

Machine Learning HW1

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1. Bayesian Linear Regression

(1)

Q: Why we need the basis function $\phi(x)$ for linear regression? And what is the benefit for applying basis function over linear regression? (5%)

A:

x 代表所有的feature集合，basis function $\phi(x)$ 可以針對要 train 的 feature 作 preprocessing，以及做 scaling，把每個 feature scale 在 0 到 1 之間。

(2)

Q: Prove that the predictive distribution just mentioned is the same with the form

$$p(t|x, X, T) = N(T|m(x), s^2(x))$$

Where

$$m(x) = \beta \phi(x)^T S \sum_{n=1}^N \phi(x_n) t_n \quad s^2(x) = \beta^{-1} + \phi(x)^T S \phi(x).$$

Here, the matrix S^{-1} is given by $S^{-1} = \alpha I + \beta \sum_{n=1}^N \phi(x_n) \phi(x_n)^T$ (15%)

A:

$$p(t|x, X, T) = \int_{-\infty}^{\infty} p(t, w|x, X, T) dw$$

Weight is given

$$= \int_{-\infty}^{\infty} p(t|w, x, X, T) p(w|x, X, T) dw$$

Target t and Training data X, T are unrelated, Weight w and testing data x also unrelated,

$$= \int_{-\infty}^{\infty} p(t|w, x) p(w|X, T) dw$$

$$p(w|X, T) = p(T|X, w) p(w)$$

$$= \int_{-\infty}^{\infty} p(t|w, x) p(T|X, w) p(w) dw$$

$$p(t|w, x) = N(t|y(w, x), \beta^{-1}I), \quad p(T|X, w) = N(T|y(X, w), \beta^{-1}I), \quad p(w) = N(w|0, \alpha^{-1}I)$$

$$= \int_{-\infty}^{\infty} N(t|w^T \phi(x), \beta^{-1}I) N(T|y(X, w), \beta^{-1}I) N(w|0, \alpha^{-1}I) dw$$

$$= N(t|\beta \phi(x)^T S \sum_{n=1}^N \phi(x_n) t_n, \beta^{-1} + \phi(x)^T S \phi(x)) \quad Q.E.D$$

(3)

Q: Could we use linear regression function for classification? Why or why not? Explain it! (10%)

A:

可以，我們可以在model的output加一個 Sigmoid Function，把輸出控制在0到1，0到0.5是一個class，0.5到1是另一個class，就可以做分類了。

2. Feature Select

(a)

Q: In the feature selection stage, please apply polynomials of order $M = 1$ and $M = 2$ over the dimension $D = 7$ input data. Please evaluate the corresponding RMS error on the training set (15%) Code Result

A:

In $M=1$, Root Mean Square (RMS) Error is 0.0595042

```
n [50]: # Gradient Descent M=1
# ydata = b + w*xdata
b = 0.0
w = np.ones(7)
lr = 1
epoch = 20000
b_lr = 0.0
w_lr = np.zeros(7)

n [51]: for e in range(epoch):
# Calculate the value of the loss function
error = Y - b - np.dot(x_data, w) #shape: (500,)
loss = np.mean(np.square(error)) # Mean Square Error

# Calculate gradient
b_grad = -2*np.sum(error)*1 #shape: ()
w_grad = -2*np.dot(error, x_data) #shape: (7,)

# update learning rate
b_lr = b_lr + b_grad**2
w_lr = w_lr + w_grad**2

# update parameters.
b = b - lr/np.sqrt(b_lr) * b_grad
w = w - lr/np.sqrt(w_lr) * w_grad

# Print "Root Mean Square Error" per 1000 epoch
if (e+1) % 1000 == 0:
    print('epoch:{}\n Loss:{}'.format(e+1, np.sqrt(loss)))

epoch:2000
Loss:0.0595042087913924
epoch:4000
Loss:0.05950420877764978
epoch:6000
Loss:0.05950420877764953
epoch:8000
Loss:0.05950420877764953
epoch:10000
Loss:0.05950420877764953
epoch:12000
Loss:0.05950420877764953
epoch:14000
Loss:0.05950420877764953
epoch:16000
Loss:0.05950420877764953
epoch:18000
Loss:0.05950420877764953
epoch:20000
Loss:0.05950420877764953
```

In M=2, Root Mean Square (RMS) Error is 0.0590381

```
In [55]: # Gradient Descent M=2
# ydata = b + w2*xdata + w1*xdata^2
b = 0.0
w1 = np.ones(7)
w2 = np.ones(7)
lr = 1
epoch = 20000
b_lr = 0.0
w1_lr = np.zeros(7)
w2_lr = np.zeros(7)

In [57]: for e in range(epoch):
# Calculate the value of the loss function
x_data_square = np.square(x_data) #shape: (500,7)
error = Y - b - np.dot(x_data, w2) - np.dot(x_data_square, w1) #shape: (500,)
loss = np.mean(np.square(error)) # Mean Square Error

# Calculate gradient
b_grad = -2*np.sum(error)*1 #shape: ()
w1_grad = -2*np.dot(error, x_data_square) #shape: (7,)
w2_grad = -2*np.dot(error, x_data) #shape: (7,)

# update learning rate
b_lr = b_lr + b_grad**2
w1_lr = w1_lr + w1_grad**2
w2_lr = w2_lr + w2_grad**2

# update parameters.
b = b - lr/np.sqrt(b_lr) * b_grad
w1 = w1 - lr/np.sqrt(w1_lr) * w1_grad
w2 = w2 - lr/np.sqrt(w2_lr) * w2_grad

# Print "Root Mean Square Error" per 1000 epoch
if (e+1) % 2000 == 0:
    print('epoch:{}\n Loss:{}'.format(e+1, np.sqrt(loss)))

epoch:2000
Loss:0.059039211771226806
epoch:4000
Loss:0.05903883567163798
epoch:6000
Loss:0.05903859268360228
epoch:8000
Loss:0.059038435591609636
epoch:10000
Loss:0.05903833399516438
epoch:12000
Loss:0.059038268276338304
epoch:14000
Loss:0.05903822576043161
epoch:16000
Loss:0.05903819825341032
epoch:18000
Loss:0.05903818045607411
epoch:20000
Loss:0.05903816894066609
```

(b)

Q: How will you analysis the weights of polynomial model $M = 1$ and select the most contributive feature? Code Result, Explain (10%)

A:

In $M=1$ model, $y = w*x_data + b$, Loss function = $Y - b - w*x$

跟據我的 gradient descent 跑出來的結果, 在 epoch=20000 時, 此時的 weight

weight = [0.0929, 0.0778, 0.0238, 0.0063, 0.0674, 0.3694, 0.0243]

X_data = [GRE, TOEFL, University ranking, SOP, LOR, CGPA, Research]

可以看出 CGPA 這個 feature 對於 school admission 最具有影響, 所以 CGPA is the most contributive feature.

Code Result:

```
In [58]: for e in range(epoch):
# Calculate the value of the loss function
error = Y - b - np.dot(x_data, w) #shape: (500,)
loss = np.mean(np.square(error)) # Mean Square Error

# Calculate gradient
b_grad = -2*np.sum(error)*1 #shape: ()
w_grad = -2*np.dot(error, x_data) #shape: (7,)

# update learning rate
b_lr = b_lr + b_grad**2
w_lr = w_lr + w_grad**2

# update parameters.
b = b - lr/np.sqrt(b_lr) * b_grad
w = w - lr/np.sqrt(w_lr) * w_grad

# Print "Root Mean Square Error" per 2000 epoch
if (e+1) % 2000 == 0:
    print('epoch:{}\n Loss:{}'.format(e+1, np.sqrt(loss)))
print("w: ",w)
print("b: ",b)

epoch:2000
Loss:0.05950420879343555
epoch:4000
Loss:0.059504208777649815
epoch:6000
Loss:0.05950420877764953
epoch:8000
Loss:0.05950420877764953
epoch:10000
Loss:0.05950420877764953
epoch:12000
Loss:0.05950420877764953
epoch:14000
Loss:0.05950420877764953
epoch:16000
Loss:0.05950420877764953
epoch:18000
Loss:0.05950420877764953
epoch:20000
Loss:0.05950420877764953
w: [0.09292532 0.07778323 0.02376547 0.00634455 0.06743497 0.36936137
0.02430748]
b: 0.3482198690275523
```

3. Maximum Likelihood Approach

(a)

Q: Which basis function will you use to further improve your regression model, Polynomial, Gaussian, Sigmoidal, or hybrid? Explain (5%)

A:

我的 Linear Regression Model 採用的是二次 Polynomial Function, 因為我使用 Gradient Descent去最佳化我的 loss function, 所以不需要Gaussian跟Sigmoidal。

(b)

Q: Introduce the basis function you just decided in (a) to linear regression model and analyze the result you get. (Hint: You might want to discuss about the phenomenon when model becomes too complex.) Code Result, Explain (10%)

A:

我採用了 Polynomial Function 一次函數跟二次函數兩種方法，

一次式： $y = w * x_data + b$ ，二次式： $y = w1 * x_data^2 + w2 * x_data + b$

$x_data = (500, 7)$ 500個人, 7個feature, $w = (7,)$ 每個feature的weight, $b =$ 常數

定義了loss function = $y - w * x_data - b$ 和

loss function = $y - w1 * x_data^2 - w2 * x_data - b$

用Gradient descent去最佳化loss function, 當Gradient越大, learning rate就越大, 下降越快, 當Gradient越小, learning rate就越小, 下降越慢, 越來越逼近最佳解

最後得到的結論是使用二次式： $y = w1 * x_data^2 + w2 * x_data + b$ 所得到的RMS Error會比較使用一次式還要小。

使用Gradient descent最佳化不能用在三次以上或更複雜的Model, 因為Gradient descent有可能找到函數的Local Minimum，這時候就不會是最佳解。

Code Result:

一次式： $y = w * x_data + b$

```
n [50]: # Gradient Descent M=1
# ydata = b + w*xdata
b = 0.0
w = np.ones(7)
lr = 1
epoch = 20000
b_lr = 0.0
w_lr = np.zeros(7)

n [51]: for e in range(epoch):
# Calculate the value of the loss function
error = Y - b - np.dot(x_data, w) #shape: (500,)
loss = np.mean(np.square(error)) # Mean Square Error

# Calculate gradient
b_grad = -2*np.sum(error)*1 #shape: ()
w_grad = -2*np.dot(error, x_data) #shape: (7,)

# update learning rate
b_lr = b_lr + b_grad**2
w_lr = w_lr + w_grad**2

# update parameters.
b = b - lr/np.sqrt(b_lr) * b_grad
w = w - lr/np.sqrt(w_lr) * w_grad

# Print "Root Mean Square Error" per 1000 epoch
if (e+1) % 1000 == 0:
    print('epoch:{}\n Loss:{}'.format(e+1, np.sqrt(loss)))

epoch:2000
Loss:0.0595042087913924
epoch:4000
Loss:0.05950420877764978
epoch:6000
Loss:0.05950420877764953
epoch:8000
Loss:0.05950420877764953
epoch:10000
Loss:0.05950420877764953
epoch:12000
Loss:0.05950420877764953
epoch:14000
Loss:0.05950420877764953
epoch:16000
Loss:0.05950420877764953
epoch:18000
Loss:0.05950420877764953
epoch:20000
Loss:0.05950420877764953
```

二次式 : $y = w1 \cdot x_data^2 + w2 \cdot x_data + b$

```
In [55]: # Gradient Descent M=2
# ydata = b + w2*xdata + w1*xdata^2
b = 0.0
w1 = np.ones(7)
w2 = np.ones(7)
lr = 1
epoch = 20000
b_lr = 0.0
w1_lr = np.zeros(7)
w2_lr = np.zeros(7)

In [57]: for e in range(epoch):
# Calculate the value of the loss function
x_data_square = np.square(x_data) #shape: (500,7)
error = Y - b - np.dot(x_data, w2) - np.dot(x_data_square, w1) #shape: (500,)
loss = np.mean(np.square(error)) # Mean Square Error

# Calculate gradient
b_grad = -2*np.sum(error)*1 #shape: ()
w1_grad = -2*np.dot(error, x_data_square) #shape: (7,)
w2_grad = -2*np.dot(error, x_data) #shape: (7,)

# update learning rate
b_lr = b_lr + b_grad**2
w1_lr = w1_lr + w1_grad**2
w2_lr = w2_lr + w2_grad**2

# update parameters.
b = b - lr/np.sqrt(b_lr) * b_grad
w1 = w1 - lr/np.sqrt(w1_lr) * w1_grad
w2 = w2 - lr/np.sqrt(w2_lr) * w2_grad

# Print "Root Mean Square Error" per 1000 epoch
if (e+1) % 2000 == 0:
    print('epoch:{}\n Loss:{}'.format(e+1, np.sqrt(loss)))

epoch:2000
Loss:0.059039211771226806
epoch:4000
Loss:0.05903883567163798
epoch:6000
Loss:0.05903859268360228
epoch:8000
Loss:0.059038435591609636
epoch:10000
Loss:0.05903833399516438
epoch:12000
Loss:0.059038268276338304
epoch:14000
Loss:0.05903822576043161
epoch:16000
Loss:0.05903819825341032
epoch:18000
Loss:0.05903818045607411
epoch:20000
Loss:0.05903816894066609
```

(c)

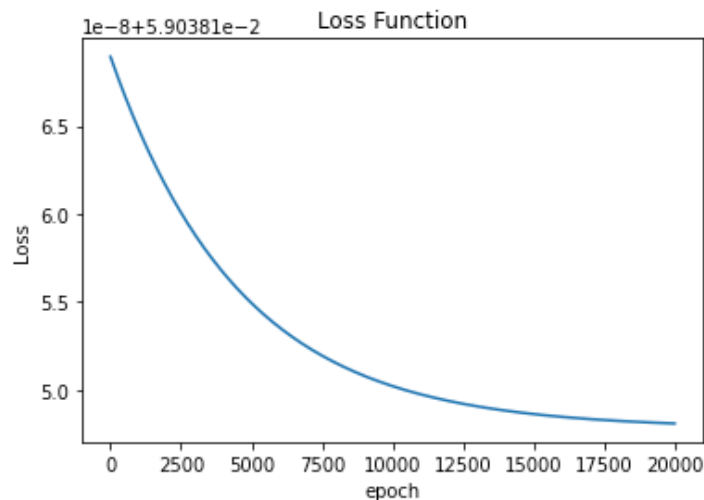
Q: Apply N-fold cross-validation in your training stage to select at least one hyperparameter(order, parameter number, ...) for model and do some discussion(underfitting, overfitting). Code Result, Explain (10%)

A:

從下圖可以看到，隨著epoch次數增加，loss 慢慢地收斂，loss越大收斂較快，loss越小時收斂越較慢，既沒有overfitting，也沒有underfitting。

Code Result:

```
In [32]: plt.plot(plt_epoch, plt_loss)
plt.title('Loss Function')
plt.ylabel('Loss')
plt.xlabel('epoch')
plt.show()
```



4. Maximum A Posterior Approach

(a)

Q: What is the key difference between maximum likelihood approach and maximum a posterior approach? Explain (5%)

A:

Maximum Likelihood 認為所有 θ 出現的機率是均等的，只考慮當下的機率，所以會把「這一次的實驗」所算出來的機率當作這整個事件的機率。

Maximum A Posterior 會先算出 θ 出現的機率，包括 θ 怎麼來的，手中先握著一個先驗機率 (Prior Probability)，再透過不斷觀察新的實驗來更新手上的機率。

(b)

Q: Use Maximum a posterior approach method to retest the model in 2 you designed. You could choose Gaussian distribution as a prior. Code Result (10%)

A:

```
In [175]: #calculate MAP theta
hypothesis = np.linspace(0, 1, 101)
theta_hat_1 = hypothesis[np.argmax(w1)]
theta_hat_2 = hypothesis[np.argmax(w2)]
print(theta_hat_1, theta_hat_2)

0.02 0.05

In [176]: # Gradient Descent M=2 for Maximum a posterior approach
# ydata = b + w2*xdata + w1*xdata^2
b = 0.0
w1 = np.ones(7)
w2 = np.ones(7)
lr = 1
epoch = 20000
b_lr = 0.0
w1_lr = np.zeros(7)
w2_lr = np.zeros(7)

In [180]: pltmap_loss = []
pltmap_epoch = []
for e in range(epoch):
    # Calculate the value of the loss function
    x_data_square = np.square(x_data) #shape: (500,7)
    error = Y - b - theta_hat_1*np.dot(x_data, w2) - theta_hat_2*np.dot(x_data_square, w1)
    loss = np.mean(np.square(error)) # Mean Square Error

    # Calculate gradient
    b_grad = -2*np.sum(error)*1 #shape: ()
    w1_grad = -2*np.dot(error, x_data_square) #shape: (7,)
    w2_grad = -2*np.dot(error, x_data) #shape: (7,)

    # update learning rate
    b_lr = b_lr + b_grad**2
    w1_lr = w1_lr + w1_grad**2
    w2_lr = w2_lr + w2_grad**2

    # update parameters.
    b = b - lr/np.sqrt(b_lr) * b_grad
    w1 = w1 - lr/np.sqrt(w1_lr) * w1_grad
    w2 = w2 - lr/np.sqrt(w2_lr) * w2_grad

    pltmap_loss.append(np.sqrt(loss))
    pltmap_epoch.append(e)
    # Print "Root Mean Square Error" per 2000 epoch
    if (e+1) % 2000 == 0:
        print('epoch:{}\n MAP Loss:{}'.format(e+1, np.sqrt(loss)))
```

```
epoch:2000
MAP Loss:0.059299922504985496
epoch:4000
MAP Loss:0.05927349890374746
epoch:6000
MAP Loss:0.05925087590137326
epoch:8000
MAP Loss:0.05923119619268617
epoch:10000
MAP Loss:0.059213856288005434
epoch:12000
MAP Loss:0.05919842368600604
epoch:14000
MAP Loss:0.05918458189042279
epoch:16000
MAP Loss:0.05917209379455025
epoch:18000
MAP Loss:0.05916077722045926
epoch:20000
MAP Loss:0.059150488517141976
```


(c)

Q: Compare the result between maximum likelihood approach and maximum a posterior approach. Is it consistent with your conclusion in (a)? Explain (5%)

A:

根據我的計算結果

maximum likelihood MSE error = 0.0590381

maximum a posterior MSE error = 0.05915

兩者的Error 差不多，使用Maximum Likelihood 較佳一點