Problem Sheet 1

Linear regression of time series data

Recall the Oxford temperature data considered in the lecture. In this lab we will try to approximate the known values of the temperature in time, and to predict the unknown values in the future. As a by-product, we will refresh our *numpy* skills.

Once again, here is the prediction rule we would like to explore:

$$h_{\boldsymbol{\theta}}(x) = \theta_0 + \theta_1 x + \cdots + \theta_n x^n,$$

where x is the time value, and $\boldsymbol{\theta} = (\theta_0, \ldots, \theta_n)$ is the vector of coefficients we will optimise. Given a dataset $D = (\mathbf{X}, \mathbf{y})$ of months $\mathbf{X} = \{x_1, \ldots, x_m\}$ and temperature values $\mathbf{y} = \{y_1, \ldots, y_m\}$, we need to minimise the sum-of-squares loss

$$L_D(\boldsymbol{\theta}) = \frac{1}{m} \sum_{i=1}^{m} (h_{\boldsymbol{\theta}}(x_i) - y_i)^2.$$

Warm-up

- Prove that a vector of m predictions $\hat{\mathbf{y}} := (h_{\boldsymbol{\theta}}(x_1), \ldots, h_{\boldsymbol{\theta}}(x_m))^\top$ can be computed as a product of the *Vandermonde* matrix

$$V = \begin{bmatrix} 1 & x_1 & \cdots & x_1^n \\ 1 & x_2 & \cdots & x_2^n \\ \vdots & & & \vdots \\ 1 & x_m & \cdots & x_m^n \end{bmatrix} \in \mathbb{R}^{m \times (n+1)}$$

  and the parameter vector $\boldsymbol{\theta}$, $\hat{\mathbf{y}} = V\boldsymbol{\theta}$.

Solution:

Let $\mathbf{v}_i = (1, x_i, \cdots, x_i^n)$, the i-th row of V. Note that
$(V\boldsymbol{\theta})_i = \mathbf{v}_i \boldsymbol{\theta} = \theta_0 + x_i\theta_1 + \cdots + x_i^n\theta_n = h_{\boldsymbol{\theta}}(x_i) = \hat{y}_i$, for any $i = 1, \ldots, m$.

Task (a): sum-of-squares minimiser

- **Prove** that any solution of Equation (1.2) in the lecture notes satisfies the first-order optimality conditions (Equation (1.1))

$$\frac{\partial L_D(\boldsymbol{\theta}^*)}{\partial \theta_0} = \cdots = \frac{\partial L_D(\boldsymbol{\theta}^*)}{\partial \theta_n} = 0$$

  in general. Recall that Equation (1.2) is a system of linear equations

$$A\boldsymbol{\theta}^* = \mathbf{b},$$

  where

$$A = V^\top V, \qquad \mathbf{b} = V^\top \mathbf{y}.$$

Solution

The elementwise gradient calculation in the lecture can be collected into a matrix notation,

$$\frac{\partial L_{\mathbf{D}}(\boldsymbol{\theta}^*)}{\partial \theta_j} = \frac{2}{m}\sum_{i=1}^{m} \underbrace{x_i^j}_{V_{i,j}}((V\boldsymbol{\theta}^*)_i - y_i) = \frac{2}{m} V_j^\top (V\boldsymbol{\theta}^* - \mathbf{y}) = \frac{2}{m}(V^\top V \boldsymbol{\theta}^* - V^\top \mathbf{y})_j = 0, \quad j = 0, \ldots, n.$$

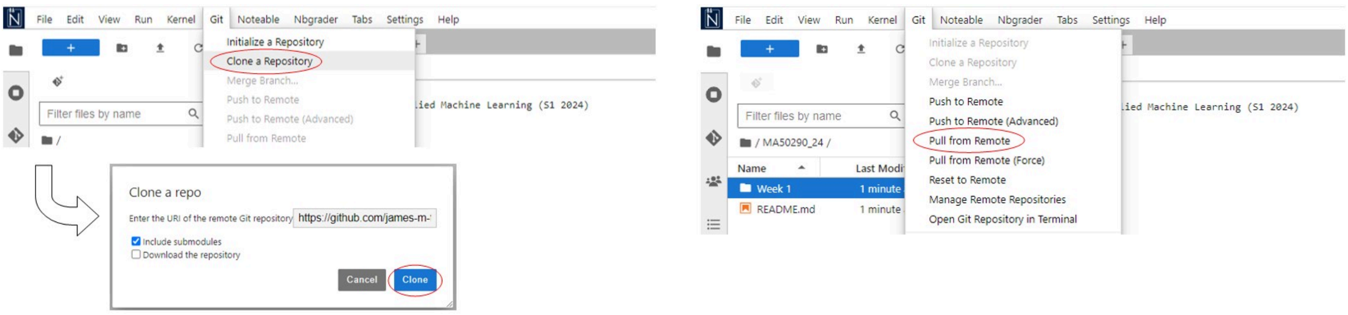
Task 0: fetching this problem sheet on the Noteable Jupyter server

The problem sheets (and solutions) will be uploaded to a Github repository: https://github.com/james-m-foster/MA50290_24

To download these materials, click **Git -> Clone a Repository**, enter https://github.com/james-m-foster/MA50290_24.git and click **Clone**.

Each week, you can download the latest materials by clicking **Git -> Pull from Remote**. Whilst this shouldn't overwrite the files that you've changed (and saved), I would still recommend that you write your problem sheet solutions in a **different folder**.

This is summerised in the following screenshots:



- Look at the sub-folder `Week 1` in the folder `MA50290_24`

Here you will find a Jupyter notebook file `ProblemSheet1.ipynb`, which is a copy of this problem sheet, and a data file `OxfordTemp.txt`, containing monthly average temperatures in Oxford starting from January 2022.

Task 1: read and split the data

- The file `OxfordTemp.txt` contains the dataset $\mathbf{D} = \{(x_1, y_1), \ldots, (x_m, y_m)\}$ in the form of two columns separated by a tab. **Read about** the *numpy* **function** `np.loadtxt` (https://numpy.org/doc/stable/reference/generated/numpy.loadtxt.html) which can be used to load simple text data as a *numpy* array.
- **Write Python code** that loads the file `OxfordTemp.txt` into a *numpy* array, and extracts the first column as a *numpy* array $\mathbf{x} \in \mathbb{R}^m$, and the second column as an array $\mathbf{y} \in \mathbb{R}^m$. You can use the cell below.

In [5]:
```
import numpy as np
D = np.loadtxt('OxfordTemp.txt')
x = D[:,0]
y = D[:,1]
```

Warm-up: polynomial features

- (Without using `np.vander`) **Write** a Python **function** `features(x,n)` that takes as input a *numpy* array $\mathbf{x} \in \mathbb{R}^m$ and an integer number $n \geq 0$, and constructs and returns the Vandermonde matrix $V \in \mathbb{R}^{m \times (n+1)}$ as a *numpy* array.

In [6]:
```
def features(x,n):
    powers = np.arange(n+1)                     # [0,1,2,...,n]
    powers = np.reshape(powers, (1, -1))  # Make it explicitly a row vector
    x = np.reshape(x, (-1, 1))              # Make it explicitly a column vector
    return x**powers                        # Python automatically broadcasts the vectors to each
                                            # and takes the power between the resulting matrices
```

Task 2: optimisation of the parameters

- **Write** a Python **function** `optimise_loss(V,y)` that takes as **input** the matrix V constructed in the previous task and the vector $\mathbf{y}$ loaded from the file. This function should compute the matrix $A = V^\top V$, the vector $\mathbf{b} = V^\top \mathbf{y}$, solve the linear equations $A\boldsymbol{\theta}^* = \mathbf{b}$, and **return** the vector $\boldsymbol{\theta}^*$.

Hint: you can recap on numpy functions `@` (matrix multiplication) and `np.linalg.solve`

In [7]:
```
def optimise_loss(V,y):
    return np.linalg.solve(V.T @ V, V.T @ y)
```

Task 3: results

- **Write** Python **code** to compute the optimised parameter $\boldsymbol{\theta}^*$ using the functions from the previous tasks and the training arrays $\mathbf{x}, \mathbf{y}$.
- **Compute** the prediction $h_{\boldsymbol{\theta}^*}(\hat{x})$ for $\hat{x}$ ranging from 1 to 17 (inclusive).

Hint: `np.arange` can produce an appropriate array $\hat{\mathbf{x}}$

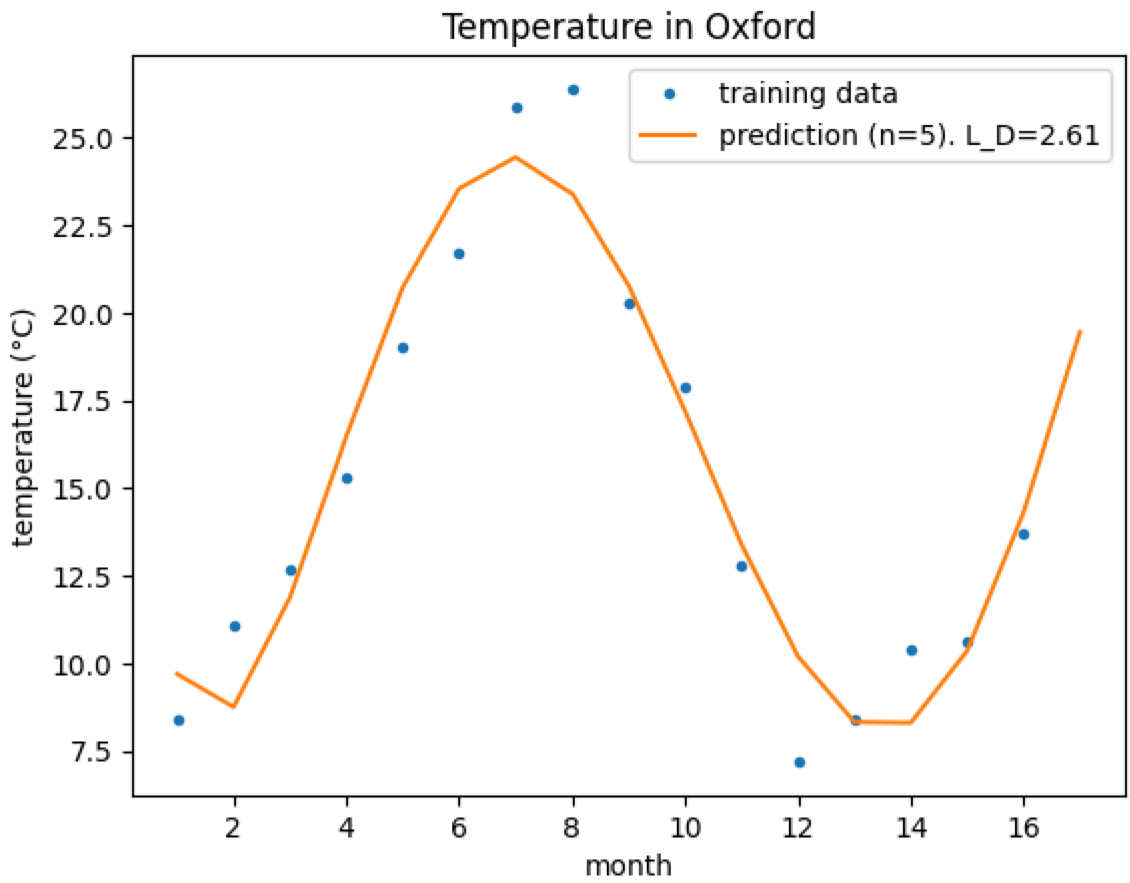
- **Plot** both the training data $\mathbf{y}$ as a function of $\mathbf{x}$, and the prediction $\hat{\mathbf{y}} = h_{\boldsymbol{\theta}^*}(\hat{\mathbf{x}})$ as a function of $\hat{\mathbf{x}}$ on the same graph.

Hint: recap on `matplotlib.pyplot.plot`

- **Vary** n from 1 to 10 and rerun this experiment. Which n gives the most accurate prediction of the known values of the temperature? Which n gives the most "reasonable" prediction for the unknown value at $x = 17$?

In [8]:
```
from matplotlib import pyplot as plt

n = 5

# Compute the optimal parameter
V = features(x, n)
theta = optimise_loss(V, y)

x_pred = np.arange(1, 18) # Prediction set of months
# Predicted temperature values are the values of the same polynomial but at x_pred time points
V_pred = features(x_pred, n)
y_pred = V_pred @ theta
```

```python
# Plot two lines on the same axis
plt.plot(x, y, '.', x_pred, y_pred)
plt.xlabel('month')
plt.ylabel('temperature (°C)')
plt.title('Temperature in Oxford')
plt.legend(("training data", f"prediction (n={n}). L_D={np.mean((y_pred[:-1] - y)**2):.2f}"))

plt.show()
```



Note that the smallest $L_D \approx 0.59$ is achieved with the largest $n = 10$, but in this case the prediction for the new 17th month looks highly erratic. The most reasonable prediction can be seen with the intermediate value $n = 5$.