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Homework - 03

Problem 01

→ i) $\min_{A_{12}\ A_{21}} \sum_{i=1}^{11} (P_i(A_{12}, A_{21}) - P_i)^2$

ii) From antoine eqn

P^{sat}_{water}; $\log_{10}(P^{sat}) = a_1 - \frac{a_2}{T + a_3}$

Consider the following

	a_1	a_2	a_3
water	8.07131	1730.62	233.426
1,4 dioxane	7.43155	1554.679	240.337

we solve for P^{sat}_{water} and $P^{sat}_{1,4\,dioxane}$

$$P^{sat}_{water} = 10^{\left(8.07131 - \frac{1730.63}{20 + 233.426}\right)}$$

$$= 17.469999884 2$$

$$P^{sat}_{dioxane} = 10^{\left(7.43155 - \frac{1554.679}{20 + 240.337}\right)}$$

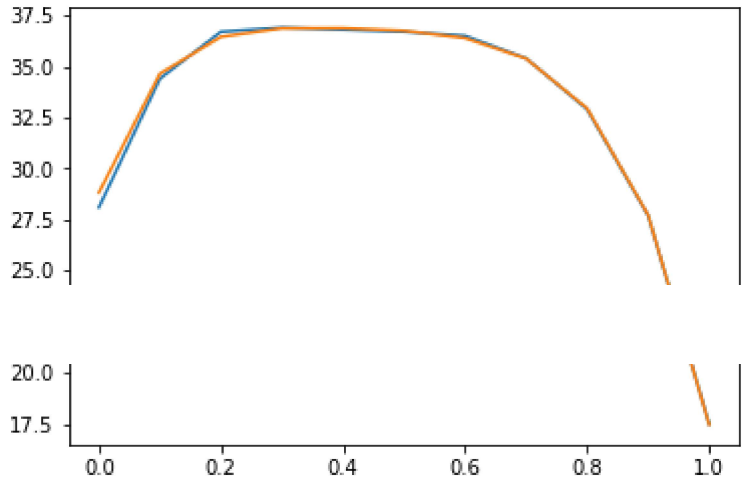
$$= 28.82409952$$

$$\therefore P = x_1 \exp\left(A_{12}\left(\frac{A_{21} x_2}{A_{12} x_1 + A_{21} x_2}\right)\right)^2 \cdot (17.47)$$

$$+ x_2 \exp\left(A_{21}\left(\frac{A_{12} x_1}{A_{12} x_1 + A_{21} x_2}\right)\right) \cdot (28.82409)$$

```
#Homework 03
#Problem 01

import torch as t
from torch.autograd import Variable
import numpy as np
import math as m
from matplotlib import pyplot
import matplotlib
import matplotlib.cm as cm
import matplotlib.pyplot as plt

x_1 = np.array([0.0,0.1,0.2,0.3,0.4,0.5,0.6,0.7,0.8,0.9,1.0])
x_2 = -x_1+1
Data_p=np.array([28.1,34.4,36.7,36.9,36.8,36.7,36.5,35.4,32.9,27.7,17.5])

water_Psat = 17.469999884208
dioxane_Psat = 28.824099527402

# Gradeint Descent
x = Variable(t.tensor([0.7, 0.3]), requires_grad=True)

#step Size
a = 0.001
for i in range(100):
    for i in range(0,11):
        obj = (((x_1[i]*t.exp(x[0]*((x[1]*x_2[i])/(x[0]*x_1[i]+x[1]*x_2[i]))**2)*water_Psat)
        obj.backward()
    x.grad.numpy()
    with t.no_grad():
       x -= a * x.grad
       x.grad.zero_()
print(x.data.numpy())
print(obj.data.numpy())

r = []
for i in range(0,11):
  P_optimized = ((x_1[i]*m.exp(x[0]*((x[1]*x_2[i])/(x[0]*x_1[i]+x[1]*x_2[i]))**2)*water_Psat)
  #print("optimized_p =",P_optimized, "     measured_p =", Data_p[i])
  #print("Error between optimuzed and measured P value =" , Data_p[i]-P_optimized)
  r.append(P_optimized)
plt.plot(x_1,Data_p)
plt.plot(x_1,r)
```

```
[1.9586585 1.6894491]
0.0009000412
[<matplotlib.lines.Line2D at 0x7f17b0f67310>]
```



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```
from bayes_opt import BayesianOptimization

#Multiplying the function by -1 inorder to get the minimum value.

def function(x_1, x_2):
    return -1*((4-2.1*x_1**2+(x_1**4)/3)*x_1**2+x_1*x_2+(-4+4*x_2**2)*x_2**2)
pbounds = {'x_1': (-3, 3), 'x_2': (-2, 2)}

optimizer = BayesianOptimization(f=function,pbounds=pbounds,random_state=1)

optimizer.maximize(init_points=2,n_iter=20)
print(optimizer.max)
```

```
|   iter    |  target   |    x_1    |    x_2    |
-------------------------------------------------
|  1        |  0.265    | -0.4979   |  0.8813   |
|  2        | -110.1    | -2.999    | -0.7907   |
|  3        | -0.4933   | -0.3849   |  1.039    |
|  4        | -0.2833   |  1.599    | -0.5696   |
|  5        | -162.9    |  3.0      |  2.0      |
|  6        | -47.77    |  0.3665   | -2.0      |
|  7        | -150.9    |  3.0      | -2.0      |
|  8        | -0.7638   |  0.4683   | -0.02769  |
|  9        | -48.27    | -2.043    |  2.0      |
|  10       | -2.236    |  1.314    |  0.6422   |
|  11       | -50.26    |  0.5766   |  2.0      |
|  12       | -52.97    | -1.299    | -2.0      |
|  13       | -1.06     | -0.7025   | -0.5363   |
|  14       | -7.993    |  2.197    |  0.07143  |
|  15       | -48.19    | -0.8016   |  2.0      |
|  16       | -1.426    | -1.507    |  0.2863   |
|  17       | -107.6    | -3.0      |  1.181    |
|  18       | -2.305    |  1.361    | -0.01254  |
|  19       |  0.03573  |  0.4022   |  0.7855   |
|  20       |  0.217    |  0.5131   | -0.8858   |
|  21       | -1.746    | -0.8282   |  0.09644  |
|  22       | -0.8247   | -1.335    |  0.9693   |
=================================================
{'target': 0.2650082867644827, 'params': {'x_1': -0.4978679717845562, 'x_2': 0.881297973
```