Case study definition

Here is a 2-variable function:

$$f\colon (x, y) \to xy + (x - 4)^2 + (y + 3)^2$$

Let's determine the arguments that minimize this function.

Code

Simple example

The relevant function is `minimize` from package `scipy.optimize`.

In [1]:
```
from scipy.optimize import minimize
import numpy as np
```

It takes 2 mandatory arguments:

- function to minimize
- initial values for the minimisation

Here after, function `f` takes as input a `numpy` array of size 2.

In [2]:
```
def f(X):
    x, y = X
    return x*y + (x-4)**2 + (y+3)**2

initial = np.array([4, -3])
```

Then `minimize` is called:

In [3]:
```
result = minimize(f, initial)
```

It returns a `OptimizeResult` object:

In [4]:
```
print(type(result))
result
```

Out[4]:
```
<class 'scipy.optimize._optimize.OptimizeResult'>
```

```
     message: Optimization terminated successfully.
     success: True
      status: 0
         fun: -24.333333333333265
           x: [ 7.333e+00 -6.667e+00]
         nit: 5
         jac: [ 0.000e+00 -4.768e-07]
    hess_inv: [[ 6.667e-01 -3.333e-01]
               [-3.333e-01  6.667e-01]]
        nfev: 21
        njev: 7
```

Let's extract the *argmin* values:

In [5]:
```
x_min, y_min = result.x
x_min, y_min
```

Out[5]:
```
(7.333333584713669, -6.666666929228556)
```

Additional arguments

It may happen that function `f` has more arguments than the one we want to minimize along, i.e. that some arguments are fixed. For instance, let's add the m variable:

$$f: (x, y, m) \rightarrow \left(xy + (x-4)^2\right)^m + (y+3)^2$$

When defining `f`, m must not be given in `X` (that holds x and y) but in a separate variable:

In [6]:
```
def f(X, m):
    x, y = X
    return (x*y + (x-4)**2)**m + (y+3)**2
```

Then an argument `args` is used in `minimize` to set m value. Note that a `tuple` is required even if there is only one fixed variable:

In [7]:
```
minimize(f, initial, args=(1, )).x
```

Out[7]:
```
array([ 7.33333358, -6.66666693])
```

In [8]:
```
minimize(f, initial, args=(2, )).x
```

Out[8]:
```
array([ 1.72508278, -3.00000009])
```

Specify the jacobian

Specifying the jacobian is a way to fasten/improve minimization in **some cases**.

This is done by modifying `f`. `f` now returns:

- the function value itself (same than previously)
- the partial derivatives that define the jacobian

Let's compute these derivatives (without the m case).

With respect to x:

$$\frac{\partial f}{\partial x} : (x, y) \rightarrow y + 2(x - 4)$$

With respect to y:

$$\frac{\partial f}{\partial y} : (x, y) \rightarrow x + 2(y + 3)$$

In [9]:
```
def f(X):
    x, y = X
    value = x*y + (x-4)**2 + (y+3)**2
    jac = np.array([y + 2 *(x-4), x+ 2 *(y+3)])
    return value, jac

x_min, y_min = minimize(f, initial, jac=True).x
x_min, y_min
```

Out[9]:
```
(7.333333333333333, -6.666666666666667)
```

Note that the order in `jac` is the same as in `X` (x first, then y).

Plot the result

In [10]:
```
import matplotlib.pyplot as plt
```

Data definition

In [11]:
```
x = np.linspace(-10, 10, 100)
y = np.linspace(-10, 10, 100)
xx, yy = np.meshgrid(x, y)
zz, _ = f([xx, yy])   # gradient is not needed here
```

Plotting

In [12]:

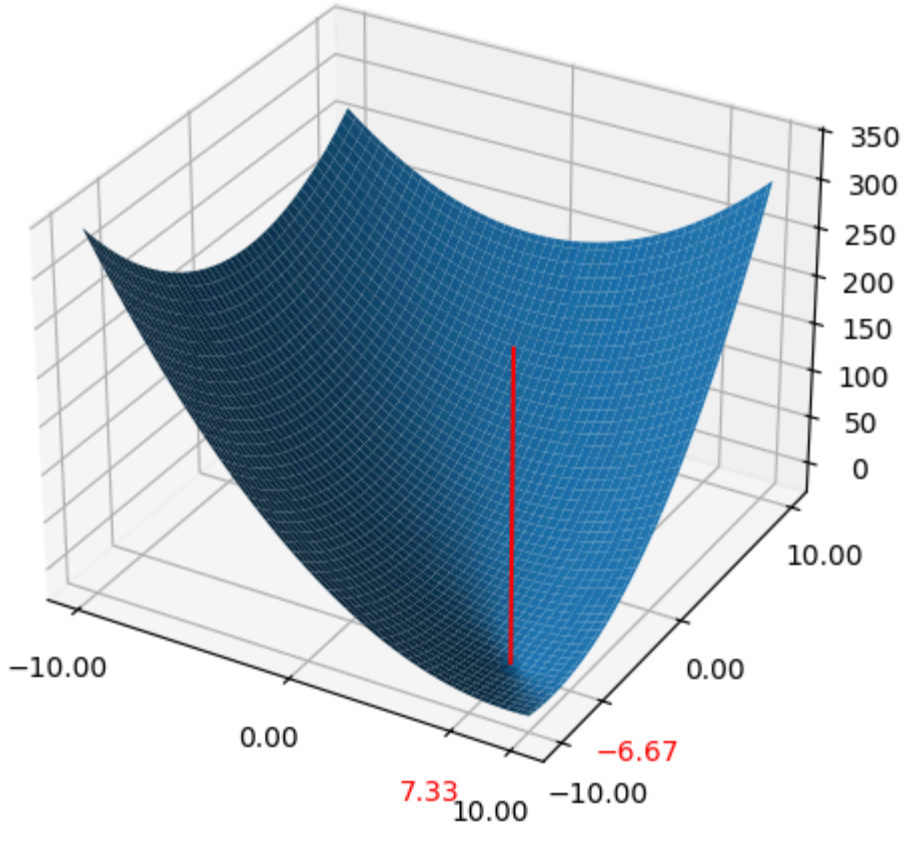
```
# surface only
fig, ax = plt.subplots(subplot_kw={'projection':'3d'})
ax.plot_surface(xx, yy, zz)


# red tick label for x_min and y_min
x_ticks = [-10, 0, 10] + [x_min]
ax.set_xticks(x_ticks)
x_ticklabels = ax.get_xticklabels()
for tick, label in zip(x_ticks, x_ticklabels):
    if tick == x_min:
        label.set_color('red')

y_ticks = [-10, 0, 10] + [y_min]
ax.set_yticks(y_ticks)
y_ticklabels = ax.get_yticklabels()
for tick, label in zip(y_ticks, y_ticklabels):
    if tick == y_min:
        label.set_color('red')

# vertical line at solution point
z, _ = f([x_min, y_min])
marker, line, _ = ax.stem([x_min], [y_min], [z], bottom=300)
line.set_color('red')
```

```
/home/nerotb/Python/3.12/lib/python3.12/site-packages/IPython/core/events.p
y:82: UserWarning: Tight layout not applied. The left and right margins cann
ot be made large enough to accommodate all Axes decorations.
  func(*args, **kwargs)
```


350
300
250
200
150
100
50
0
10.00
0.00
−6.67
−10.00
−10.00
0.00
7.33
10.00