0-Introduction

March 24, 2023

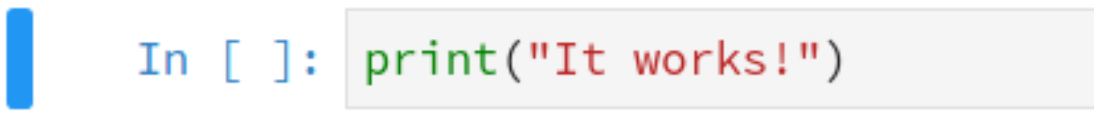
1 Advanced Python and Machine Learning Course

With this course we provide an overview of important Machine Learning concepts and introduce more advanced **Python 3** programming topcs. In the following notebooks, we will cover the areas of **regression**, **classification**, and **knowledge discovery** as well as some of the most relevant Python libraries for Machine Learning. Of course, we won't be able to provide an exhaustive presentation of all topics and their mathematical depth. The goal of this course is to give you a practical introduction with some real-world examples. There might be some additional topics, objects or commands you later find useful but have not seen in this course. However, we believe that you really become "fluent" in a programming language and the different Machine Learning tools by trying to implement your own projects and learn from difficulties you encounter along the way.

1.0.1 Small overview of working with Jupyter Lab

In this course, we make use of Jupyter Notebooks which allow us to combine executable code with text in one document, increasing code-readibility and documentation.

In Jupyter Notebooks, you have different kinds of **cells** you can make use of: **Code**, **Markdown**, and **Raw**. In order to select a cell for execution you can just click on the relevant part of the notebook and a blue bar on the left will highlight the currently selected cell like in the image below.



```
In [ ]: print("It works!")
```

Try to run the following code cell with in the panel above or *Shift+Enter*!

```
[1]: print("It works!")
```

```
It works!
```

You can stop the execution of a cell with in the panel!

1.0.2 Markdown mode

Try to add a cell below, change to **Markdown** mode and write a note!

1. Add a cell with + in the panel above or *Esc+B*
2. Change to **Markdown** in the panel above (drop-down list) or *Esc+M*
3. As before, run the cell with   in the panel above or *Shift+Enter*!

You can make notes inside the notebooks if you like! In order to edit a Markdown cell double-click somewhere in the cell!

In Markdown mode you can use the following special characters:

2 Title

2.1 Subtitle

- bullet point 1
- bullet point 2

italic font **bold**

`highlighted code`

*** (that's a separator line)

You can also use LaTeX if you want, like $\sum_{k=0}^{\infty} q^k = \frac{1}{1-q}$ (double-click here to see how it is used).

2.1.1 Code mode

Creating a **Code** cell works similarly. You can make use of it later on!

1. Add a cell with + in the panel above or *Esc+B*
2. Change to **Code** in the panel above (drop-down list) or *Esc+Y*
3. Again, run the cell with   in the panel above or *Shift+Enter*!

2.1.2 Some Remarks

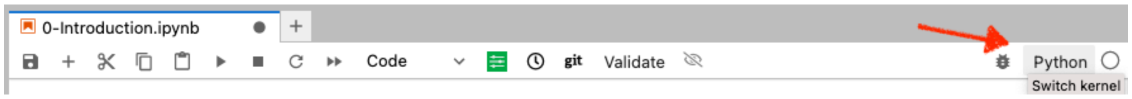
- Delete a cell with right-click on the cell and the "Delete Cells" option
- **Be careful which cells you delete** because it might not be possible to retrieve them!
- In case, you accidently deleted something try *Esc+Z* to retrieve a cell or *Ctrl+Z* to retrieve changes within a cell
- Save your notebooks with the *save icon* in the panel above or with *Ctrl+S*! **Try to save after every bigger change!** Depending on your machine, Jupyter Lab might crash from time to time.
- Try not to open too many windows in Jupyter Lab. This might lead to a crash sometimes.

2.1.3 Final Test

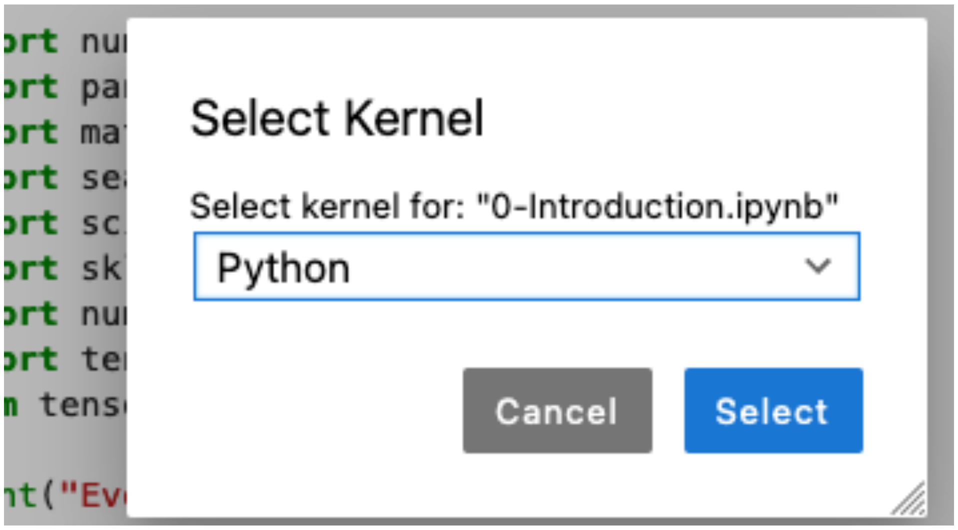
Let's see whether your setup is ready for the course. Depending on whether you (1) *use Noto* or (2) have *your own installation*, please note the following:

(1) If you are a Noto user you will need to make sure that you have the right *kernel* selected. You can do this by executing the following steps.

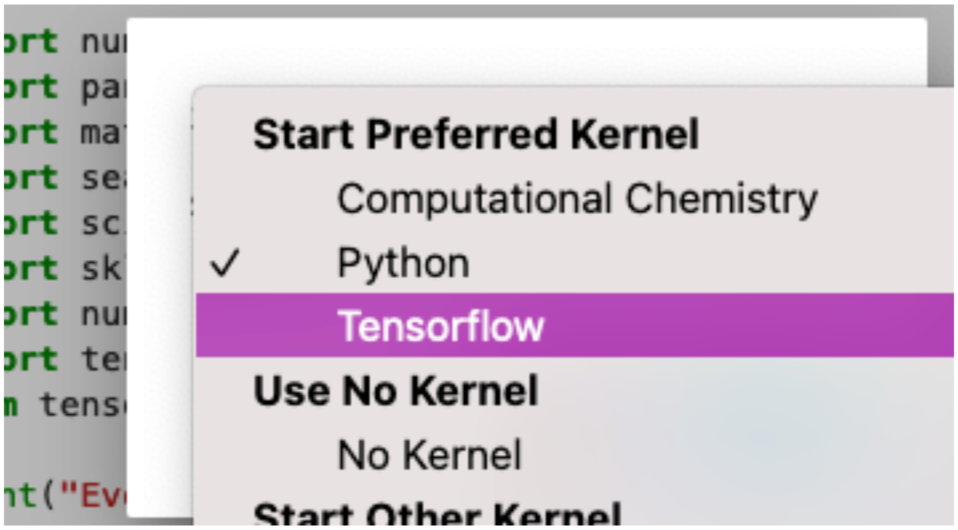
Step 1: Click in the top-right corner on the kernel name.



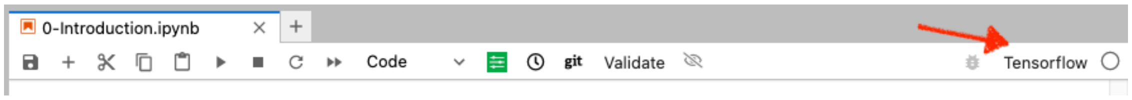
Step 2: A window pops up displaying the currently selected kernel. Click on the drop-down menu.



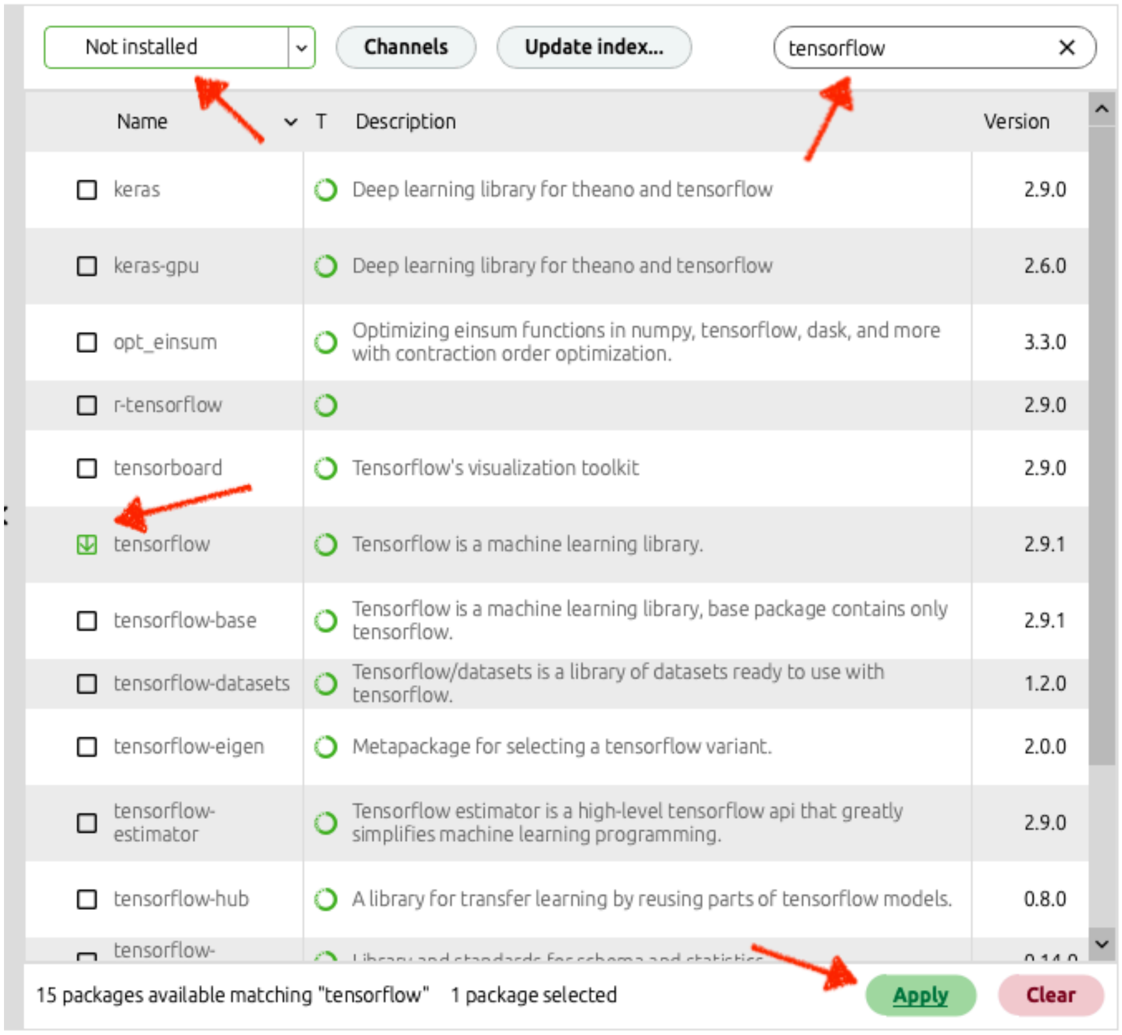
Step 3: Select the kernel called `Tensorflow` and click `Select`.



Step 4: Now, the top-right corner kernel name should read `Tensorflow`. Whenever something is not running properly, check whether the `Tensorflow` kernel is selected!



(2) If you have your own local installation you will need to install TensorFlow yourself. For this, you can follow the instructions provided in the YouTube video! In particular, you can install TensorFlow (as well as any other potentially missing library) in the Anaconda Navigator:



Name	T	Description	Version
☐ keras		Deep learning library for theano and tensorflow	2.9.0
☐ keras-gpu		Deep learning library for theano and tensorflow	2.6.0
☐ opt_einsum		Optimizing einsum functions in numpy, tensorflow, dask, and more with contraction order optimization.	3.3.0
☐ r-tensorflow			2.9.0
☐ tensorboard		Tensorflow's visualization toolkit	2.9.0
✓ tensorflow		Tensorflow is a machine learning library.	2.9.1
☐ tensorflow-base		Tensorflow is a machine learning library, base package contains only tensorflow.	2.9.1
☐ tensorflow-datasets		Tensorflow/datasets is a library of datasets ready to use with tensorflow.	1.2.0
☐ tensorflow-eigen		Metapackage for selecting a tensorflow variant.	2.0.0
☐ tensorflow-estimator		Tensorflow estimator is a high-level tensorflow api that greatly simplifies machine learning programming.	2.9.0
☐ tensorflow-hub		A library for transfer learning by reusing parts of tensorflow models.	0.8.0
☐ tensorflow-		Library and standards for schema and statistics	0.14.0

15 packages available matching "tensorflow"   1 package selected

Note that fetching specifications and downloading the package might take some time (in some cases up to an hour)!

Please execute the cell at the bottom to check whether all libraries are available which we will use later on.

[2]:
```python
import numpy
import pandas
import matplotlib
import seaborn
import scipy
import sklearn
import numba
import tensorflow
from tensorflow import keras

print("Everything is working!")
```

```
2023-03-16 10:16:55.143195: I tensorflow/core/platform/cpu_feature_guard.cc:193]
This TensorFlow binary is optimized with oneAPI Deep Neural Network Library
(oneDNN) to use the following CPU instructions in performance-critical
operations:  SSE4.1 SSE4.2 AVX AVX2 FMA
To enable them in other operations, rebuild TensorFlow with the appropriate
compiler flags.
```

```
Everything is working!
```

1-Python_Concepts

March 24, 2023

1 1. Python Concepts

We start by reviewing some more advanced Python concepts which might prove useful in implementing your Machine Learning projects. In this notebook we focus on the follwoing topics which, in particular, review some concepts related to functions in Python:

- f-strings
- subplots with Matplotlib
- lambda functions
- generators
- built-in functions map and filter
- *args and **kwargs
- decorators
- speeding up function executions with Numba

Keywords: `f"String"`, `plt.subplots`, `plt.figure.add_subplot`, `np.ravel`, `lambda x: ...`, `yield`, `map`, `filter`, `*args`, `**kwargs`, `@decorator`, `@jit`, `%timeit`

1.1 Important Python Libraries

There are several useful Python libraries for scientific computing and Machine Learning in Python.

- `NumPy` extends basic Python data structures (like lists) and provides efficient numerical functions for computations with large data arrays.
- `SciPy` builds on NumPy and provides extended functionality for numerical and statistical methods.
- `Pandas` incorporates data frames (similar to programming lanuage R) and allows for more statistical analyses.
- `Matplotlib` is the standard plotting library in Python.
- `Seaborn` builds on Matplotlib and, in particular, extends Pandas functionality to create appealing plots.
- `Scikit-learn` is a powerful Machine Learning library providing a wide range of learning algorithms. It builds upon NumPy, SciPy, and Matplotlib.
- `TensorFlow` is a library for efficient Machine Learning implementation and a standard library for Deep Learning.

- Keras is a high-level Deep Learning library build on top of TensorFlow which simplifies creating, training, and evaluating neural networks.
- PyTorch is another standard library for Deep Learning adhering more closely to basic Python principles.

In this course, we will mostly work with NumPy, Matplotlib, sckit-learn, and TensorFlow / Keras. You will be able to load these librares like this

[1]:
```
import numpy as np
import matplotlib.pyplot as plt
from sklearn import linear_model
```

1.2 f-Strings

Recommended string formatting since Python 3.6:

[4]:
```
float_var = 3.141592

print(f'String formatting allows including variables like {float_var:.2f}.')
```

```
String formatting allows including variables like 3.14.
```

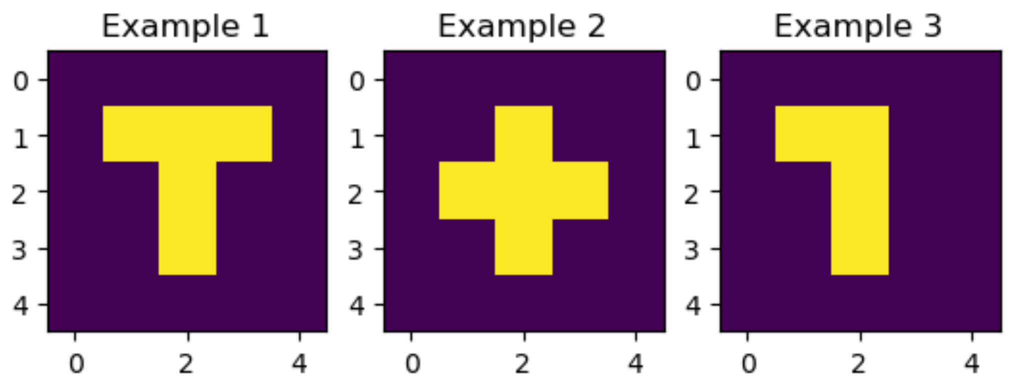
1.3 Subplots with Matplotlib

Let us create some dummy images:

[5]:
```
import numpy as np
import matplotlib.pyplot as plt

dummy_images = [[[0,0,0,0,0],
                 [0,1,1,1,0],
                 [0,0,1,0,0],
                 [0,0,1,0,0],
                 [0,0,0,0,0]],

                [[0,0,0,0,0],
                 [0,0,1,0,0],
                 [0,1,1,1,0],
                 [0,0,1,0,0],
                 [0,0,0,0,0]],

                [[0,0,0,0,0],
                 [0,1,1,0,0],
                 [0,0,1,0,0],
                 [0,0,1,0,0],
                    [0,0,0,0,0]]]
```

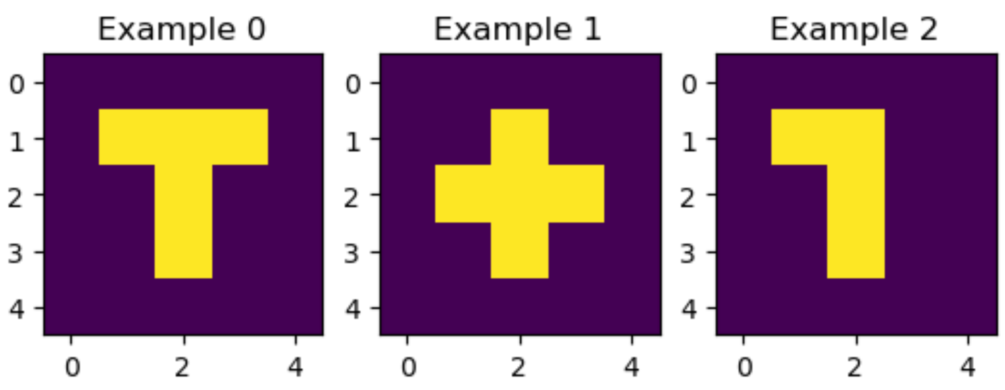
We usually use `plt.subplots` to create a figure with several sub-figures.

[6]:
```
fig, axs = plt.subplots(1,3)

axs[0].imshow(dummy_images[0])
axs[0].set_title('Example 1')

axs[1].imshow(dummy_images[1])
axs[1].set_title('Example 2')

axs[2].imshow(dummy_images[2])
axs[2].set_title('Example 3')

plt.show()
```



Another way to plot this is:

[7]:
```
fig, axs = plt.subplots(1,3)

for i, ax in enumerate(axs.ravel()):
    ax.imshow(dummy_images[i])
    ax.set_title(f"Example {i}")

plt.show()
```



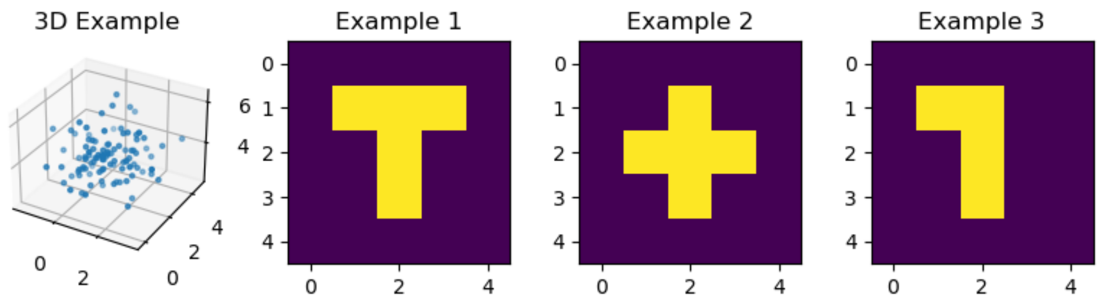
Note that you can iterate over subplots stored in object `axs`

```
In: print(axs)
Out: [<Axes: > <Axes: > <Axes: >]
```

with method `ravel` which creates a list of subplots.

There is a second way to create subplots which makes use of the `plf.figure.add_subplot` method. This is particularly useful when combining 3d and 2d sub-figures like in the following example.

```
[8]: data_3d = np.random.multivariate_normal(mean=[1,2,4], cov=np.eye(3), size=100)

fig = plt.figure(figsize=(10,2))

ax = fig.add_subplot(1,4,1, projection='3d')
ax.scatter(data_3d[:,0], data_3d[:,1], data_3d[:,2], marker='.')

ax.set_title('3D Example')

ax = fig.add_subplot(1,4,2)

ax.imshow(dummy_images[0])
ax.set_title("Example 1")

ax = fig.add_subplot(1,4,3)

ax.imshow(dummy_images[1])
ax.set_title("Example 2")

ax = fig.add_subplot(1,4,4)
ax.imshow(dummy_images[2])
ax.set_title("Example 3")

plt.show()
```



1.4 Lambda Functions

Typically, we declare a function like this in Python:

[9]:
```python
def fahrenheit_to_celsius(deg_F):
    return (deg_F - 32) * 5/9
```

[10]:
```python
fahrenheit_to_celsius(98.6)
```

[10]:
```
37.0
```

For such simple **single expression functions** a lambda function might be a convenient choice.

[11]:
```python
fahrenheit_to_celsius_lambda = lambda x: (x - 32) * 5/9
```

[12]:
```python
fahrenheit_to_celsius_lambda(98.6)
```

[12]:
```
37.0
```

They are sometimes referred to as **anonymous functions**, as they are not required to be bound to a name, e.g.

[13]:
```python
(lambda x: (x - 32) * 5/9)(98.6)
```

[13]:
```
37.0
```

We will see a more interesting example below!

1.5 Generators

Generator functions are special functions particularly suited for generating sequences of various kind.

[14]:
```
def squared_sequence(limit):
    num = 0

    while num < limit:
        yield num**2
        num += 1 # shorthand for: num = num + 1
```

[15]:
```
squared_sequence(10)
```

[15]:
```
<generator object squared_sequence at 0x7f9b3518c580>
```

[16]:
```
gen = squared_sequence(10)
```

[27]:
```
next(gen)
```

```
---------------------------------------------------------------------------
StopIteration                             Traceback (most recent call last)
Cell In[27], line 1
----> 1 next(gen)

StopIteration:
```

[32]:
```
for i in squared_sequence(10):
    print(i)

# Equivalent to:
#for i in range(10):
#    print(i**2)
```

```
0
1
4
9
16
25
36
49
64
81
```

Note the differences to standard functions:

- Generators *yield* values, suspend the function and maintain the local state
- The values are generated when they are required (called with `next()`), i.e. we do not store a whole list but generate one element at a time
- Once all elements are generated, the iteration stops

However, you can still contain all elements in a list:

[33]:
```
list(squared_sequence(10))
```

[33]:
```
[0, 1, 4, 9, 16, 25, 36, 49, 64, 81]
```

1.6 Map and Filter

The built-in functions `map` and `filter` are convenient ways to apply a function to all elements of an iterable and avoid writing a loop for that.

With `map` we apply the function to each element of the iterable(s) and return the results. We use it in the following way:

`map( function, iterable(s) )`

Let's see some examples.

[39]:
```
from matplotlib.colors import to_rgb


colours = ['green', 'red', 'blue', 'yellow']

# for c in colours:
#     print(f"{c} in RGB is: {to_rgb(c)}")

rgb_colours = map( to_rgb, colours )

print(f"Try to print rgb_colours: {rgb_colours}\n")

print(list(rgb_colours))
```

```
Try to print rgb_colours: <map object at 0x7f9b35bfafe0>

[(0.0, 0.5019607843137255, 0.0), (1.0, 0.0, 0.0), (0.0, 0.0, 1.0), (1.0, 1.0,
0.0)]
```

[42]:
```
decimals = [3.14159, 2.71828, 1.61803]

rounded = list( map( round, decimals, range(1,4) ) )

print(rounded)
```

```
[3.1, 2.72, 1.618]
```

With `filter` we apply a boolean function to an iterable and provide only the elements which returned `True`. We use it like this:

`filter( function, iterable )`

where `function` returns boolean values `True` or `False`.

```
[43]: def passed(grade):
          return grade > 4.0
```

```
[44]: grades = [5.5, 6.0, 2.0, 3.5, 4.5]

      list( filter(passed, grades) )
```

```
[44]: [5.5, 6.0, 4.5]
```

A typical use case of lambda functions is actually in connection with `map` or `filter`.

```
[46]: list( filter( lambda grade: grade > 4.0, grades ) )
```

```
[46]: [5.5, 6.0, 4.5]
```

```
[45]: list( map( lambda grade: grade > 4.0, grades ) )
```

```
[45]: [True, True, False, False, True]
```

1.7 *args and **kwargs

Sometimes you see these `*args` and `**kwargs` arguments in functions and classes. We use them to write functions with variable number of arguments of positional and keyword arguments!

Here's an example:

```
[47]: def print_arguments(first, *args, **kwargs):

          print(first)

          if args:
              print(args)

          if kwargs:
              print(kwargs)
```

```
[48]: print_arguments()
```

```
---------------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)
Cell In[48], line 1
----> 1 print_arguments()

TypeError: print_arguments() missing 1 required positional argument: 'first'
```

[49]:
```
print_arguments(1)
```

```
1
```

[50]:
```
print_arguments(1, 2, 3)
```

```
1
(2, 3)
```

[53]:
```
print_arguments(1, 2, 3, 4, color='red', marker='x')
```

```
1
(2, 3, 4)
{'color': 'red', 'marker': 'x'}
```

Note that with `*args` we collect additional positional arguments in a tuple and with `**kwargs` the additional keyword arguments in a dictionary.

1.8 Decorators

Decorators are a great way to modify the behaviour of a function or class without changing the function or class itself.

[75]:
```
def fahrenheit_to_celsius(deg_F):
    deg_C = (deg_F - 32) * 5/9
    return deg_C
```

[76]:
```
fahrenheit_to_celsius(80)
```

[76]:
```
26.666666666666668
```

Let's define a decorator and "decorate" the previous function!

[80]:
```
def just_int(func):

    def wrapper(*args, **kwargs):

        res = func(*args, **kwargs)
        print(int(res))

        return res

    return wrapper
```

[87]:
```
@just_int
def fahrenheit_to_celsius(deg_F):
    deg_C = (deg_F - 32) * 5/9
    return deg_C
```

[88]:
```
fahrenheit_to_celsius(deg_F=80)
```

```
26
```

[88]:
```
26.666666666666668
```

[90]:
```
def just_int(print_out=None):

    def just_int_inner(func):

        def wrapper(*args,**kwargs):

            if print_out:
                print(print_out)

            res = func(*args,**kwargs)
            return int(res)

        return wrapper

    return just_int_inner
```

[91]:
```
@just_int(print_out='Get rid of decimals!')
def fahrenheit_to_celsius(deg_F):
    deg_C = (deg_F - 32) * 5/9
    return deg_C
```

[92]:
```
fahrenheit_to_celsius(deg_F=80)
```

[92]:
```
26
```

1.9 Numba

Numba is a just-in-time compiler for Python which can speed up your code substantially if it is based on loops, NumPy arrays and NumPy functions. Its main feature is the `jit` decorator. Find more on Numba in the official documentation.

Let's see what it does on a small example.

[100]:
```
from numba import jit
import numpy as np
```

[101]:
```
def calc_pi(total_num_points):
    np.random.seed(1234)
    num_circle_points = 0

    for i in range(total_num_points):
        x = np.random.random()
        y = np.random.random()
        radius_squared = np.power(x,2) + np.power(y,2)

        if radius_squared < 1:
            num_circle_points += 1

    pi_estimate = 4 * num_circle_points / total_num_points
    return pi_estimate
```

[102]:
```
@jit
def calc_pi_faster(total_num_points):
    np.random.seed(1234)

    num_circle_points = 0

    for i in range(total_num_points):
        x = np.random.random()
        y = np.random.random()
        radius_squared = np.power(x,2) + np.power(y,2)

        if radius_squared < 1:
            num_circle_points += 1

    pi_estimate = 4 * num_circle_points / total_num_points
    return pi_estimate
```

The function `calc_pi_faster` is compiled to machine code when called for the first time.

[103]:
```
total_num_points = 100000

print(f"calc_pi: {calc_pi(total_num_points)}")
print(f"calc_pi_faster: {calc_pi_faster(total_num_points)}")
```

```
calc_pi: 3.14856
calc_pi_faster: 3.14856
```

[104]:
```
%timeit calc_pi(total_num_points)
```

```
609 ms ± 51.5 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

[105]:
```
%timeit calc_pi_faster(total_num_points)
```

```
1.18 ms ± 47.6 µs per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
```

Note that Jupyter (IPython) provides some built-in Python functionality through *magic commands* `%command`.

1.10 Exercise Section

Generators are very useful when loading datasets, for instance. Suppose your dataset is too large to load into memory (RAM) (e.g. several tens of GB). Typically, a possible approach is to load parts of the dataset during training as needed.

In this exercise, we implement a generator to load *batches* of images from the **MNIST dataset**. MNIST is a standard Deep Learning benchmark dataset comprising 70 000 images (usually 28 x 28 pixels) of hand-written digits with the corresponding label as the classification target.

You can load the dataset (reduced to 5 000 samples) in the next cell.

```
[106]: import numpy as np

       mnist_data = np.load('data/mnist_data_5k.npy', mmap_mode='r', allow_pickle=True)
       mnist_targets = np.load('data/mnist_labels_5k.npy', mmap_mode='r',␣
        ↪allow_pickle=True)
```

Note that `mmap_mode='r'` specifies that we do not load data into memory but instead a memory-mapped array is constructed. This means, the data is read from the disk whenever accessed. Note that

```
In[1]:  mnist_data = np.load('data/mnist_data_5k.npy', mmap_mode='r')
In[2]:  type(mnist_data)
Out[2]: numpy.memmap
```

provides a `memmap` object, while

```
In[1]:  mnist_data = np.load('data/mnist_data_5k.npy')
In[2]:  type(mnist_data)
Out[2]: numpy.ndarray
```

provides the standard NumPy array. These are two different types of objects. `memmap` lives still on the disk, while the NumPy array is loaded into RAM. Note that in a `memmap` many but not all NumPy operations will work.

(1.) Define a generator which allows passing the data, targets, and the size of the batch in the following cell. For e.g. `batch_size=10`, the generator shall slice both arrays into the first 10 samples and provide them with the `next` call. With every following call, the next 10 samples are provided. So you need to think about how to access a slice of data in NumPy arrays and how consecutively get the next slice with the next call by adjustind the indices.

```
[125]: mnist_data.shape
```

```
[125]: (5000, 784)
```

```
[127]: def batch_data(data, targets, batch_size):
           dim = len(data)

           for i in range(0, dim, batch_size):
               yield ( np.array(data[i : i + batch_size]), np.array(targets[i : i +␣
        ↪batch_size]) )
```

If you were successful, you can create the generator with

```
[128]: mnist_gen = batch_data(data=mnist_data, targets=mnist_targets, batch_size=10)
```

and retrieve a (new) batch of data with

```
[129]: new_data, new_targets = next(mnist_gen)

       print(f"Target labels in this batch: {new_targets}")
```

```
Target labels in this batch: [5 0 4 1 9 2 1 3 1 4]
```

```
[130]: type(new_data)
```

```
[130]: numpy.ndarray
```

1.11 Proposed Solutions

Generators are very useful when loading datasets, for instance. Suppose your dataset is too large to load into memory (RAM) (e.g. several tens of GB). Typically, a possible approach is to load parts of the dataset during training as needed.

In this exercise, we implement a generator to load *batches* of images from the **MNIST dataset**. MNIST is a standard Deep Learning benchmark dataset comprising 70 000 images (usually 28 x 28 pixels) of hand-written digits with the corresponding label as the classification target.

You can load the dataset (reduced to 5 000 samples) in the next cell.

```
[107]: import numpy as np

       mnist_data = np.load('data/mnist_data_5k.npy', mmap_mode='r', allow_pickle=True)
       mnist_targets = np.load('data/mnist_labels_5k.npy', mmap_mode='r',␣
        ↪allow_pickle=True)
```

Note that `mmap_mode='r'` specifies that we do not load data into memory but instead a memory-mapped array is constructed. This means, the data is read from the disk whenever accessed. Note that

```
In[1]:  mnist_data = np.load('data/mnist_data_5k.npy', mmap_mode='r')
In[2]:  type(mnist_data)
Out[2]: numpy.memmap
```

provides a `memmap` object, while

```
In[1]:  mnist_data = np.load('data/mnist_data_5k.npy')
In[2]:  type(mnist_data)
Out[2]: numpy.ndarray
```

provides the standard NumPy array. These are two different types of objects. `memmap` lives still on the disk, while the NumPy array is loaded into RAM. Note that in a `memmap` many but not all NumPy operations will work.

(1.) Define a generator which allows passing the data, targets, and the size of the batch in the following cell:

```
[111]: print(mnist_data.shape)
```

```
(5000, 784)
```

```
[112]: def batch_data(data, targets, batch_size):

           batch_num = 0
           tot_num_batches = int(data.shape[0] / batch_size)

           while batch_num < tot_num_batches:

               data_batch = data[batch_num*batch_size : (batch_num+1)*batch_size]
               targets_batch = targets[batch_num*batch_size:(batch_num+1)*batch_size]

               yield [np.array(data_batch), np.array(targets_batch)]
               batch_num = batch_num + 1
```

If you were successful, you can create the generator with

```
[113]: mnist_gen = batch_data(data=mnist_data, targets=mnist_targets, batch_size=10)
```

and retrieve a (new) batch of data with

```
[120]: new_data, new_targets = next(mnist_gen)

       print(f"Target labels in this batch: {new_targets}")
```

```
Target labels in this batch: [4 4 6 0 4 5 6 1 0 0]
```

```
[121]: type(new_data)
```

```
[121]: numpy.ndarray
```

2-Regression_and_Classification

March 24, 2023

1 2. Regression and Classification

Regression and classficiation are two fundamental tasks of supervised Machine Learning where labels allows us to guide the learning. This notebook reviews more standard approaches to regression and classification.

We provide the fundamental ideas behind

- linear regression and ridge regression
- logistic regression for classification
- decision trees and Random Forests

and apply these techniques to simulated data and a dataset example (wine quality assessment).

Keywords: `OLS`, `MSE`, `Overfittng`, `Regularisation`, `np.linalg.inv`, `sklearn.linear_model.LinearRegression`, `sklearn.linear_model.Ridge`, `sklearn.tree.DecisionTreeClassifier`, `sklearn.linear_model.LogisticRegression`, `sklearn.ensemble.RandomForestClassifier`, `sklearn.model_selection.train_test_split`

We start by fixing a random seed which controls the generation of (pseudo) random number sequences.

[1]:
```
import numpy as np
import matplotlib.pyplot as plt

np.random.seed(123)
```

Note that this enables reproducibility of our results even in the presence of "randomness". For example, the first three runs of the following cell

[2]:
```
np.random.random(size=4)
```

[2]:
```
array([0.69646919, 0.28613933, 0.22685145, 0.55131477])
```

will always produce

1. `array([0.69646919, 0.28613933, 0.22685145, 0.55131477])`
2. `array([0.71946897, 0.42310646, 0.9807642 , 0.68482974])`

3. `array([0.4809319 , 0.39211752, 0.34317802, 0.72904971])`

1.1 Standard Linear Regression and Ordinary Least Squares

We assume a linear relationship between true **response** $Y_{\text{groundtruth}} = Xw$ and **predictors / covariates** X. However, usually **our observation is not perfect**, i.e. there is some noise additional ϵ.

A simple linear regression model is then

$$Y = Xw + \epsilon. \tag{1}$$

Let us simulate $N = 10$ datapoints with Gaussian noise $\epsilon \sim \mathcal{N}(\mu = 0, \sigma = 20)$.

[3]:
```
np.random.seed(123)

num_datapoints = 10

X = np.random.random(size=num_datapoints)*50
X = np.sort(X).reshape(-1,1)

print(X)

w_groundtruth = 10
Y_groundtruth = w_groundtruth*X

epsilon_noise = np.random.normal(loc=0, scale=20.0, size=(num_datapoints,1))

Y = Y_groundtruth + epsilon_noise
```

```
[[11.34257268]
 [14.30696675]
 [19.60587591]
 [21.15532301]
 [24.04659507]
 [27.56573845]
 [34.24148693]
 [34.82345928]
 [35.97344849]
 [49.03820992]]
```

A typical objective function is given by the **mean squared error** (MSE) loss

$$\text{Loss}(w) = \frac{1}{2N}\|\epsilon\|_2^2 = \frac{1}{2N}\|Y - Xw\|_2^2 = \frac{1}{2N}\sum_{n=1}^{N}\left(y_n - x_n \cdot w\right)^2. \tag{2}$$

Under certain conditions, the solution to this equation will provide the **best linear (unbiased) estimator** for w! We identify the **minimum** through

$$\nabla \text{Loss}(w) = X^\top Y - X^\top X w \equiv 0, \tag{3}$$

which provides the **ordinary least squares** (OLS) solution

$$w_{\text{OLS}} = \left(X^\top X\right)^{-1} X^\top Y. \tag{4}$$

```
[4]: XT = np.transpose(X)
     XTX_inverse = np.linalg.inv(XT @ X)

     w_OLS = XTX_inverse @ XT @ Y

     print(f"The solution is given by w_OLS = {w_OLS.squeeze()}.")
```

```
The solution is given by w_OLS = 10.375338325958648.
```

Note

- Operator `@` provides the matrix multiplication of two numpy array (similar to `np.matmul`)
- Function `numpy.array.squeeze()` removes all dimensions of size 1 from a NumPy array, i.e.

```
In: print(w_OLS.shape)
Out: (1, 1)

In: print(w_OLS)
Out: [[10.04673211]]

In: print(w_OLS.squeeze())
Out: 10.046732109803889
```

Let's provide some predictions Y_{OLS} based on this solution.

```
[5]: Y_OLS = w_OLS * X
```

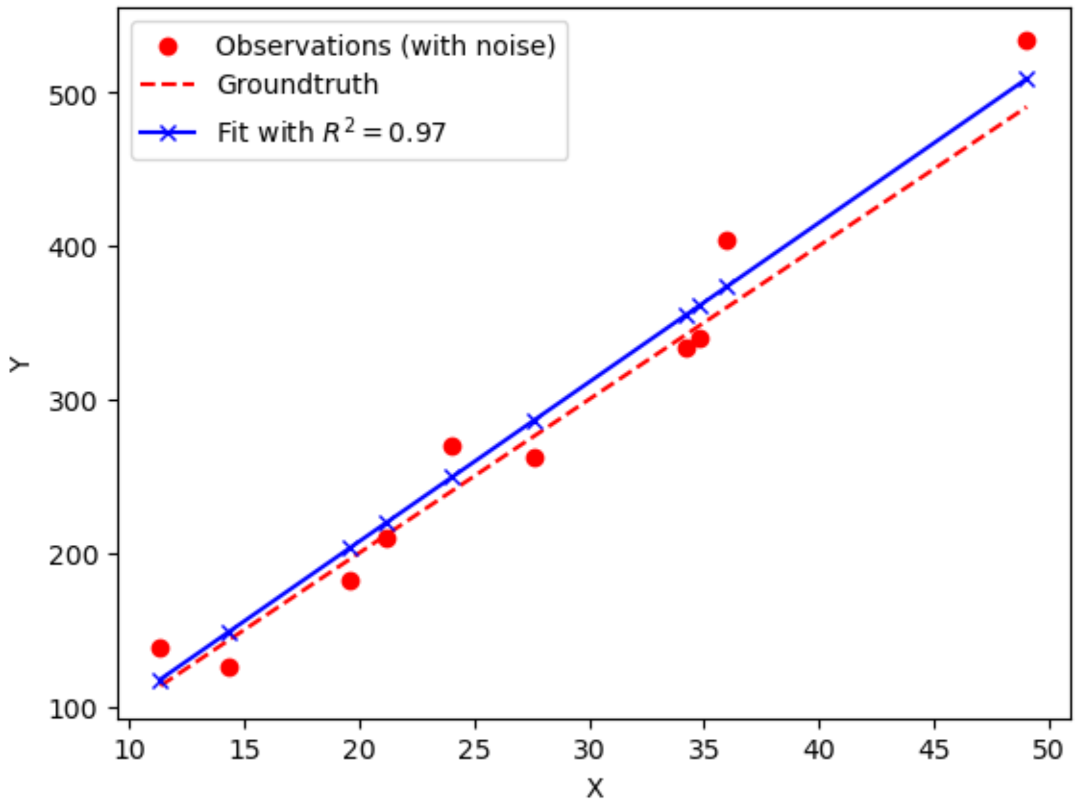
With this, we can calculate the **coefficient of determination** R^2 (Wikipedia) through

```
[6]: Rsquared = 1 - np.sum((Y - Y_OLS)**2) / np.sum((Y - np.mean(Y))**2)
     print(Rsquared)
```

```
0.965593882960831
```

```
[7]: plt.scatter(X, Y, color='red', label='Observations (with noise)')
     plt.plot(X, Y_groundtruth, color='red', linestyle='dashed',␣
       ↪label=f'Groundtruth')
     plt.plot(X, Y_OLS, marker='x', color='blue', label=f'Fit with $R^2={Rsquared:.
       ↪2f}$')
```

```
plt.xlabel('X')
plt.ylabel('Y')
plt.legend()
plt.show()
```



What happens if you have more "flexible models" at your disposal? In the following, we try to fit our observed responses Y with a polynomial model of the form

$$\begin{aligned} Y &= X_{\text{poly}} w + \epsilon & (5) \\ &= x \cdot w_1 + x^2 \cdot w_2 + x^3 \cdot w_3 + ... + x^7 \cdot w_7 + x^8 \cdot w_8 + \epsilon & (6) \end{aligned}$$

and create a hundred test datapoints.

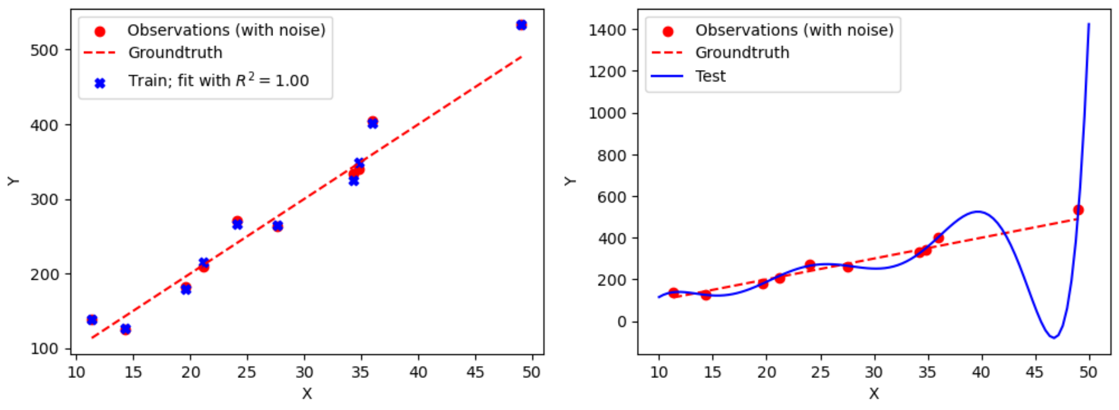
[8]:
```
X_poly = np.hstack((X, X ** 2, X ** 3, X ** 4, X ** 5, X ** 6, X ** 7, X ** 8))
print(X_poly.shape)

X_test = np.linspace(10,50,100).reshape(-1, 1)
X_test = np.hstack((X_test, X_test ** 2, X_test ** 3, X_test ** 4, X_test ** 5,␣
 ↪X_test ** 6, X_test ** 7, X_test ** 8))
```

```
(10, 8)
```

Let's see the OLS solution for that case:

```
[9]: XT = np.transpose(X_poly)
XTX_inverse = np.linalg.inv(XT @ X_poly)

w_OLS = XTX_inverse @ XT @ Y

print(f"Solution w_OLS = {w_OLS.squeeze()}")

Y_OLS = X_poly @ w_OLS
Y_OLS_test = X_test @ w_OLS

Rsquared = 1 - np.sum((Y - Y_OLS)**2) / np.sum((Y - np.mean(Y))**2)

fig, axs = plt.subplots(1,2, figsize=(12,4))

axs[0].scatter(X, Y, marker='o', color='red', label='Observations (with noise)')
axs[0].plot(X, Y_groundtruth, color='red', linestyle='dashed',␣
 ↪label=f'Groundtruth')
axs[0].scatter(X, Y_OLS, color='blue', marker='X', label=f'Train; fit with␣
 ↪$R^2={Rsquared:.2f}$')

axs[1].scatter(X, Y, marker='o', color='red', label='Observations (with noise)')
axs[1].plot(X, Y_groundtruth, color='red', linestyle='dashed',␣
 ↪label=f'Groundtruth')
axs[1].plot(X_test[:,0], Y_OLS_test, color='blue', label=f'Test')

axs[0].set_xlabel('X')
axs[0].set_ylabel('Y')
axs[0].legend()

axs[1].set_xlabel('X')
axs[1].set_ylabel('Y')
axs[1].legend()

plt.show()
```

```
Solution w_OLS = [-7.51361688e+02  2.58039804e+02 -3.52312965e+01
2.52092835e+00
 -1.02591682e-01  2.38611218e-03 -2.95006259e-05  1.50176370e-07]
```



1.2 Ridge Regression

Ridge regression adds an additional assumption on (the distribution of) weights w. We rewrite the loss as

$$\text{Loss}(w) = \frac{1}{2N}\|Y - Xw\|_2^2 + \frac{1}{2}\lambda'\|w\|_2^2 = \frac{1}{2N}\sum_{n=1}^{N}(y_n - x_n \cdot w)^2 + \frac{1}{2}\lambda'\sum_{i=1}^{d_x} w_i^2 \tag{7}$$

where the minimisation also takes into account the value (norm) of the weights w_i. Here, d_x indicates the dimensions of our input X, e.g. $d_x = 8$ in the case of the polynomial model above. The solution to this minimisation is given by

$$w_{\text{ridge}} = \left(\lambda \mathbb{1}_{d_x} + X^\top X\right)^{-1} X^\top Y. \tag{8}$$

Let's see what happens with this additional term:

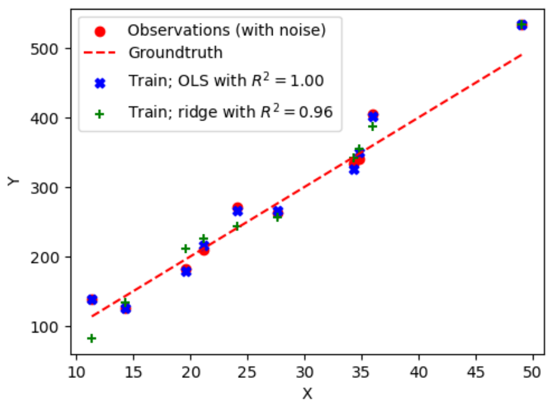
[10]:
```
lambda_ridge = 100000

XT = np.transpose(X_poly)
XTX_ridge_inverse = np.linalg.inv(XT @ X_poly + lambda_ridge * np.
  ↪identity(X_poly.shape[1]))

w_ridge = XTX_ridge_inverse @ XT @ Y

print(f"Solutions: \n w_OLS = \t {w_OLS.squeeze()},\n w_ridge = \t {w_ridge.
  ↪squeeze()}.")
```

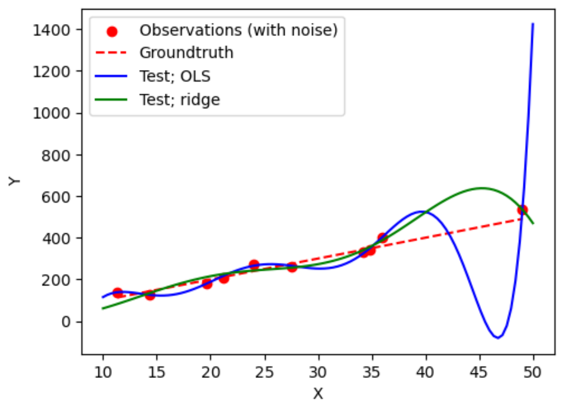
```
Solutions:
 w_OLS =          [-7.51361688e+02  2.58039804e+02 -3.52312965e+01
2.52092835e+00
```

```
 -1.02591682e-01  2.38611218e-03 -2.95006259e-05  1.50176370e-07],
 w_ridge =       [ 2.47916087e-03  1.58956294e-02  6.22240928e-02
4.74477726e-03
 -7.57974697e-04  3.01976372e-05 -4.90619797e-07  2.84986624e-09].
```

[11]:
```
Y_ridge = X_poly @ w_ridge
Y_ridge_test = X_test @ w_ridge

Rsquared_ridge = 1 - np.sum((Y - Y_ridge)**2) / np.sum((Y - np.mean(Y))**2)

print(Rsquared_ridge)

fig, axs = plt.subplots(1,2, figsize=(12,4))

axs[0].scatter(X, Y, marker='o', color='red', label='Observations (with noise)')
axs[0].plot(X, Y_groundtruth, color='red', linestyle='dashed',␣
 ↪label='Groundtruth')
axs[0].scatter(X, Y_OLS, color='blue', marker='X', label=f'Train; OLS with␣
 ↪$R^2={Rsquared:.2f}$')
axs[0].scatter(X, Y_ridge, color='green', marker='+', label=f'Train; ridge with␣
 ↪$R^2={Rsquared_ridge:.2f}$')

axs[1].scatter(X, Y, marker='o', color='red', label='Observations (with noise)')
axs[1].plot(X, Y_groundtruth, color='red', linestyle='dashed',␣
 ↪label='Groundtruth')
axs[1].plot(X_test[:,0], Y_OLS_test, color='blue', label=f'Test; OLS')
axs[1].plot(X_test[:,0], Y_ridge_test, color='green', label=f'Test; ridge')


axs[0].set_xlabel('X')
axs[0].set_ylabel('Y')
axs[0].legend()

axs[1].set_xlabel('X')
axs[1].set_ylabel('Y')
axs[1].legend()

plt.show()
```

```
0.9604147031322375
```





Note that the additional term $\lambda\|w\|_2^2 = \lambda\sum_{i=1}^{d_x=8} w_i^2$ in the loss function enables deviation from the observed noisy datapoints. That is models (i.e. weights w_i) which too closely *overfit* to the noisy observations are penalised. Parameter λ serves as a **penalty factor** biasing towards *simpler* models which **reduce overfitting**.

Generally, having terms in your loss function favouring simpler models is referred to as **regularisation** (Wikipedia). Highly-flexible models (like the blue curve in the next figure) allow fitting observations (red dots) arbitrary well. Typically, we prefer to choose simpler models (like the green curve) which usually provide better predictions to new, unseen data (**generalisation**).

Image source: Wikipedia

1.3 Using scikit-learn for Regression

You don't need to do all the work yourself! `scikit-learn` offers you the required functionality with the functions LinearRegression and Ridge!

[12]:
```
from sklearn.linear_model import LinearRegression, Ridge

linreg = LinearRegression(fit_intercept=False)
linreg.fit(X,Y)
```

[12]:
```
LinearRegression(fit_intercept=False)
```

Note that we used `fit_intercept=False` because we chose to neglect on off-set / intercept b on the y-axis. That is, we consider $Y = Xw + b + \epsilon$ with $b = 0$, which simplifies writing the equations out.

`linreg` is the linear fit which provides you the same OLS solution as seen above.

[13]:
```
w_OLS_sk = linreg.coef_
Y_OLS_sk = linreg.predict(X)
```

```
Rsquared_sk = linreg.score(X,Y)

print(f"w_OLS_sk = {w_OLS_sk.squeeze()}, Rsquared_sk = {Rsquared_sk}")
```

```
w_OLS_sk = 10.375338325958642, Rsquared_sk = 0.965593882960831
```

We can do the same for the ridge regression case.

[14]:
```
ridgereg = Ridge(fit_intercept=False)
ridgereg.fit(X,Y)

w_ridge_sk = ridgereg.coef_
Y_ridge_sk = ridgereg.predict(X)
Rsquared_ridge_sk = ridgereg.score(X,Y)

print(f"w_ridge_sk = {w_ridge_sk.squeeze()}, Rsquared_ridge_sk = {Rsquared_sk}")
```

```
w_ridge_sk = 10.374130258658917, Rsquared_ridge_sk = 0.965593882960831
```

1.4 Logistic Regression for Classification

Next, we consider binary classification where our data falls into one of two classes which we will denote with class labels $Y = 0$ (class 1) and $Y = 1$ (class 2). Let's assume that observations of class 2 occur with an unkown probability of p_2. As we only have to classes, the probablity for class 1 is $p_1 = 1 - p_2$. A natural choice in such a setting is the **Bernoulli distribution** (Wikipedia) with probability (mass) function

$$p(Y) = p_2^Y p_1^{1-Y} = p_2^Y (1 - p_2)^{1-Y}. \tag{9}$$

The idea of logistic regression is to approximate the ratio of the two class probabilites with an exponential function of the form

$$\frac{p_2}{p_1} = \exp(x_1 \cdot w_1 + x_2 \cdot w_1 \cdot w_2 + ... + x_{d_x} \cdot w_{d_x}) = \exp(Xw), \tag{10}$$

so again a linear model! Note that we can write this as

$$\exp(Xw) = \frac{p_2}{1 - p_2} \Rightarrow p_2 = \frac{1}{1 + \exp(-Xw)}. \tag{11}$$

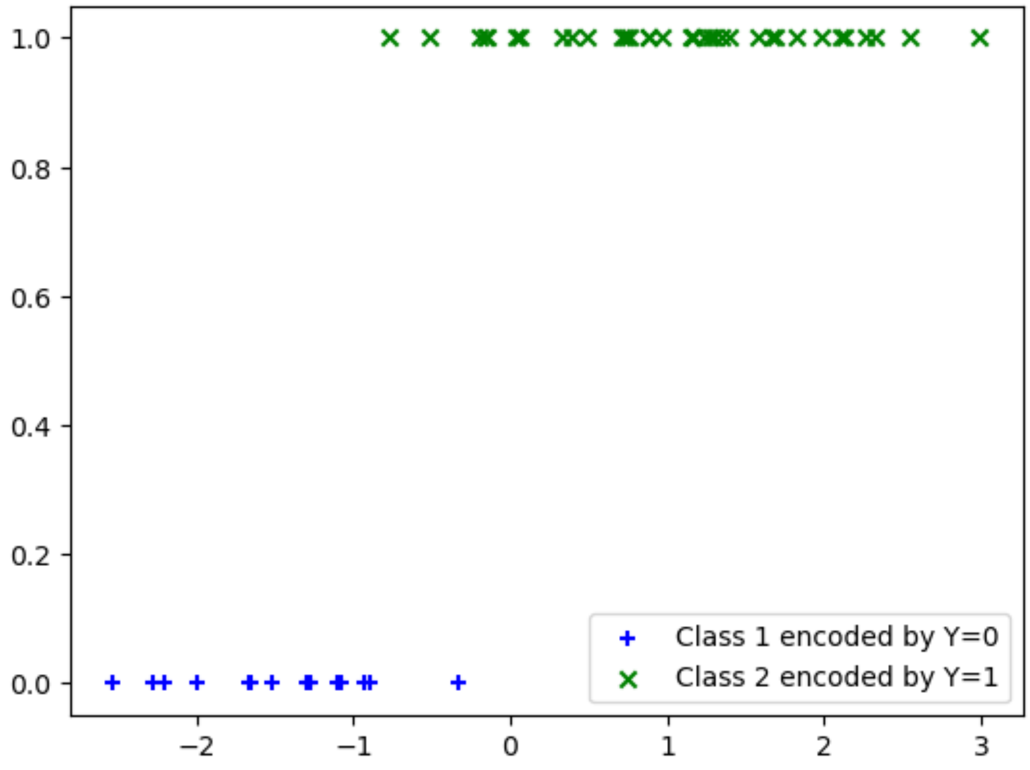
This is the **logistic function**. In order to identify the weights w, i.e. a matching model, we use the **logistic loss** (also known as **negative log-likelihood** or **cross entropy loss**, depending on the context)

$$\text{Loss}(w) = -Y\log p_2 - (1-Y)\log(1-p_2) = -\sum_{n=1}^{N} y_n \log\frac{1}{1+\exp(-x_n\cdot w)} + (1-y_n)\log\left(1-\frac{1}{1+\exp(-x_n\cdot w)}\right) \tag{12}$$

for N datapoints.

Let's create a simple binary classification problem with 50 datapoints.

[15]:
```
from sklearn.datasets import make_classification

num_datapoints = 50

X, Y = make_classification(n_samples=num_datapoints, n_features=1,␣
 ↪n_informative=1, n_redundant=0,
                           n_classes=2, n_clusters_per_class=1, weights=[0.3, 0.
 ↪7],
                           random_state=0)

plt.scatter(X[Y == 0], Y[Y == 0], color='blue', marker='+', label='Class 1␣
 ↪encoded by Y=0')
plt.scatter(X[Y == 1], Y[Y == 1], color='green', marker='x', label='Class 2␣
 ↪encoded by Y=1')
plt.legend()
plt.show()
```



Here we directly use `scikit-learn` function LogisticRegression.

```
[16]: from sklearn.linear_model import LogisticRegression

      logreg = LogisticRegression()
      logreg.fit(X, Y)
```

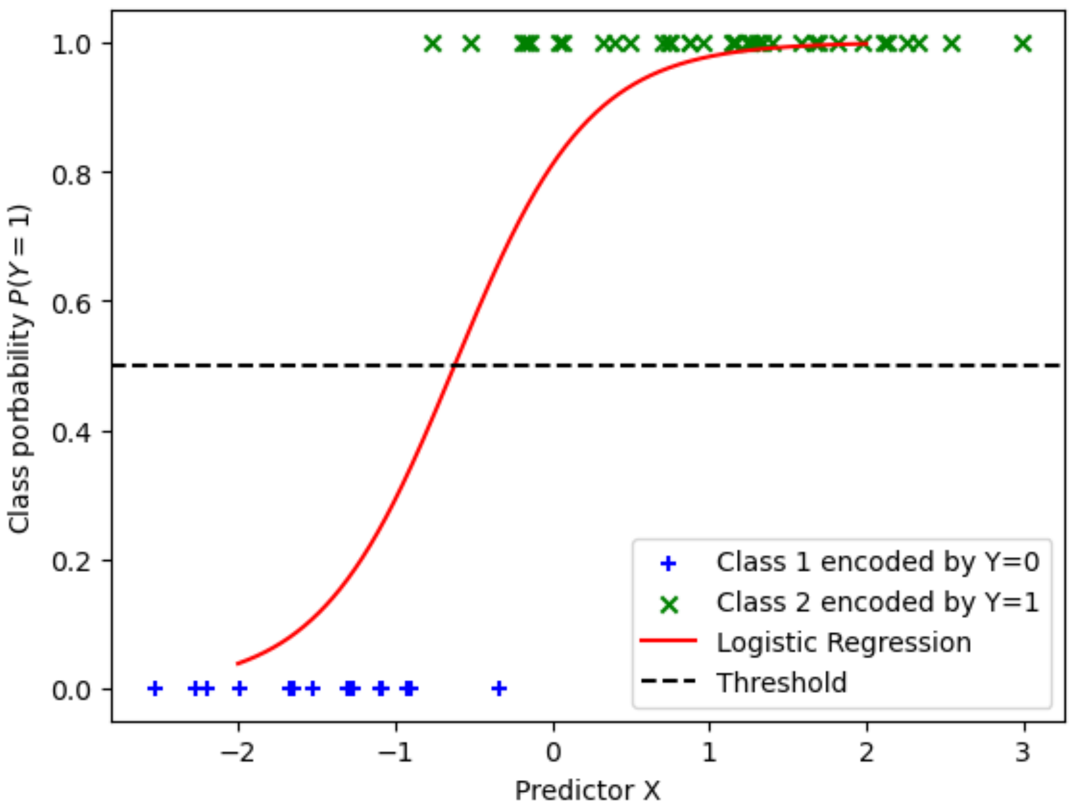
```
[16]: LogisticRegression()
```

Using the method `predict_proba` allows predicting the probability $p(Y = 1)$ for class 2 of our logistic regression model `logreg`.

```
[17]: X_logreg = np.linspace(-2, 2, 1000).reshape(-1, 1)
      Y_logreg = logreg.predict_proba(X_logreg)
```

Let's plot the result:

```
[18]: plt.scatter(X[Y == 0], Y[Y == 0], color='blue', marker='+', label='Class 1␣
        ↪encoded by Y=0')
      plt.scatter(X[Y == 1], Y[Y == 1], color='green', marker='x', label='Class 2␣
        ↪encoded by Y=1')
      plt.plot(X_logreg[:, 0], Y_logreg[:, 1], color='red', label='Logistic␣
        ↪Regression')
      plt.axhline(0.5, color='black', linestyle='--', label='Threshold')

      plt.xlabel('Predictor X')
      plt.ylabel(r'Class porbability $P(Y=1)$')
      plt.legend()
      plt.show()
```



1.5 Decision Trees and Random Forests

An more classical approach to classification problems are decision trees. In the next example, we will try to classify premium red wine from their measured propertes / features which serve as the predictors / covariates.

[19]:
```python
import pandas as pd
import matplotlib.pyplot as plt

wine_data = pd.read_csv('data/winequality-red.csv', sep=';')

# quality_threshold = 6
quality_threshold = 5

wine_data['premium'] = wine_data['quality'] > quality_threshold

wine_data
```

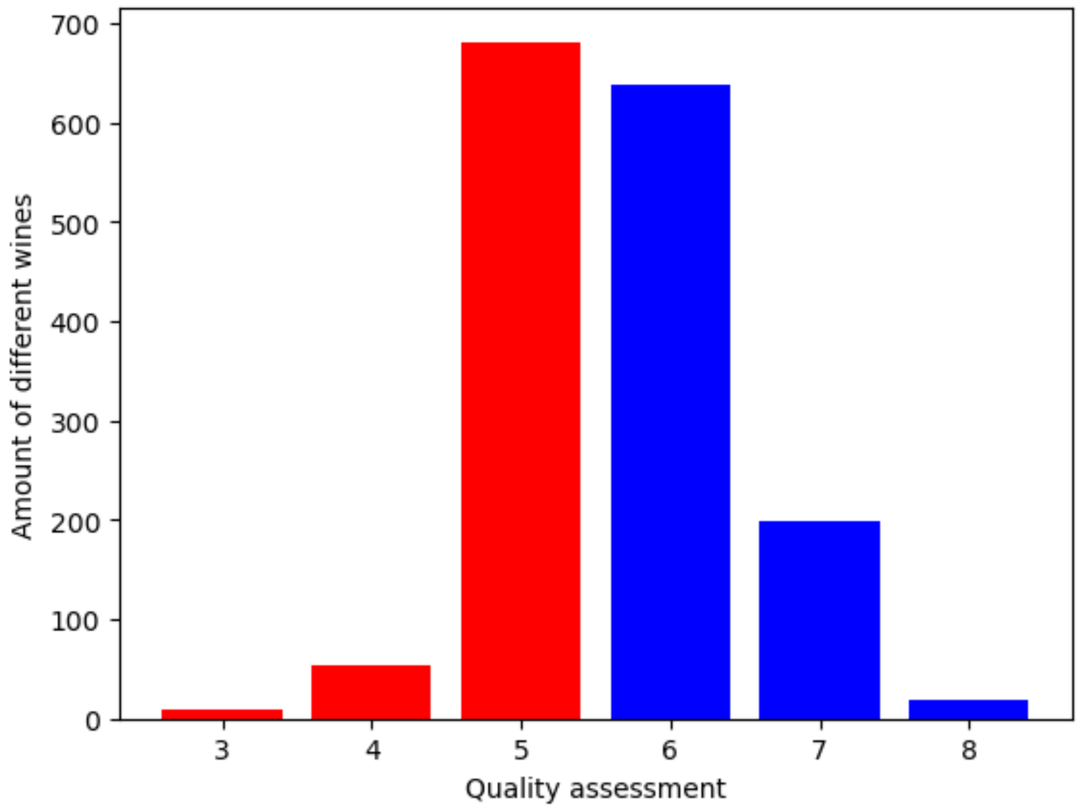
[19]:
```
      fixed acidity  volatile acidity  citric acid  residual sugar  chlorides  \
0               7.4             0.700         0.00             1.9      0.076
1               7.8             0.880         0.00             2.6      0.098
2               7.8             0.760         0.04             2.3      0.092
3              11.2             0.280         0.56             1.9      0.075
4               7.4             0.700         0.00             1.9      0.076
…                 …                 …            …               …          …
1594            6.2             0.600         0.08             2.0      0.090
1595            5.9             0.550         0.10             2.2      0.062
1596            6.3             0.510         0.13             2.3      0.076
1597            5.9             0.645         0.12             2.0      0.075
1598            6.0             0.310         0.47             3.6      0.067

      free sulfur dioxide  total sulfur dioxide  density    pH  sulphates  \
0                    11.0                  34.0  0.99780  3.51       0.56
1                    25.0                  67.0  0.99680  3.20       0.68
2                    15.0                  54.0  0.99700  3.26       0.65
3                    17.0                  60.0  0.99800  3.16       0.58
4                    11.0                  34.0  0.99780  3.51       0.56
…                       …                     …        …     …          …
1594                 32.0                  44.0  0.99490  3.45       0.58
1595                 39.0                  51.0  0.99512  3.52       0.76
1596                 29.0                  40.0  0.99574  3.42       0.75
1597                 32.0                  44.0  0.99547  3.57       0.71
1598                 18.0                  42.0  0.99549  3.39       0.66

      alcohol  quality  premium
0         9.4        5    False
1         9.8        5    False
2         9.8        5    False
3         9.8        6     True
4         9.4        5    False
…           …        …        …
1594     10.5        5    False
1595     11.2        6     True
1596     11.0        6     True
1597     10.2        5    False
1598     11.0        6     True

[1599 rows x 13 columns]
```

We focus on the quality assessment.

[20]:
```
quality_counts = wine_data['quality'].value_counts()

if quality_threshold == 5:
    colours = ['red','blue','blue','red','blue','red']
```

```python
elif quality_threshold == 6:
    colours = ['red','red','blue','red','blue','red']

print(quality_counts)

plt.bar(quality_counts.index, quality_counts, color=colours)
plt.xlabel('Quality assessment')
plt.ylabel('Amount of different wines')
plt.show()
```

```
5    681
6    638
7    199
4     53
8     18
3     10
Name: quality, dtype: int64
```



Perpare the features and target:

[21]:
```
target = wine_data['premium'].astype(int)
wine_features = wine_data.drop( ['quality','premium'], axis=1)

print("Shape of wine_features:\t{}\nShape of target:\t{}\n"
      .format(wine_features.shape, target.shape)
     )

target.head(5)
```

```
Shape of wine_features: (1599, 11)
Shape of target:        (1599,)
```

[21]:
```
0    0
1    0
2    0
3    1
4    0
Name: premium, dtype: int64
```

The Goal is to learn a classifier which predicts whether a wine is a premium / non-premium wine on the basis of the measured wine features.

Select (randomly) a set on which the classifier is calibrated / trained on and a test set on which the performance is assessed. We consider a test set size of 30% of the original data set.

[22]:
```
from sklearn.model_selection import train_test_split

feat_train, feat_test, target_train, target_test = train_test_split(
    wine_features, target, test_size = 0.3, random_state=123)

print("After splitting into train and test sets:\n\n"
      f"Shape of feat_train:\t{feat_train.shape}\nShape of target_train:
 ↪\t{target_train.shape}\n"
      f"Shape of feat_test:\t{feat_test.shape}\nShape of target_test:
 ↪\t{target_test.shape}"
     )
```

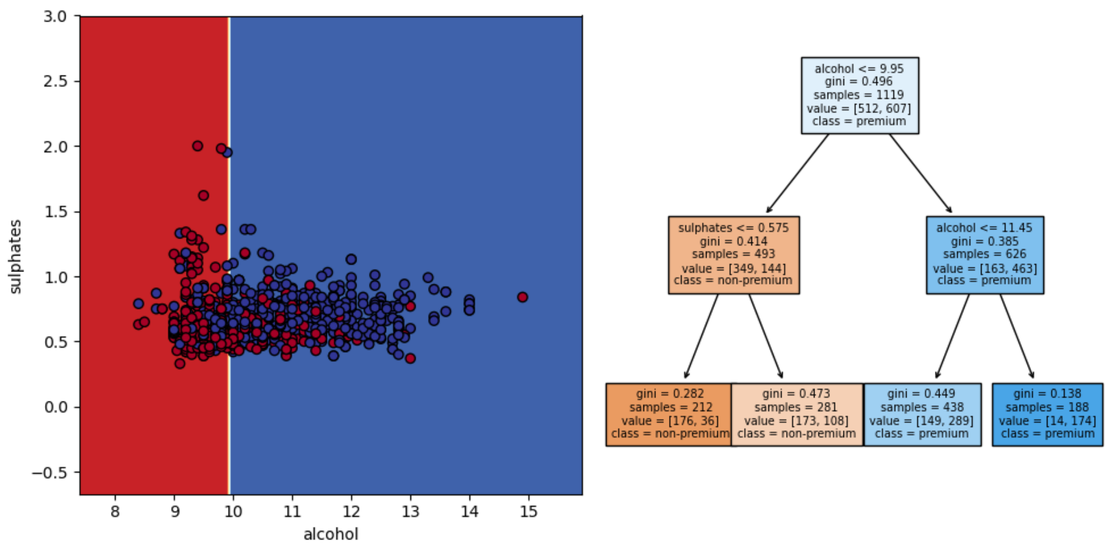
```
After splitting into train and test sets:

Shape of feat_train:    (1119, 11)
Shape of target_train:  (1119,)
Shape of feat_test:     (480, 11)
Shape of target_test:   (480,)
```

We have a first look on a decision tree and just consider the features providing the `alcohol` and `sulphates` content. We use the DecisionTreeClassifier.

[23]:
```
from sklearn.tree import DecisionTreeClassifier, plot_tree

feat_train_subset = feat_train[ ['alcohol','sulphates'] ]

wine_tree = DecisionTreeClassifier(max_depth=2)
wine_tree.fit(feat_train_subset, target_train)
```

[23]:
```
DecisionTreeClassifier(max_depth=2)
```

[24]:
```
fig, axs = plt.subplots(1,2, figsize=(10,5))

try:
    from sklearn.inspection import DecisionBoundaryDisplay

    display = DecisionBoundaryDisplay.from_estimator(
        wine_tree,
        feat_train_subset,
        cmap='RdYlBu',
        response_method="predict",
        ax=axs[0],
        xlabel='alcohol',
        ylabel='sulphates',
    )
except:
    print("Sorry, the library for plotting the decision "
          "boundary is currently missing")

plot_tree(wine_tree, max_depth=2,
          feature_names=['alcohol','sulphates'],
          class_names=['non-premium','premium'],
          ax=axs[1], fontsize=7, filled = True,
         )


axs[0].scatter(feat_train['alcohol'], feat_train['sulphates'],
               c=target_train, cmap='RdYlBu', edgecolor='black'
              )

plt.tight_layout()
plt.show()
```

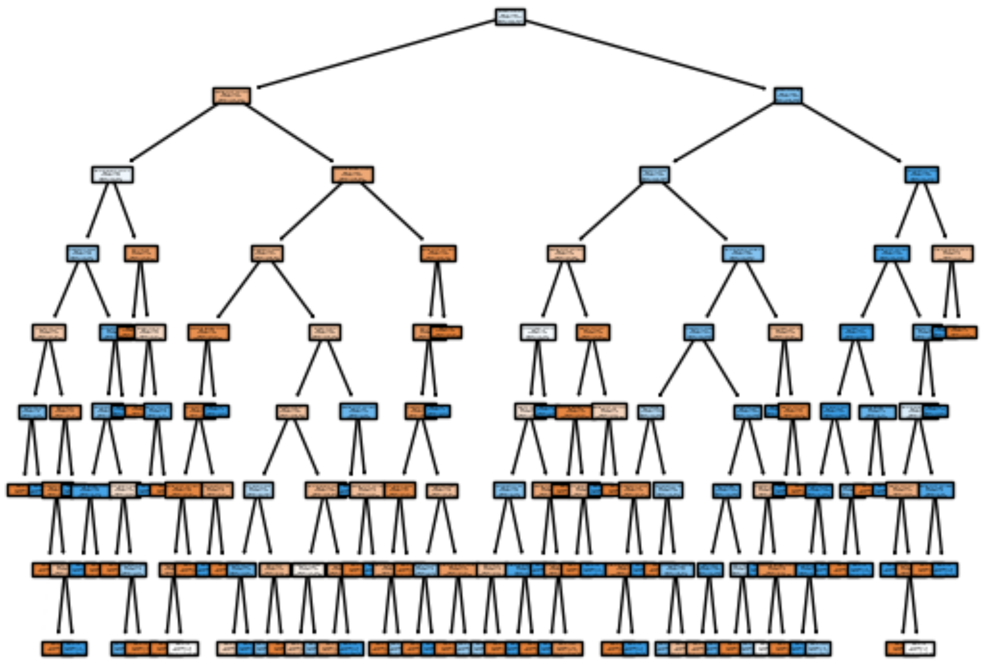


Note that decision trees partition the input space into different regions with **decision boundaries** separating different classes, like premium wines (blue data / region) and non-premium wines (red data / region)!

Now let's consider the full dataset!

[25]:
```
tree_height = 8

wine_tree = DecisionTreeClassifier(max_depth=tree_height)
wine_tree.fit(feat_train, target_train)

correct_pred = wine_tree.predict(feat_test) == target_test

correct = correct_pred.value_counts()

accuracy = (correct[True] / (correct[True] + correct[False]))*100
print(f"The random forest identified premium / non-premium wines with␣
 ↪{accuracy}% accuracy!")

plot_tree(wine_tree,
          feature_names=wine_features.columns,
          class_names=['non-premium','premium'],
          filled = True,
         )
plt.show()
```

```
The random forest identified premium / non-premium wines with 71.66666666666667%
accuracy!
```



You can learn more on decision trees from scikit-learn and the mathematical criteria for the decision splits.

Random Forests are now very powerful machine learning methods which build on decision trees. Random Forests construct a multitude of decision trees like the one above. The individual decision trees provide a classification result and by majority voting the final classification is obtained. We use the RandomForestClassifier.

[26]:
```
from sklearn.ensemble import RandomForestClassifier

num_trees = 100
tree_height = 8

wine_forest = RandomForestClassifier(n_estimators=num_trees,
                                     max_depth=tree_height,
                                     random_state=123)
wine_forest.fit(feat_train, target_train)
```

[26]:
```
RandomForestClassifier(max_depth=8, random_state=123)
```

[27]:
```
correct_pred = wine_forest.predict(feat_test) == target_test

correct = correct_pred.value_counts()
```

```
accuracy = (correct[True] / (correct[True] + correct[False]))*100
print(f"The random forest identified premium / non-premium wines with␣
  ↪{accuracy}% accuracy!")
```

```
The random forest identified premium / non-premium wines with 78.125% accuracy!
```

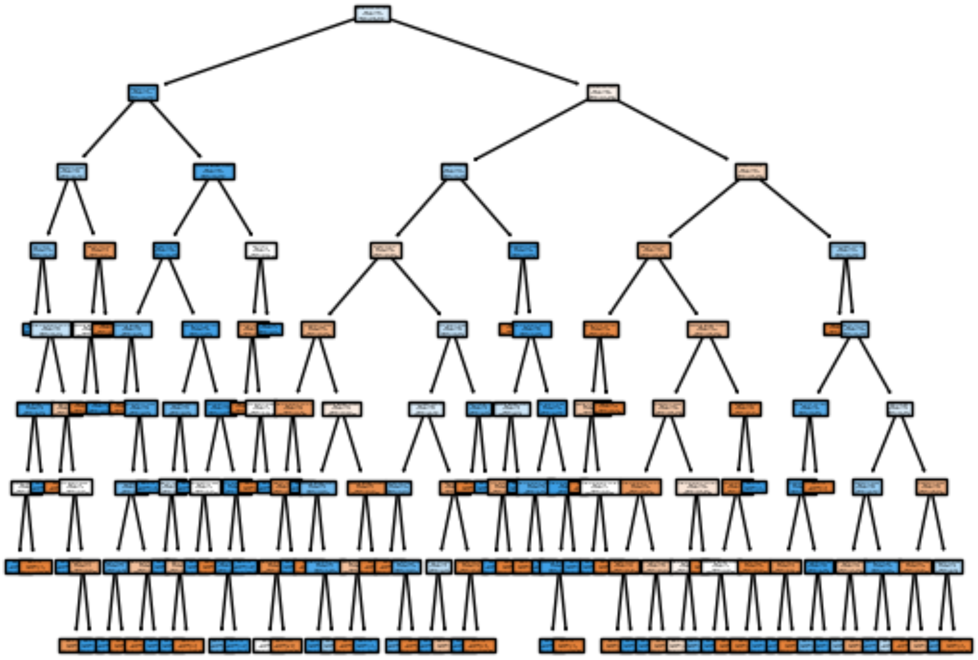
That's a great accuracy! But let's check what is actually predicted wrongly:

[28]:
```
rel_incorrect_pred = target_test[correct_pred == False].value_counts() /␣
  ↪target_test.value_counts()

print(f"Incorrect predictions by premium quality:\n{rel_incorrect_pred}")
print(f"\nRatio of premium / non-premium wines in test set:\n{target_test.
  ↪value_counts(normalize=True)}")
print(f"\nRatio of premium / non-premium wines in train set:\n{target_train.
  ↪value_counts(normalize=True)}")
```

```
Incorrect predictions by premium quality:
0    0.275862
1    0.165323
Name: premium, dtype: float64

Ratio of premium / non-premium wines in test set:
1    0.516667
0    0.483333
Name: premium, dtype: float64

Ratio of premium / non-premium wines in train set:
1    0.542449
0    0.457551
Name: premium, dtype: float64
```

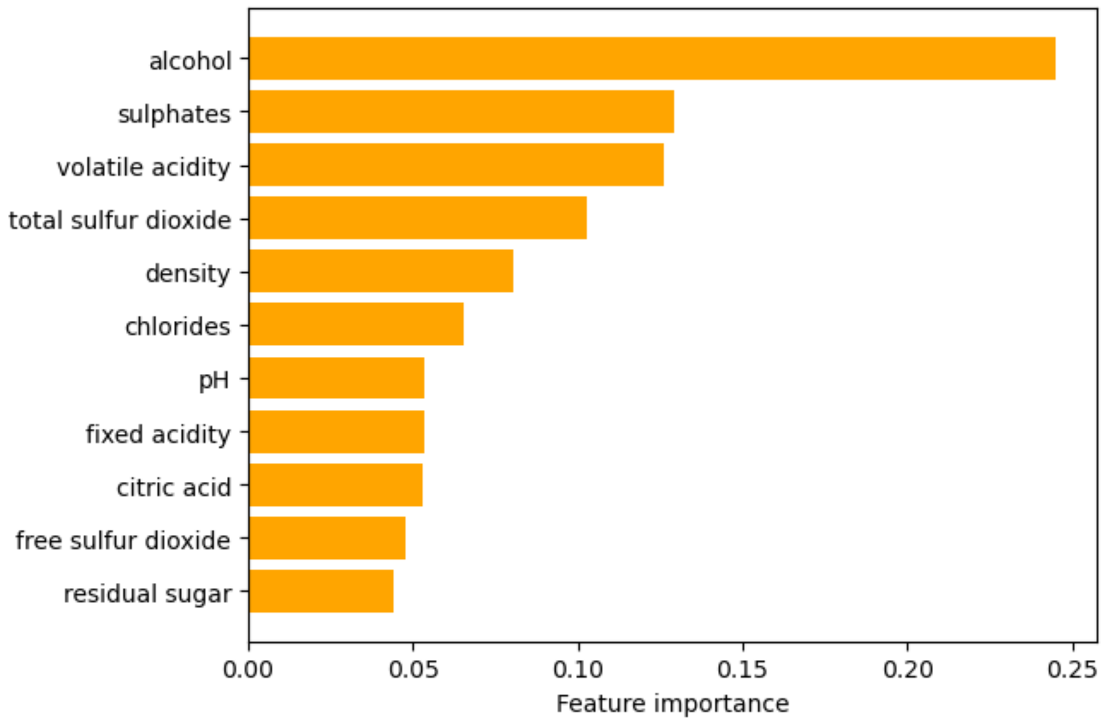
You can still plot one of the trees!

[29]:
```
single_tree = wine_forest.estimators_[5]

plot_tree(single_tree,
          feature_names=wine_features.columns,
          class_names=['non-premium','premium'],
          filled = True,
         )

plt.show()
```



However, this is less insightful, as the decision is made by vote of many (different) trees! Still, we can study the **feature importance score**:

```
[30]: feature_scores = wine_forest.feature_importances_
feature_names = list(wine_features.columns)

important_features = pd.Series(feature_scores, index=feature_names).
 ↪sort_values()

plt.barh(important_features.index, important_features, color='Orange')
plt.xlabel('Feature importance')
plt.show()
```



1.6 Exercise Section

(1.) In this exercise, we train a `Ridge` regressor for predicting the `quality` values on the test set `feat_test`. First, load the following cell:

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

from sklearn.model_selection import train_test_split

wine_data = pd.read_csv('data/winequality-red.csv', sep=';')

ex_target = wine_data['quality']
ex_features = wine_data.drop(['quality'], axis=1)

feat_train, feat_test, target_train, target_test = train_test_split(
    ex_features, ex_target, test_size = 0.3, random_state=123)
```

[ ]:
```
feat_train.head(5)
```

[ ]:
```
target_train.head(5)
```

Put your result in the next cell and use `ex_pred_ridge` for the predicted quality values.

```
[ ]: from sklearn.linear_model import Ridge

     # Fill in

     ex_pred_ridge = # Fill in
```

Execute the next cell to save the results in a summary data frame.

```
[ ]: target_test = target_test.to_frame()
     target_test['Ridge_predicted_quality'] = np.around(ex_pred_ridge, decimals=2)
     target_test['Ridge_absolut_deviation'] = abs(target_test['quality'] -␣
      ↪target_test['Ridge_predicted_quality'])
     target_test
```

(2.) You can create a Random Forest not only for classification, but also regression. Make use of the `scikit-learn` method

```
[ ]: from sklearn.ensemble import RandomForestRegressor
```

to make predictions on the wine quality based on the other features / predictors. Load the previous cell and train a the `RandomForestRegressor` for predicting the quality values on the test set `feat_test`. Put your result in the next cell and use `ex_pred_RF` for the predicted quality values.

Hint: You might want to revisit the steps for RF classification we saw above.

```
[ ]: num_trees = 100
     tree_height = 8

     # Fill in

     ex_pred_RF = # Fill in
```

```
[ ]: target_test['RF_predicted_quality'] = np.around(ex_pred_RF, decimals=2)
     target_test['RF_absolut_deviation'] = abs(target_test['quality'] -␣
      ↪target_test['RF_predicted_quality'])
     target_test
```

Finally, compare how the Random Forest and ridge regressor performed in comparison. For this, just execute the next cell.

```
[ ]: RF_pred_MSE = (target_test['RF_absolut_deviation']**2).mean()
     Ridge_pred_MSE = (target_test['Ridge_absolut_deviation']**2).mean()

     print(f"Mean squared error of RandomForestRegressor: {RF_pred_MSE:.2f}")
     print(f"Mean squared error of Ridge: {Ridge_pred_MSE:.2f}")
```

1.7 Proposed Solutions

(1.) In this exercise, we train a `Ridge` regressor for predicting the `quality` values on the test set `feat_test`. First, load the following cell:

```
[31]: import numpy as np
      import pandas as pd
      import matplotlib.pyplot as plt

      from sklearn.model_selection import train_test_split

      wine_data = pd.read_csv('data/winequality-red.csv', sep=';')

      ex_target = wine_data['quality']
      ex_features = wine_data.drop(['quality'], axis=1)

      feat_train, feat_test, target_train, target_test = train_test_split(
          ex_features, ex_target, test_size = 0.3, random_state=123)
```

Put your result in the next cell and use `ex_pred_ridge` for the predicted quality values.

```
[32]: from sklearn.linear_model import Ridge

      ridgereg = Ridge()
      ridgereg.fit(feat_train, target_train)

      ex_pred_ridge = ridgereg.predict(feat_test)

      print(f"Rsquared_ridgereg: {ridgereg.score(feat_train, target_train)}")
```

```
Rsquared_ridgereg: 0.3627326339932849
```

Execute the next cell to save the results in a summary data frame.

```
[33]: target_test = target_test.to_frame()
      target_test['Ridge_predicted_quality'] = np.around(ex_pred_ridge, decimals=2)
      target_test['Ridge_absolut_deviation'] = abs(target_test['quality'] -␣
       ↪target_test['Ridge_predicted_quality'])
      target_test
```

```
[33]:       quality  Ridge_predicted_quality  Ridge_absolut_deviation
      912         6                     6.32                     0.32
      772         5                     4.97                     0.03
      1037        5                     4.77                     0.23
      1106        6                     6.57                     0.57
      263         5                     5.51                     0.51
      …         …                      …                        …
      1466        7                     5.57                     1.43
      580         5                     5.32                     0.32
```

```
1082        6                      5.40                       0.60
1279        7                      6.31                       0.69
1155        5                      5.32                       0.32

[480 rows x 3 columns]
```

(2.) You can create a Random Forest not only for classification, but also regression. Make use of the `scikit-learn` method

[34]:
```
from sklearn.ensemble import RandomForestRegressor
```

to make predictions on the wine quality based on the other features / predictors. Load the previous cell and train a the `RandomForestRegressor` for predicting the quality values on the test set `feat_test`. Put your result in the next cell and use `ex_pred_RF` for the predicted quality values.

Hint: You might want to revisit the steps for RF classification we saw above.

[35]:
```
num_trees = 100
tree_height = 8

ex_forest = RandomForestRegressor(n_estimators=num_trees,␣
 ↪max_depth=tree_height, random_state=123)
ex_forest.fit(feat_train, target_train)
ex_pred_RF = ex_forest.predict(feat_test)

print(f"Rsquared_RF: {ex_forest.score(feat_train, target_train)}")
```

```
Rsquared_RF: 0.7545065944574373
```

[36]:
```
target_test['RF_predicted_quality'] = np.around(ex_pred_RF, decimals=2)
target_test['RF_absolut_deviation'] = abs(target_test['quality'] -␣
 ↪target_test['RF_predicted_quality'])
target_test
```

[36]:
```
      quality  Ridge_predicted_quality  Ridge_absolut_deviation  \
912         6                     6.32                     0.32
772         5                     4.97                     0.03
1037        5                     4.77                     0.23
1106        6                     6.57                     0.57
263         5                     5.51                     0.51
…       …                      …                       …
1466        7                     5.57                     1.43
580         5                     5.32                     0.32
1082        6                     5.40                     0.60
1279        7                     6.31                     0.69
1155        5                     5.32                     0.32

      RF_predicted_quality  RF_absolut_deviation
```

```
912                 6.41                0.41
772                 5.10                0.10
1037                4.98                0.02
1106                6.44                0.44
263                 5.73                0.73
…                  …                  …
1466                5.84                1.16
580                 4.98                0.02
1082                5.49                0.51
1279                6.41                0.59
1155                5.18                0.18

[480 rows x 5 columns]
```

Finally, compare how the Random Forest and ridge regressor performed in comparison. For this, just execute the next cell.

[37]:
```
RF_pred_MSE = (target_test['RF_absolut_deviation']**2).mean()
Ridge_pred_MSE = (target_test['Ridge_absolut_deviation']**2).mean()

print(f"Mean squared error of RandomForestRegressor: {RF_pred_MSE:.2f}")
print(f"Mean squared error of Ridge: {Ridge_pred_MSE:.2f}")
```

```
Mean squared error of RandomForestRegressor: 0.34
Mean squared error of Ridge: 0.42
```

3-Dim_Reduction_Clustering

March 24, 2023

1 3. Dimensionality Reduction and Clustering

In the previous notebook, we could rely on labels which supervised the learning algorithm. Next, we consider the unsupervised setting and knowledge discovery. We focus on the idea of identifying a subset of relevant dimensions which capture the most variation in the data. This is closely related to the idea of compression.

In this notebook, we cover

- Principal Component Analysis (PCA) for dimensionality reduction (with a finance application)
- k-means clustering
- Gaussian Mixture Models (GMMs)

and apply these techniques to simulated data and two dataset examples (digit recognition and financial data).

Keywords: `MNIST`, `np.linalg.eig`, `sklearn.decomposition.PCA`, `sklearn.cluster.KMeans`, `sklearn.mixture.GaussianMixture`

1.1 Dimensionality Reduction

The topic of dimensionality reduction plays a vital role in Machine Learning. Typically, our datasets collect a great number of predictors or covariates or consist of images with hundreds of pixels. Getting an idea of the input space and relevant features is challenging in these high-dimensional problems. Three main use cases include:

1. **Identifying relevant features / dimensions** in the input space which as much as possible preserves the variance in the data. In the following simplified example, the black arrows indicate the dimensions of highest variance:

   The longer arrow can be viewed as the **main direction / dimension of variance** which accounts for about 90% of total variance and thus as the "more relevant" feature.

2. **Data compression**: In many applications we can reduce the number of dimensions to capture the relevant information. In the previous image, we might choose the longer arrow as a compressed version of our data. Another compression example is shown in the next image:

   Here, we encoded an image of Maxim's cat (with an approach called *Fast Fourier Transformation*) into a much lower dimensional compressed image which only requires 9% of pixels compared to the original image. Decoding this compressed image reconstructs the orginial image almost perfectly.

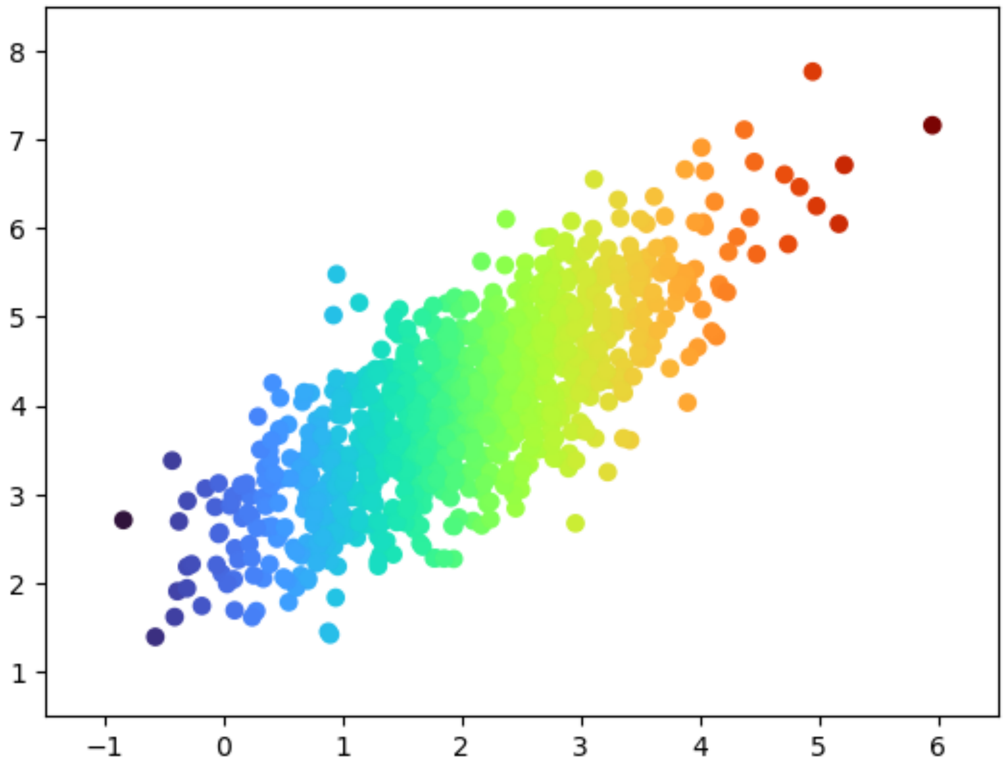
3. **Visualising** high-dimensional data is generally difficult for dimensions larger than 3. Thus, dimensionality reduction is an important tool for visualisation and identifying patterns.

1.2 Principal Component Analysis

Principal Component Analysis (PCA) (Wikipeda) is such a standard technique used for the above purposes and is of great relevance in a great variety of different disciplines.

Let us generate simple 2-dimensional dataset to identify the main dimensions of variation.

[1]:
```
import numpy as np
import matplotlib.pyplot as plt

np.random.seed(123)

num_datapoints = 1000

mu_generation = [2,4]
covariance_matrix_generation = np.array([[1,    0.75],
                                         [0.75, 1,  ]
                                        ])

gauss_2d_rotated = np.random.multivariate_normal(mean=mu_generation,
                                                  ␣
 ↪cov=covariance_matrix_generation,
                                                  size=num_datapoints)

plt.scatter(gauss_2d_rotated[:,0], gauss_2d_rotated[:,1], c=gauss_2d_rotated[:
 ↪,0], cmap='turbo')

plt.ylim(0.5,8.5)
plt.xlim(-1.5,6.5)

plt.show()
```



The fundamental idea of PCA is to perform an eigendecomposition on the data covariance matrix $\mathrm{cov}(X, X)$. If our dataset X is **centered**, i.e. the mean of all datapoints N is 0, we can write the (sample) covariance matrix as

$$\mathrm{cov}(X, X) = \frac{1}{N-1} X X^{\top}. \tag{1}$$

The corresponding eigenvectors to the largest eigenvalues of this matrix provide the main axes of variation (principle components) in our dataset X.

Let's calculate these for our example and start by centering the dataset.

```
[2]: data_mean = np.mean(gauss_2d_rotated, axis=0)
     data_centered = gauss_2d_rotated - data_mean
```

Next, calculate the eigenvalues and eigenvectors using `np.linalg.eig` and sort them in descending order.

```
[3]: cov_matrix = np.cov(data_centered, rowvar=False)

     eigenvalues, eigenvectors = np.linalg.eig(cov_matrix)

     idx = eigenvalues.argsort()[::-1]
     eigenvalues = eigenvalues[idx]
```

```
eigenvectors = eigenvectors[:, idx]
```

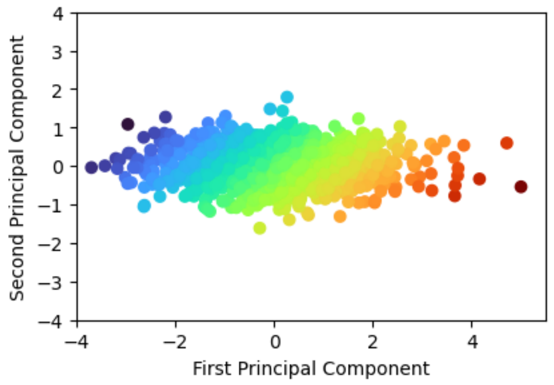
Let's compare the calculated covariance and the covariance matrix we used to generate the data:

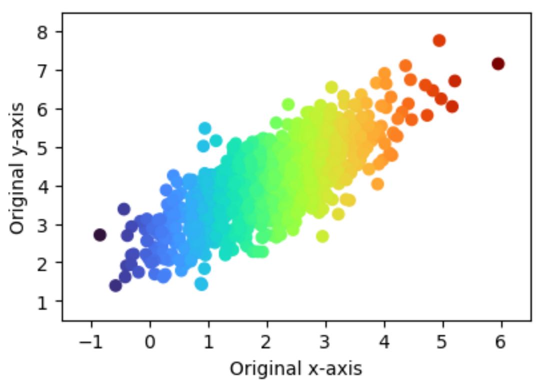
[4]:
```
print(f"Calculated covariance:\n{cov_matrix}\n\nCovariance used for generation:
 ↪\n{covariance_matrix_generation}")
```

```
Calculated covariance:
[[0.98354551 0.74236276]
 [0.74236276 0.97100139]]

Covariance used for generation:
[[1.   0.75]
 [0.75 1.  ]]
```

Choose the two eigenvectors with the highest eigenvalues and project the data onto these vectors. These are our "new" x- and y-axes.

[5]:
```
data_pca_transform = np.dot(data_centered, eigenvectors[:, :2])

fig, axs = plt.subplots(1,2, figsize=(10,3))

axs[0].scatter(data_pca_transform[:, 0], data_pca_transform[:, 1],␣
 ↪c=gauss_2d_rotated[:,0], cmap='turbo')

axs[0].set_xlabel('First Principal Component')
axs[0].set_ylabel('Second Principal Component')
axs[0].set_xlim(-4,5.5)
axs[0].set_ylim(-4,4)

axs[1].scatter(gauss_2d_rotated[:,0], gauss_2d_rotated[:,1],␣
 ↪c=gauss_2d_rotated[:,0], cmap='turbo')

axs[1].set_xlabel('Original x-axis')
axs[1].set_ylabel('Original y-axis')
axs[1].set_ylim(0.5,8.5)
axs[1].set_xlim(-1.5,6.5)

plt.show()
```





Note that in this 2d example, the **projection on the two eigenvectors corresponds to a rotation** of our dataset. This will be different, if the original dataset has more dimensions.

1.2.1 As before, we can just use scikit-learn

and its functionality with the function PCA!

[6]:
```python
from sklearn.decomposition import PCA

num_eigvectors = 2

data_pca = PCA(n_components=num_eigvectors)
data_pca.fit(gauss_2d_rotated)

data_pca_transform = data_pca.transform(gauss_2d_rotated)
```

We can even check the explained variance ratio of the first two principal components:

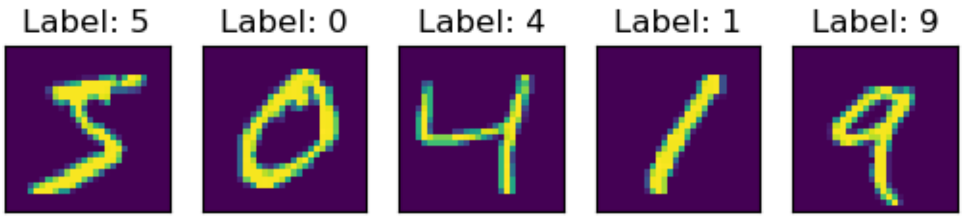
[7]:
```python
print(data_pca.explained_variance_ratio_)
```

```
[0.87982678 0.12017322]
```

1.2.2 MNIST Example

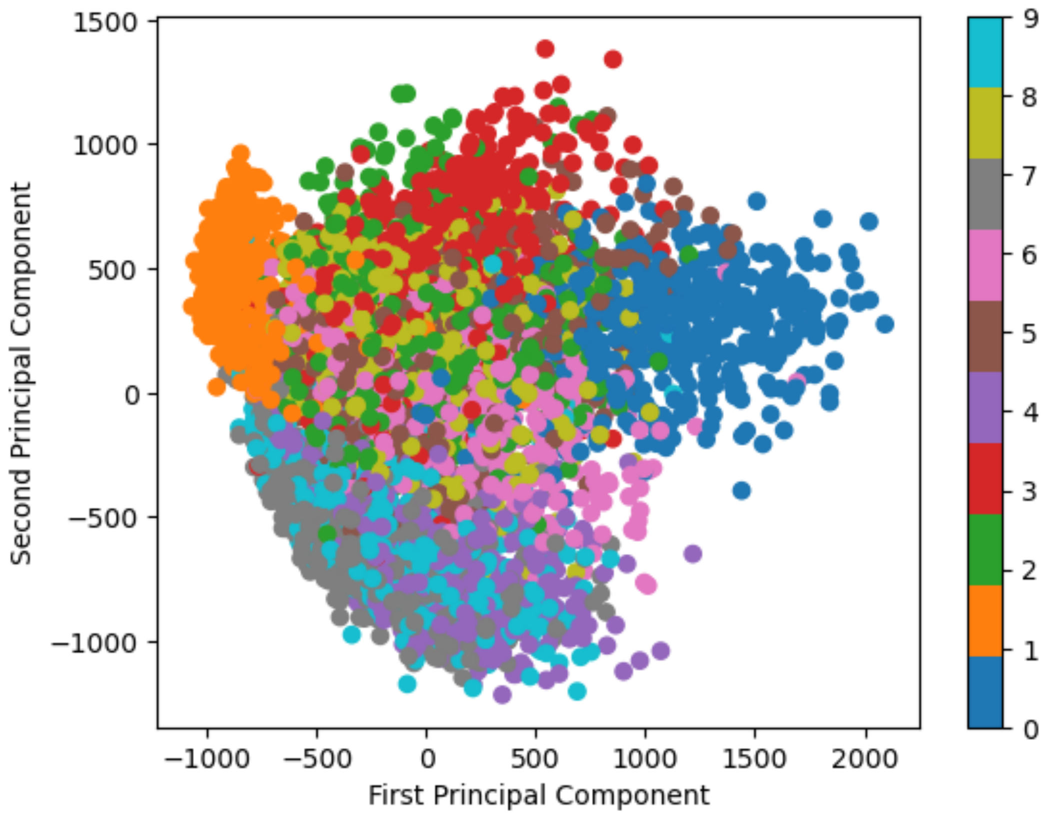
As a first, more interesting example, we examine the MNIST dataset!

[8]:
```python
mnist_data = np.load('data/mnist_data_5k.npy', allow_pickle=True)
mnist_targets = np.load('data/mnist_labels_5k.npy', allow_pickle=True)

fig, axs = plt.subplots(1,5)

for i, ax in enumerate(axs.ravel()):
    ax.imshow(mnist_data[i].reshape(28,28))
    ax.set_title(f"Label: {mnist_targets[i]}")
    ax.set_xticks([])
    ax.set_yticks([])

plt.show()
```



Let's see what the projection on the first two eigenvectors looks like in MNIST:

[9]:
```
data_pca = PCA(n_components=2)
data_pca.fit(mnist_data)
data_pca_transform_mnist = data_pca.transform(mnist_data)

plt.scatter(data_pca_transform_mnist[:, 0], data_pca_transform_mnist[:, 1],␣
  ↪c=mnist_targets, cmap='tab10')
plt.xlabel('First Principal Component')
plt.ylabel('Second Principal Component')
plt.colorbar()
plt.show()
```



The result shows that **similar numbers are clustered** and thus that samples from the **same class share similar features**.

1.2.3 Finance Example

Next, we consider an application in finance in which PCA can help to:

1. Identify clusters of similar assets.
2. Build predictive models where principal components can be used as new variables to predict some quantities.

[10]:
```python
import numpy as np
from sklearn.decomposition import PCA
import matplotlib.pyplot as plt

import pandas as pd
pd.set_option('display.precision', 2)
```

In the first analysis, we consider a portfolio of companies in four industries:

- automotive (‘MBG.DE’, ‘BMW.DE’)
- airlines (‘LHA.DE’, ‘AF.PA’)
- pharmaceuticals (‘BAYN.DE’, ‘NVS’, ‘RO.SW’)

- tech ('AAPL', 'AMZN', 'GOOG')

[11]:
```
portfolio = ['MBG.DE', 'BMW.DE', 'LHA.DE', 'AF.PA',
             'BAYN.DE', 'NVS', 'RO.SW', 'AAPL', 'AMZN', 'GOOG']

toy_df = pd.read_csv('data/finance_toy_data.csv', index_col='Date')
```

[12]:
```
toy_df
```

[12]:
```
            MBG.DE  BMW.DE  LHA.DE  AF.PA  BAYN.DE    NVS   RO.SW    AAPL  \
Date
2016-01-04   50.61   64.88   13.41   7.25    83.98  56.90  216.19   24.07
2016-01-05   50.60   64.58   13.83   7.49    84.13  57.21  219.82   23.47
2016-01-06   49.32   62.44   14.05   7.55    82.92  56.43  217.00   23.01
2016-01-07   47.42   60.09   13.91   7.58    80.81  55.70  214.58   22.04
2016-01-08   46.86   58.68   13.83   7.68    78.58  54.12  210.15   22.16
…              …      …       …      …     …       …       …
2021-12-23   64.87   82.88    6.29   3.96    45.14  79.71  395.23  175.00
2021-12-27   64.68   83.65    6.26   3.93    45.59  80.59  402.45  179.02
2021-12-28   64.41   83.61    6.30   3.94    45.65  81.07  404.21  177.98
2021-12-29   63.15   82.91    6.25   3.89    45.46  81.06  400.89  178.07
2021-12-30   62.55   82.25    6.18   3.88    45.51  80.45  399.13  176.90

              AMZN    GOOG
Date
2016-01-04   31.85   37.09
2016-01-05   31.69   37.13
2016-01-06   31.63   37.18
2016-01-07   30.40   36.32
2016-01-08   30.35   35.72
…              …      …
2021-12-23  171.07  147.14
2021-12-27  169.67  148.06
2021-12-28  170.66  146.45
2021-12-29  169.20  146.50
2021-12-30  168.64  146.00

[1522 rows x 10 columns]
```

We compute the normalised returns as well as the mean return and perform the PCA as before.

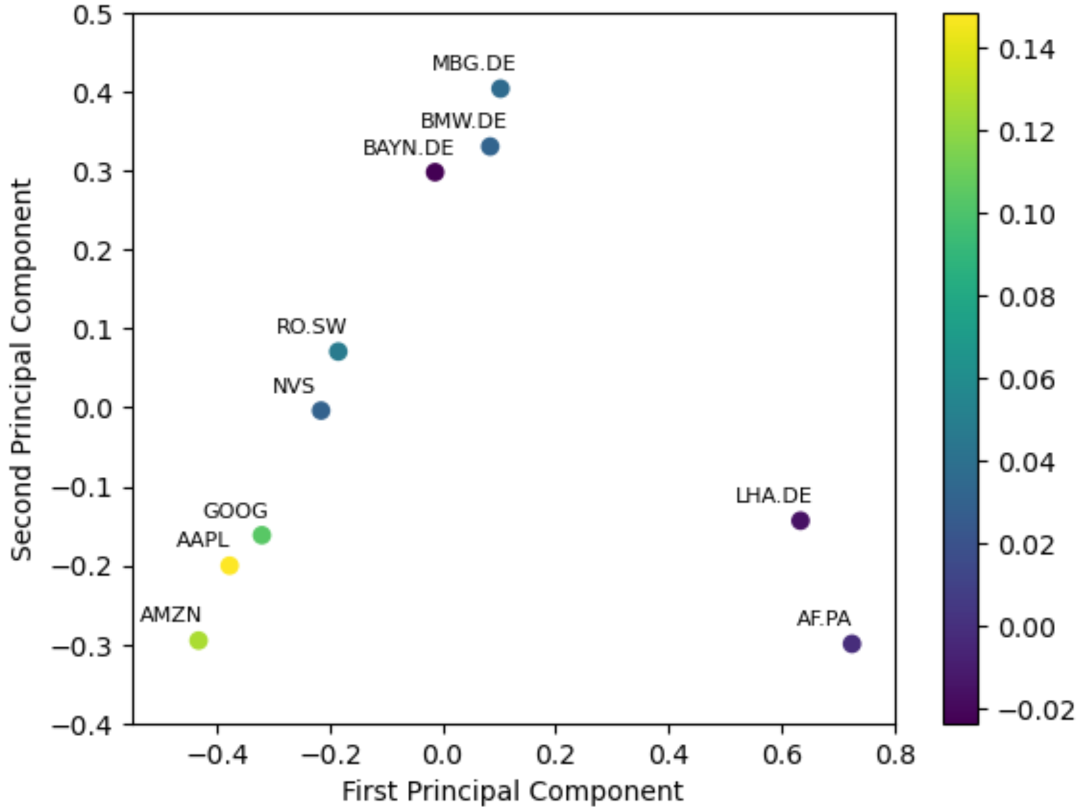
[13]:
```
norm_returns = toy_df.pct_change().dropna().T

mean_return = norm_returns.mean(axis=1)

num_eigvectors = 2

data_pca = PCA(n_components=num_eigvectors)
```

```
data_pca.fit(norm_returns)
data_pca_transform = data_pca.transform(norm_returns)

print(data_pca.explained_variance_ratio_)
```

```
[0.40273122 0.17428425]
```

Plot the first two principal components and label the individual datapoints:

```
[14]: plt.scatter(data_pca_transform[:, 0], data_pca_transform[:, 1],
                  c=mean_return.to_numpy()*100, cmap='viridis')

      for i, label in enumerate(portfolio):
          plt.annotate(label, (data_pca_transform[i, 0], data_pca_transform[i, 1]),␣
       ↪textcoords="offset points",
                       xytext=(-10, 7), ha='center', fontsize=8)

      plt.xlim(-0.55,0.8)
      plt.ylim(-0.4,0.5)

      plt.xlabel('First Principal Component')
      plt.ylabel('Second Principal Component')
      plt.colorbar()

      plt.show()
```

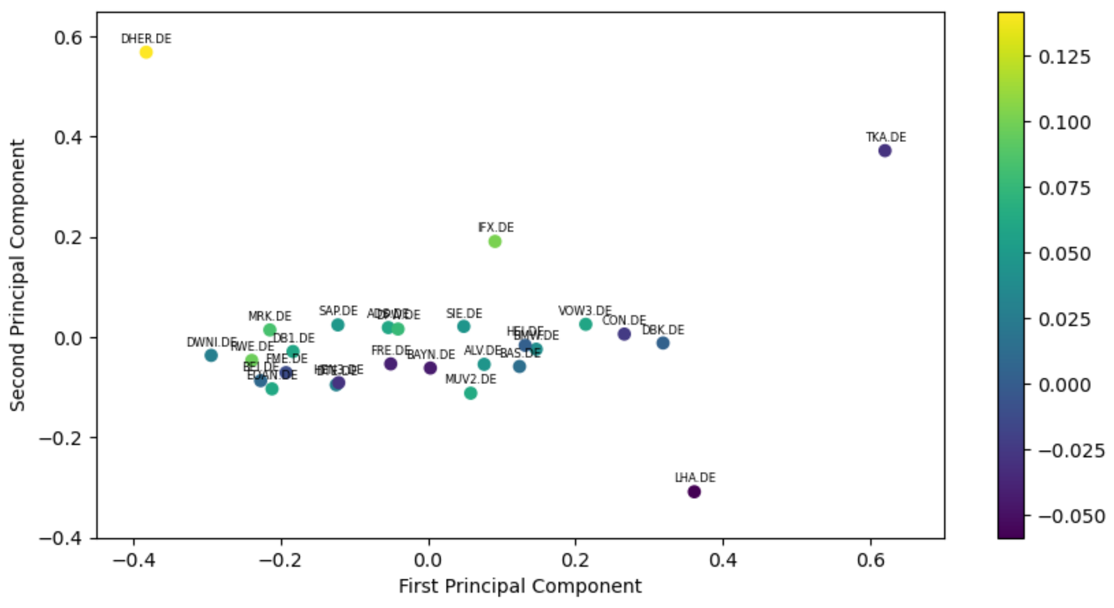


Interpretation of our results:

- Assets with similar characteristics, such as tech companies (bottom-left corner) or airlines (bottom-right corner), tend to form clusters.
- The first principal component can be interpreted as the **asset return axis**, while the second principal component represents the **volatility or variance of returns**.
- For instance, **Apple (AAPL)** had high average returns, but also high volatility. On the other hand, **Lufthansa (LHA.DE)** yields negative gains but facing also high volatility (due to a sharp price drop during the covid crisis). This is why, AAPL and LHA.DE are closely positioned on the Y-axis but substantially deviate on the X-axis.
- Companies in the upper-mid section, such as **BMW**, provided acceptable gains, and as a relatively conservative company, its volatility tends to be low. Hence, the scatter is centered on the X-axis and is at the upper part of the Y-axis.

We extend our analysis to a high amount of assets. For this, we load data of the **DAX** which is a stock index that includes the 40 biggest German companies.

[15]:
```
portfolio = ['ADS.DE', 'ALV.DE', 'BAS.DE', 'BAYN.DE', 'BEI.DE',
             'BMW.DE', 'CON.DE', 'DB1.DE', 'DBK.DE', 'DHER.DE',
             'DPW.DE', 'DTE.DE', 'DWNI.DE', 'EOAN.DE', 'FME.DE',
             'FRE.DE', 'HEI.DE', 'HEN3.DE', 'IFX.DE', 'LHA.DE',
             'MRK.DE', 'MUV2.DE', 'RWE.DE', 'SAP.DE', 'SIE.DE',
             'TKA.DE', 'VOW3.DE']

dax_df = pd.read_csv('data/finance_dax_data.csv', index_col='Date')

norm_returns = dax_df.pct_change().dropna().T

mean_return = norm_returns.mean(axis=1)

data_pca = PCA(n_components=2)
data_pca.fit(norm_returns)
data_pca_transform = data_pca.transform(norm_returns)

plt.figure(figsize=(10, 5))

plt.scatter(data_pca_transform[:, 0], data_pca_transform[:, 1],
            c=mean_return.to_numpy()*100, cmap='viridis')

for i, label in enumerate(portfolio):

    plt.annotate(label, (data_pca_transform[i, 0], data_pca_transform[i, 1]),␣
 ↪textcoords="offset points",
                 xytext=(0, 5), ha='center', fontsize=6)

plt.xlim(-0.45,0.7)
plt.ylim(-0.4,0.65)

plt.xlabel('First Principal Component')
plt.ylabel('Second Principal Component')
plt.colorbar()

plt.show()
```



The DAX example shows that **two dimensions are insuffiecient to explain the data well**, as can be seen in the explained variance ratio:

```
[16]: print('Explained variance ratio:', data_pca.explained_variance_ratio_)
```

```
Explained variance ratio: [0.19837711 0.09713147]
```

This indicates that there are more important hidden features. Still, we can at least **detect outliers** in order to identify excellent or bad performing assets.

1.3 Clustering

Another important approach to identifying patterns in an unsupervised fashion is clustering. In the previous examples, we have already seen instances where datapoints might form clusters indicating similar features.

Two popular approaches to clustering are **k-means** and **Gaussian Mixture Models** which we consider in the following.

k-means The underlying idea of k-means (Wikipedia) is assign datapoints to k cluster means / centroids in the dataset. The following GIF illustrates this for $k = 3$ centroids:

GIF source: Wikipedia

More formally, we consider a set of N datapoints $X = (x_1, ..., x_N)$ which we try to group into k groups forming sets $S_1, S_2, ..., S_k$. The objective function is given by

$$\text{argmin}_S \sum_{i=1}^{k} \sum_{x \in S_i} \|x - \mu_i\|^2 \tag{2}$$

where $\mu_i = \frac{1}{|S_i|} \sum_{x \in S_i} x$ is the mean of the datapoints in cluster S_i.

The algorithm **starts** with placing the cluster means / centroids μ_i in a random position (see GIF above at Iteration #0). Datapoints are assigned to the closest mean μ_i, i.e. to cluster S_i, and a **new cluster mean** is calculated. The algorithm **iterates** this step several times until the cluster assignments remain unchanged.

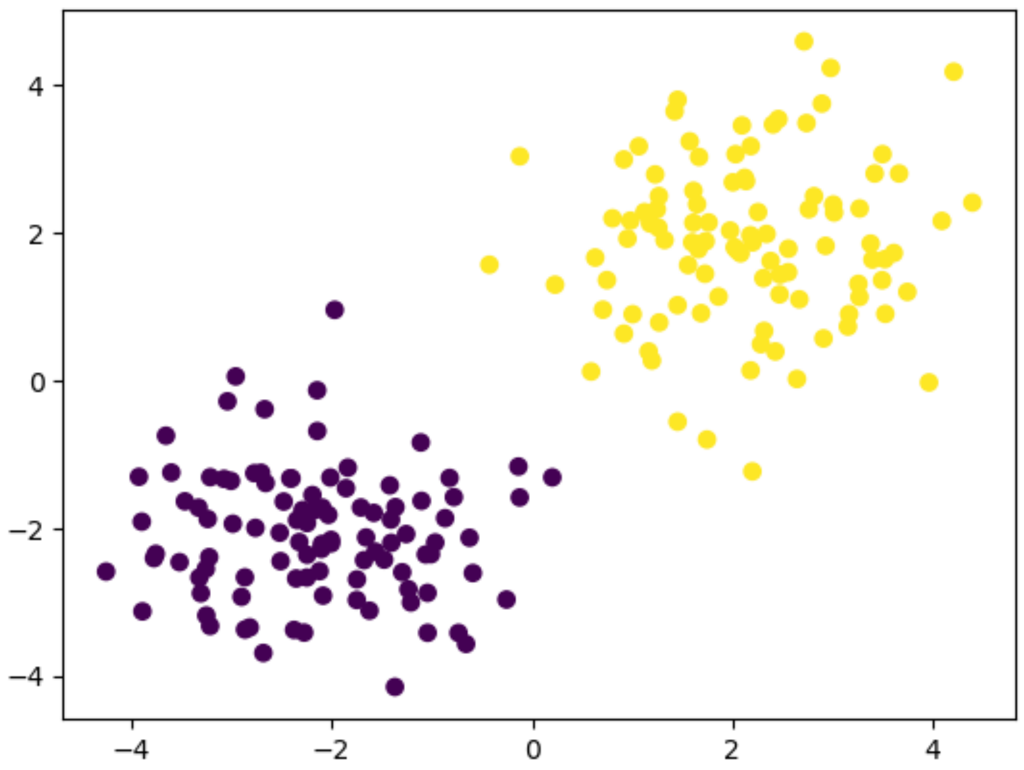
Note that in an unsupervised setting, **we generally do not know the number of clusters** k! Thus, k is a *hyper-parameter* we need to choose!

Let's create a clustered dataset with two clusters of 100 datapoints each, i.e. $N = 200$.

[17]:
```
import numpy as np
import matplotlib.pyplot as plt

np.random.seed(123)

num_datapoints = 100

cluster_1 = np.random.normal( 2, 1, size=(num_datapoints, 2))
cluster_2 = np.random.normal(-2, 1, size=(num_datapoints, 2))

cluster_data = np.concatenate([cluster_1, cluster_2])
```

We make use of the `scikit-learn` implementation of KMeans and choose $k = 2$.

[18]:
```
from sklearn.cluster import KMeans

k = 2

kmeans = KMeans(n_clusters=k, random_state=123, n_init=10)
kmeans.fit(cluster_data)

cluster_prediction = kmeans.predict(cluster_data)

plt.scatter(cluster_data[:,0], cluster_data[:,1], c=cluster_prediction)
plt.show()
```



1.3.1 Gaussian Mixture Model

A Gaussian Mixture Model (GMM) (Wikipedia) can be viewed as a (probabilistic) relaxation of k-means. Instead of "hard" cluster assignments, we consider "soft" assignments by means of probabilities.

An GMM assumes a mixture of several Gaussian distributions as the underlying distribution for the dataset and observed clustering (which can be a strong assumption, in practice). Each Gaussian distribution $\mathcal{N}(\mu_i, \Sigma_i)$ forms a cluster and is characterized by mean μ_i and covariance matrix Σ_i. The GMM (prior) distribution is then given by the mixture model

$$p(\mu, \Sigma) = \sum_{i=1}^{k} w_i \mathcal{N}(\mu_i, \Sigma_i) \tag{3}$$

where $\mu = (\mu_1, ..., \mu_k)$, $\Sigma = (\Sigma_1, ..., \Sigma_k)$, and $w = (w_1, ..., w_k)$ is the weighting of the different mixture components.

As before, we start by choosing a number of k clusters and setting the parameters μ, Σ to some initial values. The cluster assignment and parameters are then updated iteratively with the **expectation-maximisation (EM) algorithm** until cluster assignments, i.e. the parameters μ, Σ, do not change any longer.

Let's consider the same dataset as for k-means and make use of the `scikit-learn` GaussianMixture method.

[19]:
```python
from sklearn.mixture import GaussianMixture

k = 2

GMM = GaussianMixture(n_components=k)
GMM.fit(cluster_data)
```

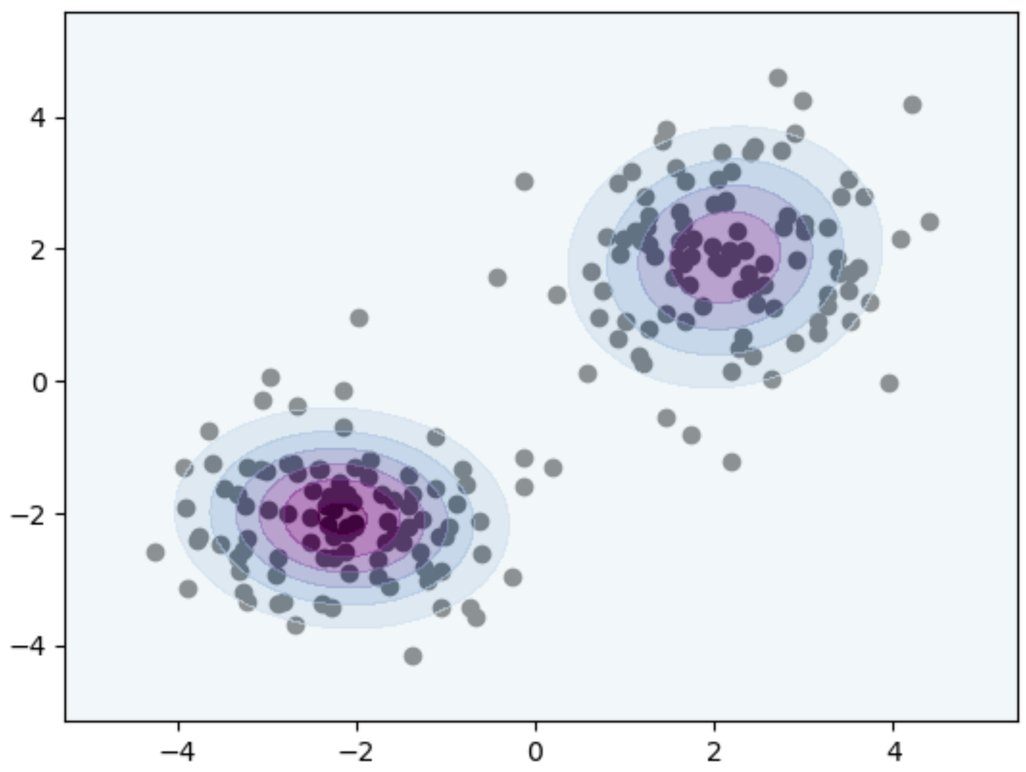
[19]:
```
GaussianMixture(n_components=2)
```

In order to provide the probabilities, we need to obtain a grid of datapoints which can do with `numpy.meshgrid`.

[20]:
```python
x_min = cluster_data[:, 0].min() - 1
x_max = cluster_data[:, 0].max() + 1

y_min = cluster_data[:, 1].min() - 1
y_max = cluster_data[:, 1].max() + 1

xx, yy = np.meshgrid(np.linspace(x_min, x_max, 100),
                     np.linspace(y_min, y_max, 100))
```

Finally, we can obtain the probability predictions with `score_samples` and plot the results. Note that this method provides the log-likelihood, i.e. we need to exponentiate these outputs!

[21]:
```python
probab = GMM.score_samples(np.c_[xx.ravel(), yy.ravel()])
probab = np.exp(probab)
probab = probab.reshape(xx.shape)

plt.scatter(cluster_data[:, 0], cluster_data[:, 1], c='black')
plt.contourf(xx, yy, probab, alpha=0.6, cmap='BuPu')

plt.xlim(x_min, x_max)
plt.ylim(y_min, y_max)

plt.show()
```



Note that `np.c_[A,B]` concatenates NumPy arrays `A` and `B` along the second axis.

1.4 Exercise Section

In the next two exercises, we use k-means and a Gaussian Mixture Model on the projection of the MNIST data on its two first principal components.

(1.) Firstly, to simplify the clustering task, we will only consider digits `0`, `3`, `6`, and `9`. For this make us of `%3` to identify all of these labels in `mnist_targets` and select only the respective elements in `data_pca_transform_mnist` and `mnist_targets` (defined above). Provide the filtered datasets `ex_data` and the corresponding labels in `ex_targets` in the following cell.

```
[ ]: ex_data = # fill in
     ex_targets = # fill in
```

If you were successful, you can plot the filtered dataset below, which should look like the following plot:

```
[ ]: plt.scatter(ex_data[:, 0], ex_data[:, 1], c=ex_targets, cmap='tab10')
     plt.xlabel('First Principal Component')
     plt.ylabel('Second Principal Component')
     plt.colorbar()
     plt.show()
```

(2.) Implement a k-means approach for clustering `ex_data` and provide the k-means object as `kmeans` and cluster predictions in `cluster_prediction`.

[ ]:
```
# fill in
```

Use `cluster_prediction` and the above defined `kmeans` to plot the clusters with the following cell.

[ ]:
```
plt.scatter(ex_data[:,0], ex_data[:,1], c=cluster_prediction)
plt.scatter(kmeans.cluster_centers_[:,0], kmeans.cluster_centers_[:,1],␣
  ↪marker='X', c='red')
plt.show()
```

(3.) Implement an Gaussian Mixture Model approach for clustering `ex_data`. Provide the Gaussian Mixture Model as object `GMM`, the grid coordinates `xx` and `yy` (as seen before) and the predictions in `probab`.

[ ]:
```
# fill in
```

If you have defined `GMM`, `xx`, `yy`, and `probab` in the cell, the next cell will allow you to plot your result.

[ ]:
```
plt.scatter(ex_data[:, 0], ex_data[:, 1], c='black')
plt.contourf(xx, yy, probab, alpha=0.6, cmap='BuPu')
plt.scatter(GMM.means_[:,0],GMM.means_[:,1], marker='X', c='orange')

plt.xlim(x_min, x_max)
plt.ylim(y_min, y_max)

plt.show()
```

1.5 Proposed Solutions

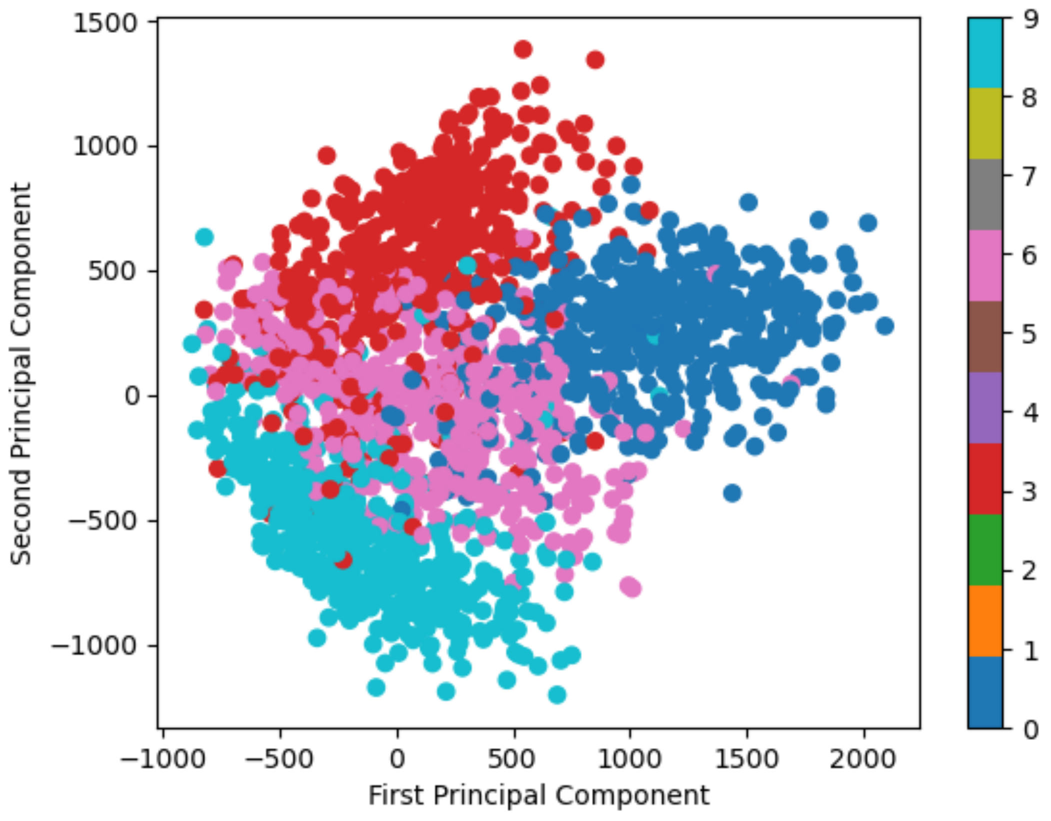
In the next two exercises, we use k-means and a Gaussian Mixture Model on the projection of the MNIST data on its two first principal components.

(1.) Firstly, to simplify the clustering task, we will only consider digits `0`, `3`, `6`, and `9`. For this make us of `%3` to identify all of these labels in `mnist_targets` and select only the respective elements in `data_pca_transform_mnist` and `mnist_targets` (defined above). Provide the filtered datasets `ex_data` and the corresponding labels in `ex_targets` in the following cell

[22]:
```
ex_data = data_pca_transform_mnist[mnist_targets%3==0]
ex_targets = mnist_targets[mnist_targets%3==0]
```

If you were successful, you can plot the filtered dataset below, which should look like the following plot:

[23]:
```python
plt.scatter(ex_data[:, 0], ex_data[:, 1], c=ex_targets, cmap='tab10')
plt.xlabel('First Principal Component')
plt.ylabel('Second Principal Component')
plt.colorbar()
plt.show()
```



(2.) Implement an k-means approach for clustering `ex_data` and provide the k-means object as `kmeans` and cluster predictions in `cluster_prediction`.

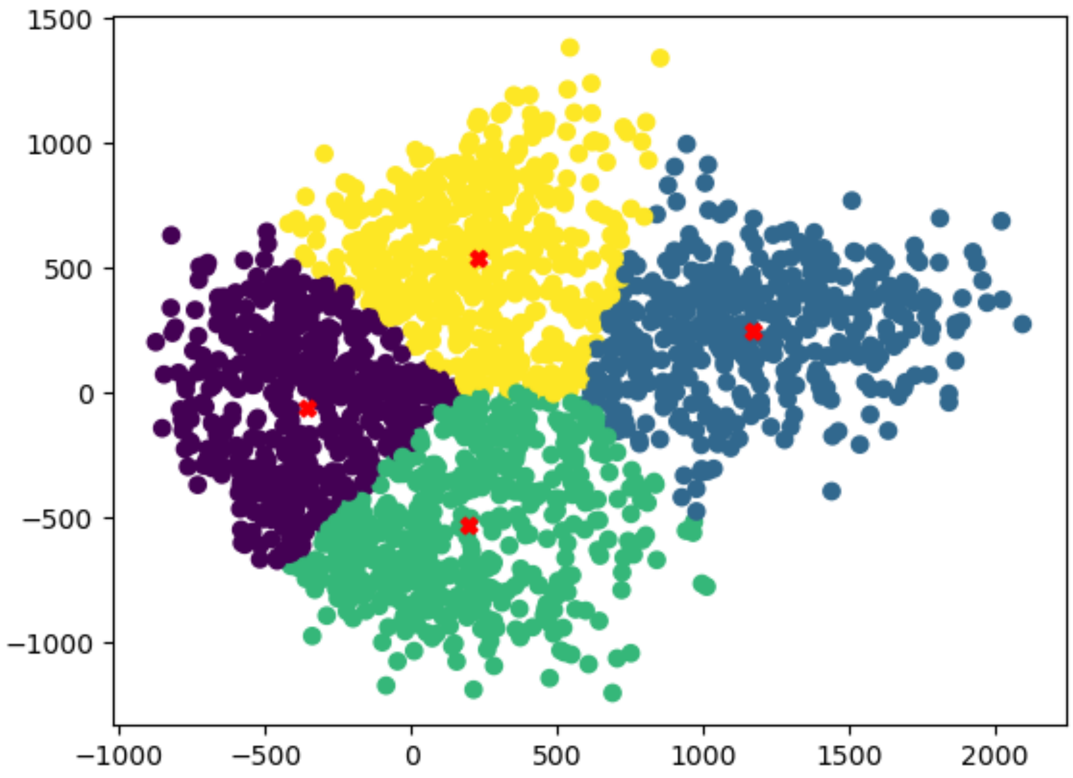
[24]:
```python
from sklearn.cluster import KMeans

k = 4

kmeans = KMeans(n_clusters=k, random_state=123)
kmeans.fit(ex_data)

cluster_prediction = kmeans.predict(ex_data)
```

```
/Users/maxim/opt/anaconda3/envs/APML/lib/python3.10/site-
packages/sklearn/cluster/_kmeans.py:870: FutureWarning: The default value of
`n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init`
```

```
explicitly to suppress the warning
  warnings.warn(
```

Use `cluster_prediction` and the above defined `kmeans` to plot the clusters with the following cell.

[25]:
```python
plt.scatter(ex_data[:,0], ex_data[:,1], c=cluster_prediction)
plt.scatter(kmeans.cluster_centers_[:,0], kmeans.cluster_centers_[:,1],␣
  ↪marker='X', c='red')
plt.show()
```



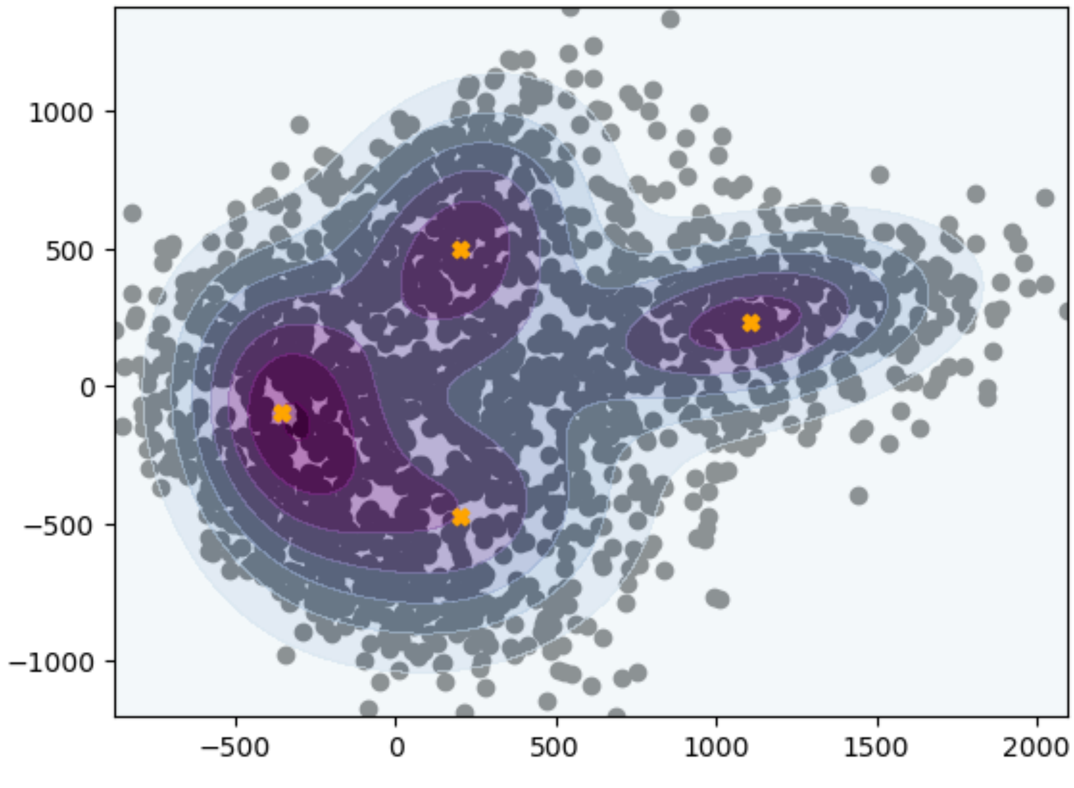
(3.) Implement an Gaussian Mixture Model approach for clustering `ex_data`. Provide the Gaussian Mixture Model as object `GMM`, the grid coordinates `xx` and `yy` (as seen before) and the predictions in `probab`.

[26]:
```python
from sklearn.mixture import GaussianMixture

k = 4

GMM = GaussianMixture(n_components=k)
GMM.fit(ex_data)

x_min = ex_data[:, 0].min() - 1
x_max = ex_data[:, 0].max() + 1
```

```
y_min = ex_data[:, 1].min() - 1
y_max = ex_data[:, 1].max() + 1

xx, yy = np.meshgrid(np.linspace(x_min, x_max, 100),
                     np.linspace(y_min, y_max, 100))

probab = GMM.score_samples(np.c_[xx.ravel(), yy.ravel()])
probab = np.exp(probab)
probab = probab.reshape(xx.shape)
```

If you have defined GMM, xx, yy, and probab in the cell, the next cell will allow you to plot your result.

[27]:
```
plt.scatter(ex_data[:, 0], ex_data[:, 1], c='black')
plt.contourf(xx, yy, probab, alpha=0.6, cmap='BuPu')
plt.scatter(GMM.means_[:,0],GMM.means_[:,1], marker='X', c='orange')

plt.xlim(x_min, x_max)
plt.ylim(y_min, y_max)

plt.show()
```



[28]:
```
print(f"GMM cluster means = \n{GMM.means_}\n")
print(f"k-means cluster means = \n{kmeans.cluster_centers_}")
```

```
GMM cluster means =
[[-353.81194024  -95.63547646]
 [ 203.63777088  502.06423334]
 [ 204.99018448 -475.32174602]
 [1104.22246709  232.42521412]]

k-means cluster means =
[[-358.89398063  -61.23607797]
 [1172.16616214  245.21794471]
 [ 196.21543053 -531.75772784]
 [ 231.10450973  539.9021651 ]]
```

4-Kernel_Methods

March 24, 2023

1 4. Kernel Methods

In contrast to the idea of dimensionality reduction and compression, another popular direction in Machine Learning considers the opposite approach of solving problems in a higher-dimensional space. In this notebook we present the general idea of **kernel methods** on the example of

- Kernel ridge regression and
- Gaussian Processes

mostly focusing on simulated data to highlight their main benefits.

Keywords: `feature mapping`, `RBF kernel`, `sklearn.kernel_ridge.KernelRidge`, `sklearn.gaussian_process.GaussianProcessRegressor`, `sklearn.gaussian_process.kernels.RBF` `sklearn.pipeline.make_pipeline`, `sklearn.preprocessing.StandardScaler`

1.1 Lifting Data into higher Dimensions

All models considered in the previous notebooks can be regarded as essentially linear models. Although linear models have their advantages (in particular with respect to mathematical derivations and guarantees), they severly limit the kind of functions we can represent. A common approach therefore is to **map** the problem from the input space into a **higher-dimensional feature space** as illustrated in the next figure for a classification setting.

The feature mapping ϕ allows us to map data from a lower-dimensional input space into a higher-dimensional feature space. The key idea is that identifying the complicated decision boundary in input space might be challenging, but **in feature space a linear model suffices** to identify the planar decision boundary.

More importantly, we can show that we do not need to ever evaluate $\phi(x)$. We can rely on the **kernel trick**! This implies that we only need to evalute scalar products of feature mappings – called kernels – $\kappa(x, x') = \langle \phi(x), \phi(x') \rangle$ for pairs of datapoints x, x' in our dataset X.

One such wildly used kernel is the **radial basis function (RBF) kernel**

$$\kappa(x, x') = \exp\Big(- \frac{1}{2\sigma^2} \|x - x'\|_2^2 \Big) \tag{1}$$

which corresponds to an infinite-dimensional feature space. In general, we can design task-dependent kernels which might extract features we deem relevant to our problem. Furthermore, we can “kernelise” standard linear approaches to become more powerful!

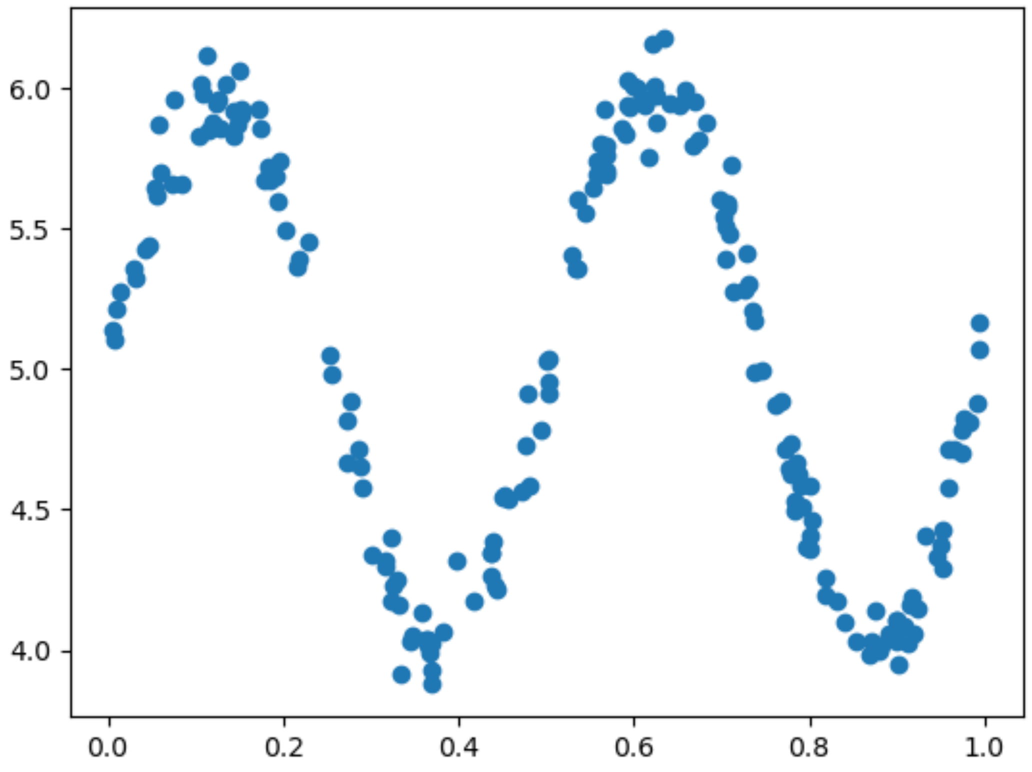
1.2 Kernel Ridge Regression

We revisit our standard regression techniques and see how the kernelised version extends what we have seen before. We formulated the linear regression model before as

$$Y = Xw + \epsilon. \tag{2}$$

Let's simulate a sinusoidal dataset (with noise) of $N = 200$ datapoints.

[1]:
```
import numpy as np
import matplotlib.pyplot as plt

np.random.seed(1234)

num_datapoints = 200
X = np.random.rand(num_datapoints)
X = np.sort(X).reshape(-1,1)

Y = np.sin(4 * np.pi * X) + np.random.randn(num_datapoints, 1) * 0.1 + 5

plt.scatter(X,Y)
plt.show()
```

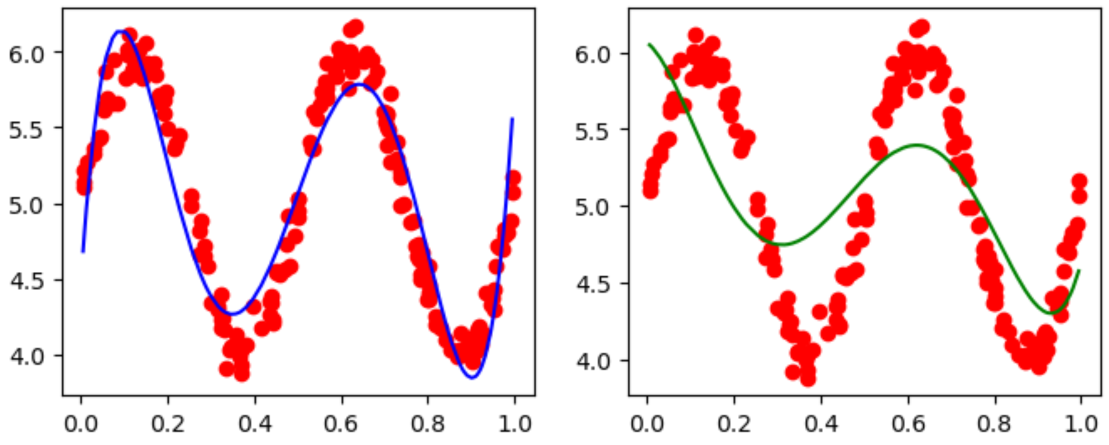


As we have seen before, we will try to fit these observations with a polynomial with linear and ridge regression.

In the following, we make use of an advanced `scikit-learn` tool. We build a **pipeline** (see documentation) which allows data processing steps to be executed with an estimator like `LinearRegression` or `Ridge`. In particular, we use the `StandardScalar` method (see documentation) which is a method to standardise our dataset, i.e. subtract the sample mean and divide by the sample standard deviation. With such a pipeline we can do some "data curation" before training!

[2]:
```
from sklearn.linear_model import LinearRegression, Ridge
from sklearn.pipeline import make_pipeline
from sklearn.preprocessing import StandardScaler

X_poly = np.hstack((X, X ** 2, X ** 3, X ** 4, X ** 5))

linreg = make_pipeline(StandardScaler(), LinearRegression())
linreg.fit(X_poly,Y)
Y_OLS = linreg.predict(X_poly)
Rsquared_lin = linreg.score(X_poly,Y)

ridgereg = make_pipeline(StandardScaler(), Ridge(alpha=0.001))
ridgereg.fit(X_poly,Y)
Y_ridge = ridgereg.predict(X_poly)
Rsquared_ridge = ridgereg.score(X_poly,Y)

print(f"Rsquared_lin = {Rsquared_lin:.2f}, Rsquared_ridge = {Rsquared_ridge:.
 ↪2f}")

fig, axs = plt.subplots(1,2, figsize=(8,3))

axs[0].scatter(X[:, 0], Y, color='red')
axs[0].plot(X[:, 0], Y_OLS, color='blue')

axs[1].scatter(X[:, 0], Y, color='red')
axs[1].plot(X[:, 0], Y_ridge, color='green')

plt.show()
```

```
Rsquared_lin = 0.89, Rsquared_ridge = 0.55
```



1.2.1 Kernel Ridge Regression (KRR)

incorporates the idea of employing a feature mapping ϕ and we rewrite the linear regression model as

$$Y = \phi(X)w + \epsilon = f(x) + \epsilon. \tag{3}$$

Similar to the ridge regression result, the solution can be shown to be

$$w_{\text{KRR}} = \phi(X)^\top \left(\phi(X)^\top \phi(X) + \lambda \mathbb{1}_N\right)^{-1} Y. \tag{4}$$

and the learned function (without going into the mathematical details) is then given by

$$f(x) = K(x, X)\left(K(X, X) + \lambda \mathbb{1}_{d_N}\right)^{-1} Y \tag{5}$$

with K being the kernel matrix $K_{nm} = \kappa(x_n, x_m) = \langle \phi(x_n), \phi(x_m) \rangle$.

Let's see how we can make use of for the above dataset and define the RBF kernel.

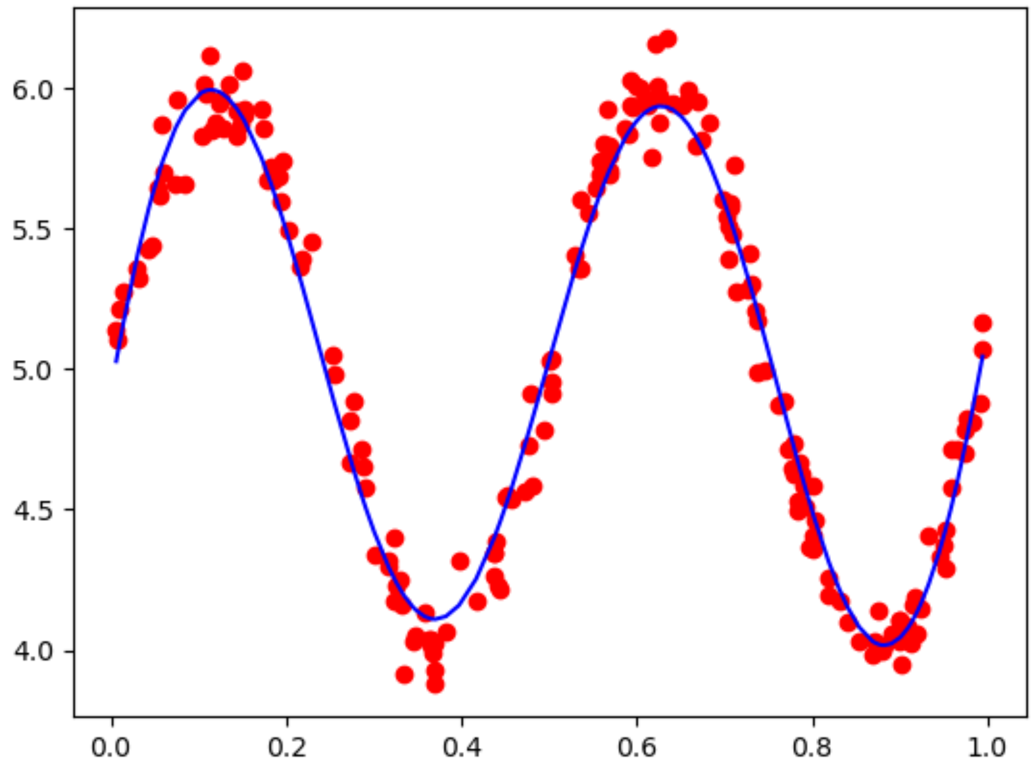
[3]:
```python
def rbf_kernel(x1, x2, sigma=1.0):
    return np.exp(-np.linalg.norm(x1 - x2) ** 2 / (2 * sigma ** 2))
```

As usually, we use a `scikit-learn` estimator: KernelRidge.

[4]:
```python
from sklearn.kernel_ridge import KernelRidge

KRR = make_pipeline(StandardScaler(), KernelRidge(kernel=rbf_kernel, alpha=0.
  ↪01, gamma=0.1))
KRR.fit(X, Y)
Y_KRR = KRR.predict(X)
```

```
Rsquared_KRR = KRR.score(X,Y)

print(f"Rsquared_lin = {Rsquared_lin:.2f}, Rsquared_ridge = {Rsquared_ridge:.
↪2f}, Rsquared_KRR = {Rsquared_KRR:.2f}")

plt.scatter(X[:, 0], Y, color='red')
plt.plot(X[:, 0], Y_KRR, color='blue')
plt.show()
```

```
Rsquared_lin = 0.89, Rsquared_ridge = 0.55, Rsquared_KRR = 0.98
```



1.3 Gaussian Processes

Kernel Ridge Regression has a close connection to **Gaussian Processes (GPs)** (Wikipedia or scikit-learn). Informally, a GP extends the notion of random variables to random functions. In a regression setting with input matrix X, the GP prior distribution $p(f \mid X) = \mathcal{N}(0, K)$ allows us to model the regression function $f(X) = [f(x_1), ..., f(x_N)]^\top$ as

$$(f(x_1), ..., f(x_N)) \sim \mathcal{N}(0, K) \tag{6}$$

with sample covariance matrix $K = \mathrm{cov}(X, X)$. Let us consider a GP regression model with noisy responses Y as before, i.e.

$$Y = f(x) + \epsilon. \tag{7}$$

Leaving the mathematical derivation aside, in order to make a prediction for function $f(x)$ with new (test) data x, we can show that the posterior predictive distribution (Wikipedia) has the form

$$p(f \mid x, X, Y) = \mathcal{N}(\mu(x), \Sigma(x, X)) \tag{8}$$

$$\mu(x) = K(x, X)\left(K(X, X) + \lambda \mathbb{1}_N\right)^{-1} Y \tag{9}$$

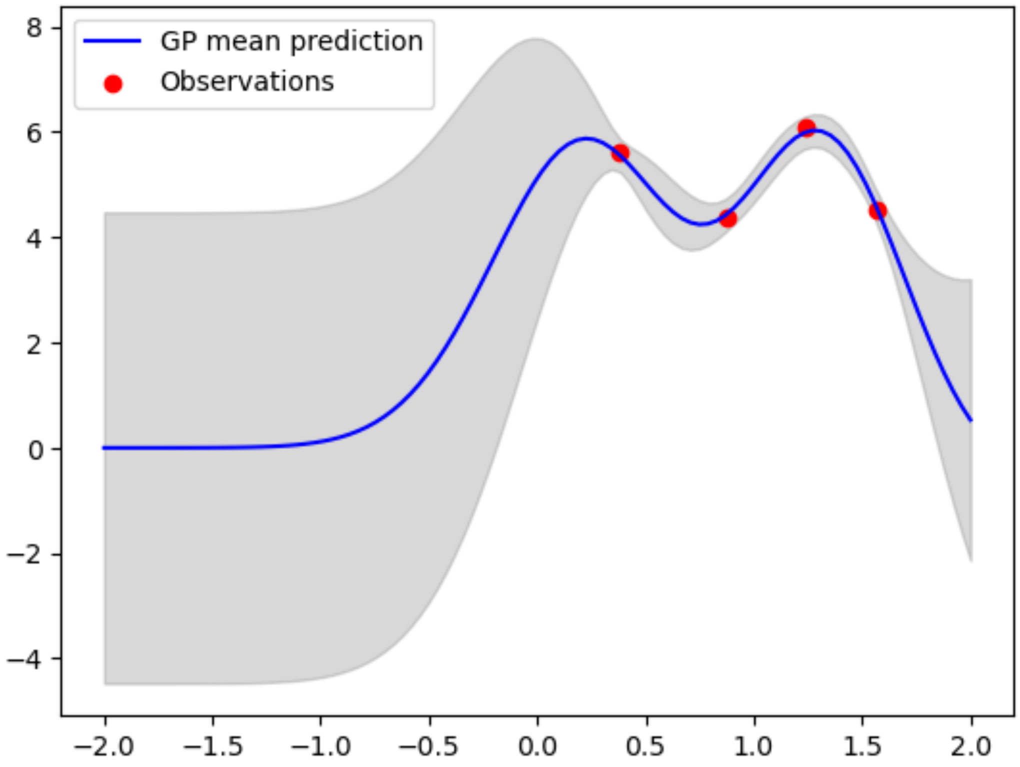
$$\Sigma(x, X) = K(x, x) - K(x, X)^\top \left(K(X, X) + \lambda \mathbb{1}_N\right)^{-1} K(x, X) \tag{10}$$

Note that what we have written earlier for $f(x)$ in KRR **corresponds exactly** to $\mu(x)$ in GP regression, i.e. there is a close connection between KRR and GP regression (see e.g. this comparison). This motivates that the **covariance matrix K is a kernel**, too! Compared to KRR, GPs can be more flexible (as we can sample functions from the posterior) and we can make use of the GP formalism for training. Also, GPs enable us to quantify the uncertainty of a prediction due to $\Sigma(x, X)$.

Let's study this in a simplified example with $N = 4$ datapoints. As always, we can use `scikit-learn` methods for the GaussianProcessRegressor and different kernels. We employ the RBF kernel as well as a ConstantKernel, i.e. $\kappa(x, x') = \mathrm{const}$.

[5]:
```
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import RBF, ConstantKernel

np.random.seed(1234)

num_datapoints = 4

X = np.random.rand(num_datapoints, 1)*2
Y = np.sin(2 * np.pi * X) + np.random.randn(num_datapoints, 1) * 0.1 + 5

kernel = ConstantKernel(constant_value=1.0, constant_value_bounds=(0.001, 1000))
kernel = kernel * RBF(length_scale=0.5, length_scale_bounds=(0.01, 100))

GPreg = GaussianProcessRegressor(kernel=kernel, alpha=0.1,␣
  ↪n_restarts_optimizer=10)
GPreg.fit(X, Y)

X_pred = np.linspace(-2.0, 2.0, 100).reshape(-1, 1)
Y_GPreg, stddev_GPreg = GPreg.predict(X_pred, return_std=True)

X_pred = X_pred.reshape(-1)
Y_GPreg = Y_GPreg.reshape(-1)
```

```
plt.fill_between(X_pred, Y_GPreg - stddev_GPreg,  Y_GPreg + stddev_GPreg,␣
 ↪alpha=0.3, color='grey')
plt.plot(X_pred, Y_GPreg, color='blue', label='GP mean prediction')
plt.scatter(X, Y, color='red', label='Observations')

plt.legend(loc='upper left')
plt.show()
```



1.4 Exercise Section

For the exercises, we consider again the red wine dataset but this time train a (1.) kernel ridge regressor and (2.) Gaussian Process regressor. As in notebook 2, we want to predict the `quality` values on the test set `feat_test` and compare the mean squared errors (MSEs) of KRR and GP regression to the previous results for ridge regression (0.42) and Random Forest regression (0.34).

In order, to prepare the data and kernel, load the following cell:

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

```
from sklearn.model_selection import train_test_split
from sklearn.pipeline import make_pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.gaussian_process.kernels import RBF, ConstantKernel

np.random.seed(1234)

ex_kernel = RBF(length_scale=5, length_scale_bounds=(0.01, 100))

wine_data = pd.read_csv('data/winequality-red.csv', sep=';')

ex_target = wine_data['quality']
ex_features = wine_data.drop(['quality'], axis=1)

feat_train, feat_test, target_train, target_test = train_test_split(
    ex_features, ex_target, test_size = 0.3, random_state=123)

target_test = target_test.to_frame()
```

[13]:
```
feat_train.head(5)
```

[13]:
```
      fixed acidity  volatile acidity  citric acid  residual sugar  chlorides  \
374            14.0             0.410         0.63             3.8      0.089
800             7.2             0.610         0.08             4.0      0.082
1441            7.4             0.785         0.19             5.2      0.094
1269            5.5             0.490         0.03             1.8      0.044
691             9.2             0.920         0.24             2.6      0.087

      free sulfur dioxide  total sulfur dioxide  density    pH  sulphates  \
374                   6.0                  47.0  1.00140  3.01       0.81
800                  26.0                 108.0  0.99641  3.25       0.51
1441                 19.0                  98.0  0.99713  3.16       0.52
1269                 28.0                  87.0  0.99080  3.50       0.82
691                  12.0                  93.0  0.99980  3.48       0.54

        alcohol
374   10.800000
800    9.400000
1441   9.566667
1269  14.000000
691    9.800000
```

[14]:
```
target_train.head(5)
```

[14]:
```
374     6
800     5
1441    6
```

```
1269    8
691     5
Name: quality, dtype: int64
```

(1.) Implement kernel ridge regression as we have seen it in this notebook. Please provide the predictions for the test set `feat_test` in `ex_pred_KRR`.

```
[ ]: # Fill in
```

We use `ex_pred_KRR` in the following cell to provide the results. You can just execute the next cell.

```
[ ]: target_test['KRR_predicted_quality'] = np.around(ex_pred_KRR, decimals=2)
     target_test['KRR_absolut_deviation'] = abs(target_test['quality'] -␣
      ↪target_test['KRR_predicted_quality'])
     print(target_test)

     KRR_pred_MSE = (target_test['KRR_absolut_deviation']**2).mean()
     print(f"\nMean squared error of KernelRidge: {KRR_pred_MSE:.2f}")
```

(2.) Implement GP regression as we have seen it in this notebook. Please provide the predictions for the test set `feat_test` in `ex_pred_GPreg`.

For Noto users: You might want to set `n_restarts_optimizer=1`(i.e. only one), as otherwise the computation might take too long.

```
[ ]: # Fill in
```

We use `ex_pred_GPreg` in the following cell to provide the results. You can just execute the next cell.

```
[ ]: target_test['GPreg_predicted_quality'] = np.around(ex_pred_GPreg, decimals=2)
     target_test['GPreg_absolut_deviation'] = abs(target_test['quality'] -␣
      ↪target_test['GPreg_predicted_quality'])
     print(target_test)

     GPreg_pred_MSE = (target_test['GPreg_absolut_deviation']**2).mean()

     print(f"\nMean squared error of GaussianProcessRegressor: {GPreg_pred_MSE:.2f}")
     print(f"Mean squared error of KernelRidge: {KRR_pred_MSE:.2f}")
```

1.5 Proposed Solutions

For the exercises, we consider again the red wine dataset but this time train a (1.) kernel ridge regressor and (2.) Gaussian Process regressor. As in notebook 2, we want to predict the `quality` values on the test set `feat_test` and compare the mean squared errors (MSEs) of KRR and GP regression to the previous results for ridge regression (0.42) and Random Forest regression (0.34).

In order, to prepare the data and kernel, load the following cell:

```
[6]: import numpy as np
     import pandas as pd
     import matplotlib.pyplot as plt

     from sklearn.model_selection import train_test_split
     from sklearn.pipeline import make_pipeline
     from sklearn.preprocessing import StandardScaler
     from sklearn.gaussian_process.kernels import RBF, ConstantKernel

     np.random.seed(1234)

     ex_kernel = RBF(length_scale=5, length_scale_bounds=(0.01, 100))

     wine_data = pd.read_csv('data/winequality-red.csv', sep=';')

     ex_target = wine_data['quality']
     ex_features = wine_data.drop(['quality'], axis=1)

     feat_train, feat_test, target_train, target_test = train_test_split(
         ex_features, ex_target, test_size = 0.3, random_state=123)

     target_test = target_test.to_frame()
```

(1.) Implement kernel ridge regression as we have seen it in this notebook. Please provide the predictions for the test set `feat_test` in `ex_pred_KRR`.

```
[7]: from sklearn.kernel_ridge import KernelRidge

     KRR_ex = make_pipeline(StandardScaler(), KernelRidge(kernel=ex_kernel, alpha=0.
      ↪1))
     KRR_ex.fit(feat_train, target_train)
     ex_pred_KRR = KRR_ex.predict(feat_test)

     Rsquared_KRR_ex = KRR_ex.score(feat_train, target_train)
```

We use `ex_pred_KRR` in the following cell to provide the results. You can just execute the next cell.

```
[8]: target_test['KRR_predicted_quality'] = np.around(ex_pred_KRR, decimals=2)
     target_test['KRR_absolut_deviation'] = abs(target_test['quality'] -␣
      ↪target_test['KRR_predicted_quality'])
     print(target_test)

     KRR_pred_MSE = (target_test['KRR_absolut_deviation']**2).mean()
     print(f"\nMean squared error of KernelRidge: {KRR_pred_MSE:.2f}")
```

```
     quality  KRR_predicted_quality  KRR_absolut_deviation
912        6                   6.32                   0.32
772        5                   4.87                   0.13
```

```
1037        5                 5.04                0.04
1106        6                 6.45                0.45
263         5                 5.58                0.58
…       …                 …                   …
1466        7                 5.60                1.40
580         5                 4.71                0.29
1082        6                 5.37                0.63
1279        7                 6.25                0.75
1155        5                 5.37                0.37

[480 rows x 3 columns]

Mean squared error of KernelRidge: 0.38
```

(2.) Implement GP regression as we have seen it in this notebook. Please provide the predictions for the test set `feat_test` in `ex_pred_GPreg`.

For Noto users: You might want to set `n_restarts_optimizer=1`(i.e. only one), as otherwise the computation might take too long.

[10]:
```
from sklearn.gaussian_process import GaussianProcessRegressor

GPreg_ex = make_pipeline(StandardScaler(),␣
  ↪GaussianProcessRegressor(kernel=ex_kernel, alpha=0.15,␣
  ↪n_restarts_optimizer=5))
GPreg_ex.fit(feat_train, target_train)
ex_pred_GPreg = GPreg_ex.predict(feat_test)

Rsquared_GPreg_ex = GPreg_ex.score(feat_train, target_train)
```

We use `ex_pred_GPreg` in the following cell to provide the results. You can just execute the next cell.

[11]:
```
target_test['GPreg_predicted_quality'] = np.around(ex_pred_GPreg, decimals=2)
target_test['GPreg_absolut_deviation'] = abs(target_test['quality'] -␣
  ↪target_test['GPreg_predicted_quality'])
print(target_test)

GPreg_pred_MSE = (target_test['GPreg_absolut_deviation']**2).mean()

print(f"\nMean squared error of GaussianProcessRegressor: {GPreg_pred_MSE:.2f}")
print(f"Mean squared error of KernelRidge: {KRR_pred_MSE:.2f}")
```

```
      quality  KRR_predicted_quality  KRR_absolut_deviation  \
912         6                   6.32                   0.32
772         5                   4.87                   0.13
1037        5                   5.04                   0.04
1106        6                   6.45                   0.45
263         5                   5.58                   0.58
```

```
…       …                    …                    …
1466        7                  5.60                     1.40
580         5                  4.71                     0.29
1082        6                  5.37                     0.63
1279        7                  6.25                     0.75
1155        5                  5.37                     0.37

      GPreg_predicted_quality  GPreg_absolut_deviation
912                      6.31                     0.31
772                      4.86                     0.14
1037                     5.04                     0.04
1106                     6.44                     0.44
263                      5.58                     0.58
…                       …                      …
1466                     5.59                     1.41
580                      4.74                     0.26
1082                     5.36                     0.64
1279                     6.23                     0.77
1155                     5.38                     0.38

[480 rows x 5 columns]

Mean squared error of GaussianProcessRegressor: 0.38
Mean squared error of KernelRidge: 0.38
```

5-Neural_Networks

March 24, 2023

1 5. Neural Networks

In the previous notebook, we have seen that we can choose feature mappings ϕ or kernels κ to design powerful non-linear models. Informally, deep learning can be characterised as trying to learn the feature mapping ϕ from data.

In this notebook we will discuss and implement our first

- feed-forward neural network / multi-layer perceptron and
- convolutional neural network

for the MNIST and wine quality classification task.

Keywords: `Gradient descent`, `Cross-entropy loss`, `ReLU`, `One-hot encoding`, `Max pooling`, `Convolution`, `keras.layers`, `model.compile`, `model.fit`, `model.evaluate`, `model.save`, `model.summary`, `models.load_model`, `keras.optimizers.SGD`

1.1 Neural Network Basics

We start with the classical **Feed-Forward Neural Networks (FFNNs)** which are also referred to as multi-layer perceptrons (MLPs). FFNNs were originally proposed as a computational model simulating mechanisms of the human brain. The general idea is that inputs are processed in a sequential manner by **artificial neurons**. The common architecture consist of an input layer, one to several hidden layers, and an output layer as illustrated in the following figure.

As before, we try to learn the function $f(X)$. The displayed three-layer FFNN **parameterises** this function in the following way

$$f(X, W) = \sigma(\sigma(XW_1)W_2)W_3 = \phi(X, W_1, W_2)W_3, \tag{1}$$

where weights $W = (W_1, W_2, W_3)$ are the matrices which we multiply layer-wise to the output of the previous layer. The outputs are called **activations**. An important part of why neural networks are so powerful is the use of **non-linear activation functions**. The **rectified linear unit (ReLU)** $\sigma(z) = \max\{0, z\}$ is a particularly popular choice, e.g. $\sigma(z = -2) = 0$ and $\sigma(z = 2) = 2$, with z being the preactivation.

We can make a connection between neural networks and what we have seen before. Let's consider a deeper L-layer FFNN. In the regression setting, our goal is again to find a model for

$$Y = f(X, W) + \epsilon = \phi(X, W_1, \dots, W_{L-1})W_L + \epsilon \tag{2}$$

where this time ϕ is learned! We calibrate our model to solve the task by using **(Stochastic) Gradient Descent** for updating the weights $W = (W_1, \dots, W_L)$:

$$W^{(t+1)} = W^{(t)} - \eta \nabla \mathrm{Loss}(W^{(t)}). \tag{3}$$

As illustrated in the figure below, the idea is to start at some position of our loss landscape described by initially random weights $W^{(t=0)}$ drawn from a Gaussian distribution. With every update step, we approach a (local) minimum until the weights do not change any longer. Note that this requires an appropriate choice of the step size or **learning rate** η (which again is a hyperparameter like λ and k which we've seen before).

As before, we can use the mean-squared error loss for regression tasks

$$\mathrm{Loss}(W) = \frac{1}{2N}\|Y - f(X, W)\|_2^2 = \frac{1}{2N}\sum_{n=1}^{N}\left(y_n - f(x_n, W)\right)^2. \tag{4}$$

In the classification setting, we use the multi-class version of the logistic loss encountered earlier. In deep learning context, we usually call it the **cross-entropy loss**

$$\mathrm{Loss}(W) = -\sum_{n=1}^{N}\sum_{c=1}^{C} y_{n,c}\log p_{n,c} = -\sum_{n=1}^{N}\sum_{c=1}^{C} y_{n,c}\log f_c(x_n, W), \tag{5}$$

where we consider C different classes our N datapoints belong to. The neural network provides in the output layer the probabilities for the different classes $p_{n,c} = f_c(x_n, W)$. For this, we use another kind of activation function knows as the **softmax activation function** which maps the activation to the values between 0 and 1. The activation $\sigma(z)_i$ at output neuron i is given by

$$\sigma(z)_i = \frac{\exp(z_i)}{\sum_{j=1}^{C}\exp(z_j)}, \tag{6}$$

where C is the number of neurons in the output layer, i.e. the number of classes, and $i, j \in 1, \dots, C$. Typically, we change the class labels into a **one-hot encoding** which provides something like a class probability associated with the label. Suppose our datapoint x_n shows the digit 9 and the corresponding target is $y_n = 9$. In the one-hot encoding we replace y_n with the vector

$$y_n = \begin{pmatrix} y_{n,0} \\ y_{n,1} \\ \vdots \\ y_{n,9} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}, \tag{7}$$

where we have 0s at every index but the class index, i.e. 9 in this case.

Let's use all of this in building a FFNN for classifying MNIST digits!

[5]:
```
import numpy as np
from tensorflow import keras

mnist_data = np.load('data/mnist_data_5k.npy', allow_pickle=True)
mnist_targets = np.load('data/mnist_labels_5k.npy', allow_pickle=True)
```

In the following, we normalise the vector of pixel values to the $[0, 1]$ interval. It is typically advisable to scale all your predictors in X (i.e. the columns) such that values range between 0 and 1. Furthermore, we split the data into training, validation, and test datasets.

[6]:
```
mnist_data_flat = mnist_data.reshape(-1, 784, 1) / 255

num_train = 3000
num_val = 1000
num_test = 1000

x_train = mnist_data_flat[:num_train]
y_train = mnist_targets[:num_train]

x_val = mnist_data_flat[num_train:num_train+num_val]
y_val = mnist_targets[num_train:num_train+num_val]

x_test = mnist_data_flat[-num_test:]
y_test = mnist_targets[-num_test:]
```

Now, we define a three-layer FFNN with the following layers sizes:

- 784 neurons in the input layer
- 1024 (hidden) neurons in the first hidden layer with ReLU activation
- 512 (hidden) neurons in the second hidden layer with ReLU activation
- 10 output neurons for our classes in the output layer with a softmax activation

[7]:
```
ffnn = keras.Sequential([
    keras.layers.Dense(1024, activation='relu', input_shape=(784,)),
    keras.layers.Dense(512, activation='relu'),
    keras.layers.Dense(10, activation='softmax')
    ], name='FFNN_example')
```

```
2023-03-23 11:39:22.757417: I tensorflow/core/platform/cpu_feature_guard.cc:193]
This TensorFlow binary is optimized with oneAPI Deep Neural Network Library
(oneDNN) to use the following CPU instructions in performance-critical
operations:  SSE4.1 SSE4.2 AVX AVX2 FMA
To enable them in other operations, rebuild TensorFlow with the appropriate
compiler flags.
```

Next, we specify hyperparameters. As outlined before, the **learning rate** η is an important hyperparameter. In addition, we typically cannot (but also do not want to) use all datapoints for training at the same time. We choose small batches of the dataset and thus need to specify the **batch size**.

[8]:
```python
learning_rate = 0.01
batch_size = 16
num_epochs = 10

print(f"Shape of training set: {x_train.shape}")
print(f"Number of batches: {x_train.shape[0] / batch_size}")
```

```
Shape of training set: (3000, 784, 1)
Number of batches: 187.5
```

A training **epoch** is concluded after we have seen the total number of batches. We set multiple epochs to iteratively refine the neural network weights, i.e. training samples are seen several times during training.

Now, let's define our optimisation method where we use Stochastic Gradient Descent.

[9]:
```python
keras.utils.set_random_seed(123)

ffnn.compile(optimizer=keras.optimizers.SGD(learning_rate=learning_rate),
             loss='sparse_categorical_crossentropy',
             metrics=['accuracy'])
```

We use as the loss the `sparse_categorical_crossentropy` where

- *categorical* means that the neural network outputs are expected to be softmax values between 0 and 1
- *sparse* indicates that we have did not one-hot encode our y-targets; the loss will take care of that

[10]:
```python
print(y_train)
```

```
[5 0 4 … 9 1 5]
```

We can now use the methods fit and evaluate to train our FFNN and evaluate it on the test set.

[11]:
```python
ffnn_history = ffnn.fit(x=x_train, y=y_train, batch_size=batch_size,
                        validation_data=(x_val, y_val), epochs=num_epochs)

test_loss, test_acc = ffnn.evaluate(x_test, y_test, verbose=0)

print(f'\nTest accuracy: {test_acc:.4f}')

ffnn.save('output/MNIST_FFNN.h5')
```

```
Epoch 1/10
188/188 [==============================] - 3s 13ms/step - loss: 1.5611 -
accuracy: 0.6623 - val_loss: 0.9880 - val_accuracy: 0.7920
Epoch 2/10
188/188 [==============================] - 2s 10ms/step - loss: 0.7085 -
accuracy: 0.8460 - val_loss: 0.6251 - val_accuracy: 0.8580
Epoch 3/10
```

```
188/188 [==============================] - 2s 11ms/step - loss: 0.4892 -
accuracy: 0.8800 - val_loss: 0.4892 - val_accuracy: 0.8760
Epoch 4/10
188/188 [==============================] - 2s 11ms/step - loss: 0.3970 -
accuracy: 0.8967 - val_loss: 0.4276 - val_accuracy: 0.8870
Epoch 5/10
188/188 [==============================] - 2s 10ms/step - loss: 0.3459 -
accuracy: 0.9117 - val_loss: 0.3802 - val_accuracy: 0.9040
Epoch 6/10
188/188 [==============================] - 2s 12ms/step - loss: 0.3083 -
accuracy: 0.9187 - val_loss: 0.3617 - val_accuracy: 0.9060
Epoch 7/10
188/188 [==============================] - 3s 14ms/step - loss: 0.2788 -
accuracy: 0.9270 - val_loss: 0.3504 - val_accuracy: 0.9070
Epoch 8/10
188/188 [==============================] - 2s 12ms/step - loss: 0.2553 -
accuracy: 0.9350 - val_loss: 0.3152 - val_accuracy: 0.9090
Epoch 9/10
188/188 [==============================] - 2s 13ms/step - loss: 0.2360 -
accuracy: 0.9343 - val_loss: 0.3116 - val_accuracy: 0.9150
Epoch 10/10
188/188 [==============================] - 2s 11ms/step - loss: 0.2181 -
accuracy: 0.9413 - val_loss: 0.2976 - val_accuracy: 0.9210

Test accuracy: 0.9100
```

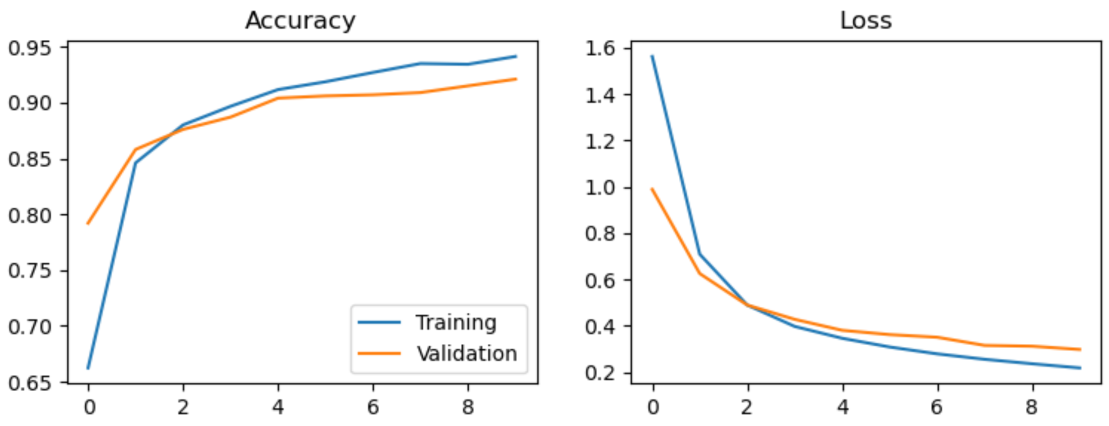
We can summarise the network parameters:

```
[12]: ffnn.summary()
```

```
Model: "FFNN_example"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense (Dense)               (None, 1024)              803840

 dense_1 (Dense)             (None, 512)               524800

 dense_2 (Dense)             (None, 10)                5130

=================================================================
Total params: 1,333,770
Trainable params: 1,333,770
Non-trainable params: 0
_________________________________________________________________
```

Let's see how the accuracy and loss developped over training making use of the `ffnn_history` object we assigned after training.

[13]:
```python
import matplotlib.pyplot as plt

fig, axs = plt.subplots(1,2, figsize=(9,3))

axs[0].plot(ffnn_history.history['accuracy'], label='Training')
axs[0].plot(ffnn_history.history['val_accuracy'], label='Validation')
axs[0].set_title('Accuracy')
axs[0].legend()

axs[1].plot(ffnn_history.history['loss'])
axs[1].plot(ffnn_history.history['val_loss'])
axs[1].set_title('Loss')

plt.show()
```



We use the predict method to provide predictions to new data. You can use the model you just trained or you can load a previously **pretrained** model.

[18]:
```python
# Our pretrained model (100 epochs):
ffnn = keras.models.load_model('output/MNIST_FFNN_pretrained.h5')

# ... or load the model you trained yourself:
# ffnn = keras.models.load_model('output/MNIST_FFNN.h5')

test_loss, test_acc = ffnn.evaluate(x_test, y_test, verbose=0)

print(f'Test accuracy: {test_acc:.4f}\n')

num_examples = 10

predictions_1hot = ffnn.predict(x_test, verbose=0)
```

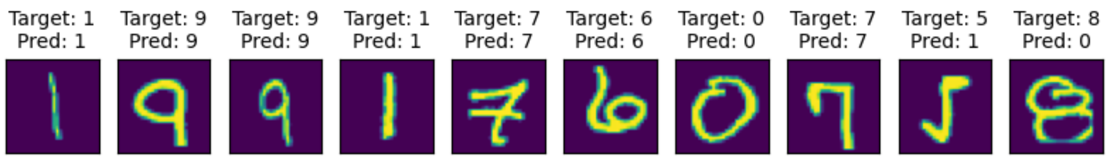
```
# print(predictions_1hot[0])

nicer_predictions_1hot_0 = list(map(np.format_float_positional,␣
 ↪predictions_1hot[0], [5]*10))

print(f"Shape of the predictions: {predictions_1hot.shape}\n")
print(f"First prediction: {nicer_predictions_1hot_0}\n")

predictions = np.argmax(predictions_1hot, axis=1)

print(f"First class prediction: {predictions[0]}")
```

```
Test accuracy: 0.9260

Shape of the predictions: (1000, 10)

First prediction: ['0.00000', '0.00000', '0.00004', '0.00043', '0.00000',
'0.00000', '0.00000', '0.99954', '0.00000', '0.00000']

First class prediction: 7
```

Note that the neural network outputs vectors with class probabilities. We choose the class with the highest probability.

Let's plot some of the predicted labels.

```
[19]: fig, axs = plt.subplots(1,num_examples, figsize=(num_examples,5))

start_index = 900

for i, ax in enumerate(axs.ravel()):
    ax.imshow(x_test[start_index+i].reshape(28,28))

    ax.set_xticks([])
    ax.set_yticks([])
    ax.set_title(f"Target: {y_test[start_index+i]}\nPred:␣
 ↪{predictions[start_index+i]}",
                 fontsize=10)

plt.show()
```



1.2 Convolutional Neural Networks

An important class of neural network architectures are **convolutional neural networks (CNNs)**. CNNs are inspired by biological models for the primary visual cortex and their resemblance to the mathemtical convolution operation. CNNs can be viewed as a particular kind of FFNNs where certain connections are missing and some neurons share the same weights. This gives rise to architectures as illustrated in the following figure.

CNNs are particularly suited to work with images and generally data **where some kind of local relationship / correlation** are present, e.g. adjacent pixels in an image or adjacent time steps in time series data. Two key components of CNNs are pooling and convolutional layers illustrated in the following.

Convolutional layers use a **convolutional filter** (sometimes called *kernel*, too) which processes the input images with respect to particular features (like edges) producing **feature maps**. Sequentially applying convolutional layers allow for **identifying increasingly complex features**. A typical size of a convolutional filter is 3×3 which can be thought of as a matrix of weights (in red above) which are adjusted during training to identify features in a data-driven fashion.

Pooling layers reduce the resolution of feature maps and don't have any associated weights. In particular, max pooling layers of size 2×2 are used to identify the main activation in adjecent pixels. This allows objects to be in different positions in the image but still be recognised as the same object.

Let's implement such a CNN and reshape the image vectors to actual images again.

[20]:
```python
mnist_data_image = mnist_data.reshape(-1, 28, 28, 1) / 255

x_train = mnist_data_image[:num_train]
x_val = mnist_data_image[num_train:num_train+num_val]
x_test = mnist_data_image[-num_test:]
```

We define a CNN with the following layers and train as before:

- 28 \$ $\times$\$ 28 \$ $\times$\$ 1 neurons in the input layer for the greyscale image
- 6 conv. filters of size 3×3 in the first hidden layer with ReLU activation followed by a 2×2 max pooling
- 16 conv. filters of size 3×3 in the first hidden layer with ReLU activation followed by a 2×2 max pooling
- flatten these feature maps in a single vector
- 1024 (hidden) neurons in the second hidden layer with ReLU activation
- 512 (hidden) neurons in the second hidden layer with ReLU activation
- 10 output neurons for our classes in the output layer with a softmax activation

[21]:
```python
keras.utils.set_random_seed(123)

cnn = keras.Sequential([
    keras.layers.Conv2D(6, (3, 3), activation='relu', input_shape=(28, 28, 1)),
    keras.layers.MaxPooling2D((2, 2)),
    keras.layers.Conv2D(16, (3, 3), activation='relu'),
    keras.layers.MaxPooling2D((2, 2)),
    keras.layers.Flatten(),
    keras.layers.Dense(1024, activation='relu'),
    keras.layers.Dense(512, activation='relu'),
    keras.layers.Dense(10, activation='softmax')
    ], name='CNN_example')

cnn.compile(optimizer=keras.optimizers.SGD(learning_rate=learning_rate),
              loss='sparse_categorical_crossentropy',
              metrics=['accuracy'])

cnn_history = cnn.fit(x=x_train, y=y_train, batch_size=batch_size,
                      validation_data=(x_val, y_val), epochs=num_epochs)

test_loss, test_acc = cnn.evaluate(x_test, y_test, verbose=0)

print(f'\nTest accuracy: {test_acc:.4f}\n')

cnn.save('output/MNIST_CNN.h5')

cnn.summary()
```

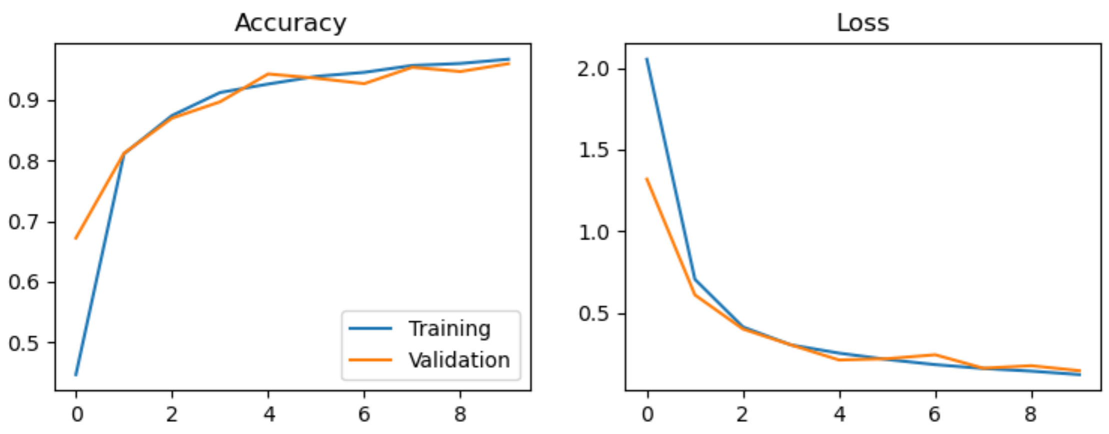
```
Epoch 1/10
188/188 [==============================] - 5s 21ms/step - loss: 2.0534 -
accuracy: 0.4463 - val_loss: 1.3186 - val_accuracy: 0.6720
Epoch 2/10
188/188 [==============================] - 4s 21ms/step - loss: 0.7040 -
accuracy: 0.8110 - val_loss: 0.6086 - val_accuracy: 0.8120
Epoch 3/10
188/188 [==============================] - 4s 20ms/step - loss: 0.4119 -
accuracy: 0.8743 - val_loss: 0.3993 - val_accuracy: 0.8700
Epoch 4/10
188/188 [==============================] - 4s 23ms/step - loss: 0.3018 -
accuracy: 0.9123 - val_loss: 0.3021 - val_accuracy: 0.8970
Epoch 5/10
188/188 [==============================] - 5s 25ms/step - loss: 0.2515 -
accuracy: 0.9263 - val_loss: 0.2094 - val_accuracy: 0.9430
Epoch 6/10
188/188 [==============================] - 4s 19ms/step - loss: 0.2127 -
accuracy: 0.9390 - val_loss: 0.2174 - val_accuracy: 0.9360
Epoch 7/10
188/188 [==============================] - 4s 23ms/step - loss: 0.1811 -
accuracy: 0.9457 - val_loss: 0.2416 - val_accuracy: 0.9270
Epoch 8/10
188/188 [==============================] - 4s 21ms/step - loss: 0.1575 -
accuracy: 0.9570 - val_loss: 0.1591 - val_accuracy: 0.9540
```

```
Epoch 9/10
188/188 [==============================] - 5s 27ms/step - loss: 0.1413 -
accuracy: 0.9603 - val_loss: 0.1745 - val_accuracy: 0.9470
Epoch 10/10
188/188 [==============================] - 4s 21ms/step - loss: 0.1200 -
accuracy: 0.9673 - val_loss: 0.1439 - val_accuracy: 0.9600

Test accuracy: 0.9310

Model: "CNN_example"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 conv2d (Conv2D)             (None, 26, 26, 6)         60

 max_pooling2d (MaxPooling2D  (None, 13, 13, 6)        0
 )

 conv2d_1 (Conv2D)           (None, 11, 11, 16)        880

 max_pooling2d_1 (MaxPooling  (None, 5, 5, 16)         0
 2D)

 flatten (Flatten)           (None, 400)               0

 dense_3 (Dense)             (None, 1024)              410624

 dense_4 (Dense)             (None, 512)               524800

 dense_5 (Dense)             (None, 10)                5130

=================================================================
Total params: 941,494
Trainable params: 941,494
Non-trainable params: 0
_________________________________________________________________
```

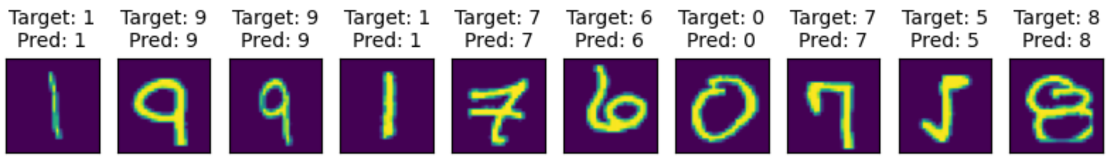
Let's study the performance of the CNN.

[22]:
```python
import matplotlib.pyplot as plt

fig, axs = plt.subplots(1,2, figsize=(9,3))

axs[0].plot(cnn_history.history['accuracy'], label='Training')
axs[0].plot(cnn_history.history['val_accuracy'], label='Validation')
axs[0].set_title('Accuracy')
axs[0].legend()
```

```
axs[1].plot(cnn_history.history['loss'])
axs[1].plot(cnn_history.history['val_loss'])
axs[1].set_title('Loss')

plt.show()

# Our pretrained model (100 epochs):
# cnn = keras.models.load_model('output/MNIST_CNN_pretrained.h5')

# ... or load your model:
cnn = keras.models.load_model('output/MNIST_CNN.h5')

test_loss, test_acc = cnn.evaluate(x_test, y_test, verbose=0)

print(f'Test accuracy: {test_acc:.4f}\n')

num_examples = 10

predictions_1hot = cnn.predict(x_test, verbose=0)
predictions = np.argmax(predictions_1hot, axis=1)

fig, axs = plt.subplots(1, num_examples, figsize=(num_examples,5))

start_index = 900

for i, ax in enumerate(axs.ravel()):
    ax.imshow(x_test[start_index+i])

    ax.set_xticks([])
    ax.set_yticks([])
    ax.set_title(f"Target: {y_test[start_index+i]}\nPred:␣
 ↪{predictions[start_index+i]}",
                 fontsize=10)

plt.show()
```



```
Test accuracy: 0.9310
```



1.3 Exercise Section

For a final time, we consider the red wine dataset with our new regression method. As before, we want to predict the `quality` values on the test set `feat_test` and compare it to the previous results:

- ridge regression MSE 0.42
- Random Forest regression MSE 0.34
- kernel ridge regression MSE 0.38
- Gaussian Process regression MSE 0.38

Prepare the data by load the following cell:

[1]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

from sklearn.model_selection import train_test_split

from tensorflow import keras
```

```
np.random.seed(123)
keras.utils.set_random_seed(123)

wine_data = pd.read_csv('data/winequality-red.csv', sep=';')

ex_target = wine_data['quality']
ex_features = wine_data.drop(['quality'], axis=1)

ex_features = (ex_features - ex_features.min()) / (ex_features.max() -␣
 ↪ex_features.min())

feat_train, feat_test, target_train, target_test = train_test_split(
    ex_features, ex_target, test_size = 0.3, random_state=123)

target_test = target_test.to_frame()
```

```
2023-03-24 08:31:42.445354: I tensorflow/core/platform/cpu_feature_guard.cc:193]
This TensorFlow binary is optimized with oneAPI Deep Neural Network Library
(oneDNN) to use the following CPU instructions in performance-critical
operations:  SSE4.1 SSE4.2 AVX AVX2 FMA
To enable them in other operations, rebuild TensorFlow with the appropriate
compiler flags.
```

(1.) Implement a feed-forward neural network with the following number of artificial neurons in the hidden layers: 1024, 512, 256, 128, 64. Use ReLU activations and the following hyperparameters:

```
[ ]: learning_rate = 0.005
     batch_size = 64
     num_epochs = 50
```

Put your result in the following cell and note:

- Provide the model as `ffnn_reg`, the history of the training in `ffnn_reg_history`, and the predicted quality values in `ex_pred_ffnn`.
- The output in the regression setting is just 1-dimensional and no activation is required.
- Use as the MSE loss `keras.losses.MeanSquaredError()` and do not use the `metrics` argument.
- You can use the test set for `validation_data`.

```
[ ]: # fill in
```

Try to check the accuracy and loss during training with the following plot.

```
[ ]: plt.plot(ffnn_reg_history.history['loss'][1:], label='Training')
     plt.plot(ffnn_reg_history.history['val_loss'][1:], label='Test')
     plt.title('Loss')
     plt.legend()

     plt.show()
```

As we have done earlier, the following cell provides a data frame with an overview of the predictions.

```
[ ]: target_test['NN_predicted_quality'] = np.around(ex_pred_ffnn, decimals=2)
     target_test['NN_absolut_deviation'] = np.around(abs(target_test['quality'] -␣
      ↪target_test['NN_predicted_quality']), decimals=2)
     print(target_test)

     NN_pred_MSE = (target_test['NN_absolut_deviation']**2).mean()
     print(f"\nMean squared error of Feedforward Neural Network regression:␣
      ↪{NN_pred_MSE:.2f}")
```

```
[1]: import numpy as np
     import pandas as pd
     import matplotlib.pyplot as plt

     from sklearn.model_selection import train_test_split

     from tensorflow import keras

     np.random.seed(123)
     keras.utils.set_random_seed(123)

     wine_data = pd.read_csv('data/winequality-red.csv', sep=';')

     ex_target = wine_data['quality']
     ex_features = wine_data.drop(['quality'], axis=1)

     ex_features = (ex_features - ex_features.min()) / (ex_features.max() -␣
      ↪ex_features.min())

     feat_train, feat_test, target_train, target_test = train_test_split(
         ex_features, ex_target, test_size = 0.3, random_state=123)

     target_test = target_test.to_frame()
```

```
2023-03-21 12:53:11.016835: I tensorflow/core/platform/cpu_feature_guard.cc:193]
This TensorFlow binary is optimized with oneAPI Deep Neural Network Library
(oneDNN) to use the following CPU instructions in performance-critical
operations:  SSE4.1 SSE4.2 AVX AVX2 FMA
To enable them in other operations, rebuild TensorFlow with the appropriate
compiler flags.
```

(1.) Implement a feed-forward neural network with the following number of artificial neurons in the hidden layers: 1024, 512, 256, 128, 64. Use ReLU activations and the following hyperparameters:

```
[2]: learning_rate = 0.005
     batch_size = 64
     num_epochs = 50
```

Put your result in the following cell and note:

- Provide the model as `ffnn_reg`, the history of the training in `ffnn_reg_history`, and the predicted quality values in `ex_pred_ffnn`.
- The output in the regression setting is just 1-dimensional and no activation is required.
- Use as the MSE loss `keras.losses.MeanSquaredError()` and do not use the `metrics` argument.
- You can use the test set for `validation_data`.

[3]:
```
ffnn_reg = keras.Sequential(
    [
    keras.layers.Dense(1024, activation='relu', input_shape=(11,)),
    keras.layers.Dense(512, activation='relu'),
    keras.layers.Dense(256, activation='relu'),
    keras.layers.Dense(128, activation='relu'),
    keras.layers.Dense(64, activation='relu'),
    keras.layers.Dense(1)
    ],
    name='FFNN_regression')

ffnn_reg.compile(optimizer=keras.optimizers.SGD(learning_rate=learning_rate),
                 loss=keras.losses.MeanSquaredError())

ffnn_reg_history = ffnn_reg.fit(x=feat_train, y=target_train,
                                validation_data=(feat_test, target_test),
                                batch_size=batch_size, epochs=num_epochs)

ex_pred_ffnn = ffnn_reg.predict(feat_test, verbose=0)

ffnn_reg.save(f'output/MNIST_FFNN_reg.h5')
```

```
Epoch 1/50
```

```
2023-03-21 12:53:13.838010: I tensorflow/core/platform/cpu_feature_guard.cc:193]
This TensorFlow binary is optimized with oneAPI Deep Neural Network Library
(oneDNN) to use the following CPU instructions in performance-critical
operations:  SSE4.1 SSE4.2 AVX AVX2 FMA
To enable them in other operations, rebuild TensorFlow with the appropriate
compiler flags.
```

```
18/18 [==============================] - 1s 15ms/step - loss: 17.3084 -
val_loss: 0.6507
Epoch 2/50
18/18 [==============================] - 0s 7ms/step - loss: 0.6783 - val_loss:
0.6384
Epoch 3/50
18/18 [==============================] - 0s 7ms/step - loss: 0.6341 - val_loss:
0.5898
Epoch 4/50
```

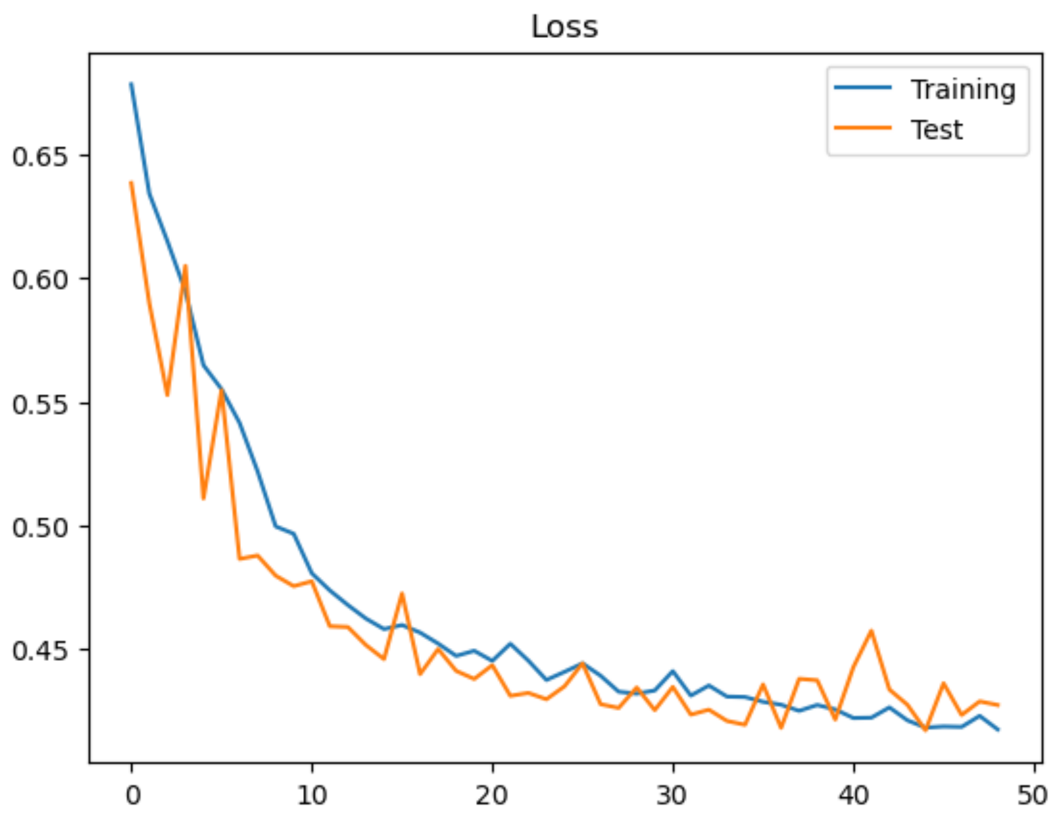
```
18/18 [==============================] - 0s 7ms/step - loss: 0.6149 - val_loss:
0.5527
Epoch 5/50
18/18 [==============================] - 0s 9ms/step - loss: 0.5946 - val_loss:
0.6049
Epoch 6/50
18/18 [==============================] - 0s 7ms/step - loss: 0.5648 - val_loss:
0.5109
Epoch 7/50
18/18 [==============================] - 0s 8ms/step - loss: 0.5551 - val_loss:
0.5547
Epoch 8/50
18/18 [==============================] - 0s 9ms/step - loss: 0.5414 - val_loss:
0.4864
Epoch 9/50
18/18 [==============================] - 0s 7ms/step - loss: 0.5218 - val_loss:
0.4878
Epoch 10/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4996 - val_loss:
0.4796
Epoch 11/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4966 - val_loss:
0.4754
Epoch 12/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4806 - val_loss:
0.4774
Epoch 13/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4737 - val_loss:
0.4592
Epoch 14/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4678 - val_loss:
0.4589
Epoch 15/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4623 - val_loss:
0.4516
Epoch 16/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4580 - val_loss:
0.4459
Epoch 17/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4597 - val_loss:
0.4725
Epoch 18/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4566 - val_loss:
0.4398
Epoch 19/50
18/18 [==============================] - 0s 9ms/step - loss: 0.4522 - val_loss:
0.4500
Epoch 20/50
```

```
18/18 [==============================] - 0s 7ms/step - loss: 0.4472 - val_loss:
0.4411
Epoch 21/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4493 - val_loss:
0.4379
Epoch 22/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4452 - val_loss:
0.4434
Epoch 23/50
18/18 [==============================] - 0s 9ms/step - loss: 0.4521 - val_loss:
0.4310
Epoch 24/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4452 - val_loss:
0.4322
Epoch 25/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4375 - val_loss:
0.4297
Epoch 26/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4407 - val_loss:
0.4349
Epoch 27/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4442 - val_loss:
0.4442
Epoch 28/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4392 - val_loss:
0.4277
Epoch 29/50
18/18 [==============================] - 0s 9ms/step - loss: 0.4327 - val_loss:
0.4261
Epoch 30/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4319 - val_loss:
0.4344
Epoch 31/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4332 - val_loss:
0.4253
Epoch 32/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4410 - val_loss:
0.4346
Epoch 33/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4311 - val_loss:
0.4234
Epoch 34/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4352 - val_loss:
0.4254
Epoch 35/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4307 - val_loss:
0.4209
Epoch 36/50
```

```
18/18 [==============================] - 0s 7ms/step - loss: 0.4306 - val_loss:
0.4193
Epoch 37/50
18/18 [==============================] - 0s 9ms/step - loss: 0.4286 - val_loss:
0.4357
Epoch 38/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4274 - val_loss:
0.4181
Epoch 39/50
18/18 [==============================] - 0s 9ms/step - loss: 0.4250 - val_loss:
0.4379
Epoch 40/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4273 - val_loss:
0.4373
Epoch 41/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4255 - val_loss:
0.4215
Epoch 42/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4221 - val_loss:
0.4426
Epoch 43/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4222 - val_loss:
0.4574
Epoch 44/50
18/18 [==============================] - 0s 9ms/step - loss: 0.4264 - val_loss:
0.4336
Epoch 45/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4211 - val_loss:
0.4274
Epoch 46/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4182 - val_loss:
0.4171
Epoch 47/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4186 - val_loss:
0.4361
Epoch 48/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4185 - val_loss:
0.4233
Epoch 49/50
18/18 [==============================] - 0s 9ms/step - loss: 0.4229 - val_loss:
0.4288
Epoch 50/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4174 - val_loss:
0.4273
```

Try to check the accuracy and loss during training with the following plot.

```
[4]: plt.plot(ffnn_reg_history.history['loss'][1:], label='Training')
     plt.plot(ffnn_reg_history.history['val_loss'][1:], label='Test')
     plt.title('Loss')
     plt.legend()

     plt.show()
```



As we have done earlier, the following cell provides a data frame with an overview of the predictions.

```
[5]: # Pretrained for 1000 epochs
     #ffnn_reg = keras.models.load_model('output/MNIST_FFNN_reg_pretrained.h5')
     #ex_pred_ffnn = ffnn_reg.predict(feat_test, verbose=0)
```

```
[6]: target_test['NN_predicted_quality'] = np.around(ex_pred_ffnn, decimals=2)
     target_test['NN_absolut_deviation'] = np.around(abs(target_test['quality'] -␣
      ↪target_test['NN_predicted_quality']), decimals=2)
     print(target_test)

     NN_pred_MSE = (target_test['NN_absolut_deviation']**2).mean()
     print(f"\nMean squared error of Feedforward Neural Network regression:␣
      ↪{NN_pred_MSE:.2f}")
      quality  NN_predicted_quality  NN_absolut_deviation
912         6                  6.52                  0.52
772         5                  5.09                  0.09
1037        5                  4.91                  0.09
1106        6                  6.60                  0.60
263         5                  5.51                  0.51
…         …                   …                   …
1466        7                  5.61                  1.39
580         5                  5.44                  0.44
1082        6                  5.47                  0.53
1279        7                  6.35                  0.65
1155        5                  5.34                  0.34

[480 rows x 3 columns]

Mean squared error of Feedforward Neural Network regression: 0.43
```

1.4 5. Neural Networks

1.5 Proposed Solutions

For a final time, we consider the red wine dataset with our new regression method. As before, we want to predict the `quality` values on the test set `feat_test` and compare it to the previous results:

- ridge regression MSE 0.42
- Random Forest regression MSE 0.34
- kernel ridge regression MSE 0.38
- Gaussian Process regression MSE 0.38

Prepare the data by load the following cell:

[1]:
```python
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

from sklearn.model_selection import train_test_split

from tensorflow import keras

np.random.seed(123)
keras.utils.set_random_seed(123)

wine_data = pd.read_csv('data/winequality-red.csv', sep=';')

ex_target = wine_data['quality']
ex_features = wine_data.drop(['quality'], axis=1)
ex_features = (ex_features - ex_features.min()) / (ex_features.max() -␣
↪ex_features.min())

feat_train, feat_test, target_train, target_test = train_test_split(
    ex_features, ex_target, test_size = 0.3, random_state=123)

target_test = target_test.to_frame()
```

```
2023-03-24 08:32:57.033994: I tensorflow/core/platform/cpu_feature_guard.cc:193]
This TensorFlow binary is optimized with oneAPI Deep Neural Network Library
(oneDNN) to use the following CPU instructions in performance-critical
operations:  SSE4.1 SSE4.2 AVX AVX2 FMA
To enable them in other operations, rebuild TensorFlow with the appropriate
compiler flags.
```

[5]:
```
feat_train
```

[5]:
```
      fixed acidity  volatile acidity  citric acid  residual sugar  chlorides  \
374        0.831858          0.198630         0.63        0.198630   0.128548
800        0.230088          0.335616         0.08        0.212329   0.116861
1441       0.247788          0.455479         0.19        0.294521   0.136895
1269       0.079646          0.253425         0.03        0.061644   0.053422
691        0.407080          0.547945         0.24        0.116438   0.125209
…               …                 …           …             …          …
1122       0.150442          0.239726         0.00        0.034247   0.071786
1346       0.132743          0.321918         0.01        0.082192   0.073456
1406       0.318584          0.082192         0.34        0.287671   0.083472
1389       0.185841          0.246575         0.02        0.089041   0.113523
1534       0.176991          0.301370         0.14        0.102740   0.086811

      free sulfur dioxide  total sulfur dioxide   density        pH  \
374              0.070423              0.144876  0.831865  0.212598
800              0.352113              0.360424  0.465492  0.401575
1441             0.253521              0.325088  0.518355  0.330709
1269             0.380282              0.286219  0.053598  0.598425
691              0.154930              0.307420  0.714391  0.582677
…                     …                     …       …         …
1122             0.366197              0.095406  0.156388  0.559055
1346             0.056338              0.024735  0.341410  0.614173
1406             0.098592              0.056537  0.538179  0.377953
1389             0.492958              0.371025  0.379589  0.283465
1534             0.169014              0.081272  0.286344  0.535433

      sulphates   alcohol
374    0.287425  0.369231
800    0.107784  0.153846
1441   0.113772  0.179487
```

```
1269    0.293413  0.861538
691     0.125749  0.215385
…          …         …
1122    0.089820  0.600000
1346    0.137725  0.461538
1406    0.365269  0.384615
1389    0.119760  0.200000
1534    0.173653  0.507692

[1119 rows x 11 columns]
```

(1.) Implement a feed-forward neural network with the following number of artificial neurons in the hidden layers: 1024, 512, 256, 128, 64. Use ReLU activations and the following hyperparameters:

[2]:
```
learning_rate = 0.005
batch_size = 64
num_epochs = 50
```

Put your result in the following cell and note:

- Provide the model as `ffnn_reg`, the history of the training in `ffnn_reg_history`, and the predicted quality values in `ex_pred_ffnn`.
- The output in the regression setting is just 1-dimensional and no activation is required.
- Use as the MSE loss `keras.losses.MeanSquaredError()` and do not use the `metrics` argument.
- You can use the test set for `validation_data`.

[3]:
```
ffnn_reg = keras.Sequential(
    [
    keras.layers.Dense(1024, activation='relu', input_shape=(11,)),
    keras.layers.Dense(512, activation='relu'),
    keras.layers.Dense(256, activation='relu'),
    keras.layers.Dense(128, activation='relu'),
    keras.layers.Dense(64, activation='relu'),
    keras.layers.Dense(1)
    ],
    name='FFNN_regression')

ffnn_reg.compile(optimizer=keras.optimizers.SGD(learning_rate=learning_rate),
                 loss=keras.losses.MeanSquaredError())

ffnn_reg_history = ffnn_reg.fit(x=feat_train, y=target_train,
                                validation_data=(feat_test, target_test),
                                batch_size=batch_size, epochs=num_epochs)

ex_pred_ffnn = ffnn_reg.predict(feat_test, verbose=0)

ffnn_reg.save(f'output/MNIST_FFNN_reg.h5')
```

```
Epoch 1/50

2023-03-21 12:53:13.838010: I tensorflow/core/platform/cpu_feature_guard.cc:193]
This TensorFlow binary is optimized with oneAPI Deep Neural Network Library
(oneDNN) to use the following CPU instructions in performance-critical
operations:  SSE4.1 SSE4.2 AVX AVX2 FMA
To enable them in other operations, rebuild TensorFlow with the appropriate
compiler flags.

18/18 [==============================] - 1s 15ms/step - loss: 17.3084 -
val_loss: 0.6507
Epoch 2/50
18/18 [==============================] - 0s 7ms/step - loss: 0.6783 - val_loss:
0.6384
Epoch 3/50
18/18 [==============================] - 0s 7ms/step - loss: 0.6341 - val_loss:
0.5898
Epoch 4/50
18/18 [==============================] - 0s 7ms/step - loss: 0.6149 - val_loss:
0.5527
Epoch 5/50
18/18 [==============================] - 0s 9ms/step - loss: 0.5946 - val_loss:
0.6049
Epoch 6/50
18/18 [==============================] - 0s 7ms/step - loss: 0.5648 - val_loss:
0.5109
Epoch 7/50
18/18 [==============================] - 0s 8ms/step - loss: 0.5551 - val_loss:
0.5547
Epoch 8/50
18/18 [==============================] - 0s 9ms/step - loss: 0.5414 - val_loss:
0.4864
Epoch 9/50
18/18 [==============================] - 0s 7ms/step - loss: 0.5218 - val_loss:
0.4878
Epoch 10/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4996 - val_loss:
0.4796
Epoch 11/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4966 - val_loss:
0.4754
Epoch 12/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4806 - val_loss:
0.4774
Epoch 13/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4737 - val_loss:
0.4592
Epoch 14/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4678 - val_loss:
```

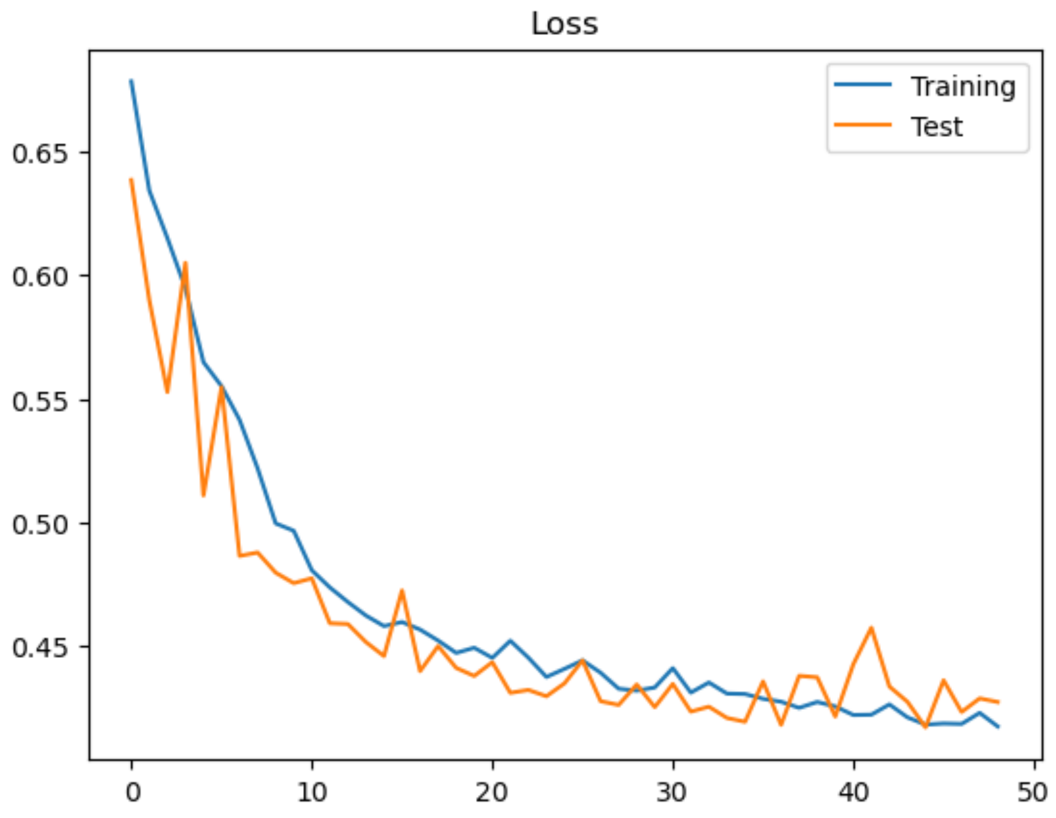
```
0.4589
Epoch 15/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4623 - val_loss:
0.4516
Epoch 16/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4580 - val_loss:
0.4459
Epoch 17/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4597 - val_loss:
0.4725
Epoch 18/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4566 - val_loss:
0.4398
Epoch 19/50
18/18 [==============================] - 0s 9ms/step - loss: 0.4522 - val_loss:
0.4500
Epoch 20/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4472 - val_loss:
0.4411
Epoch 21/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4493 - val_loss:
0.4379
Epoch 22/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4452 - val_loss:
0.4434
Epoch 23/50
18/18 [==============================] - 0s 9ms/step - loss: 0.4521 - val_loss:
0.4310
Epoch 24/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4452 - val_loss:
0.4322
Epoch 25/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4375 - val_loss:
0.4297
Epoch 26/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4407 - val_loss:
0.4349
Epoch 27/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4442 - val_loss:
0.4442
Epoch 28/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4392 - val_loss:
0.4277
Epoch 29/50
18/18 [==============================] - 0s 9ms/step - loss: 0.4327 - val_loss:
0.4261
Epoch 30/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4319 - val_loss:
```

```
0.4344
Epoch 31/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4332 - val_loss:
0.4253
Epoch 32/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4410 - val_loss:
0.4346
Epoch 33/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4311 - val_loss:
0.4234
Epoch 34/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4352 - val_loss:
0.4254
Epoch 35/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4307 - val_loss:
0.4209
Epoch 36/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4306 - val_loss:
0.4193
Epoch 37/50
18/18 [==============================] - 0s 9ms/step - loss: 0.4286 - val_loss:
0.4357
Epoch 38/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4274 - val_loss:
0.4181
Epoch 39/50
18/18 [==============================] - 0s 9ms/step - loss: 0.4250 - val_loss:
0.4379
Epoch 40/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4273 - val_loss:
0.4373
Epoch 41/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4255 - val_loss:
0.4215
Epoch 42/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4221 - val_loss:
0.4426
Epoch 43/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4222 - val_loss:
0.4574
Epoch 44/50
18/18 [==============================] - 0s 9ms/step - loss: 0.4264 - val_loss:
0.4336
Epoch 45/50
18/18 [==============================] - 0s 8ms/step - loss: 0.4211 - val_loss:
0.4274
Epoch 46/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4182 - val_loss:
```

```
0.4171
Epoch 47/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4186 - val_loss:
0.4361
Epoch 48/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4185 - val_loss:
0.4233
Epoch 49/50
18/18 [==============================] - 0s 9ms/step - loss: 0.4229 - val_loss:
0.4288
Epoch 50/50
18/18 [==============================] - 0s 7ms/step - loss: 0.4174 - val_loss:
0.4273
```

Try to check the accuracy and loss during training with the following plot.

[4]:
```
plt.plot(ffnn_reg_history.history['loss'][1:], label='Training')
plt.plot(ffnn_reg_history.history['val_loss'][1:], label='Test')
plt.title('Loss')
plt.legend()

plt.show()
```



As we have done earlier, the following cell provides a data frame with an overview of the predictions.

[7]:
```
# Pretrained for 1000 epochs
ffnn_reg = keras.models.load_model('output/MNIST_FFNN_reg_pretrained.h5')
ex_pred_ffnn = ffnn_reg.predict(feat_test, verbose=0)
```

[4]:
```
target_test['NN_predicted_quality'] = np.around(ex_pred_ffnn, decimals=2)
target_test['NN_absolut_deviation'] = np.around(abs(target_test['quality'] -␣
 ↪target_test['NN_predicted_quality']), decimals=2)
print(target_test)

NN_pred_MSE = (target_test['NN_absolut_deviation']**2).mean()
print(f"\nMean squared error of Feedforward Neural Network regression:␣
 ↪{NN_pred_MSE:.2f}")
```

```
      quality  NN_predicted_quality  NN_absolut_deviation
912         6                  6.49                  0.49
772         5                  4.94                  0.06
1037        5                  4.74                  0.26
1106        6                  6.59                  0.59
263         5                  5.40                  0.40
…         …                   …                   …
1466        7                  5.59                  1.41
580         5                  4.69                  0.31
1082        6                  5.28                  0.72
1279        7                  6.29                  0.71
1155        5                  5.19                  0.19

[480 rows x 3 columns]

Mean squared error of Feedforward Neural Network regression: 0.37
```

6-VAE

March 24, 2023

1 6. Variational Autoencoder

We have seen approaches for compression previously. In this notebook, we cover a related approach based on neural networks which also enables us to generate novel (artificial) data.

In particular, we discuss

- latent variable models and
- the Variational Autoencoder

and provide a more advanced CNN implementation for MNIST and a molecule dataset.

Keywords: `VAE`, `ELBO`, `reparameterisation trick`, `keras.Model`, `keras.layers.Conv2DTranspose`, `tensorflow.GradientTape`, `tf.sigmoid`, `model.save_weights`, `model.load_weights`, `keras.optimizers.Adam`

1.1 Latent Variable Models

Latent variable models (LVMs) are statistical models which consider random variables. Suppose that our observations X and Y are random variables following a probability distribution $p(X, Y)$. LVMs assume that there are **latent, i.e. unobserved or hidden, variables** Z which have a relationship to our observed data X and Y. A typical assumption, for instance is, that our predictors X are generated by **lower-dimensional latent variables** Z, e.g. $p(X \mid Z)$.

Note that we have seen models such as these already. For example, in a **Gaussian Mixture Model** datapoints X_i belonging to cluster i with mean μ_i and covariance matrix Σ_i are generated by sampling from $\mathcal{N}(\mu_i, \Sigma_i)$. In other words, the low-dimensional latent variables are $Z = (\mu, \Sigma)$. **PCA** is another example where few principal components can allow describing the majority of variation in a dataset. However, these **linear LVMs** assume linear relationships between latent variable Z and the observations.

Due to the highly non-linear nature of neural networks, we can use neural networks to extend models such as PCA to **non-linear LVMs**. Here, we pick up the previously encountered idea of compression:

The **Variational Autoencoder (VAE)** is an unsupervised neural network approach which attempts to identify a meaningful **latent representation** Z capable of reconstructing the original input as perfectly as possible. The VAE can be viewed as probabilistic non-linear PCA, with the general idea being illustrated in the following figure.

The VAE has three important components:

1. **Enocoder**: The encoder neural network attempts to compress the relevant information about X in latent representation Z with dimensions $d_X > d_Z$. The goal of the encoder is to parameterise a distribution $q_\phi(Z \mid X)$ which provides us a (variational) approximation for the distribution of the (compressed) latent variables Z given an input X. Here, ϕ denotes the weights of the encoder network. We typically assume that this approximation is given by a Gaussian distribution $\mathcal{N}(\mu_Z, \Sigma_Z)$ where $\mu_Z = (\mu_1, \ldots, \mu_{d_Z})$ and $\Sigma_Z = (\sigma_1, \ldots, \sigma_{d_Z})$ containing only the diagonal entries of covariance matrix Σ_Z (all other entries are 0). For technical reasons (details omitted), we require the **reparameterisation trick** to sample latent variables Z:
$$z_n(\varepsilon) = \mu_Z(x_n) + \Sigma_Z^2(x_n)\varepsilon$$
with $\varepsilon \sim \mathcal{N}(0, 1)$.

2. **Latent representation / space** Z: Datapoints from the input space are mapped into the lower-dimensional latent space Z. To start with, we typically assume that the latent variables Z are normally distributed, i.e. a prior distribution $p(Z) = \mathcal{N}(0, \mathbb{1}_{d_Z})$ with d_Z being the number of latent dimensions. We train the encoder such that the (posterior) distribution $q_\phi(Z \mid X)$ matches the prior $p(Z)$ as much as possible. The deviations from the prior distribution will capture important features of our dataset. We measure the difference in these distributions with the (non-negative) Kullback-Leibler divergence
$$D_{\text{KL}}(q_\phi(Z \mid X) \| p(Z)) = -\frac{1}{2}\sum_{i=1}^{d_Z}(1 + \log \sigma_i^2 - \mu_i^2 - \sigma_i^2),$$
where the last expression follows from the Gaussian distrubtion assumptions outlined before.

3. **Decoder**: The decoder neural network attempts so reconstruct the original input X from the compressed representation Z. The goal of the decoder is to parameterise the likelihood $p_\theta(X \mid Z)$ with decoder network weights θ. The **reconstruction error** is measured by the log-likelihood $\log(p_\theta(X \mid Z))$ which in the case of regression tasks is typically given by the mean-squared error loss and in classification tasks by the cross-entropy loss.

Combining these ingredients, we obtain the VAE loss function which is usually referred to as negative **evidence lower bound (ELBO)**
$$\text{Loss}(\phi, \theta) = \frac{1}{s}\sum_{i=1}^{s} \underbrace{\mathbb{E}_{q_\phi(z|x_i)}\big(-\log(p_\theta(x_i|z))\big)}_{\text{reconstruction loss}} + \underbrace{D_{\text{KL}}(q_\phi(z|x_i)\|p(z))}_{\text{latent loss}} \tag{1}$$
where s is the batch size (denoting that we sum the results for different batches). Note that the VAE objective has two parts which we try to balance:

1. The **reconstruction loss** measures how well we can reconstruct the input X from the compression Z. In other words, this term is an incentive to provide as much information of X in Z as possible, i.e. less compression.
2. The **latent loss** measures how well the posterior $q_\phi(Z \mid X)$ agrees with the prior $p(Z)$. This term favours stronger compressions.

With this probabilistic framework, we can now explore the latent space Z and, in particular, pick latent points in Z to generate novel artifical objects by decoding the picked latent point!

Let's implement and apply a VAE on MNIST! For this, we first define a class for the model which provides the individual parts as outlined above.

[1]:
```
import numpy as np
import matplotlib.pyplot as plt
import tensorflow as tf
from tensorflow import keras

class VAE(keras.Model):

    def __init__(self, latent_dim, batch_size):
        super(VAE, self).__init__()
        self.latent_dim = latent_dim
        self.batch_size = batch_size

        # Encoder network:
        self.encoder = keras.Sequential(
            [
                keras.layers.InputLayer(input_shape=(28, 28, 1)),
                keras.layers.Conv2D(filters=32, kernel_size=3, strides=(2, 2),␣
 ↪activation='relu'),
                keras.layers.Conv2D(filters=64, kernel_size=3, strides=(2, 2),␣
 ↪activation='relu'),
                keras.layers.Flatten(),
                keras.layers.Dense(latent_dim + latent_dim),
            ]
        )

        # Decoder network:
        self.decoder = keras.Sequential(
            [
                keras.layers.InputLayer(input_shape=(latent_dim,)),
                keras.layers.Dense(units=7 * 7 * 32, activation='relu'),
                keras.layers.Reshape(target_shape=(7, 7, 32)),
                keras.layers.Conv2DTranspose(filters=32, kernel_size=3,␣
 ↪strides=2, padding='same', activation='relu'),
                keras.layers.Conv2DTranspose(filters=64, kernel_size=3,␣
 ↪strides=2, padding='same', activation='relu'),
                keras.layers.Conv2DTranspose(filters=1, kernel_size=3,␣
 ↪strides=1, padding='same'),
            ]
        )


    def encode(self, x):
        mean, logvar = tf.split(self.encoder(x), num_or_size_splits=2, axis=1)
        return mean, logvar
    def decode(self, z, apply_sigmoid=False):
        logits = self.decoder(z)
        if apply_sigmoid:
            probs = tf.sigmoid(logits)
            return probs
        return logits


    @tf.function
    def sample(self, eps=None):
        if eps is None:
            eps = tf.random.normal(shape=(self.batch_size, self.latent_dim))
        return self.decode(eps, apply_sigmoid=True)


    # Reparameterisation trick:
    def reparameterize(self, mean, logvar):
        eps = tf.random.normal(shape=(self.batch_size, self.latent_dim))
        return eps * tf.exp(logvar * .5) + mean


    def call(self, x):
        mean, logvar = tf.split(self.encoder(x), num_or_size_splits=2, axis=1)
        z = self.reparameterize(mean, logvar)
        return self.decoder(z), mean, logvar
```

```
2023-03-24 13:15:39.884475: I tensorflow/core/platform/cpu_feature_guard.cc:193]
This TensorFlow binary is optimized with oneAPI Deep Neural Network Library
(oneDNN) to use the following CPU instructions in performance-critical
operations:  SSE4.1 SSE4.2 AVX AVX2 FMA
To enable them in other operations, rebuild TensorFlow with the appropriate
compiler flags.
```

Furthermore, we define some functions we will use for computing the loss and the training steps. Note that in the previous notebook we used some built-in `keras` functions for that.

[2]:
```
def log_normal_pdf(sample, mean, logvar, raxis=1):
    log2pi = tf.math.log(2.0 * np.pi)
    return tf.reduce_sum(-0.5 * ((sample - mean) ** 2.0 * tf.exp(-logvar) +␣
 ↪logvar + log2pi), axis=raxis)


def compute_loss(model, x):
    mean, logvar = model.encode(x)
    z = model.reparameterize(mean, logvar)
    x_logit = model.decode(z)
    cross_ent = tf.nn.sigmoid_cross_entropy_with_logits(logits=x_logit,␣
 ↪labels=x)
    logpx_z = -tf.reduce_sum(cross_ent, axis=[1, 2, 3])
    logpz = log_normal_pdf(z, 0., 0.)
    logqz_x = log_normal_pdf(z, mean, logvar)

    return -tf.reduce_mean(logpx_z + logpz - logqz_x)


@tf.function
def train_step(model, x, optimizer):

    with tf.GradientTape() as tape:
        loss = compute_loss(model, x)

    gradients = tape.gradient(loss, model.trainable_variables)
    optimizer.apply_gradients(zip(gradients, model.trainable_variables))
```

Now, we can load MNIST as before.

```
[3]: mnist_data = np.load('data/mnist_data_5k.npy', allow_pickle=True).
      ↪astype('float32')
     mnist_targets = np.load('data/mnist_labels_5k.npy', allow_pickle=True).
      ↪astype('float32')

     mnist_data = mnist_data.reshape(-1, 28, 28, 1) / 255

     num_train = 3000
     num_val = 1000
     num_test = 1000

     x_train = mnist_data[:num_train]
     y_train = mnist_targets[:num_train]

     x_val = mnist_data[num_train:num_train+num_val]
     y_val = mnist_targets[num_train:num_train+num_val]

     x_test = mnist_data[-num_test:]
     y_test = mnist_targets[-num_test:]
```

Define the hyperparameters, the model, and the optimiser, where we choose the Adam optimiser this time.

```
[4]: learning_rate = 0.0001
     batch_size = 64
     num_epochs = 20
     latent_dim = 2
```

```
vae_model = VAE(latent_dim, batch_size)
optimizer = keras.optimizers.Adam(learning_rate=learning_rate)
```

```
2023-03-24 13:15:45.891703: I tensorflow/core/platform/cpu_feature_guard.cc:193]
This TensorFlow binary is optimized with oneAPI Deep Neural Network Library
(oneDNN) to use the following CPU instructions in performance-critical
operations:  SSE4.1 SSE4.2 AVX AVX2 FMA
To enable them in other operations, rebuild TensorFlow with the appropriate
compiler flags.
```

In the following, we write our own loop for training and validation.

For Noto users: Please note that the training can take several minutes on Noto!

[5]:
```
for epoch in range(1, num_epochs + 1):

    # Training steps
    for i in range(num_train // batch_size):
        train_step(vae_model, x_train[i:i + batch_size], optimizer)

    # Validation steps
    r_val = num_val // batch_size
    loss = keras.metrics.Mean()
    elbo = 0

    for i in range(r_val):
        loss(compute_loss(vae_model, x_val[i:i + batch_size]))
        elbo += -loss.result()

    elbo /= r_val

    print(f'Epoch: {epoch}/{num_epochs}, validation loss (ELBO): {elbo}')
```

```
Epoch: 1/20, validation loss (ELBO): -529.894775390625
Epoch: 2/20, validation loss (ELBO): -455.3930358886719
Epoch: 3/20, validation loss (ELBO): -335.8797912597656
Epoch: 4/20, validation loss (ELBO): -285.97296142578125
Epoch: 5/20, validation loss (ELBO): -251.6230010986328
Epoch: 6/20, validation loss (ELBO): -234.57460021972656
Epoch: 7/20, validation loss (ELBO): -225.56549072265625
Epoch: 8/20, validation loss (ELBO): -220.42120361328125
Epoch: 9/20, validation loss (ELBO): -217.3555145263672
Epoch: 10/20, validation loss (ELBO): -215.20712280273438
Epoch: 11/20, validation loss (ELBO): -212.9918975830078
Epoch: 12/20, validation loss (ELBO): -211.4029998779297
Epoch: 13/20, validation loss (ELBO): -209.53585815429688
Epoch: 14/20, validation loss (ELBO): -207.47470092773438
Epoch: 15/20, validation loss (ELBO): -206.21136474609375
```

```
Epoch: 16/20, validation loss (ELBO): -205.02468872070312
Epoch: 17/20, validation loss (ELBO): -203.96925354003906
Epoch: 18/20, validation loss (ELBO): -202.82403564453125
Epoch: 19/20, validation loss (ELBO): -201.59617614746094
Epoch: 20/20, validation loss (ELBO): -200.6598358154297
```

For our custom model, we need to store the trained weights in the following way:

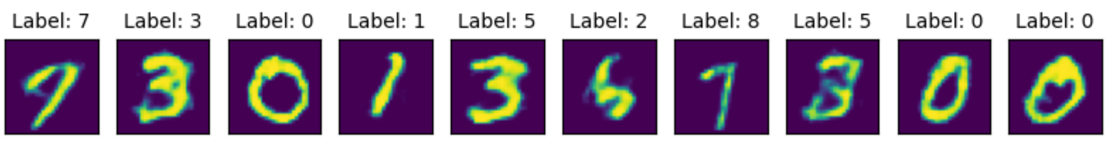
[6]:
```
vae_model.save_weights('output/MNIST_VAE.h5', save_format='h5')
```

You can load a pretrained model like this:

[7]:
```
vae_model = VAE(latent_dim, num_test)
vae_model(x_test)  # For input dimension specification

# Our pretrained model (300 epochs):
vae_model.load_weights('output/MNIST_VAE_pretrained.h5')

# ... or load your model:
# vae_model.load_weights('output/MNIST_VAE.h5')
```

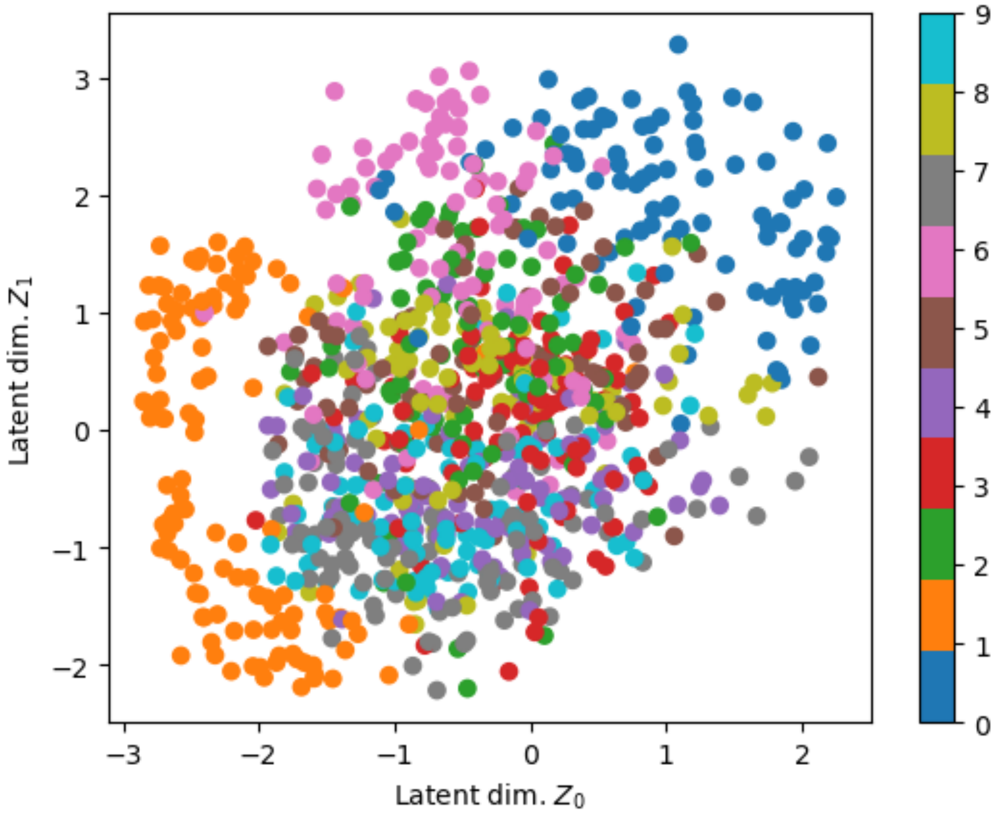
Let's check out the results for the test data.

[8]:
```
mean_z, logvar_z = vae_model.encode(x_test)
latent_z = vae_model.reparameterize(mean_z, logvar_z)
predictions = vae_model.sample(latent_z)

fig, axs = plt.subplots(1,10, figsize=(10,5))

for i, ax in enumerate(axs.ravel()):
    ax.imshow(predictions[i])

    ax.set_title(f"Label: {int(y_test[i])}", fontsize=10)
    ax.set_xticks([])
    ax.set_yticks([])

plt.show()
```



We can also investigate where the test datapoints lie in the latent space.

[9]:
```
plt.scatter(latent_z[:, 0], latent_z[:, 1], c=y_test, cmap='tab10')
plt.colorbar()
plt.xlabel(r"Latent dim. $Z_0$")
plt.ylabel(r"Latent dim. $Z_1$")
plt.show()
```



1.2 Variational Autoencoder for Molecules

(Note that in this part you might not be able to execute all cells – in particular on Noto!)

In the following we apply the VAE-idea on a molecular dataset and train a **Chemical VAE**. In addition to the standard VAE, we also predict a chemical property Y. This allow us to do a **guided search of novel molecules** which match a property of our interest.

As illustrated above, we predict a chemical property with an **additional decoder network** directly from the latent sample. This does not only provide additional information about the molecules, but also structures the latent representation Z with resprect to property Y. This will have the effect the chemical property will gradually change within the latent space.

So far, we have worked with tabular data and images as inputs. Molecules can be represented in variouse ways. A common representation is a graph. Here, the nodes of a molecular graph are the atoms and the edges are molecular bonds. A popular and simple depiction of a molecular graph is a so-called **SMILES representation**. It is a text string that encloses all the information required to convert it to a graph.

For our experiments we will use a variant called the **Deep-SMILES representation** which makes generation of valid molecular structures easier.

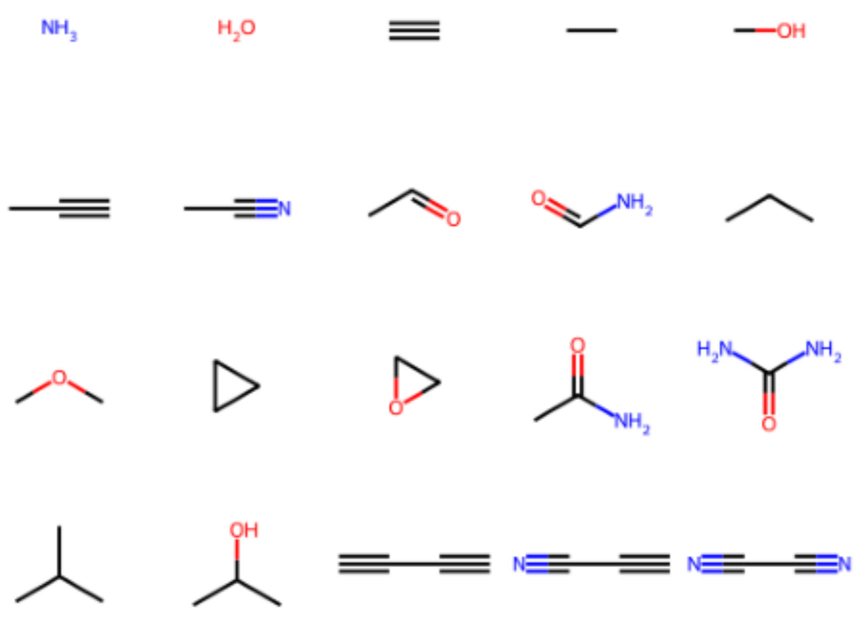
Let's have a closer look on the dataset and how these SMILES and Deep-SMILES look like.

```
[10]: import pandas as pd
      import numpy as np

      molecule_data = pd.read_pickle('data/molecule_data.pkl')
      molecule_data
```

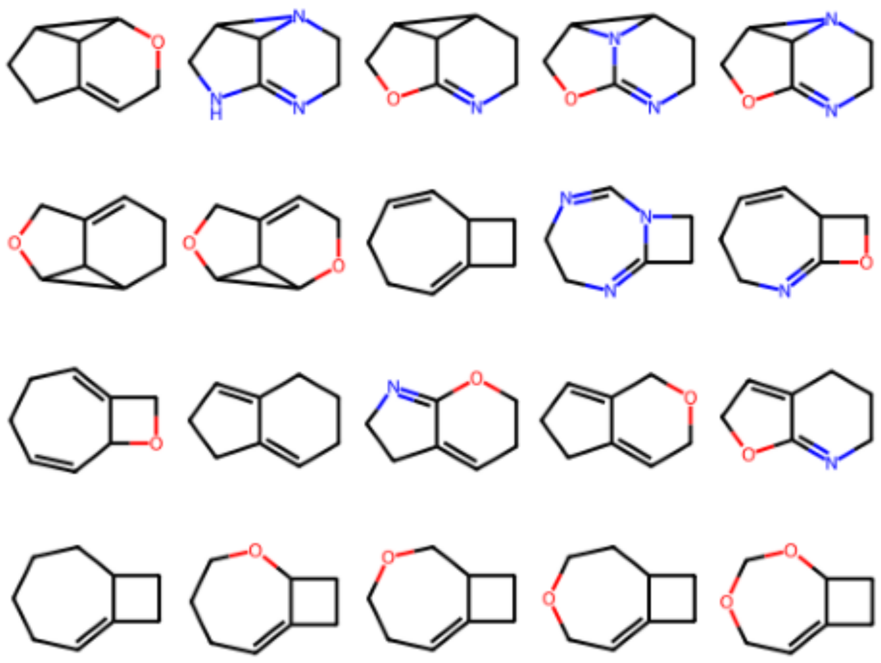
```
[10]:           id          smiles   deep_smiles  band_gap
      0          2               N             N    0.3399
      1          3               O             O    0.3615
      2          4             C#C           C#C    0.3351
      3          7              CC            CC    0.4426
      4          8              CO            CO    0.3437
      …        …             …            …        …
      31667  41529  C1CC2=CCCOCC12  CCC=CCCOCC97    0.2548
      31668  41530  C1CC2=CCOCCC12  CCC=CCOCCC97    0.2528
      31669  41531  C1CC2=CCOCOC12  CCC=CCOCOC97    0.2504
      31670  41533  C1OC2=NCCCCC12  COC=NCCCCC97    0.2701
      31671  41535  C1OC2=NCCCOC12  COC=NCCCOC97    0.2648

      [31672 rows x 4 columns]
```

We can now plot the first and the last molecules from the dataset as chemical graphs.

```
[11]: from rdkit import Chem
      from rdkit.Chem import Draw
      import matplotlib.pyplot as plt

      smiles_list = molecule_data['smiles'].values[0:20]
      molecule_list = [Chem.MolFromSmiles(smiles) for smiles in smiles_list]
      figure = Draw.MolsToGridImage(molecule_list, molsPerRow=5, subImgSize=(100,␣
       ↪100), returnPNG=False)

      plt.imshow(figure)
      plt.axis('off')
      plt.show()
```



```
[12]: smiles_list = molecule_data['smiles'].values[31650:31670]
      molecule_list = [Chem.MolFromSmiles(smiles) for smiles in smiles_list]
      figure = Draw.MolsToGridImage(molecule_list, molsPerRow=5, subImgSize=(100,␣
       ↪100), returnPNG=False)

      plt.imshow(figure)
      plt.axis('off')
      plt.show()
```



Let’s define some functions which help us to convert deep-smiles into a one-hot representation and normalise the property values.

[13]:
```python
def smiles_to_onehot(deep_smiles):

    max_len = max([len(x) for x in deep_smiles])
    data = []

    for item in deep_smiles:
        ch_lst = list(item) + (max_len - len(item)) * [stop_character]

        res = []

        for ch in ch_lst:
            r = [0] * len(chars)
            r[chars.index(ch)] = 1
            res.append(r)

        data.append(res)

    return data


def one_hot_to_smiles(data, chars, stop_character):
    res = []

    for item in data:
        ch_lst = []

        for ch in item:
            ch_lst.append(chars[np.argmax(ch)])

        res.append(''.join(ch_lst).split(stop_character)[0])

    return res


def sparse_to_smiles(data):

    res = []

    for item in data:
        ch_lst = []

        for ch in item:
            ch_lst.append(chars[ch[0]])

        res.append(''.join(ch_lst))

    return res
```

First, we shuffel the data.

[14]:
```
molecule_data = molecule_data.sample(frac=1, random_state=123)
```

Then, we use our function to convert deep smiles to a one-hot representation

[15]:
```
stop_character = 'x'

chars = sorted(list(set(''.join(molecule_data['deep_smiles'].values))))
chars = chars + [stop_character]

print('Unique characters:', chars)

data = smiles_to_onehot(molecule_data['deep_smiles'].values)
data = np.array(data).reshape((len(data), 17, 15, 1)).astype(np.float32)
```

```
Unique characters: ['#', ')', '3', '4', '5', '6', '7', '8', '9', '=', 'C', 'F',
'N', 'O', 'x']
```

and normalise the property values

[16]:
```
band_gap_mean = molecule_data['band_gap'].mean()
band_gap_std = molecule_data['band_gap'].std()
target = (molecule_data['band_gap'] - band_gap_mean) / band_gap_std
target = target.values.reshape((len(data), 1)).astype(np.float32)
```

As usual, we split the dataset into training, validation, and test sets.

[17]:
```
num_train = 28000
num_val = 1000
num_test = 1000

x_train = data[:num_train]
y_train = target[:num_train]

x_val = data[num_train:num_train + num_val]
y_val = target[num_train:num_train + num_val]

x_test = data[num_train + num_val:num_train + num_val + num_test]
y_test = target[num_train + num_val:num_train + num_val + num_test]
```

We can now create our new model `CVAE` which provides property predictions.

[18]:
```
import tensorflow as tf
from tensorflow import keras

class CVAE(keras.Model):

    def __init__(self, latent_dim, batch_size):
        super(CVAE, self).__init__()
        self.latent_dim = latent_dim
        self.batch_size = batch_size
        self.encoder = keras.Sequential(
            [
                keras.layers.InputLayer(input_shape=(17, 15, 1)),
                keras.layers.Flatten(),
                keras.layers.Dense(units=1120, activation='relu'),
                keras.layers.Dense(units=1120, activation='relu'),
                keras.layers.Dense(latent_dim + latent_dim),
            ]
        )

        self.decoder = keras.Sequential(
            [
                keras.layers.InputLayer(input_shape=(latent_dim,)),
                keras.layers.Dense(units=1120, activation='relu'),
                keras.layers.Dense(units=1120, activation='relu'),
                keras.layers.Dense(units=255),
                keras.layers.Reshape(target_shape=(17, 15, 1)),
            ]
        )

        # Our new decoder:
        self.decoder_property = keras.Sequential(
            [
                keras.layers.InputLayer(input_shape=(latent_dim,)),
                keras.layers.Dense(units=1120, activation='relu'),
                keras.layers.Dense(units=1120, activation='relu'),
                keras.layers.Dense(units=1),
            ]
        )

    def call(self, x):
        mean, logvar = tf.split(self.encoder(x), num_or_size_splits=2, axis=1)
        z = self.reparameterize(mean, logvar)
        return self.decoder(z), mean, logvar

    @tf.function
    def sample(self, eps=None):
        if eps is None:
            eps = tf.random.normal(shape=(self.batch_size, self.latent_dim))
        return self.decode(eps, apply_sigmoid=True)

    def encode(self, x):
        mean, logvar = tf.split(self.encoder(x), num_or_size_splits=2, axis=1)
        return mean, logvar

    def reparameterize(self, mean, logvar):
        eps = tf.random.normal(shape=(self.batch_size, self.latent_dim))
        return eps * tf.exp(logvar * .5) + mean

    def decode(self, z, apply_sigmoid=False):
        logits = self.decoder(z)
        if apply_sigmoid:
            probs = tf.sigmoid(logits)
            return probs
        return logits


def log_normal_pdf(sample, mean, logvar, raxis=1):
    log2pi = tf.math.log(2.0 * np.pi)

    return tf.reduce_sum(-0.5 * ((sample - mean) ** 2.0 * tf.exp(-logvar) +␣
 ↪logvar + log2pi), axis=raxis)
```

```
def compute_loss(model, x, y):
    mean, logvar = model.encode(x)
    z = model.reparameterize(mean, logvar)
    x_logit = model.decode(z)
    cross_ent = tf.nn.sigmoid_cross_entropy_with_logits(logits=x_logit,␣
↪labels=x)
    logpx_z = -tf.reduce_sum(cross_ent, axis=[1, 2, 3])
    logpz = log_normal_pdf(z, 0., 0.)
    logqz_x = log_normal_pdf(z, mean, logvar)

    # Property

    y_pred = model.decoder_property(z)
    y_mse = -tf.reduce_mean(tf.square(y - y_pred), axis = 0)

    return -tf.reduce_mean(100 * y_mse + logpx_z + logpz - logqz_x)


def compute_y_mae(model, x, y):
    mean, logvar = model.encode(x)
    z = model.reparameterize(mean, logvar)
    y_pred = model.decoder_property(z)
    y_mae = tf.reduce_mean(tf.abs(y - y_pred), axis = 0)
    return y_mae


@tf.function
def train_step(model, x, y, optimizer):
    with tf.GradientTape() as tape:
        loss = compute_loss(model, x, y)
    gradients = tape.gradient(loss, model.trainable_variables)
    optimizer.apply_gradients(zip(gradients, model.trainable_variables))
```

With this, we can now set the hyperparameters and create our model and optimiser.

[19]:
```
learning_rate = 0.0001
batch_size = 100
num_epochs = 31
latent_dim = 14

optimizer = keras.optimizers.Adam(learning_rate)
model = CVAE(latent_dim, batch_size)
```

You can try to train this model:

[ ]:
```
for epoch in range(1, num_epochs + 1):
    # Training steps
    for i in range(num_train // batch_size):
        train_step(model, x_train[i:i + batch_size], y_train[i:i + batch_size],␣
↪optimizer)

    # Validation steps
    r_val = num_val // batch_size
    loss = keras.metrics.Mean()
    elbo = 0
    y_loss = 0

    for i in range(r_val):
        loss(compute_loss(model, x_val[i:i + batch_size], y_val[i:i +␣
↪batch_size]))
        y_loss += compute_y_mae(model, x_val[i:i + batch_size], y_val[i:i +␣
↪batch_size]).numpy()[0]
        elbo += -loss.result()

    elbo /= r_val
    y_loss = y_loss / r_val * band_gap_std * 627

    # Print validation results
    print(f'Epoch: {epoch}/{num_epochs}, validation loss (ELBO): {elbo}, Y MAE:␣
↪{y_loss}')

    if epoch % 10:
        path = 'output/Molecules_VAE.h5'
        model.save_weights(path, save_format='h5')
```

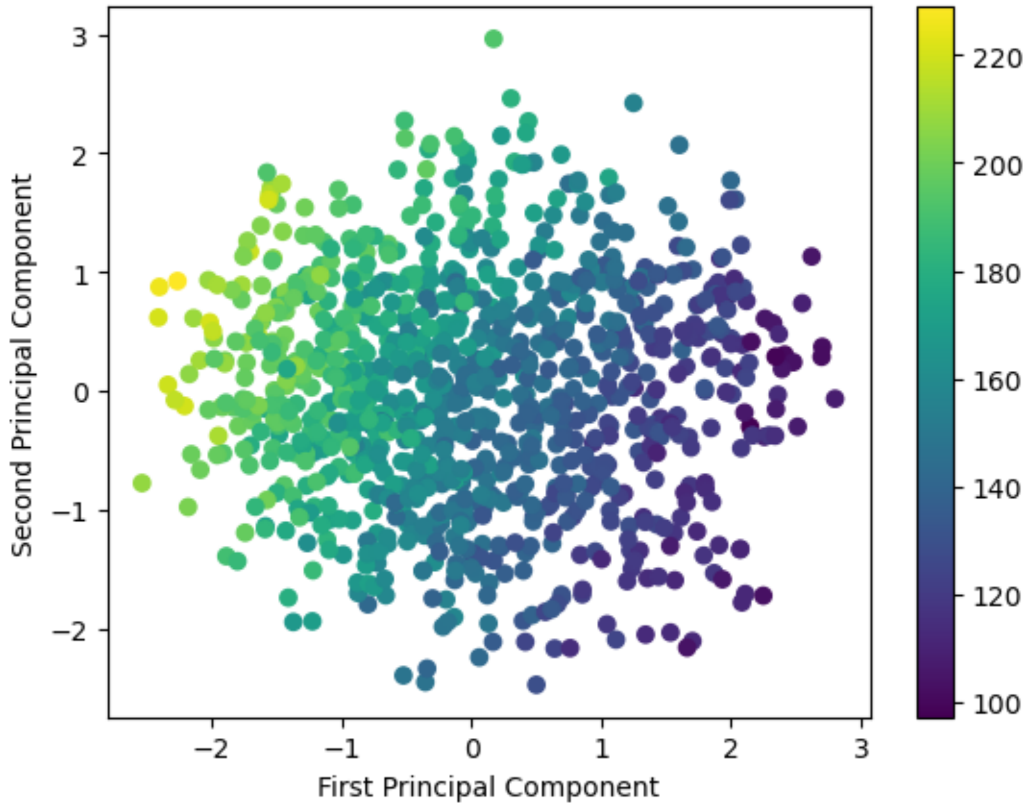
Alternatively, you can just load the pretrained model here:

[21]:
```
model = CVAE(latent_dim, num_test)
model(x_test)

# Our pretrained model (31 epochs):
model.load_weights('output/Molecules_VAE_pretrained.h5')

# ... or load your model:
# model.load_weights('output/Molecules_VAE.h5')
```

We can now make predictions with our model and use PCA for dimensionality reduction in order to visualise the latent space.

[22]:
```
from sklearn.decomposition import PCA

mean_z, logvar_z = model.encode(x_test)
latent_z = model.reparameterize(mean_z, logvar_z)
```

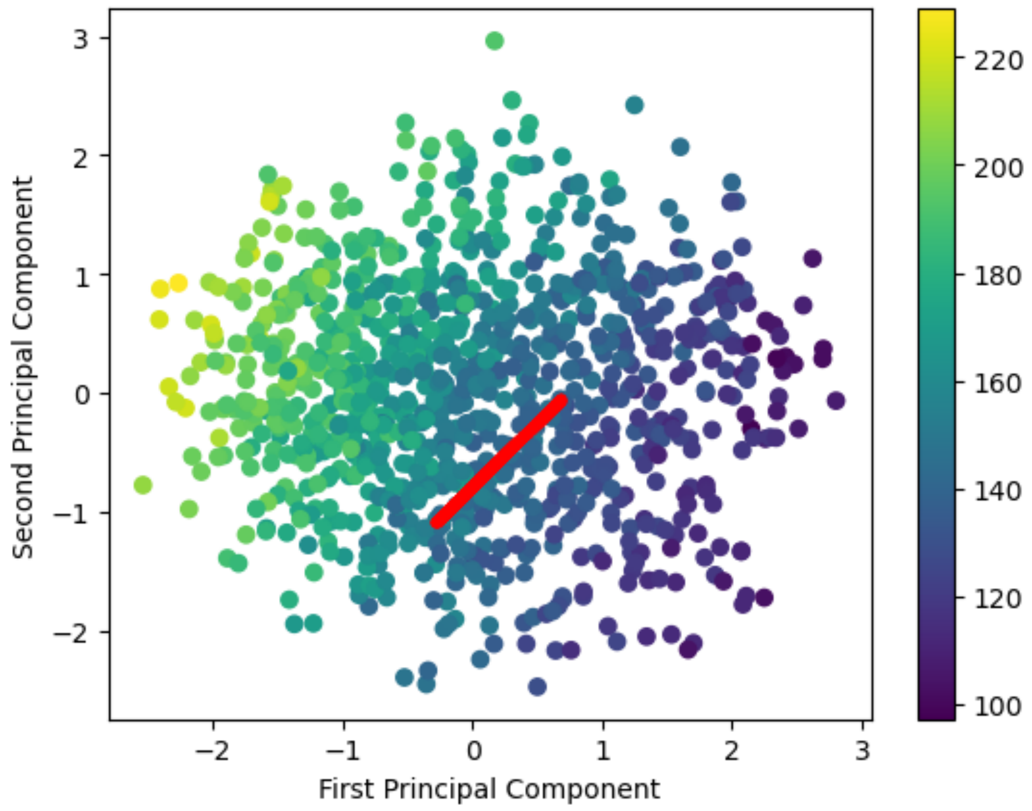
```
target_pred = model.decoder_property(latent_z).numpy().flatten()

# Invert the scaling and convert the property unit to Kcal/mol
target_pred = (target_pred * band_gap_std + band_gap_mean) * 627

data_pca = PCA(n_components=2)
data_pca.fit(mean_z.numpy())
data_pca_transform = data_pca.transform(mean_z.numpy())

plt.scatter(data_pca_transform[:, 0], data_pca_transform[:, 1], c=target_pred)
plt.xlabel('First Principal Component')
plt.ylabel('Second Principal Component')
plt.colorbar()
plt.show()
```



In this plot we can see a **smooth transition of the property correspondence making it easy to sample molecules of our interest**. To this end, we can linearly interpolate between two molecules.

Let us pick 1000 datapoints in the latent space.

[23]:
```python
num_inter_data = 1000

latent_z_inter = np.linspace(mean_z[7:8][0], mean_z[8:9][0], num_inter_data)
latent_z_inter_transform = data_pca.transform(latent_z_inter)

plt.scatter(data_pca_transform[:, 0], data_pca_transform[:, 1], c=target_pred)
plt.colorbar()

plt.scatter(latent_z_inter_transform[:, 0], latent_z_inter_transform[:, 1],
            marker='.', c='red')

plt.xlabel('First Principal Component')
plt.ylabel('Second Principal Component')

plt.show()
```



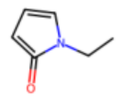
We can now take these latent datapoints and decode molecules and their corresponding property value.

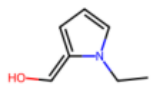
[24]:
```python
data_inter_pred = model.decoder(latent_z_inter)
target_inter_pred = model.decoder_property(latent_z_inter).numpy()
```

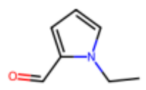
```
deep_smi_inter_pred = sparse_to_smiles(tf.argmax(data_inter_pred, axis=2).
 ↪numpy())
deep_smi_inter_pred = [item.replace(stop_character, '') for item in␣
 ↪deep_smi_inter_pred]

deep_smi_inter_pred, idx = np.unique(deep_smi_inter_pred, return_index=True)

# Invert the scaling and convert the property unit to Kcal/mol
target_inter_pred = (target_inter_pred[idx] * band_gap_std + band_gap_mean) *␣
 ↪627
```

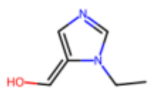
Parse generated molecules and sort out invalid samples.

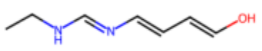
[25]:
```
import deepsmiles

converter = deepsmiles.Converter(rings=True, branches=True)

molecule_list = []
labels = []

for i, item in enumerate(deep_smi_inter_pred):
    try:
        smi = converter.decode(item)
        mol = Chem.MolFromSmiles(smi, sanitize = False)

        if mol is not None:
            molecule_list.append(mol)
            p = target_inter_pred[i][0]
            labels.append(f'{smi} - {p:.2f} kcal/mol')
    except:
        pass

figure = Draw.MolsToGridImage(molecule_list, legends=labels, molsPerRow=4,␣
 ↪subImgSize=(300, 300), returnPNG=False)

plt.figure(figsize=(10, 10))
plt.imshow(figure)
plt.axis('off')
plt.show()
```

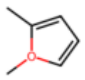

CCN1C=CC=C1=O - 139.47 kcal/mol

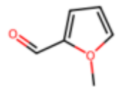

CCN1C=CC=C1=CO - 139.47 kcal/mol

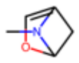

CCN1C=CC=C1C=O - 139.46 kcal/mol

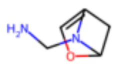

CCN1C=NC=C1=CO - 139.48 kcal/mol

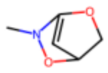

CCNC=NC=CC=CO - 139.48 kcal/mol

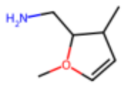

CO1C=CC=C1C - 139.41 kcal/mol

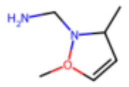

CO1C=CC=C1C=O - 139.41 kcal/mol

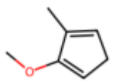

C12OC=C(C1)N2C - 140.50 kcal/mol

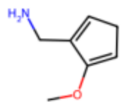

C12OC=C(C1)N2CN - 140.41 kcal/mol

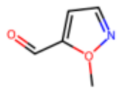

C1OC2=CC1ON2C - 140.84 kcal/mol

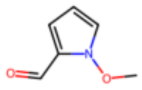

CO1C=CC(C)C1CN - 139.90 kcal/mol


CO1C=CC(C)N1CN - 140.03 kcal/mol


COC1=CCC=C1C - 139.48 kcal/mol


COC1=CCC=C1CN - 139.51 kcal/mol


CO1N=CC=C1C=O - 139.41 kcal/mol


CON1C=CC=C1C=O - 139.40 kcal/mol

7-Image_Segmentation

March 24, 2023

1 7. Image Segmentation Example

In this last notebook, we see a medical imaging example for which we can make use of neural networks. To this end, we consider the LIDC-IDRI dataset of lung CT scans where anomalities, in particular lesions, were manually outlined by experts. The goal is to design a **neural network for image segmentation** which learns from previous outlines of lesions to predict anomalities in new lung CT scans.

Keywords: `Semantic segmentation`, `U-Net`, `keras.layers.SeparableConv2D`, `keras.layers.BatchNormalization`, `keras.layers.UpSampling2D`

1.1 U-Net-based Semantic Segmentation

Semantic segmentation describes the task of grouping pixels together which (semanticly) belong to one object. In that regrad, a particularly useful architecture for biomedical imaging tasks is the U-Net illustrated in the following figure. It is a **fully-convolutional neural network** and can be used also with comparably small datasets.

The architecture we use in this notebook is based on the U-Net. We adopt the *U-Net Xception-style model* proposed in a Keras tutorial on image segmentation.

With the following cell, we load and plot the dataset. Note that we only use a small subset (119 images) of the full dataset.

[1]:
```
import numpy as np
import matplotlib.pyplot as plt

images = np.load('data/lidc_images_119.npy')
targets = np.load('data/lidc_labels_119.npy')

fig, axs = plt.subplots(10,2, figsize=(4,20))

for i in range(10):
    axs[i,0].imshow(images[i])
    axs[i,1].imshow(targets[i])

    axs[i,0].set_xticks([])
    axs[i,0].set_yticks([])
    axs[i,1].set_xticks([])
    axs[i,1].set_yticks([])

axs[0,0].set_title('Image')
axs[0,1].set_title('Groundtruth')

plt.show()

train_images = images[:100][...,np.newaxis]
train_targets = targets[:100][...,np.newaxis]

test_images = images[100:][...,np.newaxis]
test_targets = targets[100:][...,np.newaxis]
```

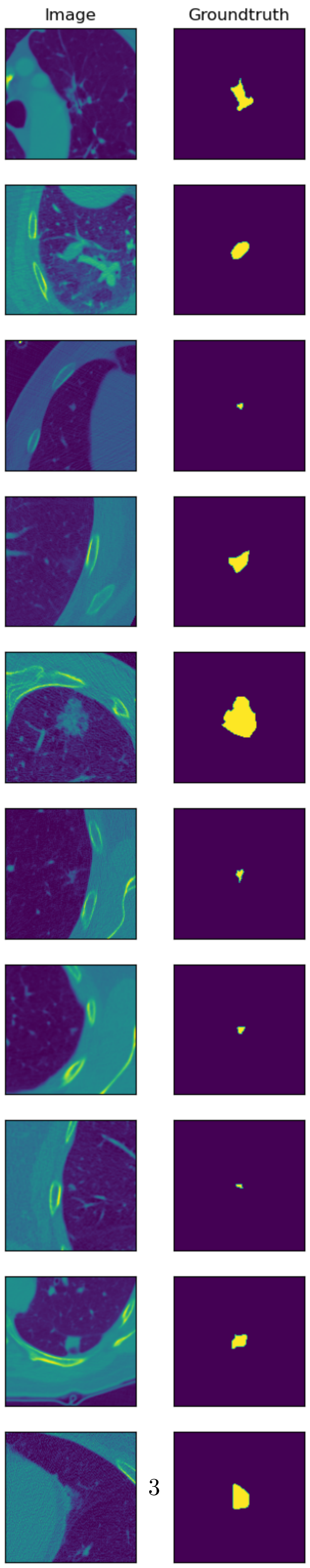


Image
Groundtruth

We use the following hyperparameters

[2]:
```
learning_rate = 0.001
batch_size = 10
num_epochs = 10
```

and define the model as follows.

[3]:
```
from tensorflow import keras

keras.utils.set_random_seed(123)

def segmentation_model(img_size=(128, 128), num_classes=2):
    inputs = keras.Input(shape=img_size + (1,))

    ### [First half of the network: downsampling inputs] ###

    # Entry block
    x = keras.layers.Conv2D(32, 3, strides=2, padding="same")(inputs)
    x = keras.layers.BatchNormalization()(x)
    x = keras.layers.Activation("relu")(x)

    previous_block_activation = x  # Set aside residual

    # Blocks 1, 2, 3 are identical apart from the feature depth.
    for filters in [64, 128, 256]:
        x = keras.layers.Activation("relu")(x)
        x = keras.layers.SeparableConv2D(filters, 3, padding="same")(x)
        x = keras.layers.BatchNormalization()(x)

        x = keras.layers.Activation("relu")(x)
        x = keras.layers.SeparableConv2D(filters, 3, padding="same")(x)
        x = keras.layers.BatchNormalization()(x)

        x = keras.layers.MaxPooling2D(3, strides=2, padding="same")(x)

        # Project residual
        residual = keras.layers.Conv2D(filters, 1, strides=2, padding="same")(
            previous_block_activation
        )
        x = keras.layers.add([x, residual])  # Add back residual
        previous_block_activation = x  # Set aside next residual

    ### [Second half of the network: upsampling inputs] ###
    for filters in [256, 128, 64, 32]:
        x = keras.layers.Activation("relu")(x)
        x = keras.layers.Conv2DTranspose(filters, 3, padding="same")(x)
        x = keras.layers.BatchNormalization()(x)

        x = keras.layers.Activation("relu")(x)
        x = keras.layers.Conv2DTranspose(filters, 3, padding="same")(x)
        x = keras.layers.BatchNormalization()(x)

        x = keras.layers.UpSampling2D(2)(x)

        # Project residual
        residual = keras.layers.UpSampling2D(2)(previous_block_activation)
        residual = keras.layers.Conv2D(filters, 1, padding="same")(residual)
        x = keras.layers.add([x, residual])  # Add back residual
        previous_block_activation = x  # Set aside next residual

    # Add a per-pixel classification layer
    outputs = keras.layers.Conv2D(num_classes, 3, activation="softmax",␣
↪padding="same")(x)

    # Define the model
    model = keras.Model(inputs, outputs)

    return model
```

```
2023-03-24 11:17:32.055524: I tensorflow/core/platform/cpu_feature_guard.cc:193]
This TensorFlow binary is optimized with oneAPI Deep Neural Network Library
(oneDNN) to use the following CPU instructions in performance-critical
operations:  SSE4.1 SSE4.2 AVX AVX2 FMA
To enable them in other operations, rebuild TensorFlow with the appropriate
compiler flags.
```

Now, we build the model.

[4]:
```
# Free up RAM in case the model definition cells were run multiple times
keras.backend.clear_session()

model = segmentation_model(img_size=(128, 128), num_classes=2)
model.summary()
```

```
2023-03-24 11:24:35.665252: I tensorflow/core/platform/cpu_feature_guard.cc:193]
This TensorFlow binary is optimized with oneAPI Deep Neural Network Library
(oneDNN) to use the following CPU instructions in performance-critical
operations:  SSE4.1 SSE4.2 AVX AVX2 FMA
To enable them in other operations, rebuild TensorFlow with the appropriate
compiler flags.
```

```
Model: "model"
```

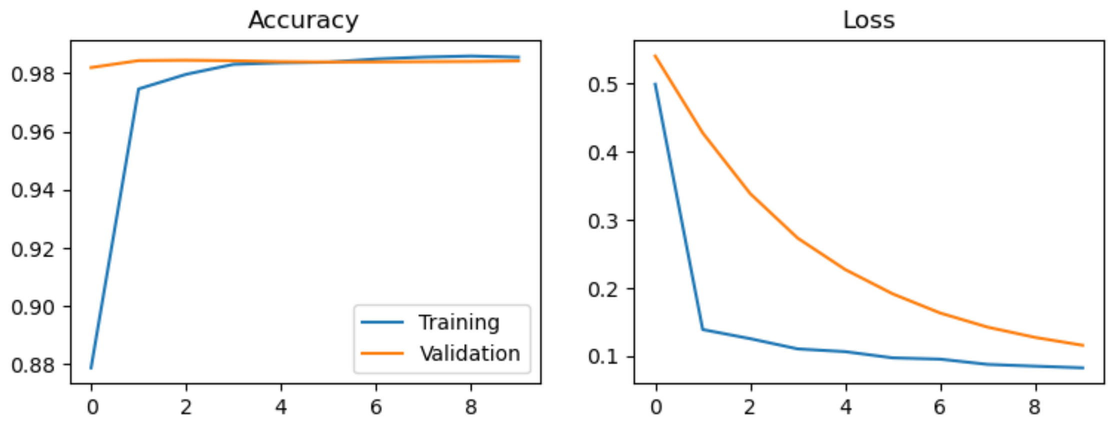
```
________________________________________________________________________________
__________________
 Layer (type)                   Output Shape         Param #     Connected to
================================================================================
==================
 input_1 (InputLayer)           [(None, 128, 128, 1  0           []
                                )]

 conv2d (Conv2D)                (None, 64, 64, 32)   320
['input_1[0][0]']

 batch_normalization (BatchNorm  (None, 64, 64, 32)  128
['conv2d[0][0]']
 alization)

 activation (Activation)        (None, 64, 64, 32)   0
['batch_normalization[0][0]']

 activation_1 (Activation)      (None, 64, 64, 32)   0
['activation[0][0]']

 separable_conv2d (SeparableCon  (None, 64, 64, 64)  2400
['activation_1[0][0]']
 v2D)

 batch_normalization_1 (BatchNo  (None, 64, 64, 64)  256
['separable_conv2d[0][0]']
 rmalization)

 activation_2 (Activation)      (None, 64, 64, 64)   0
['batch_normalization_1[0][0]']

 separable_conv2d_1 (SeparableC  (None, 64, 64, 64)  4736
['activation_2[0][0]']
 onv2D)

 batch_normalization_2 (BatchNo  (None, 64, 64, 64)  256
['separable_conv2d_1[0][0]']
 rmalization)

 max_pooling2d (MaxPooling2D)   (None, 32, 32, 64)   0
['batch_normalization_2[0][0]']

 conv2d_1 (Conv2D)              (None, 32, 32, 64)   2112
['activation[0][0]']

 add (Add)                      (None, 32, 32, 64)   0
['max_pooling2d[0][0]',
'conv2d_1[0][0]']

 activation_3 (Activation)      (None, 32, 32, 64)   0           ['add[0][0]']

 separable_conv2d_2 (SeparableC  (None, 32, 32, 128)  8896
['activation_3[0][0]']
 onv2D)

 batch_normalization_3 (BatchNo  (None, 32, 32, 128)  512
['separable_conv2d_2[0][0]']
 rmalization)

 activation_4 (Activation)      (None, 32, 32, 128)  0
['batch_normalization_3[0][0]']

 separable_conv2d_3 (SeparableC  (None, 32, 32, 128)  17664
['activation_4[0][0]']
 onv2D)

 batch_normalization_4 (BatchNo  (None, 32, 32, 128)  512
['separable_conv2d_3[0][0]']
 rmalization)

 max_pooling2d_1 (MaxPooling2D)  (None, 16, 16, 128)  0
['batch_normalization_4[0][0]']

 conv2d_2 (Conv2D)              (None, 16, 16, 128)  8320        ['add[0][0]']

 add_1 (Add)                    (None, 16, 16, 128)  0
['max_pooling2d_1[0][0]',
'conv2d_2[0][0]']

 activation_5 (Activation)      (None, 16, 16, 128)  0           ['add_1[0][0]']

 separable_conv2d_4 (SeparableC  (None, 16, 16, 256)  34176
['activation_5[0][0]']
 onv2D)

 batch_normalization_5 (BatchNo  (None, 16, 16, 256)  1024
['separable_conv2d_4[0][0]']
 rmalization)

 activation_6 (Activation)      (None, 16, 16, 256)  0
['batch_normalization_5[0][0]']

 separable_conv2d_5 (SeparableC  (None, 16, 16, 256)  68096
['activation_6[0][0]']
 onv2D)
 batch_normalization_6 (BatchNo  (None, 16, 16, 256)  1024
['separable_conv2d_5[0][0]']
 rmalization)

 max_pooling2d_2 (MaxPooling2D)  (None, 8, 8, 256)   0
['batch_normalization_6[0][0]']

 conv2d_3 (Conv2D)              (None, 8, 8, 256)    33024       ['add_1[0][0]']

 add_2 (Add)                    (None, 8, 8, 256)    0
['max_pooling2d_2[0][0]',
'conv2d_3[0][0]']

 activation_7 (Activation)      (None, 8, 8, 256)    0           ['add_2[0][0]']

 conv2d_transpose (Conv2DTransp  (None, 8, 8, 256)   590080
['activation_7[0][0]']
 ose)

 batch_normalization_7 (BatchNo  (None, 8, 8, 256)   1024
['conv2d_transpose[0][0]']
 rmalization)

 activation_8 (Activation)      (None, 8, 8, 256)    0
['batch_normalization_7[0][0]']

 conv2d_transpose_1 (Conv2DTran  (None, 8, 8, 256)   590080
['activation_8[0][0]']
 spose)

 batch_normalization_8 (BatchNo  (None, 8, 8, 256)   1024
['conv2d_transpose_1[0][0]']
 rmalization)

 up_sampling2d_1 (UpSampling2D)  (None, 16, 16, 256)  0          ['add_2[0][0]']

 up_sampling2d (UpSampling2D)   (None, 16, 16, 256)  0
['batch_normalization_8[0][0]']

 conv2d_4 (Conv2D)              (None, 16, 16, 256)  65792
['up_sampling2d_1[0][0]']

 add_3 (Add)                    (None, 16, 16, 256)  0
['up_sampling2d[0][0]',
'conv2d_4[0][0]']

 activation_9 (Activation)      (None, 16, 16, 256)  0           ['add_3[0][0]']
 conv2d_transpose_2 (Conv2DTran  (None, 16, 16, 128)  295040
['activation_9[0][0]']
 spose)

 batch_normalization_9 (BatchNo  (None, 16, 16, 128)  512
['conv2d_transpose_2[0][0]']
 rmalization)

 activation_10 (Activation)     (None, 16, 16, 128)  0
['batch_normalization_9[0][0]']

 conv2d_transpose_3 (Conv2DTran  (None, 16, 16, 128)  147584
['activation_10[0][0]']
 spose)

 batch_normalization_10 (BatchN  (None, 16, 16, 128)  512
['conv2d_transpose_3[0][0]']
 ormalization)

 up_sampling2d_3 (UpSampling2D)  (None, 32, 32, 256)  0           ['add_3[0][0]']

 up_sampling2d_2 (UpSampling2D)  (None, 32, 32, 128)  0
['batch_normalization_10[0][0]']

 conv2d_5 (Conv2D)              (None, 32, 32, 128)  32896
['up_sampling2d_3[0][0]']

 add_4 (Add)                    (None, 32, 32, 128)  0
['up_sampling2d_2[0][0]',
'conv2d_5[0][0]']

 activation_11 (Activation)     (None, 32, 32, 128)  0           ['add_4[0][0]']

 conv2d_transpose_4 (Conv2DTran  (None, 32, 32, 64)  73792
['activation_11[0][0]']
 spose)

 batch_normalization_11 (BatchN  (None, 32, 32, 64)  256
['conv2d_transpose_4[0][0]']
 ormalization)

 activation_12 (Activation)     (None, 32, 32, 64)   0
['batch_normalization_11[0][0]']

 conv2d_transpose_5 (Conv2DTran  (None, 32, 32, 64)  36928
['activation_12[0][0]']
 spose)
 batch_normalization_12 (BatchN  (None, 32, 32, 64)  256
['conv2d_transpose_5[0][0]']
 ormalization)

 up_sampling2d_5 (UpSampling2D)  (None, 64, 64, 128)  0           ['add_4[0][0]']

 up_sampling2d_4 (UpSampling2D)  (None, 64, 64, 64)  0
['batch_normalization_12[0][0]']

 conv2d_6 (Conv2D)              (None, 64, 64, 64)   8256
['up_sampling2d_5[0][0]']

 add_5 (Add)                    (None, 64, 64, 64)   0
['up_sampling2d_4[0][0]',
'conv2d_6[0][0]']

 activation_13 (Activation)     (None, 64, 64, 64)   0           ['add_5[0][0]']

 conv2d_transpose_6 (Conv2DTran  (None, 64, 64, 32)  18464
['activation_13[0][0]']
 spose)

 batch_normalization_13 (BatchN  (None, 64, 64, 32)  128
['conv2d_transpose_6[0][0]']
 ormalization)

 activation_14 (Activation)     (None, 64, 64, 32)   0
['batch_normalization_13[0][0]']

 conv2d_transpose_7 (Conv2DTran  (None, 64, 64, 32)  9248
['activation_14[0][0]']
 spose)

 batch_normalization_14 (BatchN  (None, 64, 64, 32)  128
['conv2d_transpose_7[0][0]']
 ormalization)

 up_sampling2d_7 (UpSampling2D)  (None, 128, 128, 64  0           ['add_5[0][0]']
                                )

 up_sampling2d_6 (UpSampling2D)  (None, 128, 128, 32  0
['batch_normalization_14[0][0]']
                                )

 conv2d_7 (Conv2D)              (None, 128, 128, 32  2080
['up_sampling2d_7[0][0]']
                                )
 add_6 (Add)                    (None, 128, 128, 32  0
['up_sampling2d_6[0][0]',
                                )

'conv2d_7[0][0]']

 conv2d_8 (Conv2D)              (None, 128, 128, 2)  578         ['add_6[0][0]']

================================================================================
==================
Total params: 2,058,114
Trainable params: 2,054,338
Non-trainable params: 3,776
--------------------------------------------------------------------------------
------------------
```

With all of this in place, we can train our model. Note that **this can take a substantial time**, depending on your machine and the total amount of epochs.

[5]:
```python
model.compile(optimizer=keras.optimizers.SGD(learning_rate=learning_rate),
              loss='sparse_categorical_crossentropy',
              metrics=['accuracy'])

train_history = model.fit(x=train_images, y=train_targets,␣
 ↪batch_size=batch_size,
                          validation_data = (test_images, test_targets),
                          epochs=num_epochs)

fig, axs = plt.subplots(1,2, figsize=(9,3))

axs[0].plot(train_history.history['accuracy'], label='Training')
axs[0].plot(train_history.history['val_accuracy'], label='Validation')
axs[0].set_title('Accuracy')
axs[0].legend()

axs[1].plot(train_history.history['loss'])
axs[1].plot(train_history.history['val_loss'])
axs[1].set_title('Loss')

plt.show()
```

```
Epoch 1/10
10/10 [==============================] - 21s 2s/step - loss: 0.4991 - accuracy:
0.8788 - val_loss: 0.5404 - val_accuracy: 0.9819
Epoch 2/10
10/10 [==============================] - 16s 2s/step - loss: 0.1390 - accuracy:
0.9746 - val_loss: 0.4276 - val_accuracy: 0.9843
Epoch 3/10
```

```
10/10 [==============================] - 14s 1s/step - loss: 0.1257 - accuracy:
0.9796 - val_loss: 0.3386 - val_accuracy: 0.9845
Epoch 4/10
10/10 [==============================] - 16s 2s/step - loss: 0.1107 - accuracy:
0.9830 - val_loss: 0.2732 - val_accuracy: 0.9843
Epoch 5/10
10/10 [==============================] - 14s 1s/step - loss: 0.1066 - accuracy:
0.9836 - val_loss: 0.2272 - val_accuracy: 0.9840
Epoch 6/10
10/10 [==============================] - 14s 1s/step - loss: 0.0975 - accuracy:
0.9838 - val_loss: 0.1915 - val_accuracy: 0.9838
Epoch 7/10
10/10 [==============================] - 14s 1s/step - loss: 0.0956 - accuracy:
0.9849 - val_loss: 0.1633 - val_accuracy: 0.9839
Epoch 8/10
10/10 [==============================] - 14s 1s/step - loss: 0.0879 - accuracy:
0.9855 - val_loss: 0.1426 - val_accuracy: 0.9840
Epoch 9/10
10/10 [==============================] - 14s 1s/step - loss: 0.0853 - accuracy:
0.9859 - val_loss: 0.1275 - val_accuracy: 0.9840
Epoch 10/10
10/10 [==============================] - 14s 1s/step - loss: 0.0829 - accuracy:
0.9855 - val_loss: 0.1160 - val_accuracy: 0.9842
```



Save the trained model:

[6]:
```python
model.save_weights('output/Segmentation_model.h5', save_format='h5')
```

We provide again a pretrained model (500 epochs):

[10]:
```python
model.load_weights('output/Segmentation_model_pretrained.h5')
```

Make model prediction for both the training and test images.

```
[11]: train_prediction = model.predict(train_images)
      test_prediction = model.predict(test_images)
```

```
4/4 [==============================] - 4s 1s/step
1/1 [==============================] - 1s 859ms/step
```

First, we examine how well the model predicts the segmentation result on the training set.

```
[12]: fig, axs = plt.subplots(10,3, figsize=(6,20))

      for i in range(10):

          axs[i,0].imshow(train_images[i])
          axs[i,1].imshow(train_targets[i])
          axs[i,2].imshow(train_prediction[i,...,1])

          axs[i,0].set_xticks([])
          axs[i,0].set_yticks([])
          axs[i,1].set_xticks([])
          axs[i,1].set_yticks([])
          axs[i,2].set_xticks([])
          axs[i,2].set_yticks([])

      axs[0,0].set_title('Image')
      axs[0,1].set_title('Groundtruth')
      axs[0,2].set_title('Prediction')

      plt.show()
```

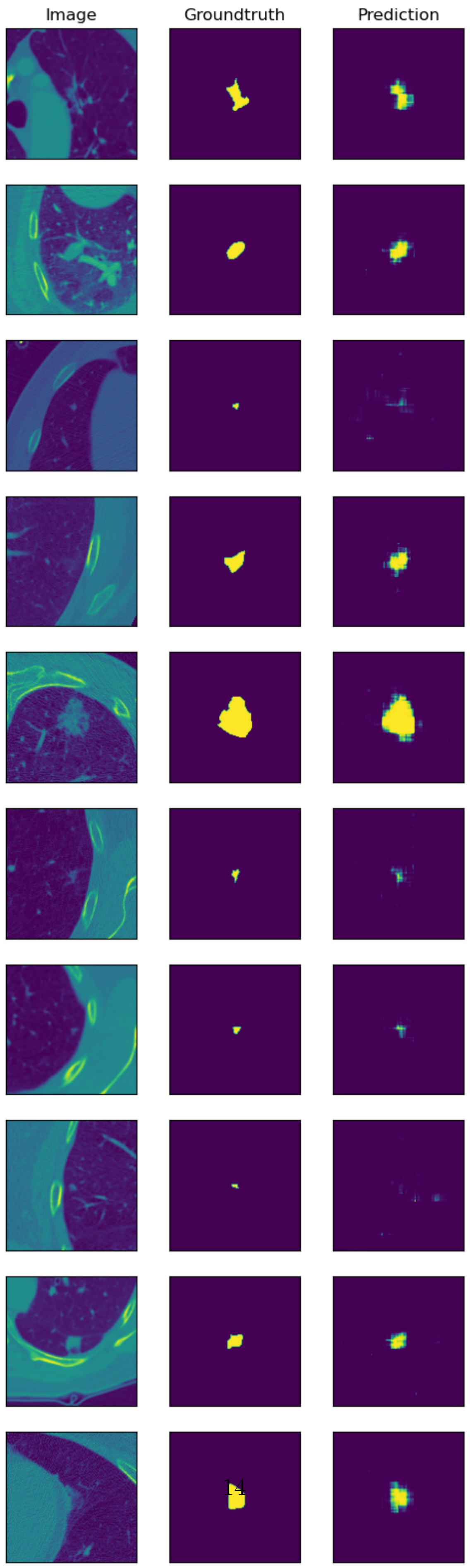


Image
Groundtruth
Prediction

Lastly, let's examine the predictions of segments on the test images.

```
[13]: fig, axs = plt.subplots(10,3, figsize=(6,20))

      for i in range(10):

          axs[i,0].imshow(test_images[i])
          axs[i,1].imshow(test_targets[i])
          axs[i,2].imshow(test_prediction[i,...,1])

          axs[i,0].set_xticks([])
          axs[i,0].set_yticks([])
          axs[i,1].set_xticks([])
          axs[i,1].set_yticks([])
          axs[i,2].set_xticks([])
          axs[i,2].set_yticks([])

      axs[0,0].set_title('Image')
      axs[0,1].set_title('Groundtruth')
      axs[0,2].set_title('Prediction')

      plt.show()
```

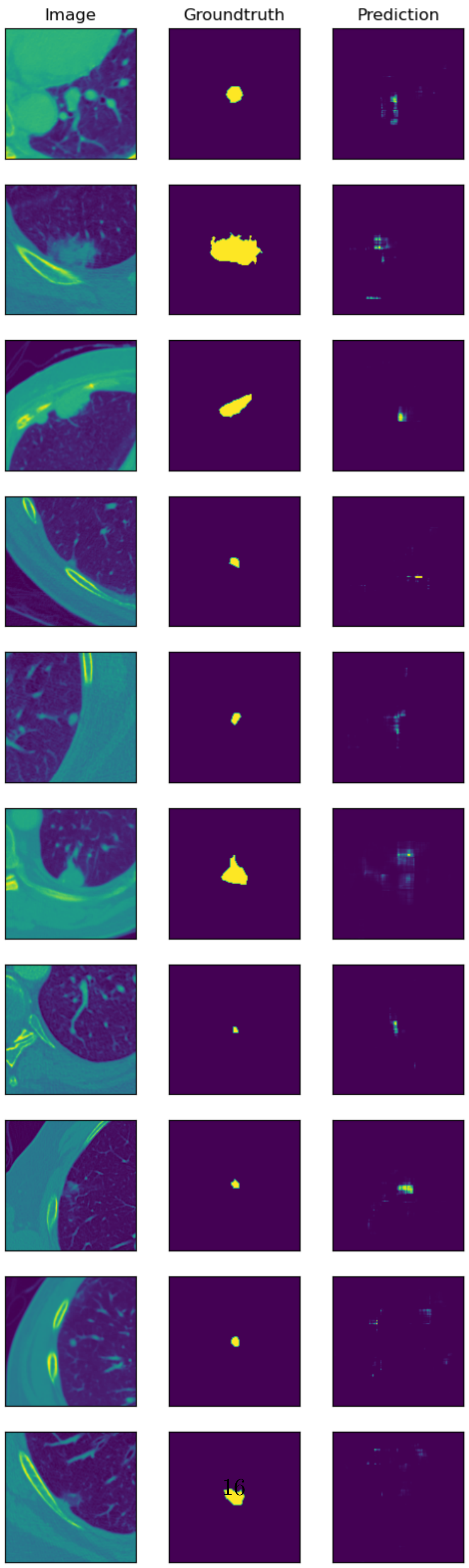


Image
Groundtruth
Prediction