mean as the average of all these means.

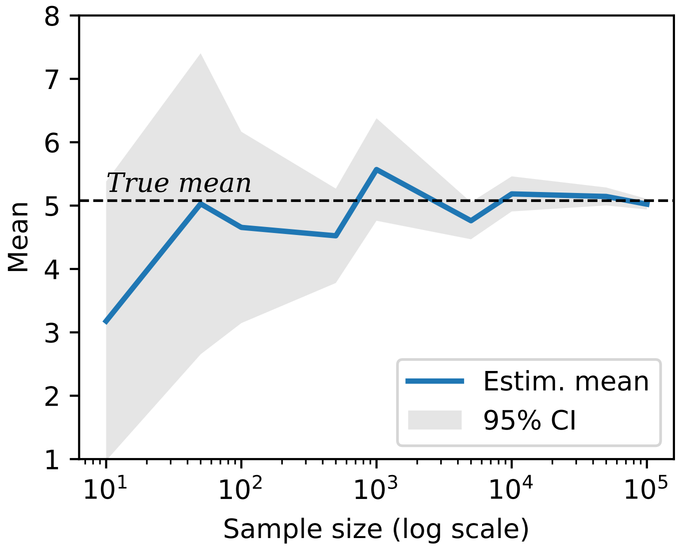
The code is substantially slower than in exercise 4 as it takes considerable time to loop over all observations in the larger samples.

Note that the jackknife is rarely used these days as it has been replaced by other resampling methods such as the bootstrap. The resulting confidence intervals look identical to the ones in exercise 4 since we have established earlier that for the sample mean the jackknife estimate of the variance is in fact identical to the standard approach.

```
[377]: import numpy as np
from numpy.random import default_rng
import matplotlib.pyplot as plt


sample_sizes = np.array([10, 50, 100, 500, 1000, 5000, 10000, 50000, 100000])
# initialize default RNG
rng = default_rng(123)

# Parameters of underlying normal distribution
mu = 0.5
sigma = 1.5

# Array to store estimated mean for each sample size
mean_hat = np.zeros(len(sample_sizes))
# Array to store std. errors for each sample size
std_err = np.zeros_like(mean_hat)

for k, N in enumerate(sample_sizes):
    data = rng.lognormal(mean=mu, sigma=sigma, size=N)

    mean_subsample = np.zeros_like(data)

    # Iterate over all elements, leaving out one element
    # and computing the mean of the resulting sub-sample
    for j in range(N):
        # Initial boolean mask: include all elements
        mask = np.ones_like(data, dtype=bool)
        # leave out j-th observation
        mask[j] = False
        subsample = data[mask]

        x_j = np.mean(subsample)
        mean_subsample[j] = x_j

    # compute sample jackknife mean estimate as average of
    # sub-sample means
    x_k = np.mean(mean_subsample)

    # Compute variance of jackknife mean estimate
    var = (N-1)/N * np.sum((mean_subsample - x_k) ** 2.0)
    # jackknife std. err. of mean estimate
    se = np.sqrt(var)

    # store sample estimates in array
    mean_hat[k] = x_k
    std_err[k] = se

# Plot results
plt.plot(sample_sizes, mean_hat, lw=2.0, label='Estim. mean')

# Add line indicating true mean of log-normal
mean = np.exp(mu + sigma ** 2.0 / 2.0)
plt.axhline(mean, lw=1.0, color='black', ls='--')
plt.text(sample_sizes[0], mean + 0.05, 'True mean', va='bottom',
         fontstyle='italic', fontfamily='serif')

plt.fill_between(sample_sizes, mean_hat - 2*std_err, mean_hat + 2*std_err,
                 color='grey', alpha=0.2, zorder=-1, lw=0.0,
                 label='95% CI')
plt.xscale('log')
plt.legend(loc='lower right')
plt.xlabel('Sample size (log scale)')
```

```
plt.ylabel('Mean')
# Use identical y-lims across ex. 4-6
plt.ylim((1.0, 8.0))
```

[377]: (1.0, 8.0)



7.5.6 Solution for exercise 6

We first define a function `bootstrap_means()` which takes as given the initial sample, and

1. Resamples the desired number of times
2. For each resample, computes the sample mean
3. Returns all sample means in an array.

[378]:
```
import numpy as np

def boostrap_mean(x, Nrounds):
    means = np.zeros(Nrounds)
    # Sample size
    N = len(x)

    for j in range(Nrounds):
        # Resample with replacement
        resampled = np.random.choice(x, size=N, replace=True)

        # Compute mean of bootstrapped sample
        m = np.mean(resampled)

        means[j] = m

    return means
```

We use the function `np.random.choice()` to sample from the initial sample with replacement (passing the argument `replace=True`).

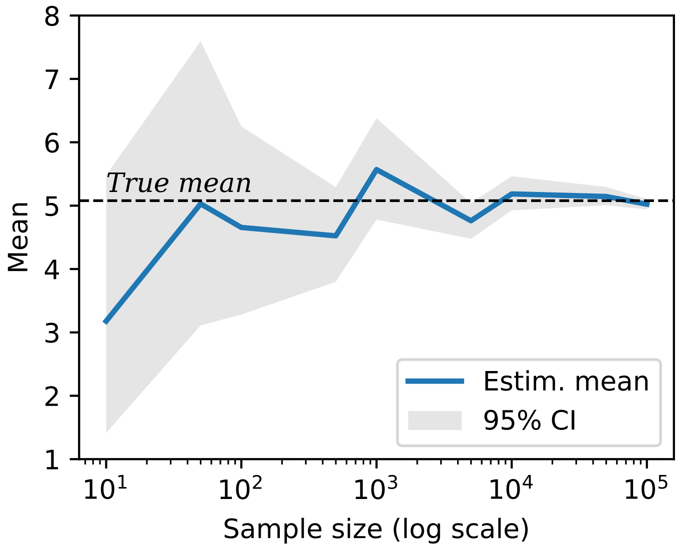
We can then use these bootstrapped means to compute the P2.5 and P97.5 percentiles using the `np.percentile()` function. These represent the bounds of the 95% confidence interval.

The remainder of the implementation looks almost identical to the previous exercises. We additionally store all bootstrapped means in the list `means_all` which we use below to create the histograms.

[379]:
```
from numpy.random import default_rng
import matplotlib.pyplot as plt

sample_sizes = np.array([10, 50, 100, 500, 1000, 5000, 10000, 50000, 100000])
# Number of bootstraps
Nbs = 999

# initialize default RNG
rng = default_rng(123)

# Parameters of underlying normal distribution
mu = 0.5
sigma = 1.5

# Array to store estimated mean for each sample size
mean_hat = np.zeros(len(sample_sizes))
# Array to store CI lower and upper bounds
bounds = np.zeros((len(sample_sizes), 2))

# Collect all bootstrapped means for each sample size
# to create histograms at the end
means_all = []

for k, N in enumerate(sample_sizes):
    data = rng.lognormal(mean=mu, sigma=sigma, size=N)

    # Mean of original sample
    x_k = np.mean(data)
    mean_hat[k] = x_k

    # bootstrap means
    mean_bs = boostrap_mean(data, Nbs)

    # CI lower and upper bounds at (p2.5, p97.5)
    rank = 2.5, 97.5
    bnd = np.percentile(mean_bs, q=rank)
    bounds[k] = bnd

    # Store in list of all bootstrapped means
    # so we can plot histogram later
    means_all.append(mean_bs)


# Plot results
plt.plot(sample_sizes, mean_hat, lw=2.0, label='Estim. mean')

# Add line indicating true mean of log-normal
mean = np.exp(mu + sigma**2.0 / 2.0)
plt.axhline(mean, lw=1.0, color='black', ls='--')
plt.text(sample_sizes[0], mean + 0.05, 'True mean', va='bottom',
         fontstyle='italic', fontfamily='serif')

plt.fill_between(sample_sizes, bounds[:, 0], bounds[:, 1],
                 color='grey', alpha=0.2, zorder=-1, lw=0.0,
                 label='95% CI')
plt.xscale('log')
plt.legend(loc='lower right')
plt.xlabel('Sample size (log scale)')
plt.ylabel('Mean')
# Use identical y-lims across ex. 4-6
```

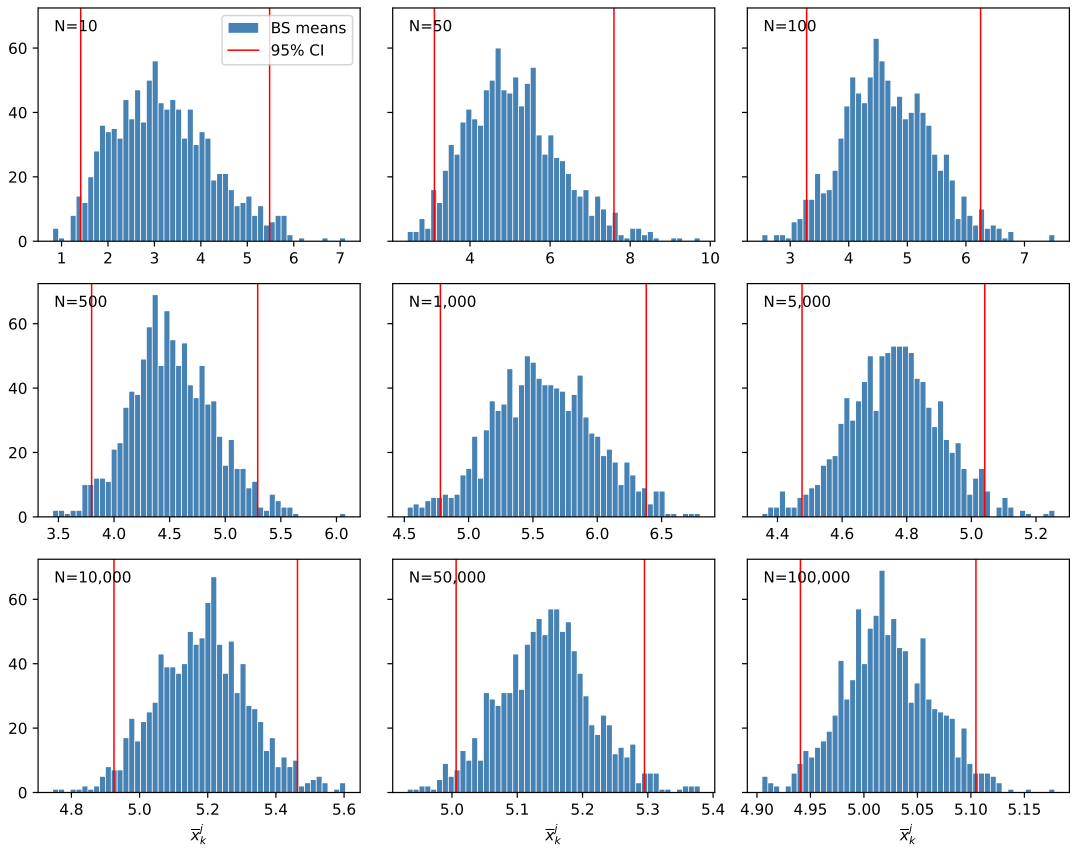
```
plt.ylim((1.0, 8.0))
```

[379]: (1.0, 8.0)



Finally, the code below creates the histograms for each sample size. Note the different plot limits on the x-axis: the bootstrapped means for larger sample sizes are much closer together.

[380]:
```
fig, axes = plt.subplots(3, 3, sharex=False, sharey=True, figsize=(10, 8))

for k, ax in enumerate(axes.flatten()):

    N_k = sample_sizes[k]
    means_k = means_all[k]
    ax.hist(means_k, bins=50, color='steelblue', lw=0.5,
            edgecolor='white', label='BS means')
    ax.axvline(bounds[k, 0], color='red', lw=1.0, label='95% CI')
    ax.axvline(bounds[k, 1], color='red', lw=1.0)

    # add sample size
    ax.text(0.05, 0.95, f'N={N_k:,d}', transform=ax.transAxes, va='top')

    if k == 0:
        ax.legend(loc='upper right')

    if k > 5:
        ax.set_xlabel(r'$\overline{x}_{k}^j$')

fig.tight_layout()
```



As an aside, the use of the bootstrap in this scenario is somewhat nonsensical and only serves to practice doing data analysis with Python. We use bootstrapping in settings where we don't know the underlying distribution, so we are forced to use the data we have as the population from which we resample with replacement. Here, we of course know that the data is log-normally distributed, so we could just draw new samples from that distribution directly.

8 Handling data with pandas

8.1 Motivation

So far, we have encountered NumPy arrays as the only way to store numerical data (we mostly ignored the built-in containers provided directly in Python). However, while NumPy arrays are great for storing homogenous data without any particular structure, they are somewhat limited when we want to use them for high-level data analysis.

For example, we usually want to process data sets with

1. several variables;
2. multiple observations, which need not be identical across variables (some values may be missing);
3. non-homogenous data types: for examples, names need to be stored as strings, birthdays as dates and income as a floating-point number.

While NumPy can in principle handle such situations, it puts all the burden on the user. Most users would prefer to not have to deal with such low-level details.

Imagine we want to store names, birth dates and annual income for two people:

Name	Date of birth	Income
Alice	1985-01-01	30,000
Bob	1997-05-12	-

No income was reported for Bob, so it's missing. With NumPy, we could do this as follows:

[381]:
```
import numpy as np
from datetime import date

date1 = date(1985, 1, 1)            # birth date for Alice
date2 = date(1997, 5, 12)           # birth date for Bob

data = np.array([['Alice', date1, 30000.0],
                 ['Bob', date2, None]])

data
```

[381]:
```
array([['Alice', datetime.date(1985, 1, 1), 30000.0],
       ['Bob', datetime.date(1997, 5, 12), None]], dtype=object)
```

[382]:
```
data.dtype          # print array data type
```

[382]:
```
dtype('O')
```

While we can create such arrays, they are almost useless for data analysis, in particular since everything is stored as a generic `object`.

- To be fair, NumPy offers an alternative array type called "record" or "structured" array which can handle fields of different data types.

  However, the pandas library offers much more beyond that, so there is little reason to use structured arrays.

Pandas was created to offer more versatile data structures that are straightforward to use for storing, manipulating and analysing heterogeneous data:

1. Data is clearly organised in *variables* and *observations*, similar to econometrics programs such as Stata.
2. Each variable is permitted to have a different data type.
3. We can use *labels* to select observations, instead of having to use a linear numerical index as with NumPy.

   We could, for example, index a data set using National Insurance Numbers.
4. Pandas offers many convenient data aggregation and reduction routines that can be applied to subsets of data.

   For example, we can easily group observations by city and compute average incomes.
5. Pandas also offers many convenient data import / export functions that go beyond what's in NumPy.

Should we be using pandas at all times, then? No!

- For low-level tasks where performance is essential, use NumPy.
- For homogenous data without any particular data structure, use NumPy.
- On the other hand, if data is heterogeneous, needs to be imported from an external data source and cleaned or transformed before performing computations, use pandas.

There are numerous tutorials on pandas on the internet, so we will keep this unit short and illustrate only the main concepts. Useful references to additional material include:

- The official user guide.
- The official pandas cheat sheet which nicely illustrates the most frequently used operations.
- The official API reference with details on every pandas object and function.
- There are numerous tutorials (including videos) available on the internet. See here for a list.

8.2 Creating pandas data structures

Pandas has two main data structures:

1. `Series` represents observations of a single variable.
2. `DataFrame` is a container for several variables. You can think of each individual column of a `DataFrame` as a `Series`, and each row represents one observation.

The easiest way to create a `Series` or `DataFrame` is to create them from pre-existing data.

To access pandas data structures and routines, we need to import them first. The near-universal convention is to make pandas available using the name `pd`:

[383]:
```
import pandas as pd
```

Examples:

We can create a `DataFrame` from a NumPy array:

[384]:
```
import numpy as np
import pandas as pd             # universal convention: import using pd
from numpy.random import default_rng

# Draw normally distributed data
rng = default_rng(123)
data = rng.normal(size=(10,3))

# Define variable (or column) names
varnames = ['A', 'B', 'C']
```

```
# Create pandas DataFrame
pd.DataFrame(data, columns=varnames)
```

[384]:
```
          A         B         C
0 -0.989121 -0.367787  1.287925
1  0.193974  0.920231  0.577104
2 -0.636464  0.541952 -0.316595
3 -0.322389  0.097167 -1.525930
4  1.192166 -0.671090  1.000269
5  0.136321  1.532033 -0.659969
6 -0.311795  0.337769 -2.207471
7  0.827921  1.541630  1.126807
8  0.754770 -0.145978  1.281902
9  1.074031  0.392621  0.005114
```

This code creates a `DataFrame` of three variables called `A`, `B` and `C` with 10 observations each.

Alternatively, we can create a `DataFrame` from non-homogenous data as follows:

[385]:
```
# Names (strings)
names = ['Alice', 'Bob']

# Birth dates (datetime objects)
bdates = pd.to_datetime(['1985-01-01', '1997-05-12'])

# Incomes (floats)
incomes = np.array([35000, np.nan])          # code missing income as NaN

# create DataFrame from dictionary
pd.DataFrame({'Name': names, 'Birthdate': bdates, 'Income': incomes})
```

[385]:
```
    Name  Birthdate   Income
0  Alice 1985-01-01  35000.0
1    Bob 1997-05-12      NaN
```

If data types differ across columns, as in the above example, it is often convenient to create the `DataFrame` by passing a dictionary as an argument. Each key represents a column name and each corresponding value contains the data for that variable.

8.3 Viewing data

With large data sets, you hardly ever want to print the entire `DataFrame`. Pandas by default limits the amount of data shown. You can use the `head()` and `tail()` methods to explicitly display a specific number of rows from the top or the end of a `DataFrame`.

To illustrate, we use a data set of 23 UK universities that contains the following variables:

- `Institition`: Name of the institution
- `Country`: Country/nation within the UK (England, Scotland, ...)
- `Founded`: Year in which university (or a predecessor institution) was founded
- `Students`: Total number of students
- `Staff`: Number of academic staff
- `Admin`: Number of administrative staff
- `Budget`: Budget in million pounds
- `Russell`: Binary indicator whether university is a member of the Russell Group, an association of the UK's top research universities.

The data was compiled based on information from Wikipedia.

We read in the data stored in the file `universities.csv` (from the `data/` folder) like this:

[386]:
```python
import pandas as pd

# relative path to CSV file
file = '../data/universities.csv'

# Load sample data set of UK universities. Individual fields are separated
# using ; so we need to pass sep=';' as an argument.
df = pd.read_csv(file, sep=';')
```

We can now display the first and last three rows:

[387]:
```python
df.head(3)       # show first three rows
```

[387]:
```
                   Institution   Country  Founded  Students   Staff   Admin  \
0     University of Glasgow  Scotland     1451     30805  2942.0  4003.0
1   University of Edinburgh  Scotland     1583     34275  4589.0  6107.0
2  University of St Andrews  Scotland     1413      8984  1137.0  1576.0

   Budget  Russell
0   626.5        1
1  1102.0        1
2   251.2        0
```

[388]:
```python
df.tail(3)       # show last three rows
```

[388]:
```
                      Institution           Country  Founded  Students   Staff  \
20       University of Stirling          Scotland     1967      9548     NaN
21  Queen's University Belfast  Northern Ireland     1810     18438  2414.0
22            Swansea University             Wales     1920     20620     NaN

     Admin  Budget  Russell
20  1872.0   113.3        0
21  1489.0   369.2        1
22  3290.0     NaN        0
```

To quickly compute some descriptive statistics for the *numerical* variables in the `DataFrame`, we use `describe()`:

[389]:
```python
df.describe()
```

[389]:
```
           Founded      Students        Staff        Admin       Budget  \
count    23.000000     23.000000    20.000000    19.000000    22.000000
mean   1745.652174  24106.782609  3664.250000  3556.736842   768.609091
std     256.992149   9093.000735  2025.638038  1550.434342   608.234948
min    1096.000000   8984.000000  1086.000000  1489.000000   113.300000
25%    1589.000000  18776.500000  2294.250000  2193.500000   340.850000
50%    1826.000000  23247.000000  3307.500000  3485.000000   643.750000
75%    1941.500000  30801.500000  4439.750000  4347.500000  1023.500000
max    2004.000000  41180.000000  7913.000000  6199.000000  2450.000000

         Russell
count  23.000000
mean    0.739130
std     0.448978
min     0.000000
25%     0.500000
50%     1.000000
75%     1.000000
max     1.000000
```

Note that this automatically ignores the columns `Institution` and `Country` as they contain strings, and computing the mean, etc. of a string variable does not make sense.

To see low-level information about the data type used in each column, we call `info()`:

```
[390]: df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 23 entries, 0 to 22
Data columns (total 8 columns):
 #   Column       Non-Null Count  Dtype
---  ------       --------------  -----
 0   Institution  23 non-null     object
 1   Country      23 non-null     object
 2   Founded      23 non-null     int64
 3   Students     23 non-null     int64
 4   Staff        20 non-null     float64
 5   Admin        19 non-null     float64
 6   Budget       22 non-null     float64
 7   Russell      23 non-null     int64
dtypes: float64(3), int64(3), object(2)
memory usage: 1.6+ KB
```

Pandas automatically discards missing information in computations. For example, the number of academic staff is missing for several universities, so the number of *non-null* entries reported in the table above is less than 23, the overall sample size.

8.4 Indexing

Pandas supports two types of indexing:

1. Indexing by position. This is basically identical to the indexing of other Python and NumPy containers.
2. Indexing by label, i.e., by the values assigned to the row or column index. These labels need not be integers in increasing order, as is the case for NumPy.

   We will see how to assign labels below.

Pandas indexing is performed either by using brackets `[]`, or by using `.loc[]` for label indexing, or `.iloc[]` for positional indexing.

Indexing via `[]` can be somewhat confusing:

- specifying `df['name']` returns the column `name` as a `Series` object.
- On the other hand, specifying a range such as `df[5:10]` returns the *rows* associated with the *positions* 5,...,9.

Examples:

```
[391]: import pandas as pd

       # Load sample data set of UK universities
       df = pd.read_csv('../data/universities.csv', sep=';')
       df['Institution']                # select a single column
```

```
[391]: 0              University of Glasgow
       1            University of Edinburgh
       2           University of St Andrews
       3             University of Aberdeen
       4          University of Strathclyde
       5                                LSE
       6                                UCL
       7            University of Cambridge
       8               University of Oxford
       9              University of Warwick
       10           Imperial College London
```

```
11              King's College London
12           University of Manchester
13              University of Bristol
14           University of Birmingham
15    Queen Mary University of London
16                 University of York
17           University of Nottingham
18               University of Dundee
19                 Cardiff University
20             University of Stirling
21          Queen's University Belfast
22                 Swansea University
Name: Institution, dtype: object
```

```
[392]: df[['Institution', 'Students']]      # select multiple columns using a list
```

```
[392]:
                        Institution  Students
0             University of Glasgow     30805
1           University of Edinburgh     34275
2          University of St Andrews      8984
3            University of Aberdeen     14775
4          University of Strathclyde     22640
5                               LSE     11850
6                               UCL     41180
7           University of Cambridge     23247
8              University of Oxford     24515
9             University of Warwick     27278
10          Imperial College London     19115
11             King's College London     32895
12         University of Manchester     40250
13            University of Bristol     25955
14         University of Birmingham     35445
15  Queen Mary University of London     20560
16               University of York     19470
17         University of Nottingham     30798
18             University of Dundee     15915
19               Cardiff University     25898
20           University of Stirling      9548
21        Queen's University Belfast     18438
22               Swansea University     20620
```

To return the rows at positions 1, 2 and 3 we use

```
[393]: df[1:4]
```

```
[393]:
                Institution   Country  Founded  Students   Staff   Admin  \
1   University of Edinburgh  Scotland     1583     34275  4589.0  6107.0
2  University of St Andrews  Scotland     1413      8984  1137.0  1576.0
3    University of Aberdeen  Scotland     1495     14775  1086.0  1489.0

   Budget  Russell
1  1102.0        1
2   251.2        0
3   219.5        0
```

Pandas follows the Python convention that indices are 0-based, and the endpoint of a slice is not included.

8.4.1 Manipulating indices

Pandas uses *labels* to index and align data. These can be integer values starting at 0 with increments of 1 for each additional element, which is the default, but they need not be. The two main methods to manipulate indices are:

- `set_index(keys=['column1', ...])`: uses the values of `column1` and optionally additional columns as indices, discarding the current index.
- `reset_index()`: resets the index to its default value, a sequence of increasing integers starting at 0.

Both methods return a new `DataFrame` and leave the original `DataFrame` unchanged. If we want to change the existing `DataFrame`, we need to pass the argument `inplace=True`.

For example, we can replace the row index and use the Roman lower-case characters `a`, `b`, `c`, ... as labels instead of integers:

[394]:
```
import pandas as pd
df = pd.read_csv('../data/universities.csv', sep=';')

# Create list of lower-case letters which has same
# length as the number of observations.
index = [chr(97+i) for i in range(len(df))]      # len(df) returns number of obs.
index
```

[394]:
```
['a',
 'b',
 'c',
 'd',
 'e',
 'f',
 'g',
 'h',
 'i',
 'j',
 'k',
 'l',
 'm',
 'n',
 'o',
 'p',
 'q',
 'r',
 's',
 't',
 'u',
 'v',
 'w']
```

[395]:
```
df['index'] = index                            # create new column 'index'
df.set_index(keys=['index'], inplace=True)     # set letters as index!

# print first 3 rows using labels
df['a':'c']                  # This is the same as df[:3]
```

[395]:
```
                    Institution   Country  Founded  Students   Staff   Admin  \
index
a         University of Glasgow  Scotland     1451     30805  2942.0  4003.0
b       University of Edinburgh  Scotland     1583     34275  4589.0  6107.0
c      University of St Andrews  Scotland     1413      8984  1137.0  1576.0

       Budget  Russell
index
a       626.5        1
b      1102.0        1
c       251.2        0
```

To add to the confusion, note that when specifying a range in terms of labels, the last element *is* included! Hence the row with index `c` in the above example is shown.

We can reset the index to its default integer values using the `reset_index()` method:

```
[396]: # Reset index labels to default value (integers 0, 1, 2, ...)
       df_new = df.reset_index(drop=True)
       df_new.head(3)            # print first 3 rows of new DataFrame
```

```
[396]:                  Institution   Country  Founded  Students   Staff   Admin  \
       0     University of Glasgow  Scotland     1451     30805  2942.0  4003.0
       1   University of Edinburgh  Scotland     1583     34275  4589.0  6107.0
       2  University of St Andrews  Scotland     1413      8984  1137.0  1576.0

          Budget  Russell
       0   626.5        1
       1  1102.0        1
       2   251.2        0
```

The `drop=True` argument tells pandas to throw away the old index values instead of storing them as a column of the resulting `DataFrame`.

8.4.2 Selecting elements

To more clearly distinguish between selection by label and by position, pandas provides the `.loc[]` and `.iloc[]` methods of indexing. To make your intention obvious, you should therefore adhere to the following rules:

1. Use `df['name']` only to select *columns* and nothing else.
2. Use `.loc[]` to select by label.
3. Use `.iloc[]` to select by position.

Selection by label

To illustrate, using `.loc[]` unambiguously indexes by label:

```
[397]: df.loc['d':'f', ['Institution', 'Students']]
```

```
[397]:                     Institution  Students
       index
       d        University of Aberdeen     14775
       e      University of Strathclyde     22640
       f                            LSE     11850
```

With `.loc[]` we can even perform slicing on column names, which is not possible with the simpler `df[]` syntax:

```
[398]: df.loc['d':'f', 'Institution':'Founded']
```

```
[398]:                     Institution   Country  Founded
       index
       d        University of Aberdeen  Scotland     1495
       e      University of Strathclyde  Scotland     1964
       f                            LSE   England     1895
```

This includes all the columns between `Institution` and `Founded`, where the latter is included since we are slicing by label.

Trying to pass in positional arguments will return an error for the given `DataFrame` since the index labels are `a`, `b`, `c`,… and not 0, 1, 2…

```
[399]: df.loc[0:4]
```

```
TypeError: cannot do slice indexing on Index with these indexers [0] of type int
```

However, we can reset the index to its default value. Then the index labels are integers and coincide with their position, so that `.loc[]` works:

[400]:
```
df.reset_index(inplace=True, drop=True)       # reset index labels to integers,
                                              # drop original index
df.loc[0:4]
```

[400]:
```
                   Institution   Country  Founded  Students   Staff   Admin  \
0      University of Glasgow  Scotland     1451     30805  2942.0  4003.0
1    University of Edinburgh  Scotland     1583     34275  4589.0  6107.0
2   University of St Andrews  Scotland     1413      8984  1137.0  1576.0
3     University of Aberdeen  Scotland     1495     14775  1086.0  1489.0
4  University of Strathclyde  Scotland     1964     22640     NaN  3200.0

   Budget  Russell
0   626.5        1
1  1102.0        1
2   251.2        0
3   219.5        0
4   304.4        0
```

Again, the end point with label `4` is included because we are selecting by label.

Somewhat surprisingly, we can also pass boolean arrays to `.loc[]` even though these are clearly not labels:

[401]:
```
df.loc[df['Country'] == 'Scotland']
```

[401]:
```
                    Institution   Country  Founded  Students   Staff   Admin  \
0       University of Glasgow  Scotland     1451     30805  2942.0  4003.0
1     University of Edinburgh  Scotland     1583     34275  4589.0  6107.0
2    University of St Andrews  Scotland     1413      8984  1137.0  1576.0
3      University of Aberdeen  Scotland     1495     14775  1086.0  1489.0
4   University of Strathclyde  Scotland     1964     22640     NaN  3200.0
18       University of Dundee  Scotland     1967     15915  1410.0  1805.0
20     University of Stirling  Scotland     1967      9548     NaN  1872.0

    Budget  Russell
0    626.5        1
1   1102.0        1
2    251.2        0
3    219.5        0
4    304.4        0
18   256.4        0
20   113.3        0
```

Indexing via `.loc[]` supports a few more types of arguments, see the official documentation for details.

Selection by position

Conversely, if we want to select items exclusively by their position and ignore their labels, we use `.iloc[]`:

[402]:
```
df.iloc[0:4, 0:2]              # select first 4 rows, first 2 columns
```

[402]:
```
                 Institution   Country
0     University of Glasgow  Scotland
1   University of Edinburgh  Scotland
2  University of St Andrews  Scotland
3    University of Aberdeen  Scotland
```

Again, `.iloc[]` supports a multitude of other arguments, including boolean arrays. See the official documentation for details.

8.5 Aggregation and reduction

8.5.1 Working with entire DataFrames

The simplest way to perform data reduction is to invoke the desired routine on the entire `DataFrame`:

[403]:
```
import pandas as pd

df = pd.read_csv('../data/universities.csv', sep=';')
df.mean(numeric_only=True)
```

[403]:
```
Founded       1745.652174
Students     24106.782609
Staff         3664.250000
Admin         3556.736842
Budget         768.609091
Russell          0.739130
dtype: float64
```

Methods such as `mean()` are by default applied column-wise to each column. The `numeric_only=True` argument is used to discard all non-numeric columns (depending on the version of pandas, `mean()` will issue a warning otherwise).

One big advantage over NumPy is that missing values (represented by `np.nan`) are automatically ignored:

[404]:
```
# mean() automatically drops 3 missing observations
df['Staff'].mean()
```

[404]:
```
3664.25
```

8.5.2 Splitting and grouping

Applying aggregation functions to the entire `DataFrame` is similar to what we can do with NumPy. The added flexibility of pandas becomes obvious once we want to apply these functions to subsets of data, i.e., groups, which we can define based on values or index labels.

For example, we can easily group our universities by country:

[405]:
```
import pandas as pd

df = pd.read_csv('../data/universities.csv', sep=';')

groups = df.groupby(['Country'])
```

Here `groups` is a special pandas objects which can subsequently be used to process group-specific data. To compute the group-wise averages, we can simply run

[406]:
```
groups.mean()
```

[406]:
```
                      Founded      Students        Staff        Admin  \
Country
England           1745.923077  27119.846154  4336.692308  4112.000000
Northern Ireland  1810.000000  18438.000000  2414.000000  1489.000000
Scotland          1691.428571  19563.142857  2232.800000  2864.571429
Wales             1901.500000  23259.000000  3330.000000  4514.500000

                       Budget   Russell
Country
England           1001.700000  1.000000
Northern Ireland   369.200000  1.000000
Scotland           410.471429  0.285714
```

```
Wales                 644.800000  0.500000
```

Groups support column indexing: if we want to only compute the total number of students for each country in our sample, we can do this as follows:

[407]:
```
groups['Students'].sum()
```

[407]:
```
Country
England             352558
Northern Ireland     18438
Scotland            136942
Wales                46518
Name: Students, dtype: int64
```

There are numerous routines to aggregate grouped data, for example:

- `mean()`, `sum()`: averages and sums over numerical items within groups.
- `std()`, `var()`: within-group std. dev. and variances
- `size()`: group sizes
- `first()`, `last()`: first and last elements in each group
- `min()`, `max()`: minimum and maximum elements within a group

Examples:

[408]:
```
groups.size()       # return number of elements in each group
```

[408]:
```
Country
England             13
Northern Ireland     1
Scotland             7
Wales                2
dtype: int64
```

[409]:
```
groups.first()      # return first element in each group
```

[409]:
```
                                 Institution  Founded  Students   Staff  \
Country
England                                  LSE     1895     11850  1725.0
Northern Ireland  Queen's University Belfast     1810     18438  2414.0
Scotland               University of Glasgow     1451     30805  2942.0
Wales                     Cardiff University     1883     25898  3330.0

                   Admin  Budget  Russell
Country
England           2515.0   415.1        1
Northern Ireland  1489.0   369.2        1
Scotland          4003.0   626.5        1
Wales             5739.0   644.8        1
```

We can create custom aggregation routines by calling `agg()` or `aggregate()` on the grouped object. To illustrate, we count the number of universities in each country that have more than 20,000 students:

[410]:
```
groups['Students'].agg(lambda x: np.sum(x >= 20000))
```

[410]:
```
Country
England             10
Northern Ireland     0
Scotland             3
Wales                2
Name: Students, dtype: int64
```

Note that we called `agg()` only on the column `Students`, otherwise the function would be applied to every column separately, which is not what we want.

The most flexible aggregation method is `apply()` which calls a given function, passing the entire group-specific subset of data (including all columns) as an argument, and glues together the results.

For example, if we want to compute the average budget per student (in pounds), we can do this as follows:

```
[411]: # Budget is in millions of pounds, rescale by 1.0e6
       groups.apply(lambda x: x['Budget'].sum() / x['Students'].sum() * 1.0e6)
```

```
[411]: Country
       England              36936.050239
       Northern Ireland     20023.863760
       Scotland             20981.875539
       Wales                13861.301002
       dtype: float64
```

We couldn't have done this with `agg()`, since `agg()` never gets to see the entire chunk of data but only one column at a time.

This section provided only a first look at pandas's "split-apply-combine" functionality implemented via `groupby`. See the official documentation for more details.

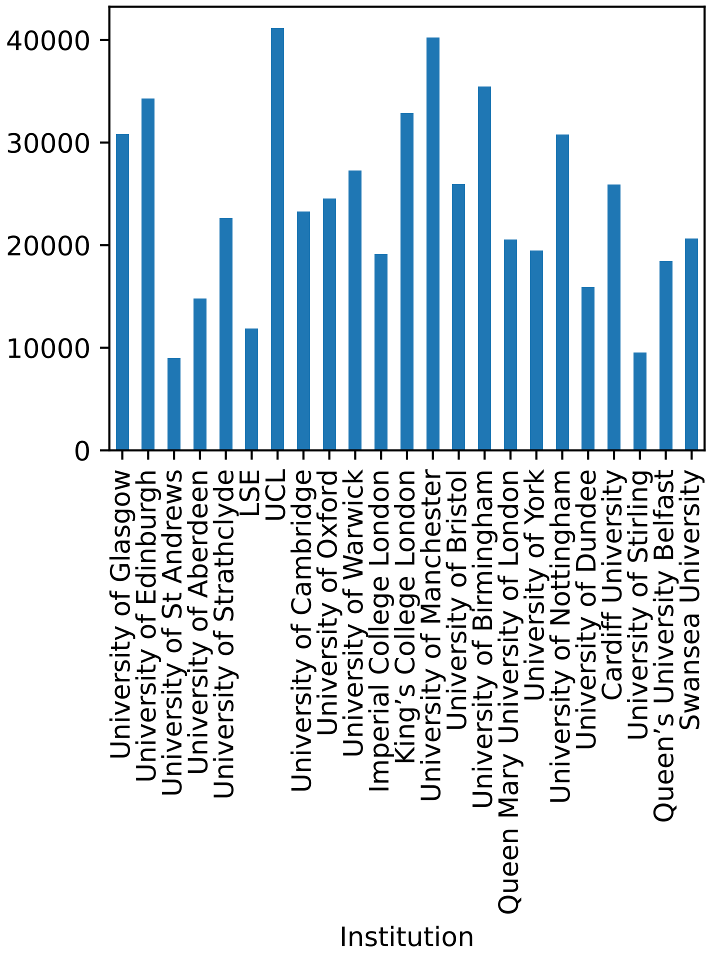
8.6 Visualisation

We covered plotting with Matplotlib in earlier units. Pandas itself implements some convenience wrappers around Matplotlib plotting routines which allow us to quickly inspect data stored in `DataFrames`. Alternatively, we can extract the numerical data and pass it to Matplotlib's routines manually.

For example, to plot student numbers as a bar chart, we can directly use pandas:

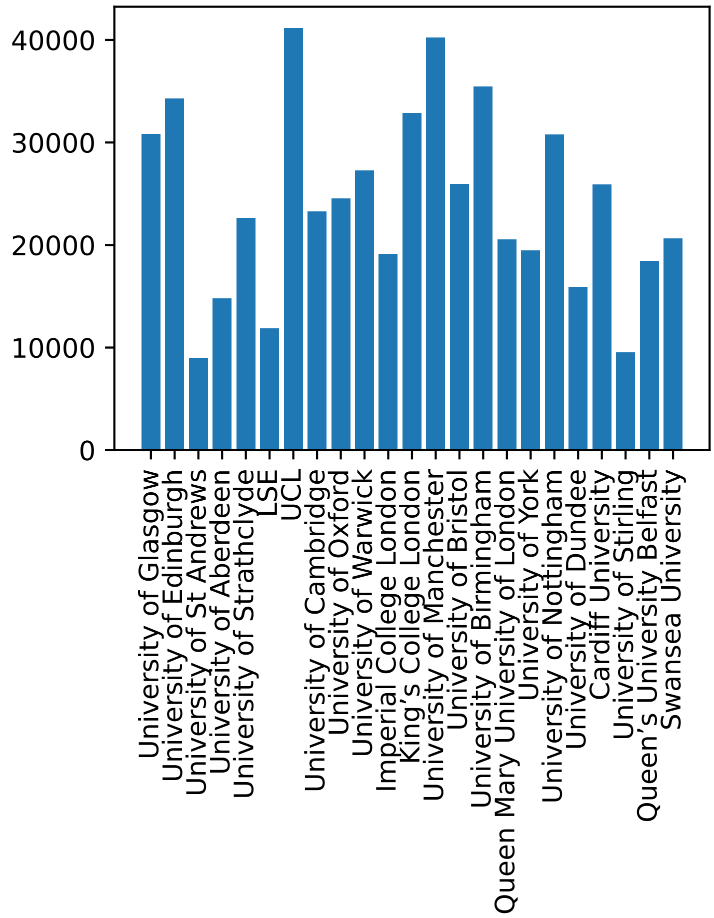
```
[412]: import pandas as pd

       df = pd.read_csv('../data/universities.csv', sep=';')

       # set institution as label so they automatically show up in plot
       df2 = df.set_index(keys=['Institution'])
       df2['Students'].plot(kind='bar')        # same as df2['Students'].plot.bar()
```

```
[412]: <AxesSubplot:xlabel='Institution'>
```



Alternatively, we can construct the graph using Matplotlib ourselves:

[413]:
```
import matplotlib.pyplot as plt

labels = df['Institution'].to_list()          # labels as list
values = df['Students'].to_numpy()            # data as NumPy array
plt.bar(labels, values)
plt.tick_params(axis='x', labelrotation=90)
```

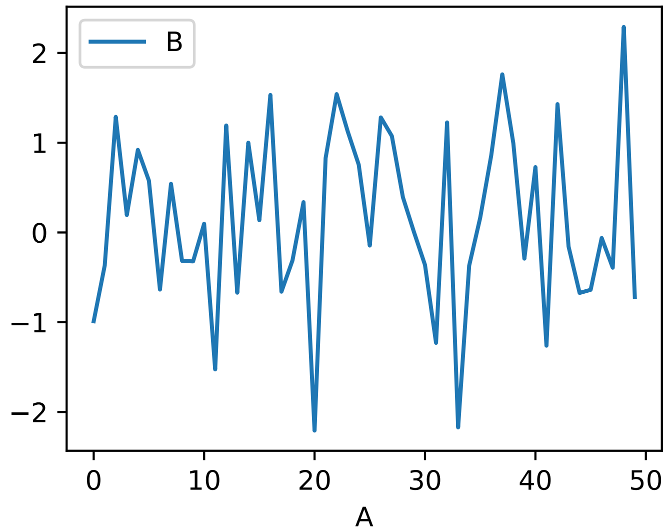


Sometimes Matplotlib's routines directly work with pandas's data structures, sometimes they don't. In cases where they don't, we can convert a `DataFrame` or `Series` object to a NumPy array using the `to_numpy()` method, and convert a `Series` to a Python list using `to_list()`, as illustrated in the example above.

To plot timeseries-like data, we can use the `plot()` method, which optionally accepts arguments to specify which columns should be used for the x-axis and which for the y-axis:

[414]:
```
import numpy as np
import pandas as pd

# Instantiate RNG
rng = np.random.default_rng(123)

# Create pandas DataFrame
nobs = 50
df = pd.DataFrame({'A': np.arange(nobs), 'B': rng.normal(size=nobs)})

df.plot(x='A', y='B')        # plot A on x-axis, B on y-axis
```

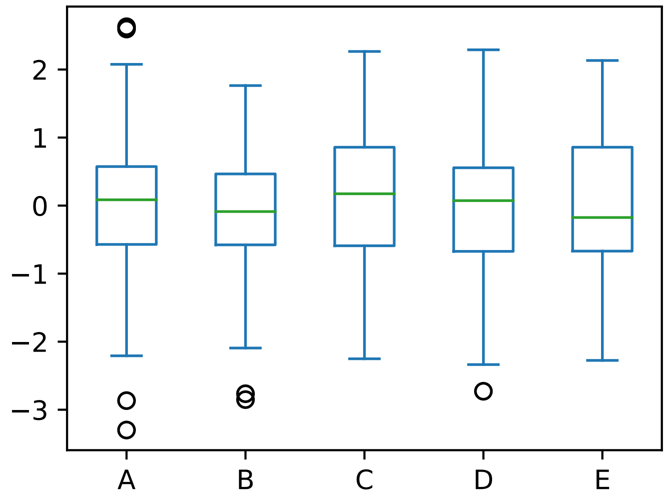
[414]:
```
<AxesSubplot:xlabel='A'>
```



To quickly generate some descriptive statistics, we can use the built-in box plot:

[415]:
```
import numpy as np
import pandas as pd

# Instantiate RNG
rng = np.random.default_rng(123)

# Create pandas DataFrame
df = pd.DataFrame(rng.normal(size=(100, 5)),
                  columns=['A', 'B', 'C', 'D', 'E'])

df.plot.box()              # same as df.plot(kind='box')
```

[415]: <AxesSubplot:>



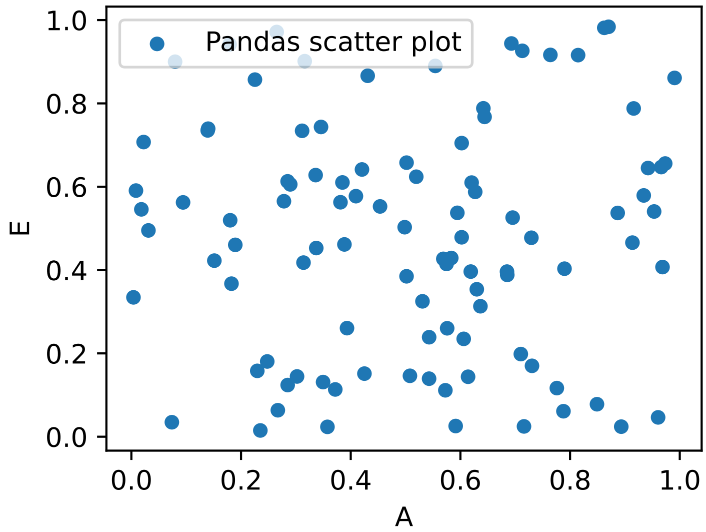
Similarly, we can generate scatter plots, plotting one column against another:

[416]:

```python
# Create pandas DataFrame
df = pd.DataFrame(rng.uniform(size=(100, 5)),
                  columns=['A', 'B', 'C', 'D', 'E'])

df.plot.scatter(x='A', y='E', label='Pandas scatter plot')
```

[416]:

```
<AxesSubplot:xlabel='A', ylabel='E'>
```

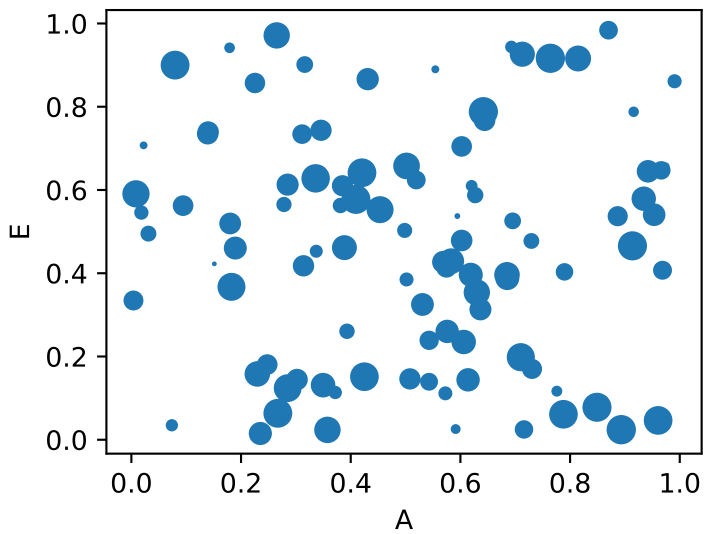


[417]:

```python
# We can even use a column to specify the dot size!
df.plot.scatter(x='A', y='E', s=df['B']*100.0)
```

[417]:

```
<AxesSubplot:xlabel='A', ylabel='E'>
```



In general, the wrappers implemented in pandas are useful to get an idea how the data looks like. For reusable code or more complex graphs, we'll usually want to directly use Matplotlib and pass the data converted to NumPy arrays.

8.7 Exercises

The following exercises use data files from the `data/` folder.

8.7.1 Exercise 1: Basic data manipulations

In this exercise, we will perform some basic data manipulation and plot the results.

1. Load the CSV file `FRED_QTR.csv` (using `sep=','`). Set the columns `Year` and `Quarter` as (joint) indices.

   Hint: You can do this by specifying these column names in the `index_col` argument of `read_csv()`. Alternatively, you can cell `set_index()` once you have loaded the data.

2. This data comes at a quarterly frequency. Convert it to annual values by computing the average values for each year.

   Hint: Group the data by `Year` using the `groupby()` function and compute the mean on the grouped data.

3. Compute two new variables from the annualised data and add them to the `DataFrame`:

   - `Inflation`, defined as the growth rate of `CPI` (consumer price index)
   - `GDP_growth`, defined as the growth rate of `GDP`

4. Drop all rows with missing values (these show up as `NaN`).

   Hint: There is no need to manually filter out `NaN` values, you can use the `dropna()` method instead.

5. Plot the columns `GDP_growth`, `Inflation`, `UNRATE` (unemployment rate) and `LFPART` (labour force participation) using the pandas plotting routines. Use the option `subplots=True` and `layout=(2,2)` to create a 2×2 grid. See the documentation for `plot()` for details.

8.7.2 Exercise 2: Decade averages

Load the FRED data from the CSV file `FRED_QTR.csv` (using `sep=','`) and perform the following tasks:

1. Compute the quarterly GDP growth rate and inflation, similar to what you did in the previous exercise.
2. Add the column `Decade` which contains the decade for every observation. Use 1940 to code the 40s, 1950 for the 50s, etc.
3. We want to retain only observations for decades for which all 40 quarters are present:
   1. Group the data by `Decade` and count the number of observations using `count()`.
   2. A decade should be kept in the data set only if *all* variables have the full 40 observations.
   3. Drop all observations for which this is not the case.
4. With the remaining observations, compute the decade averages for quarterly GDP growth, inflation and the unemployment rate (`UNRATE`). Annualise the GDP growth and inflation figures by multiplying them by 4.
5. Create a bar chart that plots these three variables by decade.

8.7.3 Exercise 3: Group averages

Load the universities data from the CSV file `universities.csv` (using `sep=';'`) and perform the following tasks:

1. Group the data by Russell Group membership using the indicator variable `Russell`. For each group, compute the averages of the following ratios using `apply()`:

   - The ratio of academic staff (`Staff`) to students (`Students`)
   - The ratio of administrative staff (`Admin`) to students.
   - The budget (`Budget`) per student in pounds.

Additionally, compute the number of universities is each group.

2. Repeat the task using a different approach:
    1. Compute the above ratios and add them as new columns to the initial `DataFrame`.
    2. Group the data by Russell Group membership.
    3. Compute the mean of each ratio using `mean()`.
    4. Compute the number of universities in each group using `count()`, and store the result in the column `Count` in the `DataFrame` you obtained in the previous step.
3. Create a bar chart, plotting the value for universities in and outside of the Russell Group for each of the four statistics computed above.

8.7.4 Exercise 4: Grouping by multiple dimensions

Load the universities data from the CSV file `universities.csv` (using `sep=';'`) and perform the following tasks:

1. Create an indicator `Pre1800` which is `True` for universities founded before the year 1800.
2. Group the data by `Country` and the value of `Pre1800`.

    Hint: You need to pass a list of column names to `groupby()`.
3. Compute the number of universities for each combination of `(Country, Pre1800)`.
4. Create a bar chart showing the number of pre- and post-1800 universities by country (i.e., create four groups of bars, each group showing one bar for pre- and one for post-1800).
5. Create a bar chart showing the number of universities by country by pre- and post-1800 period (i.e., create two groups of bars, each group showing four bars, one for each country.)

8.7.5 Exercise 5: Okun's law (advanced)

In this exercise, we will estimate Okun's law on quarterly data for each of the last eight decades.

Okun's law relates unemployment to the output gap. One version (see Jones: Macroeconomics, 2019) is stated as follows:

$$u_t - \overline{u}_t = \alpha + \beta \left(\frac{Y_t - \overline{Y}_t}{\overline{Y}_t} \right)$$

where u_t is the unemployment rate, $\overline{u}_t$ is the natural rate of unemployment, Y_t is output (GDP) and $\overline{Y}_t$ is potential output. We will refer to $u_t - \overline{u}_t$ as "cyclical unemployment" and to the term in parenthesis on the right-hand side as the "output gap." Okun's law says that the coefficient β is negative, i.e., cyclical unemployment is higher when the output gap is low (negative) because the economy is in a recession.

Load the FRED data from the CSV file `FRED_QTR.csv` (using `sep=','`) and perform the following tasks:

1. Compute the output gap and cyclical unemployment rate as defined above and add them as columns to the `DataFrame`.
2. Assign each observation to a decade as you did in previous exercises.
3. Write a function `regress_okun()` which accepts a `DataFrame` containing a decade-spefic sub-sample as the only argument, and estimates the coefficients α (the intercept) and β (the slope) of the above regression equation.

    This function should return a `DataFrame` of a single row and two columns which store the intercept and slope.

    Hint: Use NumPy's `lstsq()` to perform the regression. To regress the dependent variable `y` on regressors `X`, you need to call `lstsq(X, y)`. To include the intercept, you will manually have to create `X` such that the first column contains only ones.

4. Group the data by decade and call the `apply()` method, passing `regress_okun` you wrote as the argument.
5. Plot your results: for each decade, create a scatter plot of the raw data and overlay it with the regression line you estimated.

8.8 Solutions

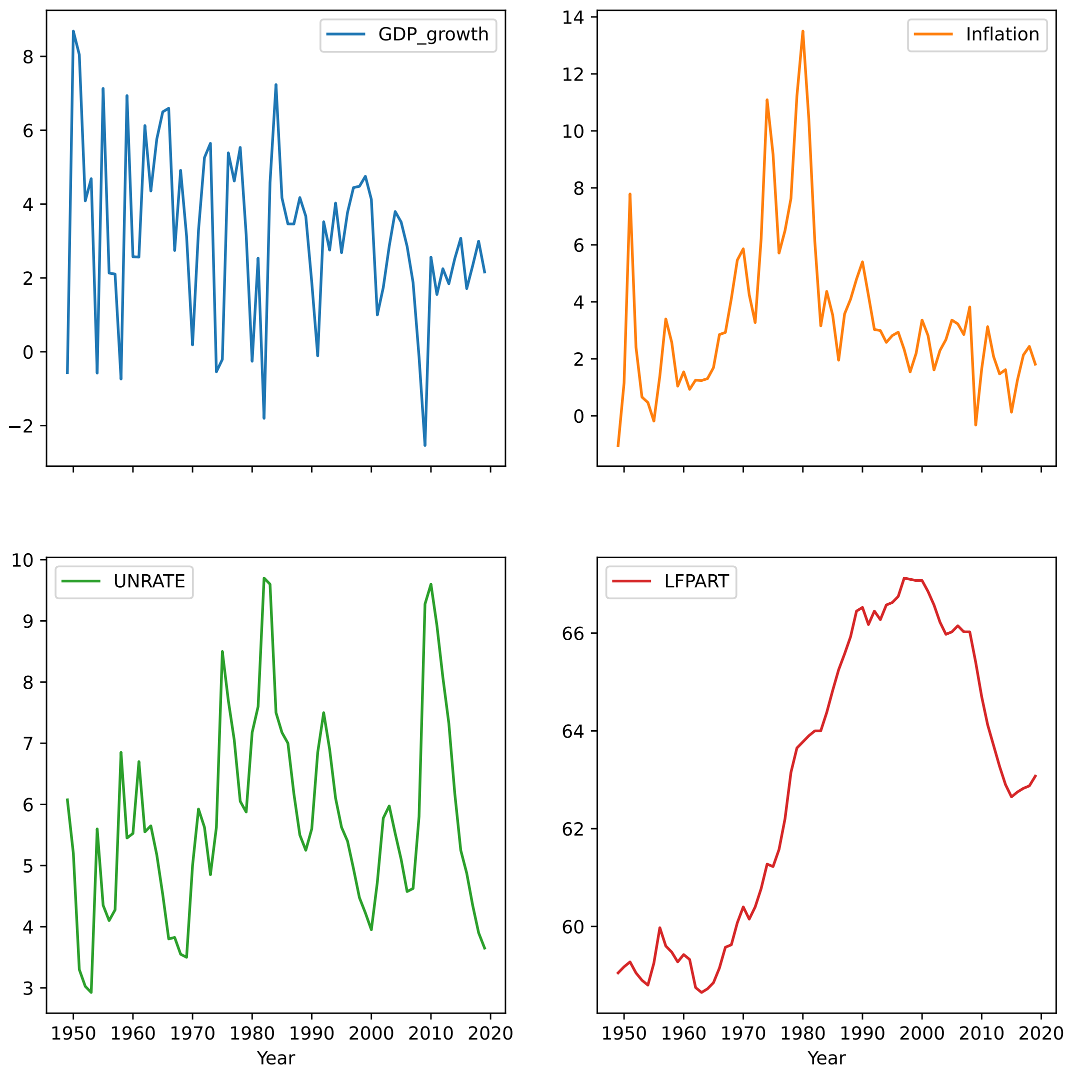
These solutions illustrate *one* possible way to solve the exercises. Pandas is extremely flexible (maybe too flexible) and allows us to perform these tasks in many different ways, so your implementation might look very different.

8.8.1 Solution for exercise 1

One possible implementation looks as follows:

[418]:
```
import pandas as pd

filepath = '../data/FRED_QTR.csv'

df = pd.read_csv(filepath, sep=',', index_col=['Year', 'Quarter'])
# Alternatively, set index columns later
# df = pd.read_csv(filepath, sep=',')
# df.set_index(keys=['Year', 'Quarter'], inplace=True)

# Convert to annual frequency
# Group by year
grp = df.groupby(['Year'])
# Compute annual data as mean of quarterly values
df_year = grp.mean()

# Alternative ways to perform the same aggregation:
# df_year = grp.agg('mean')
# df_year = grp.agg(np.mean)

# Compute CPI and GDP growth rates (in percent)
df_year['Inflation'] = df_year['CPI'].diff() / df_year['CPI'].shift() * 100.0
df_year['GDP_growth'] = df_year['GDP'].diff() / df_year['GDP'].shift() * 100.0

# Drop all rows that contain any NaNs
df_year = df_year.dropna(axis=0)

# Columns to plot
varnames = ['GDP_growth', 'Inflation', 'UNRATE', 'LFPART']
df_year.plot.line(y=varnames, subplots=True, layout=(2, 2),
                  sharex=True, figsize=(10, 10))

# Alternatively, we can call plot() directly, which
# defaults to generating a line plot:
#
# df_year.plot(y=varnames, subplots=True, layout=(2, 2),
#              sharex=True, figsize=(10, 10))
```

[418]:
```
array([[<AxesSubplot:xlabel='Year'>, <AxesSubplot:xlabel='Year'>],
       [<AxesSubplot:xlabel='Year'>, <AxesSubplot:xlabel='Year'>]],
      dtype=object)
```



A few comments:

1. We can set the index column when loading a CSV file by passing the column names as `index_col`:

   ```
   df = pd.read_csv(filepath, sep=',', index_col=['Year', 'Quarter'])
   ```

   Alternatively, we can first load the CSV file and set the index later:

   ```
   df = pd.read_csv(filepath, sep=',')
   df.set_index(keys=['Year', 'Quarter'], inplace=True)
   ```

2. There are several ways to compute the means of grouped data:

   1. We can call `mean()` on the group object directly:

      ```
      df_year = grp.mean()
      ```

   2. Alternatively, we can call `agg()` and pass it the aggregation routine that should be applied:

      ```
      df_year = grp.agg('mean')
      df_year = grp.agg(np.mean)
      ```

      Here we again have multiple options: pandas understands `'mean'` if passed as a string (which might not be the case for some other functions), or we pass an actual function such as `np.mean`.

3. The easiest way to compute differences between adjacent rows is to use the `diff()` method, which returns $x_t - x_{t-1}$. Pandas then automatically matches the correct values and sets the first observation to `NaN` as there is no preceding value to compute the difference.

   To compute a growth rate $(x_t - x_{t-1})/x_{t-1}$, we additionally need to lag a variable to get the correct period in the denominator. In pandas this is achieved using the `shift()` method (which defaults to shifting by 1 period).

8.8.2 Solution for exercise 2

This time we do not specify `index_cols` when reading in the CSV data since we need `Year` as a regular variable, not as the index.

We then compute the decade for each year, using the fact that // performs division with integer truncation. As an example, 1951 // 10 is 195, and (1951 // 10) * 10 = 1950, which we use to represent the 1950s.

[419]:
```
import pandas as pd

filepath = '../data/FRED_QTR.csv'

df = pd.read_csv(filepath, sep=',')

# Compute GDP growth rates, inflation (in percent)
df['GDP_growth'] = df['GDP'].diff() / df['GDP'].shift() * 100.0
df['Inflation'] = df['CPI'].diff() / df['CPI'].shift() * 100.0

# Assign decade using // to truncate division to
# integer part. So we have 194x // 10 = 194 for any x.
df['Decade'] = (df['Year'] // 10) * 10

grp = df.groupby(['Decade'])

# Print number of obs. by decade
print(grp.count())

# Create series that contains True for each
# decade if all variables have 40 observations.
use_decade = (grp.count() == 40).all(axis=1)
# Convert series to DataFrame, assign column name 'Keep'
df_decade = use_decade.to_frame('Keep')
# merge into original DataFrame, matching rows on value
# of column 'Decade'
df = df.merge(df_decade, on='Decade')
# Restrict data only to rows which are part of complete decade
df = df.loc[df['Keep'], :].copy()
# Drop 'Keep' column
del df['Keep']

# Compute average growth rates and unemployment rate by decade
grp = df.groupby(['Decade'])

df_avg = grp[['GDP_growth', 'Inflation', 'UNRATE']].mean()
# Convert to (approximate) annualised growth rates
df_avg['GDP_growth'] *= 4.0
df_avg['Inflation'] *= 4.0
```

```
        Year  Quarter  GDP  CPI  UNRATE  LFPART  GDPPOT  NROU  GDP_growth  \
Decade
1940       8        8    8    8       8       8       4     4           7
1950      40       40   40   40      40      40      40    40          40
1960      40       40   40   40      40      40      40    40          40
1970      40       40   40   40      40      40      40    40          40
```

```
1980        40         40    40    40      40      40      40    40          40
1990        40         40    40    40      40      40      40    40          40
2000        40         40    40    40      40      40      40    40          40
2010        40         40    40    40      40      40      40    40          40

        Inflation
Decade
1940            7
1950           40
1960           40
1970           40
1980           40
1990           40
2000           40
2010           40
```

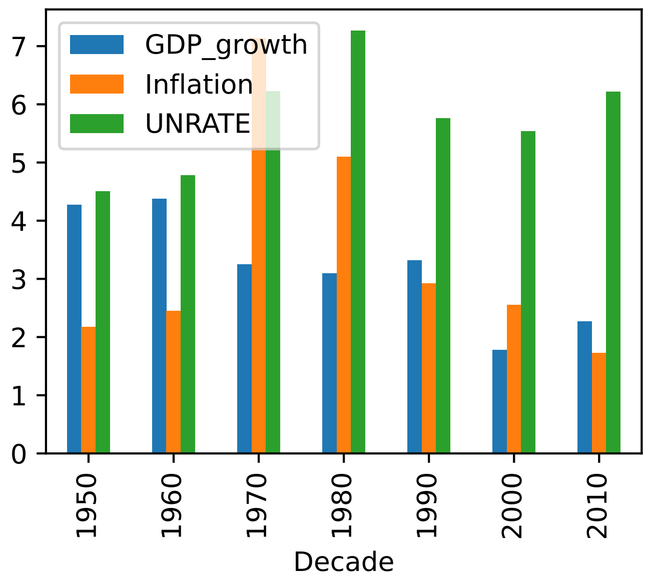
The tricky part is to keep only observations for "complete" decades that have 40 quarters of data. We see that this is not the case for the 1940s:

1. We group by `Decade` and use `count()` to determine the number of non-missing observations for each variable.
2. `count() == 40` evaluates to `True` for some variable if it has 40 observations.
3. We then use `all()` to aggregate across all variables, i.e., we require 40 observations for every variable to keep the decade.
4. Finally, we merge the indicator whether a decade should be kept in the data set using `merge()`, where we match on the value of the column `Decade`. Note that the argument to `merge()` must be a `DataFrame`, so we first have to convert our indicator data.
5. Finally, we keep only those observations which have a flag that is `True`.

The rest of the exercise is straightforward as it just repeats what we have done previously. You can create the bar chart directly with pandas as follows:

[420]:
```
df_avg.plot.bar(y=['GDP_growth', 'Inflation', 'UNRATE'])
```

[420]:
```
<AxesSubplot:xlabel='Decade'>
```



8.8.3 Solution for exercise 3

We first read in the CSV file, specifying `';'` as the field separator:

[421]:
```
import pandas as pd

# Load CSV file
filepath = '../data/universities.csv'
df = pd.read_csv(filepath, sep=';')
```

For the first task we use `apply()` to create a new `Series` object for each ratio of interest.

We compute the ratios for each institution which will result in NaNs if either the numerator of denominator is missing. We thus use `np.nanmean()` to compute averages, ignoring any NaNs.

Finally, we combine all `Series` into a `DataFrame`. We do this by specifying the data passed to `DataFrame()` as a dictionary, since then we can specify the column names as keys.

[422]:
```
# Variant 1
# Compute means using apply()

grp = df.groupby(['Russell'])

# Create Series objects with the desired means
staff = grp.apply(lambda x: np.nanmean(x['Staff'] / x['Students']))
admin = grp.apply(lambda x: np.nanmean(x['Admin'] / x['Students']))
# Budget in millions of pounds
budget = grp.apply(lambda x: np.nanmean(x['Budget'] / x['Students']))
# Convert to pounds
budget *= 1.0e6
# Count number of institutions in each group.
# We can accomplish this by calling size() on the group object.
count = grp.size()

# Create a new DataFrame. Each column is a Series object.
df_all = pd.DataFrame({'Staff_Student': staff,
                       'Admin_Student': admin,
                       'Budget_Student': budget,
                       'Count': count})

df_all
```

[422]:

	Staff_Student	Admin_Student	Budget_Student	Count
Russell				
0	0.096219	0.147762	16847.834366	6
1	0.155131	0.169079	35406.453649	17

For the second task, we first insert additional columns which contain the ratios of interest for each university.

We then drop all unused columns, group by the `Russell` indicator and compute the means by directly calling `mean()` on the group object.

[423]:
```
# Variant 2:
# Compute ratios first, apply aggregation later

# Create new variables directly in original DataFrame
df['Staff_Student'] = df['Staff'] / df['Students']
df['Admin_Student'] = df['Admin'] / df['Students']
# Budget in pounds (original Budget is in million pounds)
df['Budget_Student'] = df['Budget'] / df['Students'] * 1.0e6

# Keep only newly constructed ratios
columns_keep = [name for name in df.columns
```

```
                 if name.endswith('_Student')]
# Also keep Russell indicator
columns_keep += ['Russell']
df = df[columns_keep].copy()

# Aggregate by Russell indicator
grp = df.groupby(['Russell'])
# Count number of institutions in each group.
# We can accomplish this by calling size() on the group object.
count = grp.size()

df_all = grp.mean()
# Add counter
df_all['Count'] = count

df_all
```

[423]:

```
         Staff_Student  Admin_Student  Budget_Student  Count
Russell
0             0.096219       0.147762    16847.834366      6
1             0.155131       0.169079    35406.453649     17
```

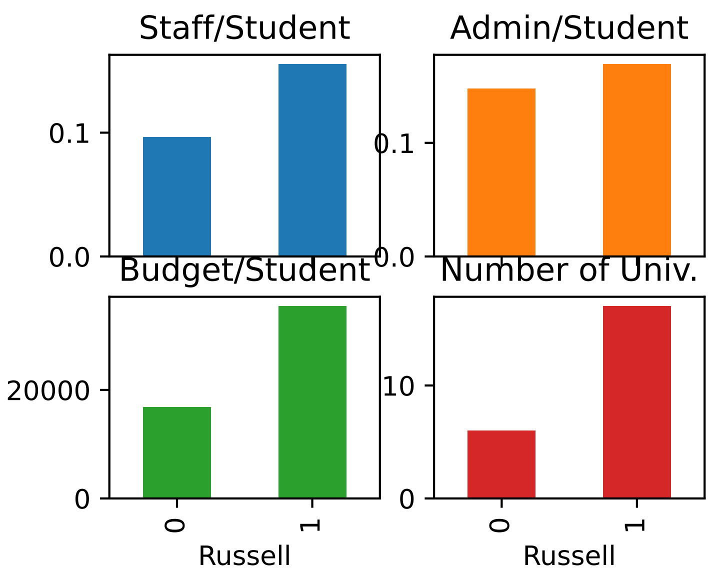
We plot the results using pandas's `bar()` function. Since the data is of vastly different magnitudes, we specify `sharey=False` so that each panel will have its own scaling on the y-axis.

[424]:

```
# Plot results as bar charts, one panel for each variable

# Pretty titles
title = ['Staff/Student', 'Admin/Student', 'Budget/Student', 'Number of Univ.']
# Create bar chart using pandas's bar() function
df_all.plot.bar(sharey=False, subplots=True, layout=(2, 2), legend=False,
                title=title)
```

[424]:

```
array([[<AxesSubplot:title={'center':'Staff/Student'}, xlabel='Russell'>,
        <AxesSubplot:title={'center':'Admin/Student'}, xlabel='Russell'>],
       [<AxesSubplot:title={'center':'Budget/Student'}, xlabel='Russell'>,
        <AxesSubplot:title={'center':'Number of Univ.'}, xlabel='Russell'>]],
      dtype=object)
```



8.8.4 Solution for exercise 4

We create an indicator variable called `Pre1800` which is set to `True` whenever the founding year in column `Founded` is lower than 1800.

We then group the data by `Country` and `Pre1800` and count the number of universities in each group using `count()`.

[425]:
```
import pandas as pd

# Load CSV file
filepath = '../data/universities.csv'
df = pd.read_csv(filepath, sep=';')

# Create mask for founding period
df['Pre1800'] = (df['Founded'] < 1800)

# Create group by country and founding period;
grp = df.groupby(['Country', 'Pre1800'])

# Number of universities by country and founding period.
# Since we are grouping by two attributes, this will create a
# Series with a multi-level (hierarchical) index
count = grp.size()

count
```

[425]:
```
Country           Pre1800
England           False      8
                  True       5
Northern Ireland  False      1
Scotland          False      3
                  True       4
Wales             False      2
dtype: int64
```

The resulting `Series` only contains values for those combinations that are actually present in the data. For example, the combination `(Wales, True)` does not show up because there are no Welsh universities founded before 1800 in our sample. We will have to "complete" the data and add zero entries in all such cases.

First, we create a `DataFrame` with countries in rows and the number of universities for the pre- and post-1800 periods in columns. To accomplish this, we need to pivot the second row index using the `unstack()` method. The `level=-1` argument tells it to use the last row index, and `fill_value=0` will assign zeros to all elements that were not present in the initial `DataFrame`, such as the combination `(Wales, True)`.

[426]:
```
# DataFrame with countries in rows, Pre-1800 indicator in columns

# Pivot inner index level to create separate columns for True/False
# values of Pre1800 indicator
df_count = count.unstack(level=-1, fill_value=0)

# Set name of column index to something pretty: this will
# be used as the legend title
df_count.columns.rename('Founding year', inplace=True)
# Rename columns to get pretty labels in legend
df_count.rename(columns={True: 'Before 1800', False: 'After 1800'},
                inplace=True)

df_count
```

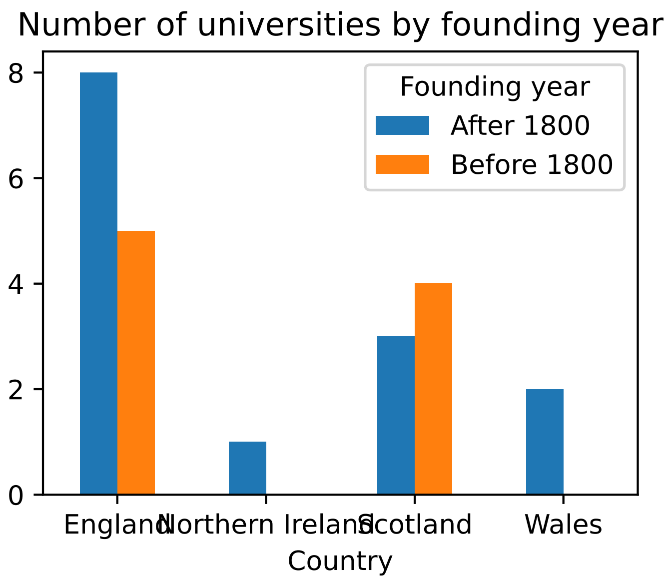
[426]:
```
Founding year     After 1800  Before 1800
Country
England                    8            5
Northern Ireland           1            0
Scotland                   3            4
Wales                      2            0
```

Whenever we use pandas's built-in plotting functions, these use index names and labels to automatically label the graph. We therefore first have to assign these objects "pretty" names.

We can then generate the bar chart as follows:

[427]:
```
# Create bar chart by country
title = 'Number of universities by founding year'
# pass rot=0 to undo the rotation of x-tick labels
# which pandas applies by default
df_count.plot.bar(xlabel='Country', rot=0, title=title)
```

[427]:
```
<AxesSubplot:title={'center':'Number of universities by founding year'},
xlabel='Country'>
```



Note how the legend title is automatically set to the column index name and the legend labels use the column index labels.

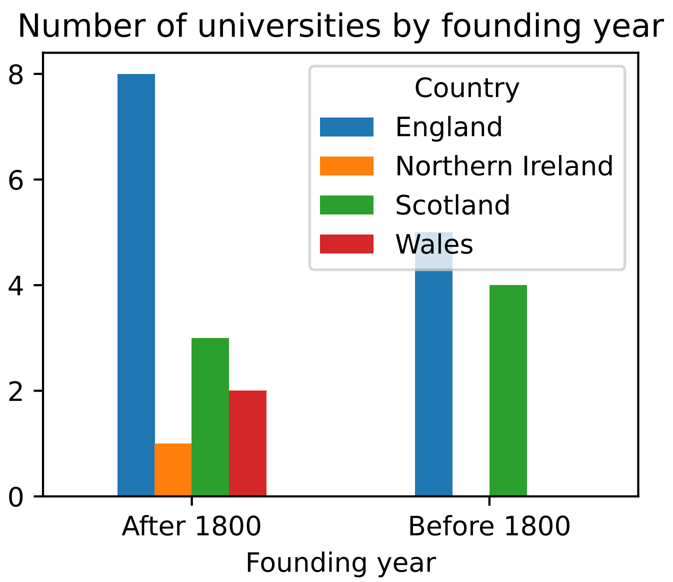
We create the second `DataFrame` with the founding period in rows and country names in columns in exactly the same way, but now call `unstack(level=0)` so that the first index level will be pivoted.

[428]:
```
# Pivot first row index level to create separate columns for each country
df_count = count.unstack(level=0, fill_value=0)

# Set index name to something pretty
df_count.index.rename('Founding year', inplace=True)
# Rename index labels to get pretty text in legend
df_count.rename(index={True: 'Before 1800', False: 'After 1800'},
                inplace=True)

df_count
```

```
[428]: Country         England  Northern Ireland  Scotland  Wales
       Founding year
       After 1800            8                 1         3      2
       Before 1800           5                 0         4      0
```

```
[429]: # Create bar chart by founding year
       # pass rot=0 to undo the rotation of x-tick labels
       # which pandas applies by default
       df_count.plot.bar(rot=0, title=title)
```

```
[429]: <AxesSubplot:title={'center':'Number of universities by founding year'},
       xlabel='Founding year'>
```



8.8.5 Solution for exercise 5

This exercise is quite involved, so we will discuss it in parts. First, we write the function that will be called by `apply()` to process sub-sets of the data which belong to a single decade:

```
[430]: def regress_okun(x):
           # x is a DataFrame, restricted to rows for the current decade

           # Extract dependent and regressor variables
           outcome = x['unempl_gap'].to_numpy()
           GDP_gap = x['GDP_gap'].to_numpy()

           # Regressor matrix including intercept
           regr = np.ones((len(GDP_gap), 2))
           # overwrite second column with output gap
           regr[:,1] = GDP_gap

           # Solve least-squares problem (pass rcond=None to avoid a warning)
           coefs, *rest = np.linalg.lstsq(regr, outcome, rcond=None)

           # Construct DataFrame which will be returned to apply()
           # Convert data to 1 x 2 matrix
           data = coefs[None]
           columns = ['Const', 'GDP_gap']
```

```
    df_out = pd.DataFrame(data, columns=columns)

    return df_out
```

This function is passed in a single argument which is a `DataFrame` restricted to the sub-sample that is currently being processed.

- Our task is to perform the required calculations and to return the result as a `DataFrame`. `apply()` then glues together all decade-specific DataFrames to form the result of the operation.
- We first extract the relevant variables as NumPy arrays, and we create a regressor matrix which has ones in the first column. This column represents the intercept.
- We invoke `lstsq()` to run the regression. `lstsq()` returns several arguments which we mop up in the tuple `*rest` since we are only interested in the regression coefficients.

  Note that we wouldn't be using `lstsq()` to run OLS on a regular basis, but it's sufficient for this use case.
- Finally, we build the `DataFrame` to be returned by this function. It has only one row (since we ran only one regression) and two columns, one for each regression coefficient.

This was the hard part. We now need to perform some standard manipulations to prepare the data:

1. We construct the output gap (in percent), which we store in the column `GDP_gap`.
2. We construct the cyclical unemployment rate and store it in the column `unempl_gap`.
3. We determine the decade each observation belongs to using the same code as in previous exercises.
4. We then drop all unused variables from the `DataFrame` and also all observations which contain missing values.

Lastly, we can call `apply()` to run the regression for each decade.

[431]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt

# Load CSV file
filepath = '../data/FRED_QTR.csv'
df = pd.read_csv(filepath, sep=',')

# Generate output gap (in percent)
df['GDP_gap'] = (df['GDP'] - df['GDPPOT']) / df['GDPPOT'] * 100.0

# Generate deviations of unempl. rate from natural unempl. rate
df['unempl_gap'] = df['UNRATE'] - df['NROU']

# Assign decade using // to truncate division to
# integer part. So we have 194x // 10 = 194 for any x.
df['Decade'] = (df['Year'] // 10) * 10

# Keep only variables of interest
df = df[['Decade', 'GDP_gap', 'unempl_gap']]
# Drop rows with any missing obs.
df = df.dropna(axis=0)

# Group by decade
grp = df.groupby(['Decade'])

# Apply regression routine to sub-set of data for each decade
df_reg = grp.apply(regress_okun)
# Get rid of second row index introduced by apply()
df_reg = df_reg.reset_index(level=-1, drop=True)

# Display intercept and slope coefficients
# estimated for each decade.
```

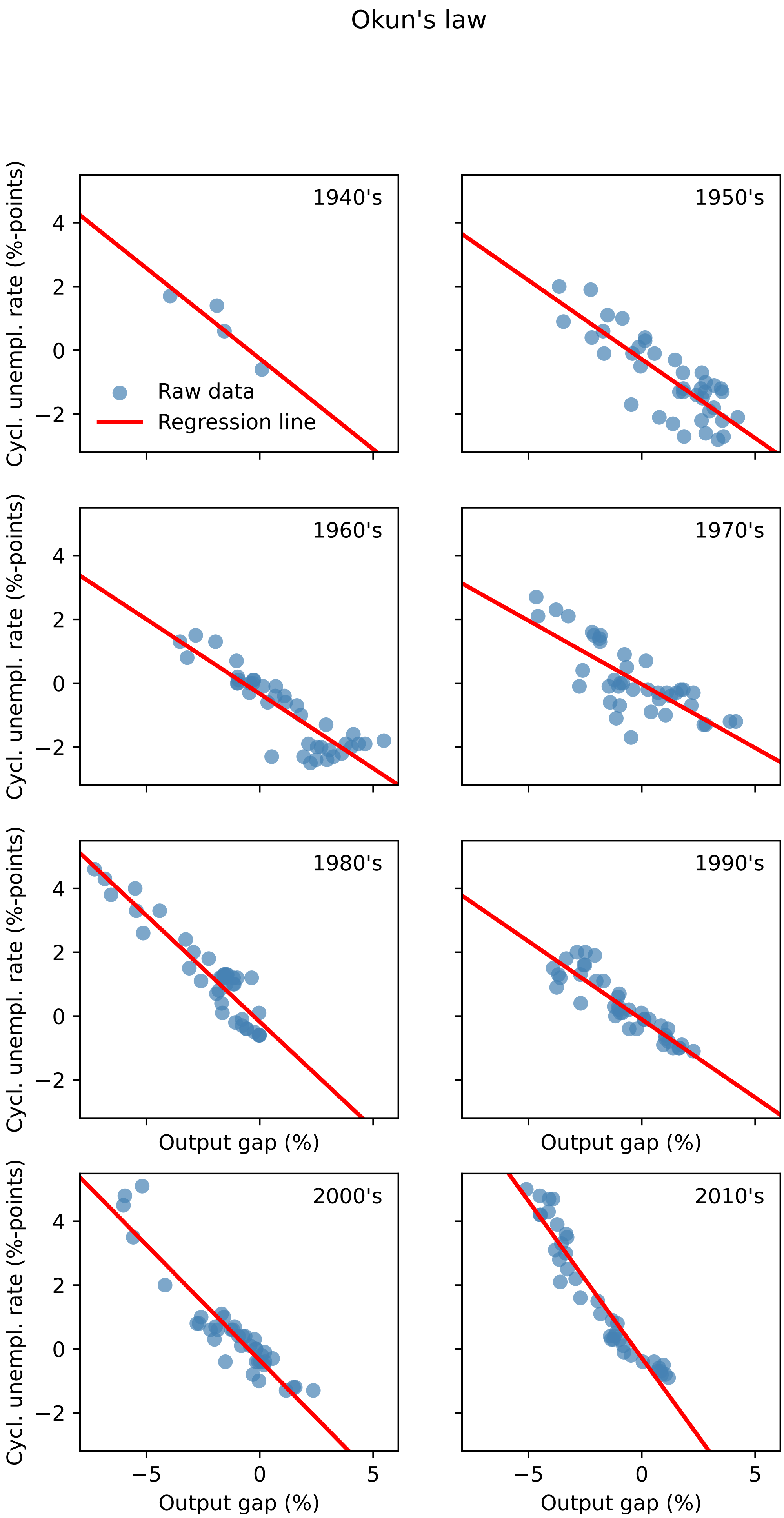
```
df_reg
```

[431]:
```
            Const   GDP_gap
Decade
1940   -0.259986 -0.567257
1950   -0.277104 -0.494637
1960   -0.331665 -0.467206
1970   -0.032063 -0.398751
1980   -0.178001 -0.666688
1990   -0.102465 -0.489427
2000   -0.355138 -0.723567
2010   -0.279333 -0.983768
```

The following code creates 8 panels of scatter plots showing the raw data and overlays a regression line for each decade.

[432]:
```
# Number of plots (= number of decades)
Nplots = len(df_reg)

# Fix number of columns, determine rows as needed
ncol = 2
nrow = int(np.ceil(Nplots / ncol))

fig, axes = plt.subplots(nrow, ncol, sharey=True, sharex=True,
                         figsize=(6, 11))

for i, ax in enumerate(axes.flatten()):

    # decade in current iteration
    decade = df_reg.index.values[i]
    # restrict DataFrame to decade-specific data
    dfi = df.loc[df['Decade'] == decade]
    # Scatter plot of raw data
    ax.scatter(dfi['GDP_gap'], dfi['unempl_gap'], color='steelblue',
               alpha=0.7, label='Raw data')
    # Extract regression coefficients
    const = df_reg.loc[decade, 'Const']
    slope = df_reg.loc[decade, 'GDP_gap']

    # plot regression line:
    # We need to provide one point and a slope to define the line to be plotted.
    ax.axline((0.0, const), slope=slope, color='red',
              lw=2.0, label='Regression line')

    # Add label containing the current decade
    ax.text(0.95, 0.95, f"{decade}'s", transform=ax.transAxes,
            va='top', ha='right')

    # Add legend in the first panel only
    if i == 0:
        ax.legend(loc='lower left', frameon=False)

    # Add x- and y-labels, but only for those panels
    # that are on the left/lower boundary of the figure
    if i >= nrow * (ncol - 1):
        ax.set_xlabel('Output gap (%)')
    if (i % ncol) == 0:
        ax.set_ylabel('Cycl. unempl. rate (%-points)')

fig.suptitle("Okun's law")
```

[432]:
```
Text(0.5, 0.98, "Okun's law")
```


Okun's law
1940's
1950's
1960's
1970's
1980's
1990's
2000's
2010's
Raw data
Regression line
Cycl. unempl. rate (%-points)
Output gap (%)
4
2
0
−2
−5
0
5

9 Data input and output

In this unit we discuss input and output, or I/O for short. We focus exclusively on I/O routines used to load and store data from files that are relevant for numerical computation and data analysis.

9.1 I/O with NumPy

9.1.1 Loading text data

We have already encountered the most basic, and probably most frequently used NumPy I/O routine, `np.loadtxt()`. We often use files that store data as text files containing character-separated values (CSV) since virtually any application supports this data format. The most important I/O functions to process text data are:

- `np.loadtxt()`: load data from a text file.
- `np.genfromtxt()`: load data from a text file and handle missing data.
- `np.savetxt()`: save a NumPy array to a text file.

There are a few other I/O functions in NumPy, for example to write arrays as raw binary data. We won't cover them here, but you can find them in the official documentation.

Imagine we have the following tabular data from FRED, where the first two rows look as follows:

Year	GDP	CPI	UNRATE
1948	2118.5	24.0	3.8
1949	2106.6	23.8	6.0

To load this CSV file as a NumPy array, we use `loadtxt()`:

[433]:
```
import numpy as np

# relative path to CSV file
file = '../data/FRED.csv'

# load CSV
data = np.loadtxt(file, skiprows=1, delimiter=',')
data[:2]          # Display first two rows
```

[433]:
```
array([[1948. , 2118.5,   24. ,    3.8],
       [1949. , 2106.6,   23.8,    6. ]])
```

The default settings will in many cases be appropriate to load whatever CSV file we might have. However, we'll occasionally want to specify the following arguments to override the defaults:

- `delimiter`: Character used to separate individual fields (default: space).
- `skiprows=n`: Skip the first `n` rows. For example, if the CSV file contains a header with variable names, `skiprows=1` needs to be specified as NumPy by default cannot process these names.
- `dtype`: Enforce a particular data type for the resulting array.
- `encoding`: Set the character encoding of the input data. This is usually not needed, but can be required to import data with non-latin characters that are not encoded using Unicode.

While `loadtxt()` is simple to use, it quickly reaches its limits with more complex data sets. For example, when we try to load our sample of universities with `loadtxt()`, we get the following error:

[434]:
```python
import numpy as np

file = '../data/universities.csv'

# Try to load CSV data that contains strings
# This will result in an error!
data = np.loadtxt(file, delimiter=';', skiprows=1)
```

```
ValueError: could not convert string to float: '"University of Glasgow"'
```

This code fails for two reasons:

1. The file contains strings and floats, and `loadtxt()` by default cannot load mixed data.
2. There are missing values (empty fields), which `loadtxt()` cannot handle either.

We can address the first issue by creating a so-called structured array, i.e., an array that contains fields with mixed data. This is accomplished by constructing a special `dtype` object that specifies the field names and their data types:

[435]:
```python
# Define names and data types for fields in CSV file
#   Data types are defined using two tokens:
#       1.  The main data type (U: unicode string, f: float, i: integer)
#       2.  The precision or field width
dtypes = np.dtype([('Institution', 'U30'),       # unicode string of length 30
                   ('Country', 'U20'),           # unicode string of length 20
                   ('Founded', 'i4'),            # integer, 4 bytes
                   ('Students', 'i4'),
                   ('Staff', 'i4'),
                   ('Admin', 'i4'),
                   ('Budget', 'f8'),             # float, 8 bytes
                   ('Russell', 'i1')])           # integer, 1 byte

data = np.loadtxt(file, delimiter=';', skiprows=1, dtype=dtypes)
```

```
ValueError: could not convert string to float: ''
```

However, this still fails because the of a few missing values.

We can get around this by using `genfromtxt()`, which is more flexible and can also deal with missing data:

[436]:
```python
# load data using genfromtxt()
# We still need to specify the dtype defined above!
data = np.genfromtxt(file, delimiter=';', dtype=dtypes, encoding='utf8',
                     skip_header=1)

# Determine rows with missing data:
#    - missing integers are coded as -1
#    - missing floats are coded as np.nan
missing = (data['Staff'] < 0) | (data['Admin'] < 0) | np.isnan(data['Budget'])

# print rows with missing values
data[missing]
```

[436]:
```
array([('"University of Strathclyde"', '"Scotland"', 1964, 22640,   -1, 3200,
304.4, 0),
       ('"University of Oxford"', '"England"', 1096, 24515, 7000,   -1, 2450. ,
1),
       ('"University of Manchester"', '"England"', 2004, 40250, 3849,   -1,
```

```
1095.4, 1),
       ('"University of Birmingham"', '"England"', 1825, 35445, 4020,   -1,
673.8, 1),
       ('"University of Nottingham"', '"England"', 1798, 30798, 3495,   -1,
656.5, 1),
       ('"University of Stirling"', '"Scotland"', 1967,  9548,   -1, 1872,
113.3, 0),
       ('"Swansea University"', '"Wales"', 1920, 20620,   -1, 3290,    nan, 0)],
      dtype=[('Institution', '<U30'), ('Country', '<U20'), ('Founded', '<i4'),
('Students', '<i4'), ('Staff', '<i4'), ('Admin', '<i4'), ('Budget', '<f8'),
('Russell', 'i1')])
```

While the CSV file can now be processed without errors, you see that NumPy does not remove the double quotes around strings such as the university names. Instead of trying to fix this, it is advisable to just use pandas to load this kind of data which handles all these problems automatically. We examine this alternative below.

9.1.2 Saving data to text files

To save a NumPy array to a CSV file, there is a logical counterpart to `np.loadtxt()` which is called `np.savetxt()`.

[437]:
```
import numpy as np
import os.path
import tempfile

# Generate some random data on [0,1)
data = np.random.default_rng(123).random(size=(10, 5))

# create temporary directory
d = tempfile.TemporaryDirectory()

# path to CSV file
file = os.path.join(d.name, 'data.csv')

# Print destination file - this will be different each time
print(f'Saving CSV file to {file}')

# Write NumPy array to CSV file. The fmt argument specifies
# that data should be saved as floating-point using a
# field width of 8 characters and 5 decimal digits.
np.savetxt(file, data, delimiter=';', fmt='%8.5f')
```

```
Saving CSV file to /tmp/tmpmswyueb3/data.csv
```

The above code creates a 10×5 matrix of random floats and stores these in the file `data.csv` using 5 significant digits.

We store the destination file in a temporary directory which we create as follows:

- Because we cannot know in advance on which system this code is run (e.g., the operating system and directory layout), we cannot hard-code a file path.
- Moreover, we do not know whether the code is run with write permissions in any particular folder.
- We work around this issue by asking the Python runtime to create a writeable temporary directory *for the system where the code is being run.*
- We use the routines in the `tempfile` module to create this temporary directory.

Of course, on your own computer you do not need to use a temporary directory, but can instead use any directory where your user has write permissions. For example, on Windows you could use something along the lines of

```
file = 'C:/Users/Path/to/file.txt'
np.savetxt(file, data, delimiter=';', fmt='%8.5f')
```

You can even use relative paths. To store a file in the current working directory it is sufficient to just pass the file name:

```
file = 'file.txt'
np.savetxt(file, data, delimiter=';', fmt='%8.5f')
```

9.2 I/O with pandas

Pandas's I/O routines are more powerful than those implemented in NumPy:

- They support reading and writing numerous file formats.
- They support heterogeneous data without having to specify the data type in advance.
- They gracefully handle missing values.

For these reasons, it is often preferable to directly use pandas to process data instead of NumPy.

The most important routines are:

- `read_csv()`, `to_csv()`: Read or write CSV text files
- `read_fwf()`: Read data with fixed field widths, i.e., text data that does not use delimiters to separate fields.
- `read_excel()`, `to_excel()`: Read or write Excel spreadsheets
- `read_stata()`, `to_stata()`: Read or write Stata's `.dta` files.

For a complete list of I/O routines, see the official documentation.

To illustrate, we repeat the above examples using pandas's `read_csv()`. Since the FRED data contains only floating-point data, the result is very similar to reading in a NumPy array.

[438]:
```
import pandas as pd

# relative path to CSV file
file = '../data/FRED.csv'

df = pd.read_csv(file, sep=',')
df.head(2)          # Display the first 2 rows of data
```

[438]:
```
   Year     GDP   CPI  UNRATE
0  1948  2118.5  24.0     3.8
1  1949  2106.6  23.8     6.0
```

The difference between NumPy and pandas become obvious when we try to load our university data: this works out of the box, without the need to specify any data types or to handle missing values:

[439]:
```
import pandas as pd

# relative path to CSV file
file = '../data/universities.csv'

df = pd.read_csv(file, sep=';')
df.tail(3)      # show last 3 rows
```

[439]:
```
                   Institution           Country  Founded  Students   Staff  \
20      University of Stirling          Scotland     1967      9548     NaN
21  Queen's University Belfast  Northern Ireland     1810     18438  2414.0
22          Swansea University             Wales     1920     20620     NaN

     Admin  Budget  Russell
20  1872.0   113.3        0
21  1489.0   369.2        1
22  3290.0     NaN        0
```

Note that missing values are correctly converted to `np.nan` and the double quotes surrounding strings are automatically removed!

Unlike NumPy, pandas can also process other popular data formats such as MS Excel files (or OpenDocument spreadsheets):

[440]:
```
import pandas as pd

# Excel file containing university data
file = '../data/universities.xlsx'

df = pd.read_excel(file, sheet_name='universities')
df.head(3)
```

[440]:
```
                   Institution   Country  Founded  Students   Staff   Admin  \
0      University of Glasgow  Scotland     1451     30805  2942.0  4003.0
1    University of Edinburgh  Scotland     1583     34275  4589.0  6107.0
2  University of St Andrews  Scotland     1413      8984  1137.0  1576.0

   Budget  Russell
0   626.5        1
1  1102.0        1
2   251.2        0
```

The routine `read_excel()` takes the argument `sheet_name` to specify the sheet that should be read.

- Note that the Python package `openpyxl` needs to be installed in order to read files from Excel 2003 and above.
- To read older Excel files (`.xls`), you need the package `xlrd`.

Finally, we often encounter text files with fixed field widths, since this is a commonly used format in older applications (for example, fixed-width files are easy to create in Fortran). To illustrate, the fixed-width variant of our FRED data looks like this:

```
Year GDP     CPI  UNRATE
1948 2118.5   24     3.8
1949 2106.6 23.8       6
1950 2289.5 24.1     5.2
1951 2473.8   26     3.3
1952 2574.9 26.6       3
```

You see that the column `Year` occupies the first 5 characters, the `GDP` column the next 7 characters, and so on. To read such files, the width (i.e., the number of characters) has to be explicitly specified:

[441]:
```
import pandas as pd

# File name of FRED data, stored as fixed-width text
file = '../data/FRED-fixed.csv'

# field widths are passed as list to read_fwf()
df = pd.read_fwf(file, widths=[5, 7, 5, 8])
df.head(3)
```

[441]:
```
   Year     GDP   CPI  UNRATE
0  1948  2118.5  24.0     3.8
1  1949  2106.6  23.8     6.0
2  1950  2289.5  24.1     5.2
```

Here the `widths` argument accepts a list that contains the number of characters to be used for each field.

9.3 Pickling

A wholly different approach to data I/O is taken by Python's built-in `pickle` module. Almost any Python object can be dumped into a binary file and read back using `pickle.dump()` and `pickle.load()`.

The big advantage over other methods is that hierarchies of objects are automatically supported. For example, we can pickle a list containing a `tuple`, a string and a NumPy array:

[442]:
```
import numpy as np
import pickle
import tempfile
import os.path

# Generate 2d array of integers
arr = np.arange(10).reshape((2, -1))
tpl = (1, 2, 3)
text = 'Pickle is very powerful!'

# data: several nested containers and strings
data = [tpl, text, arr]

# create temporary directory
d = tempfile.TemporaryDirectory()
# Binary destination file
file = os.path.join(d.name, 'data.bin')

# print destination file path
print(f'Pickled data written to {file}')

with open(file, 'wb') as f:
    pickle.dump(data, f)
```

```
Pickled data written to /tmp/tmp9zsxng8z/data.bin
```

We can then read back the data as follows:

[443]:
```
# load pickle data from above
with open(file, 'rb') as f:
    data = pickle.load(f)

# expand data into its components
tpl, text, arr = data
arr          # prints previously generated 2d array
```

[443]:
```
array([[0, 1, 2, 3, 4],
       [5, 6, 7, 8, 9]])
```

The above example introduces a few concepts we have not encountered so far:

1. The built-in function `open()` is used to open files for reading or writing.
    - The second argument indicates whether a file should be read-only, `r`, or writeable, `w`.
    - The `b` sets the file mode to *binary*, i.e., its contents are *not* human-readable text.
2. We usually access files using a so-called *context manager*. A context manager is created via the `with` statement.

    A big advantage of using a context manager is that the file resource made available as `f` in the block following `with` is automatically cleaned up as soon as the block exits. This is particularly important when writing data.

So why not always use `pickle` to load and store data?

1. Pickling is Python-specific and no other application can process pickled data.

2. The pickle protocol can change in a newer version of Python, and you might not be able to read back your old pickled objects.
3. Even worse, because projects such as NumPy and pandas implement their own pickling routines, you might not even be able to unpickle old DataFrames when you upgrade to a newer pandas version!
4. `pickle` is not secure: It is possible to construct binary data that will execute arbitrary code when unpickling, so you don't want to unpickle data from untrusted sources.
5. Some objects cannot be pickled automatically. For example, this applies to any classes defined with Numba or Cython, unless special care is taken to implement the pickle protocol.

`pickle` is great for internal use when you do not need to exchange data with others and have complete control over your computing environment (i.e., you can enforce a specific version of Python and the libraries you are using). For anything else, you should avoid it.

10 Error handling

In this unit we will briefly look at error handling in Python. The Python approach to error handling is "to ask for forgiveness rather than for permission." This means that when writing Python code, we frequently don't check whether some data satisfies certain requirements, but we instead attempt to clean up once something does not work as expected.

10.1 Exceptions

If something goes wrong in a function, we in principle have two options to communicate the error to the caller:

1. We can return some special value (a status code or error flag) that signals when something fails.

   This approach is quite inelegant, since error codes can overlap with the actual result a function would return in the absence of error. For this reasons, functions need to implement two different return values and reserve one for the status code.

   In Python, this could look like this:

   ```
   def func(x):
       # process x
       # Two return values: actual result and error flag
       return result, flag
   ```

2. We can use so-called exceptions for error handling. This is the approach taken by almost all modern languages such as Java, C++ and also Python (see here for the official documentation on error and exception handling).

   Exceptions provide means to communicate errors that are completely independent of regular return values. Furthermore, exceptions propagate along the entire call stack: If we call `func1()`, which in turn calls `func2()`, and an error occurs in `func2()`, there is no need to handle this error in `func1()`: the exception will automatically be propagated to the caller of `func1()`.

10.1.1 Common exceptions

We have already encountered numerous exceptions throughout this course, but so far we did not know how to handle them other than fixing the code that produced the exception.

There are numerous exceptions in Python, see here for a list of built-in ones. We provide a few examples of exceptions that you are most likely to encounter below.

Examples:

Trying to access an element in a collection outside of the permissible ranger produces an `IndexError`.

[444]:
```
# access to out-of-bounds index in a collection
items = 1, 2, 3
items[5]
```

```
IndexError: tuple index out of range
```

Retrieving a non-existent key in a dictionary raises another type of exception, a `KeyError`.

[445]:
```python
# Access non-existant dictionary key
dct = {'language': 'Python', 'version': 3.8}
dct['course']
```

```
KeyError: 'course'
```

Mistakenly trying to access a non-existent attribute will trigger an `AttributeError`:

[446]:
```python
value = 1.0
value.shape
```

```
AttributeError: 'float' object has no attribute 'shape'
```

When we try to apply an operation to data that does not support that particular operation, we get a `TypeError`:

[447]:
```python
items = 1, 2, 3
items + 1
```

```
TypeError: can only concatenate tuple (not "int") to tuple
```

Division by zero also triggers an exception of type `ZeroDivisionError`:

[448]:
```python
1/0
```

```
ZeroDivisionError: division by zero
```

Attempting to import a module or symbol from within a module that does not exist raises an `ImportError`:

[449]:
```python
from numpy import function_that_does_not_exist
```

```
ImportError: cannot import name 'function_that_does_not_exist' from 'numpy' (/home/
↪richard/.conda/envs/py3-default/lib/python3.10/site-packages/numpy/__init__.py)
```

Performing an operation on arrays of non-conforming shape produces a `ValueError`:

[450]:
```python
import numpy as np

a = np.arange(3)
b = np.arange(2)
a + b
```

```
ValueError: operands could not be broadcast together with shapes (3,) (2,)
```

Trying to open a non-existing file will raise an `FileNotFoundError`.

[451]:
```python
open('file_does_not_exists.txt', 'rt')
```

```
FileNotFoundError: [Errno 2] No such file or directory: 'file_does_not_exists.txt
```

In other cases, for example when using NumPy's `loadtxt`, trying to open a non-existing file will instead raise a `OSError`.

[452]:
```
import numpy as np

data = np.loadtxt('path/to/nonexisting/file.txt')
```

```
OSError: path/to/nonexisting/file.txt not found.
```

10.2 Handling errors

As you just saw, there are numerous types of exceptions raised by Python libraries we use every day. We can handle these in two ways:

1. Avoid errors before they arise.
2. Catch exceptions once they arise in special exception-handling blocks.

10.2.1 Avoiding errors

We could have avoided almost all of the above exception if we had surrounded them with `if` statements and checked whether an operation could actually be performed.

This, however, is usually not the way we write Python code, unless we are implementing library functions that need to work in situations over which we have little control. We certainly don't want to clutter "regular" code with `if` statements everywhere. There are other ways to avoid errors.

Examples:

Returning to the dictionary example, we could write something like this:

[453]:
```
# Access non-existant dictionary key
dct = {'language': 'Python', 'version': 3.10}
if 'course' in dct:
    print(dct['course'])
```

However, if we have a default value that should be used whenever a key is not present, we can more elegantly use the `get()` method which accepts a default value. No `if`'s needed:

[454]:
```
# access non-existing key
dct.get('course', 'Default programming language')
```

[454]: 'Default programming language'

If a key does exist, the default will of course be ignored:

[455]:
```
# access existing key
dct.get('language', 'Default programming language')
```

[455]: 'Python'

Another easily avoidable exception is the `IndexError`. There is hardly ever a reason to attempt retrieving elements at arbitrary indices. Usually, we first check the size of a collection:

[456]:
```
items = 1, 2, 3

# Assume idx was passed as an argument to a function
# so we need to handle unforeseen cases
idx = 1000

# Enforce valid upper bound in case the index is
# out of bounds.
items[min(idx, len(items) - 1)]
```

[456]: 3

When operating on NumPy arrays, we frequently have to retrieve their dimensions first, so there is no risk of accessing an invalid position:

[457]:
```
import numpy as np

mat = np.arange(6).reshape(2, 3)

# Retrieve array dimensions
nrow, ncol = mat.shape

# Loop makes sure to never step out of bounds
for i in range(nrow):
    for j in range(ncol):
        print(mat[i, j])
```

```
0
1
2
3
4
5
```

There are also many helper routines that allow for “robust” programming. Imagine we want a function that returns the element at position `[0,0]`:

[458]:
```
def get_elem(x):
    return x[0,0]
```

Calling this on a matrix works as intended:

[459]:
```
get_elem(np.ones((2,2)))
```

[459]: 1.0

But what if we pass a nested list or tuple?

[460]:
```
get_elem([[1,2], [3,4]])
```

```
TypeError: list indices must be integers or slices, not tuple
```

With very little effort, we can make this function more robust by using `np.atleast_2d()` which ensures that its result is at least a 2-dimensional NumPy array (it returns higher-dimensional arrays unmodified):

[461]:
```
import numpy as np

def get_elem(x):
    x = np.atleast_2d(x)
    return x[0,0]
```

[462]:
```
get_elem([[1,2], [3,4]])          # Now works on nested lists
```

[462]: 1

This function suddenly becomes much more flexible, maybe too flexible since it works on all sorts of arguments:

[463]:
```
get_elem([1, 2])          # simple list
get_elem(1.0)             # scalar
```

[463]: 1.0

NumPy also implements `np.atleast_1d()` and `np.atleast_3d()` which serve the same purpose, but return 1-dimensional or 3-dimensional arrays instead.

10.2.2 Raising exceptions

There are situations when we explicitly want to ensure that some condition is met, instead of letting the code fail somewhere down the line. This is particularly important when we write library functions that might be called from many different contexts or by many different users. Raising an exception with a clear error message is beneficial in such situations.

To illustrate the benefit of clear error messages, consider the following (highly artificial) example:

[464]:
```
def get_row(mat, i):
    # restrict to valid row indices
    irow = min(mat.shape[0] - 1, max(0, i))

    # return row
    row = mat[irow]
    return row
```

We define the function `get_row` that returns the `i`-th row of a matrix. The function ensures that the row index is within the admissible range for the given array.

Let's call this function as follows:

[465]:
```
import numpy as np
mat = np.arange(6).reshape((3, 2))
get_row(mat, 1.0)
```

```
IndexError: only integers, slices (`:`), ellipsis (`...`), numpy.newaxis (`None`),
↪and integer or boolean arrays are valid indices
```

This raises an `IndexError`, notifying the user that the statement `row = mat[irow]` was problematic. However, the caller does not know what `irow` is since this is not the name of the original argument. In the worst case, the user would have to inspect the implementation of `get_row()` to figure out what is wrong.

How can we rectify this situation? We cannot prevent someone from calling this function with an inadmissible value, but we can raise an exception once such a value is encountered.

We raise exceptions using the `raise` statement which is followed by an exception:

[466]:
```
def get_row(mat, i):
    # Check whether i is an integer
    if not isinstance(i, int):
        msg = f'Integer argument required, received {i}'
        raise ValueError(msg)
    # restrict to valid row indices
```

```
    irow = min(mat.shape[0] - 1, max(0, i))

    # return row
    row = mat[irow]
    return row
```

To check whether `i` is of integer type, we use the `isinstance()` function.

The convention is to raise a `ValueError` when a function argument does not satisfy some requirement. We can optionally pass an error message, as in the example above. There is no need or possibility to add an explicit `return` statement: as soon as an exception is raised, any remaining code is skipped. We will examine the details below.

[467]:
```
get_row(mat, 1)      # Call with integer argument; works as intended.
```

[467]:
```
array([2, 3])
```

[468]:
```
get_row(mat, 1.0)    # Call with float argument; raises exception
```

```
ValueError: Integer argument required, received 1.0
```

As you see, an exception is raised and a clear error message is returned to the caller.

10.2.3 Catching exceptions

If we are unable or unwilling to take measures to avoid an error, we have to deal with the resulting exception, should one occur. If we fail to do so, the entire program will be terminated.

We handle exceptions using the `try` statement (we sometimes say we "catch" exceptions, which is the keyword used in some other programming languages):

- The code that potentially raises an exception is placed in the `try` clause.
- If an error occurs, control is immediately passed on to the `except` clause and any remaining statements in the `try` clause are skipped.
- The `except` clause takes care of handling the exception, should one occur. If no exception is raised, the `except` clause is never executed.

Examples:

Say we need to process an integer value but are unsure about the data type of the input; calling `int()` might therefore work, or it might not:

[469]:
```
x = 1.2345
int(x)          # Works, float is truncated to integer
```

[469]:
```
1
```

[470]:
```
x = 'abc'
int(x)          # Does not work
```

```
ValueError: invalid literal for int() with base 10: 'abc'
```

Calling `int()` with a string such as `'abc'` which cannot be interpreted as an integer will raise a `ValueError`. We could handle such a situation as follows:

[471]:
```
x = 'abc'

try:
```

```
    i = int(x)
    print('Conversion to integer works!')
except ValueError:
    print(f'{x} cannot be converted to an integer')
```

```
abc cannot be converted to an integer
```

We see that the execution of the `try` clause terminates as soon as the exception is raised, so the `print()` function is never called. Instead, execution is passed on to the `except` clause which matches the exception type.

We can have multiple `except` clauses covering all sorts of exceptions:

[472]:
```
def func(x):
    try:
        i = int(x)
        print('Conversion to integer works!')
        # Return some value
        return 10/i
    except ValueError:
        print(f'{x} cannot be converted to an integer')
    except ZeroDivisionError:
        print('Division by zero')
    except:
        print('Other exception type occured')
```

[473]:
```
func('abc')          # ValueError: cannot convert integer
```

```
abc cannot be converted to an integer
```

[474]:
```
func(0)              # ZeroDivisionError
```

```
Conversion to integer works!
Division by zero
```

An `except` clause without an exception type catches any exceptions which do not match any preceding `except` clause. For example, this code raises a `TypeError` which is not specifically handled:

[475]:
```
func([1, 2, 3])      # TypeError, caught by default clause
```

```
Other exception type occured
```

If there is no default `except` clause and an unhandled exception occurs, it will be propagated back to the caller as if no error handling was present at all:

[476]:
```
# Define func to only handle ValueError
def func(x):
    try:
        i = int(x)
        print('Conversion to integer works!')
        # Return some value
        return 10/i
    except ValueError:
        print(f'{x} cannot be converted to an integer')
```

[477]:
```
func(0)          # Raises ZeroDivisionError, which is passed to caller
```

```
Conversion to integer works!
```

```
ZeroDivisionError: division by zero
```

This even works across multiple levels of the call stack:

[478]:
```
# inner function converts to integer
def inner(x):
    i = int(x)
    return i

# outer function divides by integer value
def outer(x):
    i = inner(x)
    return 10 /i
```

[479]:
```
outer('abc')              # ValueError raised in inner()
```

```
ValueError: invalid literal for int() with base 10: 'abc'
```

Here we call `outer()`, which in turn calls `inner()`, passing on its argument. Conversion to an integer fails in `inner()`, but since `outer()` does not handle this exception, it is automatically passed on the the original call site.

10.3 Exercises

10.3.1 Exercise 1: Sign function

Revisit the sign function you implemented in Unit 4, Exercise 1. To refresh your memory, the suggested solution looks as follows:

[480]:
```
import numpy as np

def sign(x):
    if x < 0.0:
        return -1.0
    elif x == 0.0:
        return 0.0
    elif x > 0.0:
        return 1.0
    else:
        # Argument is not a proper numerical value, return NaN
        # (NaN = Not a Number)
        return np.nan
```

This implementation is not very robust, as it returns all sorts of exceptions when passed non-numeric arguments:

[481]:
```
sign('abc')              # pass in string
```

```
TypeError: '<' not supported between instances of 'str' and 'float'
```

[482]:
```
sign(np.array([1, 2, 3]))            # Pass in NumPy array
```

```
ValueError: The truth value of an array with more than one element is ambiguous.␣
↪Use a.any() or a.all()
```

Modify the `sign()` function such that it only accepts built-in numerical Python types (integers, floats) and raises a `ValueError` in all other cases

10.3.2 Exercise 2: Factorials

Consider the `factorial()` function you wrote in Unit 4, Exercise 4:

[483]:
```
def factorial(n):
    if n == 0:
        return 1
    else:
        # Use recursion to compute factorial
        return n * factorial(n-1)
```

This implementation is also not very robust to nonsensical arguments, for example:

[484]:
```
factorial(1.123)
```

```
RecursionError: maximum recursion depth exceeded in comparison
```

Modify this function such that it only accepts *numerical* arguments that are either integers, or can be interpreted as integers without loss of data, such as a float `1.0` or a scalar array `np.array(1.0)`.

The function should raise a `ValueError` for all other inputs.

10.3.3 Exercise 3: Bisection

Recall the `bisect()` function from Unit 4, Exercise 5:

[485]:
```
def bisect(f, a, b, tol=1.0e-6, xtol=1.0e-6, maxiter=100):

    for iteration in range(maxiter):
        # Compute candidate value as midpoint between a and b
        mid = (a + b) / 2.0
        if abs(b-a) < xtol:
            # Remaining interval is too small
            break

        fmid = f(mid)

        if abs(fmid) < tol:
            # function value is close enough to zero
            break

        print(f'Iteration {iteration}: f(mid) = {fmid:.4e}')
        if fmid*f(b) > 0.0:
            # f(mid) and f(b) have the same sign, update upper bound b
            print(f'  Updating upper bound to {mid:.8f}')
            b = mid
        else:
            # f(mid) and f(a) have the same sign, or at least one of
            # them is zero.
            print(f'  Updating lower bound to {mid:.8f}')
            a = mid

    return mid
```

This function accepts quite a few arguments, but we never implemented any input validation. Add the following input checks at the top of the function and raise a `ValueError` if any of them is violated:

1. Check that `f(a)` and `f(b)` are of opposite sign, a precondition for the bisection algorithm to work.
2. Check that `tol` and `xtol` are positive and can be interpreted as floating-point numbers.
3. Check that `maxiter` is positive and can be interpreted as an integer.

10.4 Solutions

10.4.1 Solution for exercise 1

We can use the built-in `float()` function to determine whether something can be represented as a floating-point number.

We use only the default `except` clause without any type specification as the code in the `try` clause raises several types of exceptions, depending on the input argument.

[486]:
```python
import numpy as np

def sign(x):
    try:
        # Convert to float, which is more generic than int
        x = float(x)
    except:
        # The above statement raises at least two types
        # of exceptions: ValueError and TypeError
        raise ValueError('Numerical argument required!')

    if x < 0.0:
        return -1.0
    elif x == 0.0:
        return 0.0
    elif x > 0.0:
        return 1.0
    else:
        # Argument is not a proper numerical value, return NaN
        # (NaN = Not a Number)
        return np.nan
```

[487]:
```python
sign(123)            # integer argument
```

[487]: 1.0

[488]:
```python
sign('abc')          # string argument
```

```
ValueError: could not convert string to float: 'abc'


During handling of the above exception, another exception occurred:

ValueError: Numerical argument required!
```

[489]:
```python
sign(np.array([1, 2, 3]))        # NumPy array argument
```

```
TypeError: only size-1 arrays can be converted to Python scalars


During handling of the above exception, another exception occurred:

ValueError: Numerical argument required!
```

10.4.2 Solution for exercise 2

One possible solution looks as follows:

[490]:
```python
def factorial(n):
    try:
        i = int(n)
        assert i == n
    except:
        raise ValueError(f'Not an integer argument: {n}')

    if i == 0:
        return 1
    else:
        # Use recursion to compute factorial
        return i * factorial(i-1)
```

We perform input validation in two steps:

1. We use the `int()` function to convert the input to an integer. This will eliminate some inadmissible arguments such as `'abc'` or `[1, 2, 3]` but will accept others such as `'1'` or `1.1`. We want to eliminate these as well, since `'1'` is not numeric and `1.1` cannot be represented as an integer without loss of data.
2. We achieve this with the `assert` statement where we check whether `i == n`: this will only be true if `n` is numerical and does not have a fractional part.

   The `assert` statement will raise an `AssertionError` whenever a condition is not `True`, which will also be handled by the `except` clause.

[491]:
```python
factorial(1)            # integer argument
```

[491]: 1

[492]:
```python
factorial(1.0)          # not an integer argument, but can be
                        # represented as an integer.
```

[492]: 1

[493]:
```python
factorial(1.1)          # Floating-point argument that
                        # cannot be represented as an integer
```

```
AssertionError


During handling of the above exception, another exception occurred:

ValueError: Not an integer argument: 1.1
```

[494]:
```python
factorial('1')          # String argument
```

```
AssertionError


During handling of the above exception, another exception occurred:

ValueError: Not an integer argument: 1
```

[495]:
```python
factorial(np.array(10.0))        # Scalar array argument
```

[495]: 3628800

10.4.3 Solution for exercise 3

We modify the function as follows:

```
[496]: def bisect(f, a, b, tol=1.0e-6, xtol=1.0e-6, maxiter=100):

    fa = f(a)
    fb = f(b)

    if fa*fb > 0.0:
        raise ValueError(f'Not a bracketing interval [{a}, {b}]')
    try:
        tol = float(tol)
        assert tol > 0.0
    except:
        raise ValueError('Argument tol must be a positive number!')

    try:
        xtol = float(xtol)
        assert xtol > 0.0
    except:
        raise ValueError('Argument xtol must be a positive number!')

    try:
        maxiter = int(maxiter)
        assert maxiter > 0
    except:
        raise ValueError('Argument maxiter must be a positive integer!')


    for iteration in range(maxiter):
        # Compute candidate value as midpoint between a and b
        mid = (a + b) / 2.0
        if abs(b-a) < xtol:
            # Remaining interval is too small
            break

        fmid = f(mid)

        if abs(fmid) < tol:
            # function value is close enough to zero
            break

        print(f'Iteration {iteration}: f(mid) = {fmid:.4e}')
        if fmid*f(b) > 0.0:
            # f(mid) and f(b) have the same sign, update upper bound b
            print(f'  Updating upper bound to {mid:.8f}')
            b = mid
        else:
            # f(mid) and f(a) have the same sign, or at least one of
            # them is zero.
            print(f'  Updating lower bound to {mid:.8f}')
            a = mid

    return mid
```

As in the main loop of the function, we check whether two values are non-zero and have the same sign using the condition `fa * fb > 0`, in which case we have no bracketing interval and need to raise a `ValueError`.

The remaining checks are performed using the same code as in earlier exercises.

[497]:
```
# Function call with valid argument
x0 = bisect(lambda x: x**2.0 - 4.0, -3.0, 0.0, tol=1.0e-3)
```

```
Iteration 0: f(mid) = -1.7500e+00
  Updating upper bound to -1.50000000
Iteration 1: f(mid) = 1.0625e+00
  Updating lower bound to -2.25000000
Iteration 2: f(mid) = -4.8438e-01
  Updating upper bound to -1.87500000
Iteration 3: f(mid) = 2.5391e-01
  Updating lower bound to -2.06250000
Iteration 4: f(mid) = -1.2402e-01
  Updating upper bound to -1.96875000
Iteration 5: f(mid) = 6.2744e-02
  Updating lower bound to -2.01562500
Iteration 6: f(mid) = -3.1189e-02
  Updating upper bound to -1.99218750
Iteration 7: f(mid) = 1.5640e-02
  Updating lower bound to -2.00390625
Iteration 8: f(mid) = -7.8087e-03
  Updating upper bound to -1.99804688
Iteration 9: f(mid) = 3.9072e-03
  Updating lower bound to -2.00097656
Iteration 10: f(mid) = -1.9529e-03
  Updating upper bound to -1.99951172
```

[498]:
```
# Function call with f(a) and f(b) both positive
x0 = bisect(lambda x: x**2.0 - 4.0, 10.0, 20.0)
```

```
ValueError: Not a bracketing interval [10.0, 20.0]
```

[499]:
```
# Function call with invalid tolerance criterion
x0 = bisect(lambda x: x**2.0 - 4.0, -3.0, 0.0, tol=0.0)
```

```
AssertionError


During handling of the above exception, another exception occurred:

ValueError: Argument tol must be a positive number!
```

11 Applications: Econometrics

In this unit, we study a few more advanced examples of how to use Python to perform common econometric tasks. We will go beyond just calling existing functions that someone implemented, but we instead will implement these ourselves to understand the underlying concepts.

11.1 Preliminaries: Drawing bivariate samples

In most of the exercises below, we'll need to draw a random sample that serves as an input. We therefore first define a routine which returns a sample drawn from a bivariate normal distribution.

In line with what we learned in unit 10, we check arguments and raise an exception if a an invalid value is encountered.

[500]:
```
import numpy as np
from numpy.random import default_rng

def draw_bivariate_sample(mean, std, rho, n, seed=123):
    """
    Draw a bivariate normal random sample.

    Parameters
    ----------
    mean : array_like
        Length-2 array of means
    std : array_like
        Length-2 array of standard deviations
    rho : float
        Correlation parameter
    n : int
        Sample size
    """

    if not -1 <= rho <= 1:
        raise ValueError(f'Invalid correlation parameter: {rho}')

    if np.any(np.array(std) <= 0):
        raise ValueError(f'Invalid standard deviation: {std}')

    if n <= 0:
        raise ValueError(f'Invalid sample size: {n}')

    # initialize default RNG with given seed
    rng = default_rng(seed)

    # Unpack standard deviations for each dimension
    std1, std2 = std

    # Compute covariance
    cov = rho * std1 * std2

    # Create variance-covariance matrix
    vcv = np.array([[std1**2.0, cov],
                    [cov, std2**2.0]])
```

```
    # Draw MVN random numbers:
    # each row represents one sample draw.
    X = rng.multivariate_normal(mean=mean, cov=vcv, size=n)

    return X
```

11.2 Singular value decomposition (SVD) and principal components

Singular value decomposition is a matrix factorisation that is commonly used in econometrics and statistics. For example, we can use it to implement principal component analysis (PCA), principal component regression, OLS or Ridge regression.

Let $\mathbf{X} \in \mathbb{R}^{m \times n}$ be a matrix. For our purposes, we will assume that $m \geq n$ since $\mathbf{X}$ will be the matrix containing the data with observations in rows and variables in column. The (compact) SVD of $\mathbf{X}$ is given by

$$\mathbf{X} = \mathbf{U}\Sigma\mathbf{V}'$$

where $\mathbf{U} \in \mathbb{R}^{m \times n}$ and $\mathbf{V} \in \mathbb{R}^{n \times n}$ are orthogonal matrices, and $\Sigma \in \mathbb{R}^{n \times n}$ is a diagonal matrix

$$\Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_n \end{bmatrix}$$

The elements σ_i are called singular values of $\mathbf{X}$, and Σ is arranged such that $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$. Since $\mathbf{U}$ is not necessarily square, it's not truly orthogonal, but its columns are still orthogonal to each other.

These matrices satisfy the following useful properties:

$$\begin{aligned} \mathbf{U}'\mathbf{U} &= \mathbf{I}_n \\ \mathbf{V}'\mathbf{V} = \mathbf{V}\mathbf{V}' &= \mathbf{I}_n \\ \mathbf{V}' &= \mathbf{V}^{-1} \end{aligned}$$

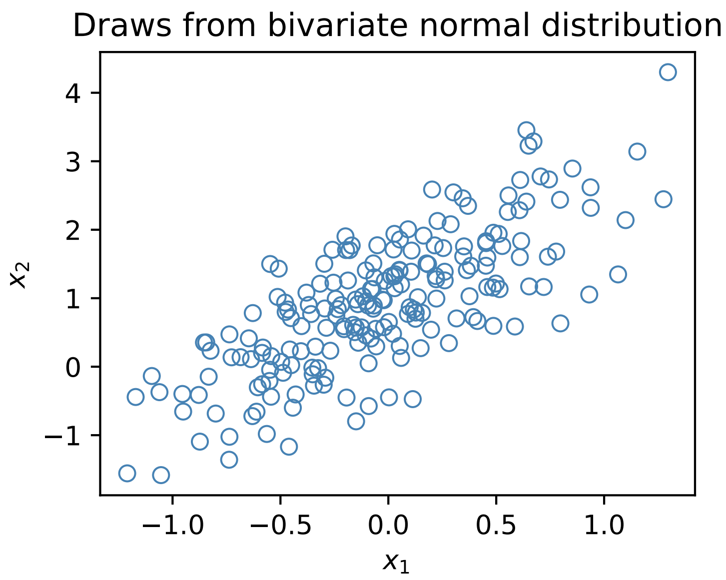
In Python, we compute the SVD using the `svd()` function from `numpy.linalg`.

11.2.1 Example: Bivariate normal

Imagine we construct X as 200 random draws from a bivariate normal:

[501]:
```
import numpy as np
import matplotlib.pyplot as plt
from numpy.random import default_rng

# Draw a bivariate normal sample using the function we defined above
mu = [0.0, 1.0]          # Vector of means
sigma = [0.5, 1.0]       # Vector of standard deviations
rho = 0.75               # Correlation coefficient
Nobs = 200               # Sample size
X = draw_bivariate_sample(mu, sigma, rho, Nobs)
x1, x2 = X.T

# Scatter plot of sample
plt.scatter(x1, x2, linewidths=0.75, c='none', edgecolors='steelblue')
plt.xlabel(r'$x_1$')
plt.ylabel(r'$x_2$')
plt.title('Draws from bivariate normal distribution')
```

[501]:
```
Text(0.5, 1.0, 'Draws from bivariate normal distribution')
```



We can now perform the SVD as follows:

[502]:
```
from numpy.linalg import svd

# svd() returns transposed V!
# We use full_matrices=False to get the compact factorisation, otherwise
# U is 200 x 200.
U, S, Vt = svd(X, full_matrices=False)
```

[503]:
```
# Check that U'U is a 2x2 identity matrix
U.T @ U          # or np.dot(U.T, U)
```

[503]:
```
array([[ 1.00000000e+00, -6.12878704e-17],
       [-6.12878704e-17,  1.00000000e+00]])
```

[504]:
```
# Check that V'V = VV' is a 2x2 identity matrix
Vt.T @ Vt        # or np.dot(Vt.T, Vt)
```

[504]:
```
array([[ 1.00000000e+00, -2.26167254e-18],
       [-2.26167254e-18,  1.00000000e+00]])
```

[505]:
```
# svd() does not return S as a matrix but only its diagonal!
S
```

[505]:
```
array([19.73152572,  5.99498933])
```

[506]:
```
# We can convert it to a diagonal matrix using np.diag()
np.diag(S)
```

[506]:
```
array([[19.73152572,  0.        ],
       [ 0.        ,  5.99498933]])
```

Finally, we can multiply the output of `svd()` to verify that the result is equal to **X**:

[507]:
```
X_svd = U * S @ Vt

# Compute the max. absolute difference
diff = np.amax(np.abs(X - X_svd) )
```

```
print(f"Max. absolute difference between X and USV': {diff:.2e}")
```

```
Max. absolute difference between X and USV': 2.89e-15
```

11.2.2 Example: Principal components

We use principal component analysis (PCA) as a dimension reduction technique, which allows us to identify an alternate set of axes along which the data in **X** varies the most. In machine learning, PCA is one of the most basic unsupervised learning techniques.

To perform the PCA, it is recommended to first demean the data:

[508]:
```
X = draw_bivariate_sample(mu, sigma, rho, Nobs)

# Demean variables in X
Xmean = np.mean(X, axis=0)

# Matrix Z stores the demeaned variables
Z = X - Xmean[None]
```

We can now use the SVD factorisation to compute the principal components. Once we have computed the matrices $\mathbf{U}$, Σ and $\mathbf{V}$, the matrix of principal components (one in each column) is given by

$$PC = \mathbf{U}\Sigma$$

[509]:
```
# Apply SVD to standardised values
U, S, Vt = svd(Z, full_matrices=False)

# Compute principal components
PC = U * S           # same as U @ np.diag(S)

# Variance is highest for first component
var_PC = np.var(PC, axis=0, ddof=1)
print(f'Principal component variances: {var_PC}')
```

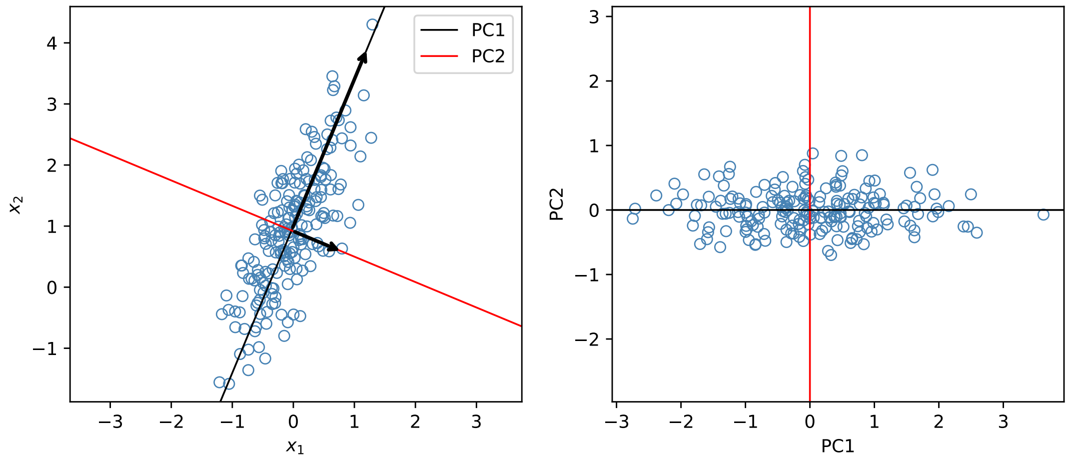
```
Principal component variances: [1.17607859 0.09444617]
```

We can plot the principal component axes in the original data space (left columns). Moreover, the right column shows the data rotated and rescaled so that each axes corresponds to a principal component. Most of the variation clearly occurs along the first axis!

[510]:
```
# Plot principal components

# Scatter plot of sample
fig, axes = plt.subplots(1, 2, figsize=(10,4))
axes[0].scatter(X[:, 0], X[:, 1], linewidths=0.75, c='none',␣
 ↪edgecolors='steelblue')
axes[0].axis('equal')
axes[0].set_xlabel(r'$x_1$')
axes[0].set_ylabel(r'$x_2$')
axes[0].axline(Xmean, Xmean + Vt[0], label='PC1', lw=1.0, c='black', zorder=1)
axes[0].axline(Xmean, Xmean + Vt[1], label='PC2', lw=1.0, c='red', zorder=1)

PC_arrows = Vt * np.sqrt(var_PC[:, None])
for v in PC_arrows:
    # Scale up arrows by 3 so that they are visible!
    axes[0].annotate('', Xmean + v*3, Xmean, arrowprops=dict(arrowstyle='->',␣
 ↪linewidth=2))

axes[0].legend()

# Plot in principal component coordinate system
```

```
axes[1].scatter(PC[:, 0], PC[:, 1], linewidths=0.75, c='none',␣
↪edgecolors='steelblue')
axes[1].set_xlabel('PC1')
axes[1].set_ylabel('PC2')
axes[1].axis('equal')
axes[1].axvline(0.0, lw=1.0, c='red')
axes[1].axhline(0.0, lw=1.0, c='black')
```

[510]: <matplotlib.lines.Line2D at 0x7f9db48531c0>



Of course, in real applications we don't need to manually compute the principal components, but can use a library such as scikit-learn to do it for us:

[511]:
```
from sklearn.decomposition import PCA

# Draw the same sample as before
X = draw_bivariate_sample(mu, sigma, rho, Nobs)

# Create PCA with 2 components (which is the max, since we have only two
# variables)
pca = PCA(n_components=2)

# Perform PCA on input data
pca.fit(X)

# The attribute components_ can be used to retrieve the V' matrix
print("Principal components (matrix V'):")
print(pca.components_)

# The attribute explained_variance_ stores the variances of all PCs
print(f'Variance of each PC: {pca.explained_variance_}')

# Fraction of variance explained by each component:
print(f'Fraction of variance of each PC: {pca.explained_variance_ratio_}')
```

```
Principal components (matrix V'):
[[ 0.38420018  0.92324981]
 [ 0.92324981 -0.38420018]]
Variance of each PC: [1.17607859 0.09444617]
Fraction of variance of each PC: [0.92566365 0.07433635]
```

11.3 Ordinary least squares (OLS)

Consider the regression

$$y_i = \mathbf{x}_i'\beta + u_i$$

where $\mathbf{x}_i$ is a vector of regressors (explanatory variables) that is assumed to include a constant. Recall that the OLS estimator $\widehat{\beta}$ is given by

$$\widehat{\beta} = \left(\mathbf{X}'\mathbf{X}\right)^{-1}\mathbf{X}'\mathbf{y}$$

where $\mathbf{X}$ is the regressor matrix that contains all stacked $\mathbf{x}_i'$, and $\mathbf{y}$ contains all observations of the dependent variable.

11.3.1 Example 1: Bivariate data

We first demonstrate how to run OLS using bivariate normal data. With only one regressor, the regression simplifies to

$$y_i = \alpha + \beta x_i + u_i$$

where α is the intercept and β is the slope coefficient. In this special case, the population coefficient β can be computed using the formula

$$\beta = \frac{E[(Y-\overline{Y})(X-\overline{X})]}{E[(X-\overline{X})]} = \frac{Cov(Y,X)}{Var(X)}$$

where the numerator contains the covariance of the random variables Y and X, and the denominator contains the variance of X. Given a sample of values, the estimator $\widehat{\beta}$ is computed using the corresponding sample moments:

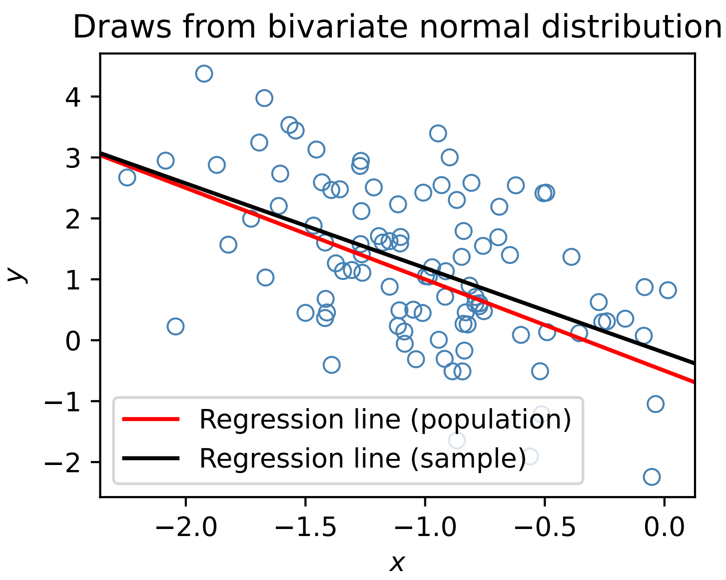
$$\widehat{\beta} = \frac{\widehat{Cov}(y,x)}{\widehat{Var}(x)}$$

[512]:
```python
import numpy as np
import matplotlib.pyplot as plt

mu = [-1.0, 1.0]                # Mean of X and Y
std = [0.5, 1.5]                # Std. dev. of X and Y
rho = -0.5                      # Correlation coefficient
Nobs = 100                      # Sample size

# We transpose the return value and unpack individual rows into X and Y
x, y = draw_bivariate_sample(mu, std, rho, Nobs).T

# Compute beta (slope coefficient) from distribution moments.
# This is the true underlying relationship given our data generating process.
cov = rho * np.prod(std)
beta = cov / std[0]**2.0
print(f'Slope of population regression line: {beta}')

# Compute beta from sample moments
# Sample variance-covariance matrix (ddof=1 returns the unbiased estimate)
cov_hat = np.cov(x, y, ddof=1)[0, -1]
var_x_hat = np.var(x, ddof=1)
beta_hat = cov_hat / var_x_hat
# Sample intercept
alpha_hat = np.mean(y) - beta_hat * np.mean(x)

print(f'Slope of sample regression line: {beta_hat}')

# Scatter plot of sample
plt.scatter(x, y, linewidths=0.75, c='none', edgecolors='steelblue')
plt.xlabel(r'$x$')
plt.ylabel(r'$y$')
```

```
plt.title('Draws from bivariate normal distribution')
plt.axline(mu, slope=beta, color='red', label='Regression line (population)')
plt.axline((0, alpha_hat), slope=beta_hat, color='black', label='Regression line␣
↪(sample)')
plt.legend()
```

```
Slope of population regression line: -1.5
Slope of sample regression line: -1.3889613032802288
```

[512]: <matplotlib.legend.Legend at 0x7f9e082f7580>



11.3.2 Example 2: OLS using matrix algebra

With more than one regressor, we need to use matrix algebra to perform the OLS estimation. For demonstration purposes, we continue using the bivariate data generated above, but now we write the OLS regression as

$$y_i = \mathbf{x}_i'\gamma + u_i$$

where $\gamma = (\alpha, \beta)$, and the regressors now contain a constant, $\mathbf{x_i} = (1, x_i)'$. As stated above, the OLS estimator is given by

$$\hat{\gamma} = \left(\mathbf{X}'\mathbf{X}\right)^{-1}\mathbf{X}'\mathbf{y}$$

Naive solution You might be tempted to solve the above equation system by explicitly computing the inverse of $\mathbf{X}'\mathbf{X}$ using NumPy's `inv()` like this:

[513]:
```
from numpy.linalg import inv

# We transpose the return value and unpack individual rows into X and Y
x, y = draw_bivariate_sample(mu, std, rho, Nobs).T

# Create vector of ones (required to estimate the intercept)
ones = np.ones((len(x), 1))
# Prepend constant to vector of regressors to create regressor matrix X
X = np.hstack((ones, x[:, None]))

# Compute inverse of X'X
```

```
XXinv = inv(X.T @ X)

print("Explicitly computed (X'X)^(-1):")
print(XXinv)

# Compute naive estimate of gamma
gamma_naive = XXinv @ X.T @ y
print(f'Naive estimate of gamma: {gamma_naive}')
```

```
Explicitly computed (X'X)^(-1):
[[0.05633363 0.04521468]
 [0.04521468 0.04412275]]
Naive estimate of gamma: [-0.20352351 -1.3889613 ]
```

This might seems like a straightforward way to implement OLS, but in practice you should *never* do this. Explicitly taking the inverse of a matrix to solve an equation system is rarely a good idea and numerically unstable, even though in this particular case it yields the same result!

Solving as a linear equation system One numerically acceptable way to run OLS is to view it as a linear equation system. Recall that a linear equation system can be written in matrix notation as

$$\mathbf{A}\mathbf{z} = \mathbf{b}$$

where $\mathbf{A} \in \mathbb{R}^{k \times k}$ is a coefficient matrix of full rank, $\mathbf{b} \in \mathbb{R}^k$ is a vector, and $\mathbf{z} \in \mathbb{R}^k$ is a vector of k unknows we want to solve for. The OLS estimator can be written in this form if we set

$$\begin{aligned} \mathbf{A} &= \mathbf{X}'\mathbf{X} \\ \mathbf{b} &= \mathbf{X}'\mathbf{y} \\ \mathbf{z} &= \widehat{\gamma} \end{aligned}$$

so that we have

$$(\mathbf{X}'\mathbf{X})\widehat{\gamma} = \mathbf{X}'\mathbf{y}$$

We can use NumPy's `solve()` to find $\widehat{\gamma}$:

[514]:
```
from numpy.linalg import solve

# Compute X'X
A = X.T @ X
# Compute X'y
b = X.T @ y

# Solve for coefficient vector
gamma_solve = solve(A, b)
print(f'Estimate of gamma using solve(): {gamma_solve}')
```

```
Estimate of gamma using solve(): [-0.20352351 -1.3889613 ]
```

Of course, running OLS (or equivalently: solving an overdetermined linear equation system) is a common task, so NumPy has the function `lstsq()` which allows you do to it without explicitly computing $\mathbf{X}'\mathbf{X}$ or $\mathbf{X}'\mathbf{y}$:

[515]:
```
from numpy.linalg import lstsq

# Estimate using lstsq(). Pass rcond=None to suppress a warning.
gamma_lstsq, *rest = lstsq(X, y, rcond=None)

print(f'Estimate of gamma using lstsq(): {gamma_lstsq}')
```

```
Estimate of gamma using lstsq(): [-0.20352351 -1.3889613 ]
```

11.3.3 Example 3: Implementing OLS yourself

NumPy's `lstsq()` uses SVD to compute the solution. Since we covered SVD in a previous exercise, we already have the tools to build our own implementation.

Recall that SVD factorises a regressor matrix $\mathbf{X}$ into three matrices,

$$\mathbf{X} = \mathbf{U}\Sigma\mathbf{V}'$$

We can use the orthogonality properties of $\mathbf{U}$ and $\mathbf{V}$ described above to transform the OLS estimator. We will be using the fact that the transpose of $\mathbf{X}$ is

$$\mathbf{X}' = \mathbf{V}\Sigma'\mathbf{U}' = \mathbf{V}\Sigma\mathbf{U}'$$

which follows since Σ is a diagonal (and thus symmetric) matrix. The OLS estimator can then be expressed as follows:

$$\begin{aligned}
\widehat{\gamma} &= (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} \\
&= \left(\mathbf{V}\Sigma\mathbf{U}'\mathbf{U}\Sigma\mathbf{V}'\right)^{-1}\mathbf{V}\Sigma\mathbf{U}'\mathbf{y} \\
&= \left(\mathbf{V}\Sigma\mathbf{I}_k\Sigma\mathbf{V}'\right)^{-1}\mathbf{V}\Sigma\mathbf{U}'\mathbf{y} \\
&= \left(\mathbf{V}\Sigma^2\mathbf{V}'\right)^{-1}\mathbf{V}\Sigma\mathbf{U}'\mathbf{y}
\end{aligned}$$

This follows since $\mathbf{U}'\mathbf{U} = \mathbf{I}_k$ is an identity matrix where $k = 2$ is the number of coefficients we are estimating. Next, we can compute the inverse using the orthogonality properties of $\mathbf{V}$,

$$\begin{aligned}
\mathbf{V}\mathbf{V}' &= \mathbf{V}'\mathbf{V} = \mathbf{I} \\
\mathbf{V}' &= \mathbf{V}^{-1}
\end{aligned}$$

Therefore,

$$\left(\mathbf{V}\Sigma^2\mathbf{V}'\right)^{-1} = (\mathbf{V}')^{-1}\Sigma^{-2}\mathbf{V}^{-1} = \mathbf{V}\Sigma^{-2}\mathbf{V}'$$

Plugging this into the expression for the OLS estimator, we see that

$$\begin{aligned}
\widehat{\gamma} &= \left(\mathbf{V}\Sigma^2\mathbf{V}'\right)^{-1}\mathbf{V}\Sigma\mathbf{U}'\mathbf{y} \\
&= \mathbf{V}\Sigma^{-2}\mathbf{V}'\mathbf{V}\Sigma\mathbf{U}'\mathbf{y} \\
&= \mathbf{V}\Sigma^{-2}\mathbf{I}_k\Sigma\mathbf{U}'\mathbf{y} \\
&= \mathbf{V}\Sigma^{-1}\mathbf{U}'\mathbf{y}
\end{aligned}$$

Why is this preferable to the original expression? Since Σ is a diagonal matrix, its inverse is trivially computed as the element-wise inverse of its diagonal elements!

[516]:
```python
from numpy.linalg import svd

# Request "compact" SVD, we don't need the full matrix U.
U, S, Vt = svd(X, full_matrices=False)

# Note that S returned by svd() is a vector that contains the diagonal
# of the matrix Sigma.
gamma_svd = Vt.T * S**(-1) @ U.T @ y
print(f'Estimate of gamma using SVD: {gamma_svd}')
```

```
Estimate of gamma using SVD: [-0.20352351 -1.3889613 ]
```

11.3.4 Example 4: OLS standard errors

All of the above methods only computed the *point estimates*, i.e., the coefficient vector. Usually, we are interested in performing inference, i.e., testing some hypothesis, for example whether our estimate is significantly different from zero. To this end, we need to compute standard errors which reflect the sampling uncertainty of our estimates.

Under the assumption of homoskedastic errors, the variance-covariance matrix of the OLS estimator $\widehat{\gamma}$ is given by the expression

$$Var(\widehat{\gamma}) = \widehat{\sigma}^2 \left(\mathbf{X}'\mathbf{X}\right)^{-1}$$
$$\widehat{\sigma}^2 = \frac{1}{n-k} \sum_{i=1}^{n} \widehat{u}_i^2$$

where $\widehat{\sigma}^2$ is the sample variance of the residuals (recall that we have included an intercept in the model, so the mean of $\widehat{u}_i$ is zero!). Note the degree-of-freedom correction in the denominator for a model with k parameters (including any intercept).

Luckily, we can directly use our insights from the previous section and instead of computing $\left(\mathbf{X}'\mathbf{X}\right)^{-1}$ directly (which is numerically undesirable), we can rewrite it using the SVD factorisation as follows:

$$\begin{aligned}
\left(\mathbf{X}'\mathbf{X}\right)^{-1} &= \left(\mathbf{V}\Sigma\mathbf{U}'\mathbf{U}\Sigma\mathbf{V}'\right)^{-1} \\
&= \left(\mathbf{V}\Sigma\mathbf{I}_k\Sigma\mathbf{V}'\right)^{-1} \\
&= \left(\mathbf{V}\Sigma^2\mathbf{V}'\right)^{-1} \\
&= \mathbf{V}\Sigma^{-2}\mathbf{V}'
\end{aligned}$$

Extending the code from above, we can now compute the point estimate and the standard errors:

[517]:
```
from numpy.linalg import svd

# Request "compact" SVD, we don't need the full matrix U.
U, S, Vt = svd(X, full_matrices=False)

# Compute point estimate as before
gamma = Vt.T * S**(-1) @ U.T @ y

# Compute (X'X)^-1
XXinv = Vt.T * S**(-2) @ Vt

# Residuals are given as u = y - X*gamma
residuals = y - X @ gamma

# Variance of residuals
k = X.shape[1]
var_u = np.var(residuals, ddof=k)

# Variance-covariance matrix of estimates
var_gamma = var_u * XXinv

# Standard errors are square roots of diagonal elements of Var(gamma)
gamma_se = np.sqrt(np.diag(var_gamma))

print(f'Point estimate of gamma: {gamma}')
print(f'Standard errors of gamma: {gamma_se}')
```

```
Point estimate of gamma: [-0.20352351 -1.3889613 ]
Standard errors of gamma: [0.26527596 0.23477147]
```

11.3.5 Example 5: Complete OLS estimation routine

We can combine all our previous code and encapsulate it in a function called `ols`, which makes sure the input data are NumPy arrays and have the same number of observations. We also add the optional parameter `add_const` which allows callers to automatically include a constant in the model.

[518]:
```
def ols(X, y, add_const=False):
    """
    Run the OLS regression y = X * beta + u
```

```
    and return the estimated coefficients beta and their variance-covariance
    matrix.

    Parameters
    ----------
    X : array_like
        Matrix (or vector) of regressors
    y : array_like
        Vector of observations of dependent variable
    add_const : bool, optional
        If True, prepend a constant to regressor matrix X.
    """

    from numpy.linalg import svd

    # Make sure that y is a one-dimensional array
    y = np.atleast_1d(y)

    # Number of obs.
    Nobs = y.size

    # Make sure that X is a matrix and the leading dimension contains the
    # observations
    X = np.atleast_2d(X).reshape((Nobs, -1))

    # Check that arrays are of conformable dimensions, and raise an exception
    # if that is not the case
    if X.shape[0] != Nobs:
        raise ValueError('Non-conformable arrays X and y')

    # Check whether we need to prepend a constant
    if add_const:
        ones = np.ones((Nobs, 1))
        X = np.hstack((ones, X))

    # Request "compact" SVD, we don't need the full matrix U.
    U, S, Vt = svd(X, full_matrices=False)

    # Compute point estimate using SVD factorisation
    beta = Vt.T * S**(-1) @ U.T @ y

    # Compute (X'X)^-1 using SVD factorisation
    XXinv = Vt.T * S**(-2) @ Vt

    # Residuals are given as u = y - X*beta
    residuals = y - X @ beta

    # Number of model parameters
    k = X.shape[1]

    # Variance of residuals
    var_u = np.var(residuals, ddof=k)

    # Variance-covariance matrix of estimates
    var_beta = var_u * XXinv

    return beta, var_beta
```

We can now draw our random sample and repeat the OLS estimation using only a few lines of code!

[519]:
```
# Test our custom OLS function

# Draw random sample, split into x and y
```

```
x, y = draw_bivariate_sample(mu, std, rho, Nobs).T

# Call OLS estimator. Note that we don't need to manually add a constant!
beta, vcv = ols(x, y, add_const=True)

# Compute standard errors
beta_SE = np.sqrt(np.diag(vcv))

print(f'Point estimate: {beta}')
print(f'Standard errors: {beta_SE}')
```

```
Point estimate: [-0.20352351 -1.3889613 ]
Standard errors: [0.26527596 0.23477147]
```

11.4 OLS using housing data

We now proceed to run a more meaningful regression using the `ols()` function developed above. To this end, we use monthly observations from the file `HOUSING.csv` which contains various variables related to the US housing market. In particular, we will take the number of housing unit construction starts (variable `NHSTART`) in a given month and regress it on the average sales price of new homes (variable `ASPNHS`) lagged by 3, 6 and 12 months. We run the regression in logs, so the estimated coefficient should be interpreted as elasticities.

If you are familiar with Stata, the regression we are trying to run will look like this:

```
. regress log_nhstart L3.log_aspnhs L6.log_aspnhs L12.log_aspnhs if year >= 2000

      Source |       SS           df       MS      Number of obs   =       259
-------------+----------------------------------   F(3, 255)       =     19.27
       Model |  7.50833492         3  2.50277831   Prob > F        =    0.0000
    Residual |  33.1247614       255  .129901025   R-squared       =    0.1848
-------------+----------------------------------   Adj R-squared   =    0.1752
       Total |  40.6330963       258  .157492621   Root MSE        =    .36042

------------------------------------------------------------------------------
 log_nhstart |      Coef.   Std. Err.      t    P>|t|     [95% Conf. Interval]
-------------+----------------------------------------------------------------
  log_aspnhs |
         L3. |   2.293265   .5024764     4.56   0.000     1.303733    3.282797
         L6. |   .8001798   .5538507     1.44   0.150    -.2905242    1.890884
        L12. |   -1.94804   .4377757    -4.45   0.000    -2.810156   -1.085924
             |
       _cons |  -6.484041   2.783441    -2.33   0.021     -11.9655   -1.002581
------------------------------------------------------------------------------
```

11.4.1 Load and visually inspect the data

We first load and inspect the data using pandas's `read_csv()` function:

[520]:
```
import numpy as np
import pandas as pd

file = '../data/HOUSING.csv'
df = pd.read_csv(file)

# Inspect first and last rows of the DataFrame
df
```

[520]:

```
      Year  Month  NHSTART  MORTGAGE30  CSHPRICE  HSN1F    ASPNHS    CPI  \
0     1975      1   1032.0         9.4       NaN  416.0   39500.0   52.3
1     1975      2    904.0         9.1       NaN  422.0   40600.0   52.6
2     1975      3    993.0         8.9       NaN  477.0   42100.0   52.8
3     1975      4   1005.0         8.8       NaN  543.0   42000.0   53.0
4     1975      5   1121.0         8.9       NaN  579.0   43200.0   53.1
..     ...    ...      ...         ...       ...    ...       ...    ...
554   2021      3   1725.0         3.1     245.5  873.0  414700.0  264.8
555   2021      4   1514.0         3.1     249.8  796.0  434800.0  266.8
556   2021      5   1594.0         3.0     254.4  720.0  442500.0  268.6
557   2021      6   1650.0         3.0     259.0  701.0  429600.0  271.0
558   2021      7   1534.0         2.9       NaN  708.0  446000.0  272.3

     HSUPPLY
0        9.9
1       10.4
2        8.9
3        7.2
4        6.8
..       ...
554      4.2
555      4.8
556      5.5
557      6.0
558      6.2

[559 rows x 9 columns]
```

The data contains several variables which we won't be using in this analysis, such as the Case-Shiller house price index (CSHPRICE) which has missing values for some of the earlier dates (missing values are denoted as NaN).

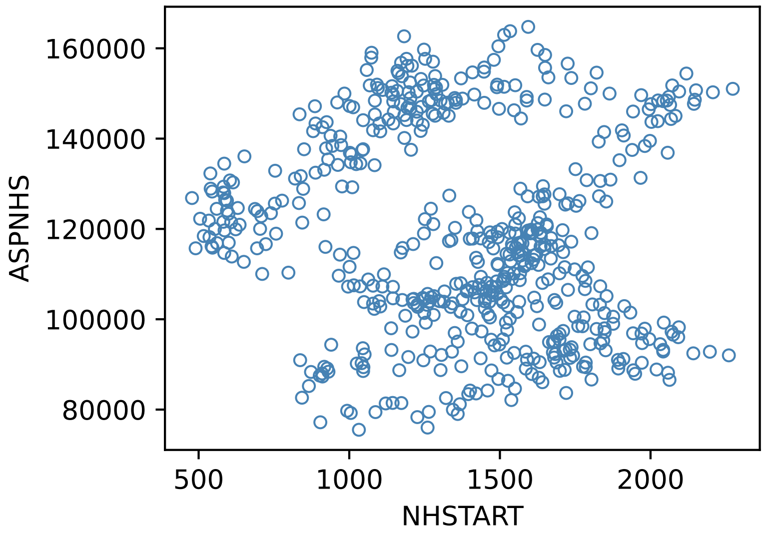
Let's first plot the bivariate relationship between new house starts and the (concurrent) average sales price. The price is in current dollars, so we first need to deflate it (using the CPI) to make the values comparable across this 45-year period.

[521]:

```python
import matplotlib.pyplot as plt

# Convert average selling price to 1982-1984 dollars.
# The value of 100 corresponds to the average price level between 1982-1984.
df['ASPNHS'] /= df['CPI'] / 100.0

df.plot.scatter('NHSTART', 'ASPNHS', linewidths=0.75,␣
 ↪color='none',edgecolor='steelblue')
```

[521]:

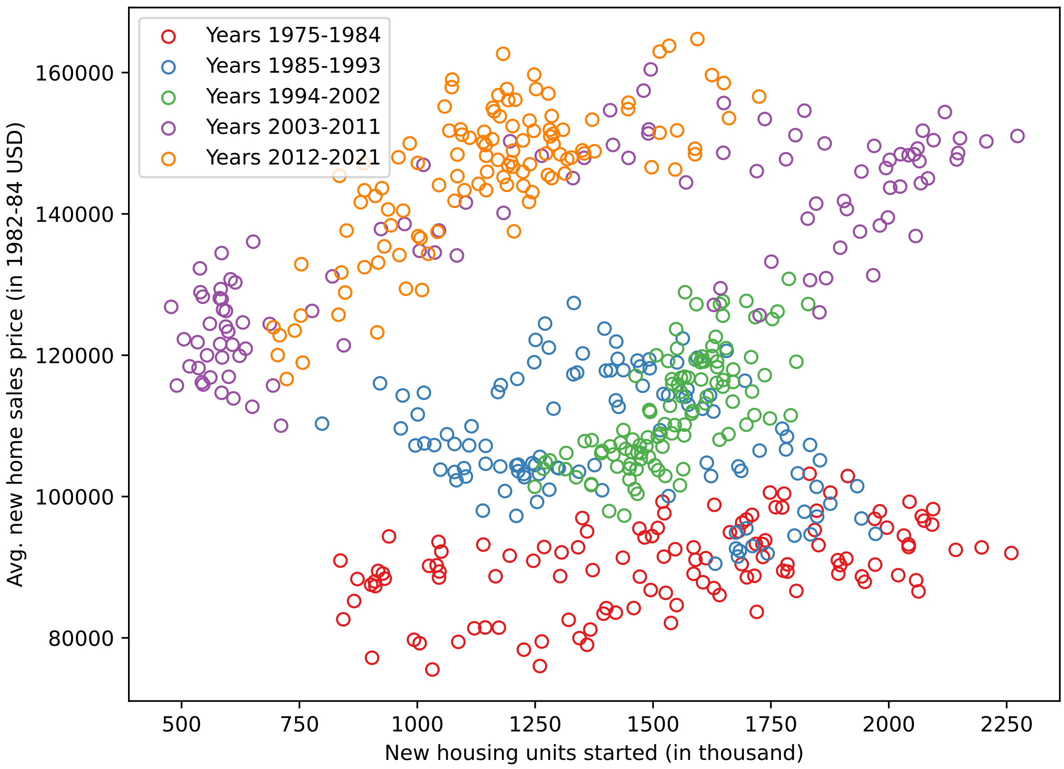
```
<AxesSubplot:xlabel='NHSTART', ylabel='ASPNHS'>
```



This scatter plot looks somewhat unexpected as there seems to be no clear relationship between housing supply and house prices. This might be because the relationship has not remained stable over the decades covered by our data.

To see this more clearly, we bin the time periods into five blocks and recreate the plots using different colours:

[522]:
```
# Create 5 approximately equally-sized bins based on the calendar year
df['Year_bin'] = pd.cut(df['Year'], bins=5, labels=False)

# Plot each group of years using a different color
fig, ax = plt.subplots(1,1, figsize=(8,6))
colors = ['#e41a1c','#377eb8','#4daf4a','#984ea3','#ff7f00']

# Iterate over bins, plot each one separately
bins = df['Year_bin'].unique()
for bin in bins:
    # Restrict data set to relevant years
    df_i = df.loc[df['Year_bin'] == bin].copy()

    # Extract initial and terminal year of this block
    yfrom, yto = df_i['Year'].min(), df_i['Year'].max()

    ax.scatter(df_i['NHSTART'], df_i['ASPNHS'],
        label=f'Years {yfrom:.0f}-{yto:.0f}',
        edgecolors=colors[bin], color='none')

ax.set_xlabel('New housing units started (in thousand)')
ax.set_ylabel('Avg. new home sales price (in 1982-84 USD)')
ax.legend()

del df['Year_bin']
```



As you see, our suspicion was correct and there are clear changes across the sample of 45 years. At this point we could do something more elaborate, but for illustrative purposes we just restrict our analysis to the period after the year 2000, where we have an upwards-sloping relationship.

11.4.2 Prepare the data

Before we can call the function `ols()`, we need to pre-process the data so that we end up with NumPy arrays (the only type of data our function accepts).

[523]:
```
# Keep only relevant variables, rest just clutters the DataFrame
varlist = ['Year', 'Month', 'ASPNHS', 'NHSTART']
df = df[varlist].copy()

# Create YYYY-MM date index
df['Date'] = pd.PeriodIndex(year=df['Year'], month=df['Month'], freq='M')
df = df.set_index('Date')

# Create 3-month, 6-month and 12-month lags of house prices
lags = 3, 6, 12
for lag in lags:
    df[f'L{lag}ASPNHS'] = df['ASPNHS'].shift(lag)

# Restrict data to year >= 2000
df = df.loc[df['Year'] >= 2000].copy()

# Drop year, month, these are no longer needed
df = df.drop(columns=['Year', 'Month'])

# Plot first 13 rows, which clearly shows the lagged values
df.head(13)
```

[523]:

```
            ASPNHS  NHSTART       L3ASPNHS       L6ASPNHS      L12ASPNHS
Date
2000-01  118310.691081   1636.0  119095.776324  113437.312537  111050.394657
2000-02  117176.470588   1737.0  125593.824228  115559.545183  116211.293260
2000-03  119824.561404   1604.0  119727.488152  116090.584029  114866.504854
2000-04  121299.005266   1626.0  118310.691081  119095.776324  115852.923448
2000-05  116822.429907   1575.0  117176.470588  125593.824228  113192.771084
2000-06  114808.362369   1559.0  119824.561404  119727.488152  116807.228916
2000-07  117081.644470   1463.0  121299.005266  118310.691081  113437.312537
2000-08  115923.566879   1541.0  116822.429907  117176.470588  115559.545183
2000-09  119988.479263   1507.0  114808.362369  119824.561404  116090.584029
2000-10  123691.776883   1549.0  117081.644470  121299.005266  119095.776324
2000-11  120952.927669   1551.0  115923.566879  116822.429907  125593.824228
2000-12  119186.712486   1532.0  119988.479263  114808.362369  119727.488152
2001-01  119020.501139   1600.0  123691.776883  117081.644470  118310.691081
```

Now that we have created all the lagged variables, we drop all rows with missing data and convert the relevant columns to NumPy arrays.

[524]:

```python
# List of variables to include in model
var_X = [f'L{lag}ASPNHS' for lag in lags]
var_y = 'NHSTART'

# Restrict to relevant variables
df = df[var_X + [var_y]].copy()

# drop all rows with missing observations
df = df.dropna()

# Extract raw data from data frame
X = df[var_X].to_numpy()
y = df[var_y].to_numpy()

# Estimate as elasticity in logs
log_X = np.log(X)
log_y = np.log(y)

# Print first 5 observations
log_X[:5]
```

[524]:

```
array([[11.68768329, 11.63900565, 11.61773938],
       [11.74080836, 11.65754122, 11.66316531],
       [11.69297351, 11.66212606, 11.65152591],
       [11.68106942, 11.68768329, 11.66007676],
       [11.67143637, 11.74080836, 11.63684758]])
```

11.4.3 Estimating the model

We are now ready to run the OLS regression.

[525]:

```python
# Run our own ols() function. This returns the coefficient vector and the
# variance-covariance matrix.
coefs, vcv = ols(log_X, log_y, add_const=True)

# Compute standard errors from the VCV matrix
se = np.sqrt(np.diag(vcv))

print(f'Estimated coefficients: {coefs}')
print(f'Standard errors: {se}')
print(f'Number of obs: {len(log_y)}')
```

```
Estimated coefficients: [-6.48405842  2.2932615   0.80018127 -1.94803646]
Standard errors: [2.78344134 0.50247618 0.55385034 0.43777545]
Number of obs: 259
```

11.4.4 Running OLS using statsmodels

As you can imagine, estimating an OLS regression is a common task so there are packages which already implement this functionality for you. One such package is `statsmodels`, which we will now use to verify our results.

[526]:
```python
import statsmodels.api as sm

# Explicitly augment the regressor matrix with a constant
log_X1 = sm.add_constant(log_X)

# Define the linear model
model = sm.OLS(log_y, log_X1)

# Estimate the model
result = model.fit()

# Print a summary of the results
result.summary()
```

[526]:
```
<class 'statsmodels.iolib.summary.Summary'>
"""
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.185
Model:                            OLS   Adj. R-squared:                  0.175
Method:                 Least Squares   F-statistic:                     19.27
Date:                Sat, 10 Sep 2022   Prob (F-statistic):           2.72e-11
Time:                        17:39:35   Log-Likelihood:                -101.18
No. Observations:                 259   AIC:                             210.4
Df Residuals:                     255   BIC:                             224.6
Df Model:                           3
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const         -6.4841      2.783     -2.330      0.021     -11.966      -1.003
x1             2.2933      0.502      4.564      0.000       1.304       3.283
x2             0.8002      0.554      1.445      0.150      -0.291       1.891
x3            -1.9480      0.438     -4.450      0.000      -2.810      -1.086
==============================================================================
Omnibus:                       31.603   Durbin-Watson:                   0.184
Prob(Omnibus):                  0.000   Jarque-Bera (JB):                9.818
Skew:                          -0.144   Prob(JB):                      0.00738
Kurtosis:                       2.090   Cond. No.                     2.55e+03
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
[2] The condition number is large, 2.55e+03. This might indicate that there are
strong multicollinearity or other numerical problems.
"""
```

As you can see, the point estimates and standard errors are exactly the same as the ones we computed.

As for the interpretation, the regression says that a 1% increase in the average sales price is associated with a 2.3% increase in new house construction starts in three months time. The elasticity is only 0.8% if we consider a lag of 6 months (albeit not statistically significant), and even reverses its sign at a 12-month horizon. This interpretation of course assumes that prices are independent over time, which is not overly plausible.