Assignment 1

Assignment 1: Optimization

Goal: Get familiar with gradient-based and derivative-free optimization by implementing these methods and applying them to a given function.

In this assignment we are going to learn about **gradient-based** (GD) optimization methods and **derivative-free optimization** (DFO) methods. The goal is to implement these methods (one from each group) and analyze their behavior. Importantly, we aim at noticing differences between these two groups of methods.

Here, we are interested in minimizing the following function:

$$f(\mathbf{x}) = x_1^2 + 2x_2^2 - 0.3\cos(3\pi x_1) - 0.4\cos(4\pi x_2) + 0.7$$

in the domain $\mathbf{x} = (x_1, x_2) \in [-100, 100]^2$ (i.e., $x_1 \in [-100, 100]$, $x_2 \in [-100, 100]$).

In this assignemnt, you are asked to implement:

1. The gradient-descent algorithm.
2. A chosen derivative-free algorithm. *You are free to choose a method.*

After implementing both methods, please run experiments and compare both methods. Please find a more detailed description below.

1. Understanding the objective

Please run the code below and visualize the objective function. Please try to understand the objective function, what is the optimum (you can do it by inspecting the plot).

If any code line is unclear to you, please read on that in numpy or matplotlib docs.

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

In [2]:
```
# PLEASE DO NOT REMOVE!
# The objective function.
def f(x):
    return x[:,0]**2 + 2*x[:,1]**2 -0.3*np.cos(3.*np.pi*x[:,0])-0.4*np.cos(4.*np.pi*x[:,
```

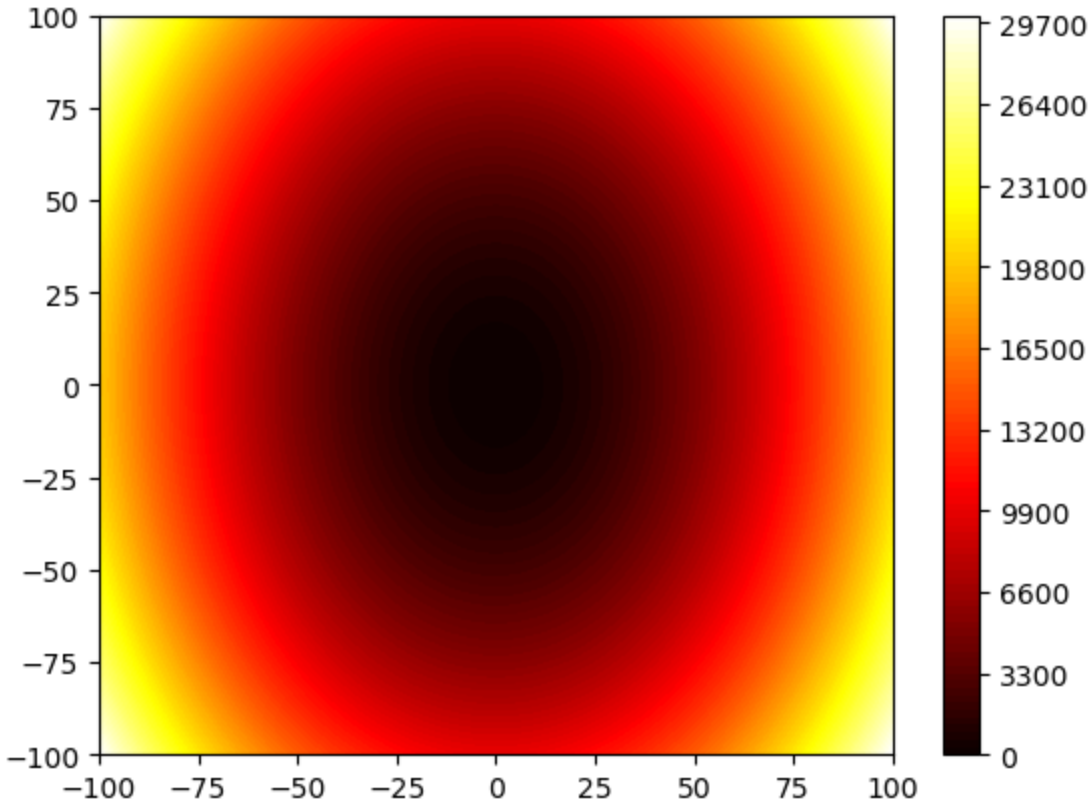
In [3]:
```
# PLEASE DO NOT REMOVE!
# Calculating the objective for visualization.
def calculate_f(x1, x2):
  f_x = []
  for i in range(len(x1)):
    for j in range(len(x2)):
      f_x.append(f(np.asarray([[x1[i], x2[j]]])))

  return np.asarray(f_x).reshape(len(x1), len(x2))
```

In [4]:
```
# PLEASE DO NOT REMOVE!
# Define coordinates
```

```
x1 = np.linspace(-100., 100., 400)
x2 = np.linspace(-100., 100., 400)

# Calculate the objective
f_x = calculate_f(x1, x2).reshape(len(x1), len(x2))
```

In [5]:
```
# PLEASE DO NOT REMOVE!
# Plot the objective
plt.contourf(x1, x2, f_x, 100, cmap='hot')
plt.colorbar()
```

Out[5]:
```
<matplotlib.colorbar.Colorbar at 0x7fc772418e50>
```



2. The gradient-descent algorithm

First, you are asked to implement the gradient descent (GD) algorithm. Please take a look at the class below and fill in the missing parts.

NOTE: Please pay attention to the inputs and outputs of each function.

NOTE: To implement the GD algorithm, we need a gradient with respect to $\mathbf{x}$ of the given function. Please calculate it on a paper and provide the solution below. Then, implement it in an appropriate function that will be further passed to the GD class.

Question 1 (0-1pt): What is the gradient of the function $f(\mathbf{x})$?

Answer:

$$\nabla_{\mathbf{x}_1} f(\mathbf{x}) = 2\mathbf{x}_1 + 0.9sin(3\pi\mathbf{x}_1)\pi$$
$$\nabla_{\mathbf{x}_2} f(\mathbf{x}) = 4\mathbf{x}_2 + 1.6sin(4\pi\mathbf{x}_2)\pi$$

In [6]:
```
#=========
# GRADING:
```

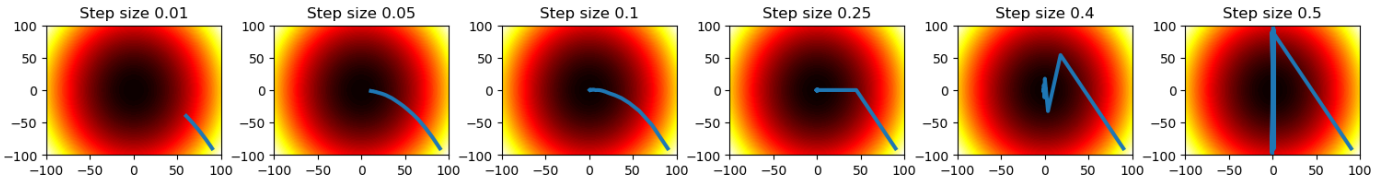
```
# 0
# 0.5pt - if properly implemented and commented well
#=========
# Implement the gradient for the considered f(x).
def grad(x):
  #------
  # PLEASE FILL IN:
  # implemented gradient of function f(x)
    grad = [2*x[0,0] + 0.9*np.sin(3*np.pi*x[0,0])*np.pi, 4*x[0,1] + 1.6*np.sin(4*np.pi*x
  #------
    return grad
```

In [7]:
```
#=========
# GRADING:
# 0
# 0.5pt if properly implemented and commented well
#=========
# Implement the gradient descent (GD) optimization algorithm.
# It is equivalent to implementing the step function.
class GradientDescent(object):
    def __init__(self, grad, step_size=0.1):
        self.grad = grad
        self.step_size = step_size

    def step(self, x_old):
        #------
        # PLEASE FILL IN:
        # Implement gradient descent algorithm
        x_new = np.subtract(x_old, np.multiply(self.step_size, self.grad(x_old)))
        #------
        return x_new
```

In [8]:
```
# PLEASE DO NOT REMOVE!
# An auxiliary function for plotting.
def plot_optimization_process(ax, optimizer, title):
  # Plot the objective function
  ax.contourf(x1, x2, f_x, 100, cmap='hot')

  # Init the solution
  x = np.asarray([[90., -90.]])
  x_opt = x
  # Run the optimization algorithm
  for i in range(num_epochs):
    x = optimizer.step(x)
    x_opt = np.concatenate((x_opt, x), 0)

  ax.plot(x_opt[:,0], x_opt[:,1], linewidth=3.)
  ax.set_title(title)
```

In [9]:
```
# PLEASE DO NOT REMOVE!
# This piece of code serves for the analysis.
# Running the GD algorithm with different step sizes
num_epochs = 20 # the number of epochs
step_sizes = [0.01, 0.05, 0.1, 0.25, 0.4, 0.5] # the step sizes

# plotting the convergence of the GD
fig_gd, axs = plt.subplots(1,len(step_sizes),figsize=(15, 2))
fig_gd.tight_layout()

for i in range(len(step_sizes)):
  # take the step size
  step_size = step_sizes[i]
  # init the GD
  gd = GradientDescent(grad, step_size=step_size)
```

```
# plot the convergence
plot_optimization_process(axs[i], optimizer=gd, title='Step size ' + str(gd.step_size)
```



Question 2 (0-0.5pt): Please analyze the plots above and comment on the behavior of the gradient-descent for different values of the step size.

Answer: Looking at the results, we observe that the gradients change with respect to step size. If step size is low, gradients slow and can't attain the optimum point. If step size is high, the gradients jump between values and can't reach optimum value, because it skips the optimum value. Thus, step size should not be too low or too high, it should be moderate.

Question 3 (0-0.5pt): What could we do to increase the convergence when the step size equals 0.01? What about when the step size equals 0.5?

Answer: When the step size equals 0.01, number of epochs could be increased in order to have better results with gradient descent algorithm. When the step size equals 0.5, a solution could be the randomization of the initial point of the algorithm. Then, the algorithm could be run several times to have better results.

3. The derivative-free optimization

In the second part of this assignment, you are asked to implement a derivative-free optimziation (DFO) algorithm. Please notice that you are free to choose any DFO method you wish. Moreover, you are encouraged to be as imaginative as possible! Do you have an idea for a new method or combine multiple methods? Great!

Question 4 (0-0.5-1-1.5-2-2.5-3pt): Please provide a description (a pseudocode) of your DFO method here.

NOTE (grading): Please keep in mind: start simple, make sure your approach works. You are encouraged to use your creativity and develop more complex approaches that will influence the grading. TAs will also check whether the pseudocode is correct.

Answer: I used local search algorithm to solve this problem. I have neighbor points for the current best solution. In the step method, a list of neighbors is created with points. Points are calculated by adding step size and direction values. The algorithm evaluates the objective function for every neighbor. In the end, the minimum value neighbor is selected.

Input: Current best solution

1. Find the best solution for the neighborhood of the current best solution
2. Find minimum from neighbor points and see the solution as the best current solution
3. Go to 1 until STOP

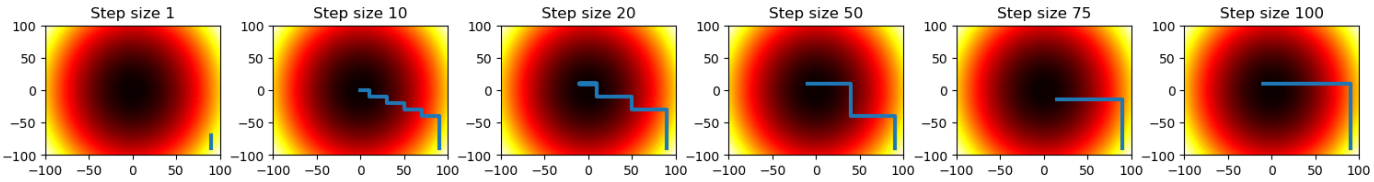
In [10]:
```
#=========
# GRADING: 0-0.5-1-1.5-2pt
# 0
```

```
# 0.5pt the code works but it is very messy and unclear
# 1.0pt the code works but it is messy and badly commented
# 1.5pt the code works but it is hard to follow in some places
# 2.0pt the code works and it is fully understandable
#=========
# Implement a derivative-free optimization (DFO) algorithm.
# REMARK: during the init, you are supposed to pass the obj_fun and other objects that a
class DFO(object):
    def __init__(self, obj_fun, step_size):
        self.obj_fun = obj_fun
        # PLEASE FILL IN: You will need some other variables
        self.step_size = step_size

    ## PLEASE FILL IN IF NECESSARY
    ## Please remember that for the DFO you may need extra functions.
    #def ...

    # This function MUST be implemented.
    # No additional arguments here!
    def step(self, x_old):
    ## PLEASE FILL IN.
        #create directions lists dir_x and dir_y
        dir_x = [step_size, 0, -step_size, 0, 0]
        dir_y = [0, step_size, 0, -step_size, 0]
        neighbors = []
        values = []
        #add neighbors to list
        for i in range(len(dir_x)):
            neighbor = x_old + np.array([dir_x[i], dir_y[i]])
            neighbors.append(neighbor)
        #add values for each neighbor, evaluate objective function
        for neighbor in neighbors:
            value = self.obj_fun(neighbor)
            values.append(value)
        #select neighbor with minimum objective function value
        x_new = neighbors[np.argmin(values)]
        return x_new
```

In [11]:

```
# PLEASE DO NOT REMOVE!
# Running the DFO algorithm with different step sizes
num_epochs = 20 # the number of epochs (you may change it!)

## PLEASE FILL IN
## Here all hyperparameters go.
## Please analyze at least one hyperparameter in a similar manner to the
## step size in the GD algorithm.
# analyzed step size parameter

step_sizes = [1, 10, 20, 50, 75, 100]

## plotting the convergence of the DFO
## Please uncomment the two lines below, but please provide the number of axes (replace
fig_dfo, axs = plt.subplots(1, len(step_sizes), figsize=(15, 2))
fig_dfo.tight_layout()

# the for-loop should go over (at least one) parameter(s) (replace HERE appriopriately)
# and uncomment the line below
#iterate over step_sizes to get step_sie and then dfo of each one
for i in range(len(step_sizes)):
  ## PLEASE FILL IN
    step_size = step_sizes[i]
    dfo = DFO(f, step_size)
  # plot the convergence
  # please change the title accordingly!
```

```
    plot_optimization_process(axs[i], optimizer=dfo, title='Step size '+ str(dfo.step_si
```



Question 5 (0-0.5-1pt) Please comment on the behavior of your DFO algorithm. What are the strong points? What are the (potential) weak points? During working on the algorithm, what kind of problems did you encounter?

Answer: DFO algorithm is done with Local Search. I guess it has weak points as the step sizes could be different. As seen above figure, when the step size is too small, the algorithm is too far away from the optimum value. And when the step size is too big, the algorithm skips the values between and can't attain optimum value. Maybe I could use more suitable step size values. However, it can reach near the optimum value with the local search algorithm. Finding suitable step size values was a challenge for me while trying to see the results. Also, creating directions list and calculating the neighbors values with a function was challenging.

4. Final remarks: GD vs. DFO

Eventually, please answer the following last question that will allow you to conclude the assignment draw conclusions.

Question 6 (0-0.5pt): What are differences between the two approaches?

Answer: Gradient descent uses gradient of the function, however in derivative free optimization derivatives of the function is not used. Gradient descent is used when the function is a differentiable function and derivative free optimization is used when the function is not differentiable. Derivative free optimization can be applied to a broader types of functions, it is more adaptable. However, derivative free optimization lacks precision compared to graident descent algorithm, as gradient descent is based on mathematical calculations.

Question 7 (0-0.5): Which of the is easier to apply? Why? In what situations? Which of them is easier to implement in general?

Answer: I think that, in general, gradient descent is easier to apply when the function is precise and differentiable. It can be done by calculating the gradient of the function. Derivative free optimization is harder to implement, as it uses algorithms to evaluate the function. When the function is not differentiable or too complex to calculate the gradient, derivative-free optimization is easier to implement.