Computer Methods in Engineerings Exercise on gradient descent

Problem 1

Consider the one dimensional function

$$f(x) = 2x^3 + 2x^2 - 4x$$
 for $x \in [-1, 1]$. (1)

a) Find the roots of f(x) and check your result using the numpy roots() function. Hint: The roots() function take the polynomial coefficients as a vector input, e.g. for $h(x) = 2x^2 - 1$ you would write: np.roots([2.0,0.0,-1]).

Solution:

```
''' Solution to problem 1 in exercise on gradient descent
import numpy as np
import matplotlib.pyplot as plt
from math import *
#Function to find root
def f(x):
  rval = 2*x**3+2*x**2-4*x
  return rval
#Find root :
coeff = np.array([2.0, 2.0, -4.0, 0.0])
r = np.roots(coeff)
print(r)
dx = 0.01
xv = np.arange(-3, 2.0, dx)
ff = f(xv)
plt.plot(xv,ff)
plt.xlim(-3.0, 2.0)
plt.ylim(-3.0,5.0)
plt.plot(r[0],f(r[0]),'ro',label='first root')
plt.plot(r[1],f(r[1]),'bo',label='second root')
plt.plot(r[2],f(r[2]),'go',label='third root')
plt.plot([-3,2], [0,0])
plt.legend()
plt.xlabel('x')
plt.ylabel('f(x)')
plt.savefig('root.pdf')
```

```
plt.show()
def gradf(x):
 return 6*x**2+4*x-4
#Error tolerance
eps = 1e-4
#Maximum number of iterations
maxIt = 100
#Initial point
xx = 0.75
itr=0
diff=2*eps
while(itr<(maxIt-1) and diff>eps):
   xxnew=xx-f(xx)/gradf(xx)
   diff=np.abs(xxnew-xx)
   xx=xxnew
   print(itr,xx)
    itr+=1
print('Root: ',xx, '\n Number of iterations: ',itr)
def ddf(x):
  return 12*x+4
#Initial point
xx = -0.25
itr=0
diff=2*eps
while(itr<(maxIt-1) and diff>eps):
   xxnew=xx-gradf(xx)/ddf(xx)
   diff=np.abs(xxnew-xx)
   xx=xxnew
   print(itr,xx)
   itr+=1
print('Extremum: ',xx, '\n Number of iterations: ',itr)
plt.plot(xv,ff)
plt.xlim(-3.0,2.0)
plt.ylim(-3.0,5.0)
plt.plot(xx, f(xx), 'ro', label='extremum')
plt.plot([-3,2], [0,0])
plt.legend()
plt.xlabel('x')
plt.ylabel('f(x)')
plt.savefig('extremum.pdf')
plt.show()
```

b) Plot f(x) in python using plot (). Use an appropriate sampling interval Δx on the

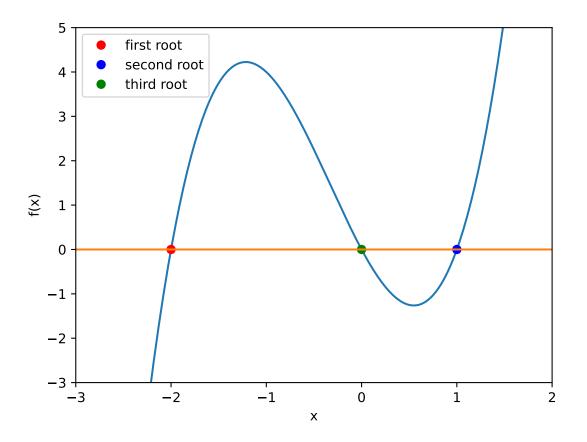


Figure 1: Roots of the function f(x) = 2x(x - 1.0)(x + 1.0)

x-axis. Give your plot a title and label the axes. Indicate the roots with a red dot and blue dot. Plot also the line y = 0

Solution:

See figure 1.

c) Use Netwon's method to find a root of the function f. Suggested starting-points are 0.5 and 0.75. As there are several roots, explain why you get the root you get when using the Netwon method.

Solution:

See the code in the solution of problem 1a.

d) Use Netwon's method to find a maximum or minimum value of the function f. Suggested starting-points are somewhere in the range [-0.5, 0.0]. Explain why you get the solution you get when using the Netwon method and your chosen starting-point.

Solution:

See the code in the solution of problem 1a. See figure 2.

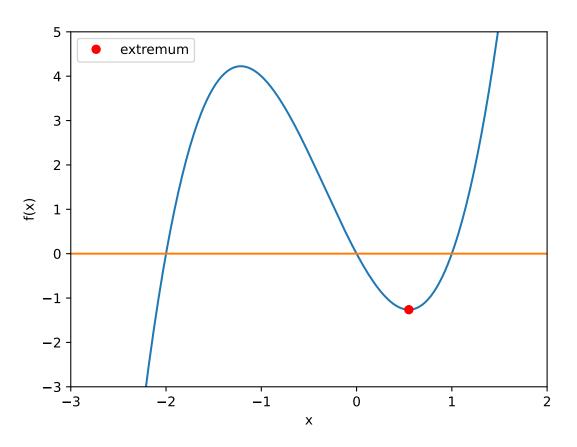


Figure 2: Extremum of the function f(x)

.

Problem 2

We will now continue with the exercise from the bracket search, where we assumed we were going to build a pipeline to transport CO2 from a capture site to an offshore storage site. A code for calculating the profit from the pipeline as a function of the radius of the pipe was given in the previous exercise.

a) Create a code to find the gradient of the profit with respect to radius.

Solution:

We can calculate the derivatives as follows:

```
def derCostPipe(self, radius):
    return 2*m.pi*radius*self.length*self.materialPrice

def derCostUse(self, radius):
    derDeltaP=-4*8*self.viscosity* ...
        self.length*self.flowRate/(m.pi*radius**5)
    return derDeltaP*self.pricePerPascalperCubed

def derProfit(self, radius, time):
    return -self.derCostUse(radius)* self.flowRate*time - ...
    self.derCostPipe(radius)
```

b) Use the derivate to make a more efficient bracket search. Compare the number of iterations with the barcket search conducted in the previous exercise.

Solution:

We can replace the test values α and β by the derivative, as shown in the following code:

```
def bracketDer(self, time):
   from random import random
   #Maximum number of iterations
   self.iN = 100
   #Error tolerance
   self.feps = 1e-3
    #Storing values during run for later plotting
   self.afA=np.zeros(self.iN)
   self.afB=np.zeros(self.iN)
    #Starting values for our interval [a,b] and internal points ...
       alpha and beta
   self.afA[0] = 0.1
   self.afB[0] = 0.4
    # This is an iterative algorithm, and we iterate over ii
    while(ii<self.iN and (self.afB[ii]-self.afA[ii])>self.feps):
        fTestRadius=(self.afA[ii]+self.afB[ii])/2
        # If derivative is positive change b value
       if self.derProfit(fTestRadius, time)>0:
           self.afA[ii+1]=fTestRadius
            self.afB[ii+1]=self.afB[ii]
        else:
```

When running this code, the optimum was found after 9 iterations. A couple of tests with the old bracket search code resulted in between 14 and 21 iterations.

c) Create a code where you do a gradient descent to find the optimum.

Solution:

We can add a code similar to this to our class:

```
def gradientDescent(self, time, initRadius=0.3):
    fRadius = initRadius
    fOldRadius = initRadius*1.2 # Ensure the loop starts
    fStepSize=1e-9
    self.iN=100
    self.eps=1e-3
    ii=0
    while ii < self.iN and abs(fRadius-fOldRadius)>self.eps:
        grad = self.derProfit(fRadius, time)
        fOldRadius = fRadius
        fRadius = fRadius + fStepSize * grad
        ii+=1
    return fRadius, self.profit(fRadius, time), ii+1
```

When running this code, the optimum was found after 11 iterations, a similar number to the bracket method. However, this code is very dependent on the step-size used.