Machine Learning

Answer Sheet for Homework 3

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Problem 1

Set $\sigma = 0.1$ and d = 8, then we can rewrite the formula to be

$$\mathbb{E}_{\mathcal{D}}\left[E_{\text{in}}\left(\mathbf{w}_{\text{lin}}\right)\right] = 0.01 \left(1 - \frac{9}{N}\right) > 0.008 \Rightarrow 0.2 > \frac{9}{N} \Rightarrow N > 45 \Rightarrow N \ge 46 \tag{1}$$

Problem 2

- (a) \mathbf{H} is positive semi-definite \Leftrightarrow All eigenvalues is non-negative. Refer to choice (c), we have shown the properties.
- (b) Refer to (e), \mathbf{H} is idempotent matrix. Suppose \mathbf{H}^{-1} exists, we have

$$\mathbf{H}^{-1}\left(\mathbf{H}^{2}\right) = \mathbf{H}^{-1}\left(\mathbf{H}\right) \Rightarrow \mathbf{H} = \mathbf{I} \tag{2}$$

Hence, **H** is invertible if and only if $\mathbf{H} = \mathbf{I}$. Hence, **H** is not always invertible.

(c) Refer to choice (e), we have $\mathbf{H}^2 = \mathbf{H}$. Suppose λ is the eigenvalue of some non-zero vector \vec{v} ,

$$\mathbf{H}\vec{v} = \lambda \vec{v} = \mathbf{H}^2 \vec{v} = \mathbf{H} (\lambda \vec{v}) = \lambda (\mathbf{H}\vec{v}) = \lambda^2 \vec{v} \Rightarrow \lambda^2 = \lambda$$
 (3)

Hence, the possible results of λ is 1 or 0.

(d) For a symmetric and idempotent matrix \mathbf{H} , rank $(\mathbf{H}) = \operatorname{trace}(\mathbf{H})$, the number of non-zero eigenvalues of \mathbf{H} .

$$\operatorname{trace}\left(\mathbf{H}\right) = \operatorname{trace}\left(\mathbf{X}\left(\mathbf{X}^{T}\mathbf{X}\right)^{-1}\mathbf{X}^{T}\right) = \operatorname{trace}\left(\left(\mathbf{X}^{T}\mathbf{X}\right)^{-1}\mathbf{X}^{T}\mathbf{X}\right) \tag{4}$$

$$=\operatorname{trace}\left(\mathbf{I}_{d+1}\right)=d+1\tag{5}$$

where we have used trace $(\mathbf{AB}) = \operatorname{trace}(\mathbf{BA})$.

Since eigenvalue can only be 0 or 1, so there are d+1 eigenvalues of 1.

(e) By the definition of \mathbf{H} , we have

$$\mathbf{H}^{2} = \left(\mathbf{X} \left(\mathbf{X}^{T} \mathbf{X}\right)^{-1} \mathbf{X}^{T}\right) \left(\mathbf{X} \left(\mathbf{X}^{T} \mathbf{X}\right)^{-1} \mathbf{X}^{T}\right)$$
(6)

$$= \mathbf{X} \left(\mathbf{X}^{T} \mathbf{X} \right)^{-1} \left(\left(\mathbf{X}^{T} \mathbf{X} \right) \left(\mathbf{X}^{T} \mathbf{X} \right)^{-1} \right) \mathbf{X}^{T}$$
 (7)

$$= \mathbf{X} \left(\mathbf{X}^T \mathbf{X} \right)^{-1} \mathbf{X}^T = \mathbf{H} \tag{8}$$

So

$$\mathbf{H}^2 = \mathbf{H} \Rightarrow \mathbf{H}^{1126} = \mathbf{H} \tag{9}$$

Problem 3

If sign $(\mathbf{w}^T \mathbf{x}) \neq y$, then $y \mathbf{w}^T \mathbf{x} < 0$ since the sign of y and $\mathbf{w}^T \mathbf{x}$ are different. Similarly, if sign $(\mathbf{w}^T \mathbf{x}) = y$, then $y \mathbf{w}^T \mathbf{x} \geq 0$.

Claim: $(\max(0, 1 - y\mathbf{w}^T\mathbf{x}))^2$ is an upper bound.

Proof of claim:

Consider the following cases.

- 1. $\left[\operatorname{sign}\left(\mathbf{w}^{T}\mathbf{x}\right) \neq y\right] = 0$ Then $y\mathbf{w}^{T}\mathbf{x} \geq 0$. Hence $\left(\max\left(0, 1 - y\mathbf{w}^{T}\mathbf{x}\right)\right)^{2} \geq 0$, which bounds $\left[\operatorname{sign}\left(\mathbf{w}^{T}\mathbf{x}\right) \neq y\right]$.
- 2. $\left[\operatorname{sign}\left(\mathbf{w}^{T}\mathbf{x}\right) \neq y\right] = 1$ Then $y\mathbf{w}^{T}\mathbf{x} < 0$. Hence $\left(\max\left(0, 1 - y\mathbf{w}^{T}\mathbf{x}\right)\right)^{2} = \left(1 - y\mathbf{w}^{T}\mathbf{x}\right)^{2} > 1$, which bounds $\left[\operatorname{sign}\left(\mathbf{w}^{T}\mathbf{x}\right) \neq y\right]$.

Set $y\mathbf{w}^T\mathbf{x} := z$. Consider $\max\left(0, -y\mathbf{w}^T\mathbf{x}\right) = \max\left(0, -z\right) := f\left(z\right)$. We have $f\left(z\right) = -z$ if $z \le 0$, else $f\left(z\right) = 0$. So

$$\lim_{z \to 0^{-}} \frac{f(z) - f(0)}{z - 0} = \frac{-z - 0}{z - 0} = -1, \quad \lim_{z \to 0^{+}} \frac{f(z) - f(0)}{z - 0} = \frac{0 - 0}{z - 0} = 0 \tag{10}$$

Hence, f(z) is not differentiable at z = 0.

Problem 5

<u>Calim</u>: $\max (0, -y\mathbf{w}^T\mathbf{x})$ results in PLA.

Proof of claim:

Consider following cases.

1. $y = \text{sign}(\mathbf{w}^T \mathbf{x})$. PLA update term is 0.

Then we have $y\mathbf{w}^T\mathbf{x} > 0$. So

$$\max\left(0, -y\mathbf{w}^T\mathbf{x}\right) = 0\tag{11}$$

2. $y \neq \text{sign}(\mathbf{w}^T \mathbf{x})$. PLA update term is $y\mathbf{x}$.

Then we have $y\mathbf{w}^T\mathbf{x} < 0$. So

$$\max(0, -y\mathbf{w}^T\mathbf{x}) = -y\mathbf{w}^T\mathbf{x} \Rightarrow -\nabla_{\mathbf{w}}\max(0, -y\mathbf{w}^T\mathbf{x}) = y\mathbf{x}$$
 (12)

Problem 6

$$\nabla E(0,0) = \left. \left(\frac{\partial E}{\partial u}, \frac{\partial E}{\partial v} \right) \right|_{(0,0)} \tag{13}$$

$$= \left(e^{u} + ve^{uv} + 2u - 2v - 3, 2e^{2v} + ue^{uv} - 2u + 4v - 2\right)\Big|_{(0,0)}$$
 (14)

$$= (-2,0) \tag{15}$$

I write a program Q07.py to calculate the result by using

$$(u_{t+1}, v_{t+1}) = (u_t, v_t) - 0.01\nabla E(u_t, v_t)$$
(16)

iteratively.

$$(u_1, v_1) = (0, 0) - 0.01 \nabla E(0, 0) = (0.02, 0)$$
(17)

$$(u_2, v_2) = (0.02, 0) - 0.01 \nabla E(0.02, 0) \approx (0.039398, 0.0002)$$
 (18)

$$(u_3, v_3) \approx (0.039398, 0.0002) - 0.01\nabla E(0.039398, 0.0002)$$
 (19)

$$\approx (0.0582102, 0.000577975) \tag{20}$$

$$(u_4, v_4) \approx (0.0764524, 0.00111381) \tag{21}$$

$$(u_5, v_5) \approx (0.09414, 0.00178911)$$
 (22)

$$E\left(u_5, v_5\right) \approx 2.825\tag{23}$$

Problem 8

$$\nabla E(0,0) = \left(\frac{\partial E}{\partial u}, \frac{\partial E}{\partial v}\right) \tag{24}$$

$$= (e^{u} + ve^{uv} + 2u - 2v - 3, 2e^{2v} + ue^{uv} - 2u + 4v - 2)$$
(25)

From this we compute the Hessian matrix

$$\nabla^{2}E(u,v) = \begin{pmatrix} e^{u} + v^{2}e^{uv} + 2 & (uv+1)e^{uv} - 2\\ (uv+1)e^{uv} - 2 & 4e^{2v} + u^{2}e^{uv} + 4 \end{pmatrix}$$
 (26)

So

$$\hat{E}(\Delta u, \Delta v) = E(0, 0) + \nabla E(0, 0) \cdot (\Delta u, \Delta v) + \frac{1}{2}(\Delta u, \Delta v) \nabla^{2} E(0, 0) \begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix}$$
(27)

$$= 3 - 2\Delta u + \frac{1}{2} (\Delta u, \Delta v) \begin{pmatrix} 3 & -1 \\ -1 & 8 \end{pmatrix} \begin{pmatrix} \Delta u \\ \Delta v \end{pmatrix}$$
 (28)

$$= \frac{3}{2} (\Delta u)^{2} + 4 (\Delta v)^{2} - \Delta u \Delta v - 2\Delta u + 0\Delta v + 3$$
 (29)

Claim: $-(\nabla^2 E(u,v))^{-1} \nabla E(u,v)$ is the Newton direction.

Proof of claim:

$$\frac{\partial \hat{E}\left(\Delta u, \Delta v\right)}{\partial \left(\Delta u, \Delta v\right)} = \nabla E\left(u, v\right) + \nabla^{2} E\left(u, v\right) \left(\Delta u, \Delta v\right) = 0 \tag{30}$$

$$\Rightarrow (\Delta u, \Delta v) = -\left(\nabla^2 E(u, v)\right)^{-1} \nabla E(u, v) \tag{31}$$

Problem 10

I write a program Q10.py to calculate the result by using

$$(u_{t+1}, v_{t+1}) = (u_t, v_t) - (\nabla^2 E(u_t, v_t))^{-1} \nabla E(u_t, v_t)$$
(32)

iteratively.

$$(u_1, v_1) \approx (0.695652173913, 0.0869565217391)$$
 (33)

$$(u_2, v_2) \approx (0.613762221112, 0.0711078990173)$$
 (34)

$$(u_3, v_3) \approx (0.611812859879, 0.0705000613365)$$
 (35)

$$(u_4, v_4) \approx (0.611811717261, 0.0704995471019)$$
 (36)

$$(u_5, v_5) \approx (0.61181171726, 0.0704995471016)$$
 (37)

$$E(u_5, v_5) \approx 2.36082334564 \tag{38}$$

This equals to the value of Problem 7 after 746 updates.

Problem 11

Write a program Q11.py to test, $\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_5, \mathbf{x}_6\}$ is the biggest subset that can be shattered by the union of quadratic, linear, or constant hypotheses of \mathbf{x} by feature form of

$$\Phi(\mathbf{x}) = (1, x_1, x_2, x_1^2, x_1 x_2, x_2^2) \tag{39}$$

Then I ran the PLA and all cases of $\{+1, -1\}^6$ are stasified. The w for $2^6 = 64$ cases are

```
[0,0,0,0,0,0]
                         [0, 1, 0, 1, 0, -4]
                                                   [1,0,1,-2,-1,-1],
                                                                              [2,0,0,0,0,-2],
                                                   [1, -1, 2, -1, -2, 0],
[-1, -2, 0, 0, -2, 0]
                         [0,0,1,2,-1,-3]
                                                                              [2,-1,1,1,-1,-3],
                         [0,0,-3,2,3,-3],
                                                   [1, -1, -2, -1, 2, 0],
                                                                               [2,0,-2,0,2,-2],
[0,0,-2,0,2,0],
                         [0, -2, -1, 4, 1, -3]
                                                   [1, -2, -1, 0, 1, 1],
                                                                              [3, -2, 0, 2, 0, -4],
[-1, -4, 0, 0, 0, 0]
[-1, 1, 0, -1, -2, 0],
                         [0, 2, 0, 0, -2, 0],
                                                   [1, 1, -2, -3, -2, 0],
                                                                              [1, 1, -1, -1, -3, -1],
                         [0, 1, 0, 1, -4, 0],
                                                   [1, -1, 1, -1, -3, 1],
                                                                               [1,0,0,0,-4,0],
[-1, 0, 1, 0, -3, 1],
[0,0,-3,0,1,1],
                         [0, 1, -4, 1, 0, 0],
                                                   [1, -1, -3, -1, 1, 1]
                                                                               [1,0,-4,0,0,0],
                                                   [1, -1, -1, -1, -1, 1],
[0, -1, -2, 1, 0, 2],
                         [0,0,-3,2,-1,1],
                                                                              [1, -1, -3, 1, -1, 1],
[0,0,2,0,2,0],
                         [0, 2, 3, 0, 1, -1],
                                                   [1,0,3,-2,1,-1],
                                                                              [1, 1, 3, -1, 1, -1],
                                                   [1, -1, 4, -1, 0, 0],
[-1, 0, 4, 0, 0, 0],
                         [0, 1, 4, 1, 0, 0]
                                                                               [1, 0, 4, 0, 0, 0]
[0,0,0,0,4,0]
                         [0, 1, 0, 1, 4, 0],
                                                   [1, -1, 0, -1, 4, 0],
                                                                               [1,0,0,0,4,0],
                                                   [1, -2, 1, 0, 3, 1],
[0,-1,1,1,3,1],
                         [0,0,1,2,3,1],
                                                                              [1, -1, 1, 1, 3, 1]
                                                   [1, 2, 1, -4, -1, 3],
[-2, 2, 0, -2, 0, 4],
                         [0,4,0,0,0,0]
                                                                              [2,4,0,0,0,0]
[-1, 0, 2, 0, -2, 2],
                         [0, 1, 3, 1, -1, 1],
                                                   [1,0,3,-2,-3,3],
                                                                              [1, 1, 3, 1, -1, 1]
                                                   [1,0,-1,-2,1,3],
[-1, 1, -1, -1, 1, 3],
                         [0,3,-1,1,1,1]
                                                                              [1, 2, 0, 0, 2, 0],
                                                   [1, -1, 0, -1, 0, 4]
[-1, 0, 0, 0, 0, 2],
                         [0, 1, 1, 1, 1, 1]
                                                                              [1, 1, 1, 1, 1, 1]
                                                                                             (40)
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Problem 12

By the transform, we have $(\Phi(\mathbf{x}))_i = z_i = (0, \dots, \underbrace{1}_{i\text{-th term}}, \dots, 0)$. To shatter the original

N points, we can assign w_i to be positive or negative to get $\mathbf{x}_i \circ \text{or } \times$.

So, this transform shatter any N points. Hence $d_{vc}(\mathcal{H}_{\Phi}) = \infty$.

The average $E_{\rm in}$ is 0.503979.

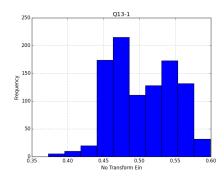


Figure 1: Q13 histogram

After feature transform, we have

$$\tilde{\mathbf{w}} = \left[-0.991720295, -3.00273423 \times 10^{-4}, -1.31851902 \times 10^{-3}, \right.$$

$$\left. 1.09524038 \times 10^{-3}, 1.55703088, 1.55594342 \right]$$

$$(41)$$

with new average $E_{\rm in}=0.124126.$

Problem 14

The average $\tilde{\mathbf{w}}_3 = 0.06306984$.

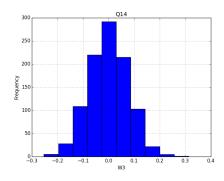


Figure 2: Q14 histogram

The average $E_{\text{out}} = 0.126195$.

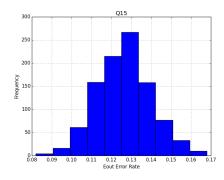


Figure 3: Q15 histogram

Problem 16

Sum the minimized negative log likelihood h_y , which is $\min_y (-\ln{(h_y)})$, we have

$$E_{\text{in}} = \frac{1}{N} \sum_{n=1}^{N} \left(-\ln \left(\frac{\exp \left(\mathbf{w}_{y_n}^T \mathbf{x}_n \right)}{\sum_{i=1}^{K} \exp \left(\mathbf{w}_i^T \mathbf{x}_n \right)} \right) \right)$$
(42)

$$= \frac{1}{N} \sum_{n=1}^{N} \left(\ln \left(\sum_{i=1}^{K} \exp \left(\mathbf{w}_{i}^{T} \mathbf{x}_{n} \right) \right) - \mathbf{w}_{y_{n}}^{T} \mathbf{x}_{n} \right)$$
(43)

Problem 17

 $\frac{\partial E_{\text{in}}}{\partial \mathbf{w}_i} = \frac{1}{N} \sum_{i=1}^{N} \frac{\partial}{\partial \mathbf{w}_i} \left(\ln \left(\sum_{i=1}^{K} \exp \left(\mathbf{w}_i^T \mathbf{x}_n \right) \right) - \mathbf{w}_{y_n}^T \mathbf{x}_n \right)$ (44)

$$= \frac{1}{N} \sum_{n=1}^{N} \left(\frac{1}{\sum_{i=1}^{K} \exp\left(\mathbf{w}_{i}^{T} \mathbf{x}_{n}\right)} \frac{\partial}{\partial \mathbf{w}_{i}} \exp\left(\mathbf{w}_{i}^{T} \mathbf{x}_{n}\right) - \frac{\partial}{\partial \mathbf{w}_{i}} \mathbf{w}_{y_{n}}^{T} \mathbf{x}_{n} \right)$$
(45)

$$= \frac{1}{N} \sum_{n=1}^{N} \left(\frac{\exp\left(\mathbf{w}_{i}^{T} \mathbf{x}_{n}\right)}{\sum_{i=1}^{K} \exp\left(\mathbf{w}_{i}^{T} \mathbf{x}_{n}\right)} \mathbf{x}_{n} - \left[y_{n} = i \right] \mathbf{x}_{n} \right)$$

$$(46)$$

$$= \frac{1}{N} \sum_{n=1}^{N} \left(h_i \left(\mathbf{x}_n \right) - \left[\left[y_n = i \right] \right] \right) \mathbf{x}_n \tag{47}$$

The $E_{\rm out} = 0.475$ with

$$\tilde{\mathbf{w}} = \begin{bmatrix} 0.01878417, -0.01260595, 0.04084862, -0.03266317, 0.01502334, \\ -0.03667437, 0.01255934, 0.04815065, -0.02206419, 0.02479605, \\ 0.06899284, 0.0193719, -0.01988549, -0.0087049, 0.04605863, \\ 0.05793382, 0.061218, -0.04720391, 0.06070375, -0.01610907, -0.03484607 \end{bmatrix}$$

Problem 19

The $E_{\text{out}} = 0.220$ with

$$\tilde{\mathbf{w}} = \begin{bmatrix} -0.00385379, -0.18914564, 0.26625908, -0.35356593, 0.04088776, \\ -0.3794296, 0.01982783, 0.33391527, -0.26386754, 0.13489328, \\ 0.4914191, 0.08726107, -0.25537728, -0.16291797, 0.30073678, \\ 0.40014954, 0.43218808, -0.46227968, 0.43230193, -0.20786372, -0.36936337 \end{bmatrix}$$

Problem 20

The $E_{\rm out} = 0.473$ with

$$\tilde{\mathbf{w}} = [0.01826899, -0.01308051, 0.04072894, -0.03295698, 0.01498363, \\ -0.03691042, 0.01232819, 0.04791334, -0.02244958, 0.02470544, \\ 0.06878235, 0.01897378, -0.02032107, -0.00901469, 0.04589259, \\ 0.05776824, 0.06102487, -0.04756147, 0.06035018, -0.01660574, -0.03509342]$$

$$\mathbf{h}^{T}\mathbf{y} = \sum_{i=1}^{N} h\left(\mathbf{x}_{i}\right) y_{i}$$
(51)

We just need two times queries to obtain $\mathbf{h}^T \mathbf{y}$.

First, take some h' such that $h'(\mathbf{x}_i) = 0$, $\forall i$. Then we have

RMSE
$$(h') = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (y_i - h'(\mathbf{x_i}))^2} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} y_i^2} \Rightarrow \sum_{i=1}^{N} y_i^2 = N (\text{RMSE}(h'))^2$$
 (52)

Second, query for some h,

RMSE
$$(h) = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (y_i - h(\mathbf{x_i}))^2}$$
 (53)

$$N \left(\text{RMSE}(h)\right)^{2} = \sum_{i=1}^{N} (y_{i} - h(\mathbf{x}_{i}))^{2} = \sum_{i=1}^{N} y_{i}^{2} - 2h(\mathbf{x}_{i}) y_{i} + h^{2}(\mathbf{x}_{i})$$
 (54)

$$\Rightarrow \mathbf{h}^{T}\mathbf{y} = -\frac{1}{2} \left(N \left(\text{RMSE} \left(h \right) - \text{RMSE} \left(h' \right) \right)^{2} - \sum_{i=1}^{N} h^{2} \left(\mathbf{x_{i}} \right) \right)$$
 (55)

where we have known the value of $\sum_{i=1}^{N} h^{2}(\mathbf{x_{i}})$ since we have already known all \mathbf{x}_{i} .

Problem 22

To find $\min_{\mathbf{w}} \text{RMSE}(H)$, we need to find $\nabla \text{RMSE}(H) = 0$.

$$\nabla \text{RMSE}(H) = 0 \Rightarrow \frac{\partial}{\partial w_k} \sum_{i=1}^{N} \left(y_i - \sum_{k=1}^{K} w_k h_k(\mathbf{x_i}) \right)^2 = 0, \forall k$$
 (56)

$$\Rightarrow 2\sum_{i=1}^{N} \left(h_k(\mathbf{x}_i) y_i - h_k(\mathbf{x}_i) \sum_{k=1}^{K} w_k h_k(\mathbf{x}_i) \right) = 0, \forall k$$
 (57)

Hence, we need to know the value of $\mathbf{h}_k^T \mathbf{y}$ for all k. Hence, follow the conclusion above, we need to query for K+1 times, where the +1 is for querying the value of $\sum_{i=1}^N y_i^2$. The derivation steps are

- 1. First, use some hypothesis h' such that $h'(\mathbf{x}_i) = 0$, $\forall i$ to get the value of $\sum_{i=1}^{N} y_i^2$.
- 2. Second, query for RMSE (h_k) , $\forall k$, costs K times query. Then we have all $\mathbf{h}_k^T \mathbf{y}$.

Hence, we have

$$\mathbf{h}_{k}^{T}\mathbf{y} - \sum_{i=1}^{N} \left(h_{k} \left(\mathbf{x}_{i} \right) \sum_{k=1}^{K} w_{k} h_{k} \left(\mathbf{x}_{i} \right) \right) = 0, \ \forall k$$
 (58)

Then we can solve the value of ${\bf w}$ to get the minimized value.

Reference

[1] Lecture Notes by Hsuan-Tien LIN, Department of Computer Science and Information Engineering, National Taiwan University, Taipei 106, Taiwan.