CS547 HW1 Group 32

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Problem 1

(1)

$$\nabla f(\boldsymbol{x}) = \begin{pmatrix} 18x_1 \\ 2x_2 \end{pmatrix}$$

(2) From fundemantal definition of calculus, we have

$$\boldsymbol{X_t'} = \frac{d\boldsymbol{X_t}}{dt} = \lim_{\Delta t \to 0} \frac{\boldsymbol{X}_{t+\Delta t} - \boldsymbol{X}_t}{\Delta t} = \lim_{\delta \to 0} \frac{\boldsymbol{X}_{t+\delta} - \boldsymbol{X}_t}{\delta} = \lim_{\delta \to 0} \frac{\boldsymbol{x}_{\lfloor \frac{t}{\delta} \rfloor + 1} - \boldsymbol{x}_{\lfloor \frac{t}{\delta} \rfloor}}{\delta}$$

Now we have

$$\boldsymbol{x}_{\lfloor \frac{t}{\delta} \rfloor + 1} - \boldsymbol{x}_{\lfloor \frac{t}{\delta} \rfloor} = \boldsymbol{x}_{n+1} - \boldsymbol{x}_n = -\delta \nabla f(\boldsymbol{x}_n)$$

Therefore

$$\begin{aligned} \boldsymbol{X_t'} &= \lim_{\delta \to 0} \frac{-\delta \nabla f(\boldsymbol{x}_n)}{\delta} = \lim_{\delta \to 0} -\nabla f(\boldsymbol{x}_n) = -\nabla f(\boldsymbol{x}_n) \\ &= -\begin{pmatrix} 18x_1 \\ 2x_2 \end{pmatrix}_{\lfloor t/\delta \rfloor} = -\begin{pmatrix} 18X_1 \\ 2X_2 \end{pmatrix}_t \end{aligned}$$

The system of ODE for $\lim_{\delta \to 0} \boldsymbol{X}_t$ at the optimal location is

$$\begin{aligned} X_1' + 18X_1 = 0 \\ X_2' + 2X_2 = 0 \end{aligned}$$

(3) Sove the system of ODE

$$\begin{aligned} X_1' + 18X_1 = 0 \\ \frac{dX_1}{dt}\frac{1}{X_1} = -18 \\ \frac{1}{X_1}dX_1 = -18dt \\ \ln X_1 = -18t + C_1 \\ X_1 = Ae^{-18t} \end{aligned}$$

Similarly we have $X_2 = Be^{-2t}$. Now substitute the initial condition of $\boldsymbol{x}_0 = \boldsymbol{X}_0 = (1, 2)$, we have

$$\begin{aligned} A = 1 \\ B = 2 \end{aligned}$$

The solution for the ODE is

$$\begin{aligned} X_1 = e^{-18t} \\ X_2 = 2e^{-2t} \end{aligned}$$

From the solution of ODE, we can conclude that X converges exponentially to the minimum point of (0,0) from initial point of (1,2) at step 0 when t tends to infinity. This is the minimum converges rate of gradient decent when we choose a step size tending to 0.

In [ ]:

```

```

Problem 2

(1) Explicitly describe the gradient descent iteration $x_{n+1} = x_n - \delta f'(x_n)$.

First compute the gradient:

$$f'(x_n) = 2\lambda x_n$$

Then we have the explicit expression for the gradient descent iteration:

$$x_{n+1} = x_n - \delta f'(x_n) = x_n - 2\delta\lambda x_n$$
$$x_{n+1} = (1 - 2\delta\lambda)x_n$$

(2) Describe the stability of gradient descent iteration for different values of δ.

Regardless of the sign of x_n, then the gradient descent is stable, x_{n+1} always tend to approach the optimal point $x = 0$. Hence, $\|1 - 2\lambda\delta\| < 1$ should be satisfied.

$$\|1 - 2\lambda\delta\| < 1$$
$$0 < \delta < \frac{1}{\lambda}, \lambda > 0.$$

Therefore, the gradient descent will be stable when $0 < \delta < \frac{1}{\lambda}$ and converges to 0. The gradient descent is unstable and diverges for all other values of δ.

Problem 3

In [8]:

```
import os
import numpy as np
import pandas as pd
from IPython.display import Markdown as md
import time
import random
import matplotlib
#%matplotlib notebook
import matplotlib.pyplot as plt
import scipy.stats
#from pandas.plotting import autocorrelation_plot
import matplotlib.offsetbox as offsetbox
from matplotlib.ticker import StrMethodFormatter

import imageio
import PIL

def saver(fname):
    plt.savefig(fname+".png",bbox_inches="tight")

def legend(pos="bottom",ncol=3,extra=False):
    if pos=="bottom":
        extra = 0.15 if extra else 0
        plt.legend(bbox_to_anchor=(0.5,-0.2-extra), loc='upper center',facecolor="lightgray",ncol=ncol)
    elif pos=="side":
        plt.legend(bbox_to_anchor=(1.1,0.5), loc='center left',facecolor="lightgray",ncol=1)

def textbox(txt,fname=None):
    plt.figure(figsize=(1,1))
    plt.gca().add_artist(offsetbox.AnchoredText("\n".join(txt), loc="center",prop=dict(size=30)))
    plt.axis('off')
    if fname is not None:
        saver(fname)
    plt.show()
    plt.close()
```

Load the data.

In [2]:

```
# tries to get local version and then defaults to google drive version
def getfile(location_pair, **kwargs):
    (loc, gdrive) = location_pair
    try:
        out = pd.read_csv(loc, **kwargs)
    except FileNotFoundError:
        print("local file not found; accessing Google Drive")
        loc = 'https://drive.google.com/uc?export=download&id=' + \
            gdrive.split('/')[-2]
        out = pd.read_csv(loc, **kwargs)
    return out
```

In [3]:

```
columns=[
"CIC0",
"SM1_Dz(Z)",
"GATS1i",
"NdsCH",
"NdssC",
"MLOGP",
"LC50" #response
]
fname = ("qsar_fish_toxicity.csv",
         "https://drive.google.com/file/d/1xd30VCQ2clQPzHDXpDi-VPU6pGTIUmQg/view?usp=sharing")

data_raw = getfile(fname, sep=";", names=columns)
```

```
local file not found; accessing Google Drive
```

In [4]:

```
data_raw.head()
```

Out[4]:

	CIC0	SM1_Dz(Z)	GATS1i	NdsCH	NdssC	MLOGP	LC50
0	3.260	0.829	1.676	0	1	1.453	3.770
1	2.189	0.580	0.863	0	0	1.348	3.115
2	2.125	0.638	0.831	0	0	1.348	3.531
3	3.027	0.331	1.472	1	0	1.807	3.510
4	2.094	0.827	0.860	0	0	1.886	5.390

In [5]:

```
feature, response = ["CIC0", "SM1_Dz(Z)", "GATS1i", "MLOGP"], "LC50"
data=data_raw.copy()
X=data[feature]
Y=data[response]
display(X.head())
display(Y.head())
```

	CIC0	SM1_Dz(Z)	GATS1i	MLOGP
0	3.260	0.829	1.676	1.453
1	2.189	0.580	0.863	1.348
2	2.125	0.638	0.831	1.348
3	3.027	0.331	1.472	1.807
4	2.094	0.827	0.860	1.886

```
0    3.770
1    3.115
2    3.531
3    3.510
4    5.390
Name: LC50, dtype: float64
```

(1) Sklearn

Use sklearn to find the formula (i.e., coefficients) for the linear regression.

In [6]:

```
from sklearn.linear_model import LinearRegression
reg = LinearRegression().fit(X, Y)
coe_sklearn = reg.coef_
display(coe_sklearn)
intrcpt_slkearn = reg.intercept_
display(intrcpt_slkearn)
```

```
array([ 0.44750162,  1.22068139, -0.77463965,  0.38310065])
2.1943526381758236
```

The expression of the linear regression is

LC50 = 0.4475 $\times$ CIC0 + 1.2207 $\times$ SM1 Dz(Z) - 0.7746 $\times$ GATS1i + 0.3831 $\times$ MLOGP + 2.1944

(2) Numpy Implementation

Derive the explicit formula for multidimensional linear regression and implement it in numpy to get explicit coefficients.

Implementing the normal equation.

When there are more than one varibale as input x in the linear regression, we have the design matrix $X_{n\times(p+1)}$, where n is the number of the training samples and p is the number of the variables considered in the linear regression model. Each training same is a row in the design matrix. The additional column in the design matrix is 1's to account for the intercept of the linear regression. Thus, we have parameter vector $P_{(p+1)\times 1} = \left(m^T, b\right)^T$. In summary, the linear regression model should look like

$$y_n = X_{n\times(p+1)}\ P_{(p+1)\times 1}$$

To obtain the optimal parameters P^* of the linear regression model, one can compute the mean squared error (MSE) of the predicted y_n and the ground truth y_{train}, which is

$$\Lambda(P) = \frac{1}{n}\sum_{i=1}^{N}\left(y_{train,\,i} - X_i\ P_{(p+1)\times 1}\ \right)^2$$

Take the derivative of the MSE $\Lambda(P)$ with respect to the parameters P and make it equal to 0, the solution of which is the solution for the multivariate linear regression.

$$\begin{gathered}\nabla_P\ \Lambda(P) = 0\\ \nabla_P\ \left(y_{train} - XP\ \right)^T\left(y_{train} - XP\ \right) = 0\\ 2X^TXP - 2X^Ty_{train} = 0\\ P = \left(X^TX\right)^{-1}X^Ty_{train}\end{gathered}$$

The Pyhton implementation of the normal equation is shown in the cell below.

In [13…

```
XX = np.hstack([np.array(X), np.array(
    [1]*X.shape[0]).reshape((X.shape[0], 1))])
m = np.linalg.inv(XX.T@XX)@(XX.T)@(Y)
print(f'----- Method 3 ------')
print(f'The coefficients of the linear regression model are:')
display(m[:-1])
print(f'The intercept of the linear regression model is:')
display(m[-1])
```

```
----- Method 3 ------
The coefficients of the linear regression model are:
array([ 0.44750162,  1.22068139, -0.77463965,  0.38310065])
The intercept of the linear regression model is:
2.1943526381757947
```

The results are same as (1):

LC50 = 0.4475 $\times$ CIC0 + 1.2207 $\times$ SM1 Dz(Z) - 0.7746 $\times$ GATS1i + 0.3831 $\times$ MLOGP + 2.1944

Gradient Descent

The gradient decent is implemented in the cell below.

More specifically, a class named **LinearRegression_multi** is defined to get multivariate linear regression models. The method **gradient_descent** in the class conducts the gradient decent inparticular.

For each iteration of the gradient descent, all training data are used (1 epoch). The cost, i.e. the difference between the predicted y and the ground truth y_{train},

$$\epsilon_i(P)\ =\ y_{train,\,i}\ -\ X_iP$$

as well as the gradient of the cost fucntion $\Lambda(P)$ with respect to the learning rate δ at $\delta = 0$

$$\nabla\Lambda(P) \;=\; -\frac{2}{n}\sum_{i=1}^{n}\epsilon_i(P)X_i$$

is computed in the function **Cost**.

The parameters P is then updated by δ and the computed gradient $\nabla\Lambda(P)$:

$$P_{i+1} = P_i - \delta\nabla\Lambda(P)$$

where i is the iteration step number.

The number of the iterations for the gradient descent is controlled by two factors: (1) maximum allowable number of iterations; (2) the gradient step L2 norm $\|\nabla\Lambda(P)\|^2$. Both factors are compared with the input tolerance during each iteration.

The detailed Python implementation is presented below, as well as the computed optimal parameters P.

In [25…

```
class LinearRegression_multi:
    def __init__(self, x, y):
        self.xvals = np.array(x)
        self.nsamples = self.xvals.shape[0]
        self.nvars = self.xvals.shape[1]

        self.yvals = np.array(y).reshape((self.nsamples, 1))

        self.XXvals = np.hstack(
            [self.xvals, np.array(([1]*self.nsamples)).reshape((self.nsamples, 1))])
        self.reset()

    def reset(self):
        self.ctr = 0
        self.callbacktext = []
        self.p = [np.zeros([self.nvars, 1]), 0.]
        self.lr = 0.0001
        #self.b = 0.

    @staticmethod
    def linear_function(p):
        (m, b) = p

        def l_f(x):
            return x@m + b
        return l_f

    def Cost(self, p, include_gradient=False):
        err = self.yvals-self.linear_function(p)(self.xvals)
        cost = np.mean(err**2)
        # print(err)
        if include_gradient:
            out = -2*np.mean(err*self.XXvals, axis=0)
            return (cost, out)
        else:
            return cost

    def gradient_descent(self, epochs, p=None, lr=None,
                         precision=0.01):
        if lr == None:
            lr = self.lr
        if p == None:
            p = self.p
        m = p[0]
        b = p[1]
        step_size = 1.
        i = 0
        cost_history = np.array([])
        m_history = np.array([m])
        b_history = np.array([b])
        while step_size > precision and i < epochs:
            cost, gradient = self.Cost([m, b], True)
            cost_history = np.append(cost_history, cost)
            m = m - lr*gradient[:-1].reshape((self.nvars, 1))
```

```
            b = b - lr*gradient[-1]
            m_history = np.append(m_history, m.T)
            b_history = np.append(b_history, b)
            step_size = np.linalg.norm(gradient)
            i += 1
        #
        print(f'Gradient descent total iterations: {i}')
        return m.T, b, cost_history, m_history, b_history

    def metric(self, p):
        (m, b) = p
        err = self.yvals-self.linear_function(p)(self.xvals)
        return np.mean(np.abs(err))

    def callback(self, x, verbose=False):
        (m, b) = p
        outstr = "ctr={0:}; (m,b)=({1:.3f},{2:.2E}); error={3:.2E}".format(
            self.ctr, m, b, self.Cost(p))
        self.callbacktext.append(outstr)
        if verbose:
            print(outstr)
        self.ctr += 1
```

Now carry out the gradient descent for the linear regration given the X and y data. The maximum iteration number is set to be 10000. The tolerance for the L2 norm of the gradient update step size is 10^{-10}. By trying several different learning rate or δ, it was found that $\delta = 0.05$ could be a good choice with stable condition and reseaonable number of iterations.

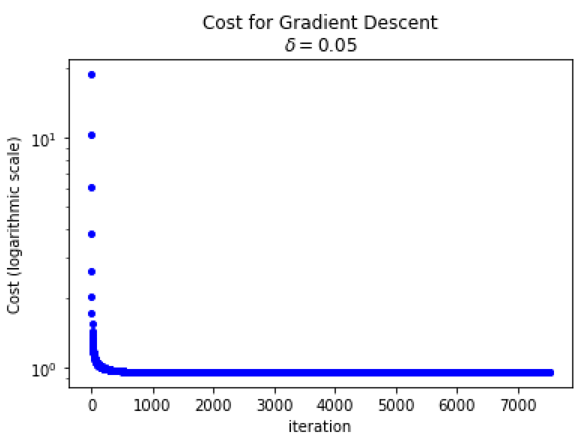
In [24…

```
LR = LinearRegression_multi(X, Y)

delta = 0.05
m_gd, b_gd, cost_his, m_his, b_his = LR.gradient_descent(10000, lr=delta,
                                                          precision=1e-10)
display(m_gd)
display(b_gd)

title = []
title.append("Cost for Gradient Descent")
title.append(r"$\delta={:.2f}$".format(delta))
plt.figure()
plt.semilogy(cost_his, 'bo', ms=4)
plt.ylabel("Cost (logarithmic scale)")
plt.xlabel("iteration")
plt.title("\n".join(title))
saver("increasing_cost")
plt.show()
plt.close()
```

```
Gradient descent total iterations: 7521
array([[ 0.44750162,  1.22068139, -0.77463965,  0.38310065]])
2.1943526365103576
```



The results agree with (1) and (2):

LC50 = 0.4475 $\times$ CIC0 + 1.2207 $\times$ SM1 Dz(Z) - 0.7746 $\times$ GATS1i + 0.3831 $\times$ MLOGP + 2.1944