

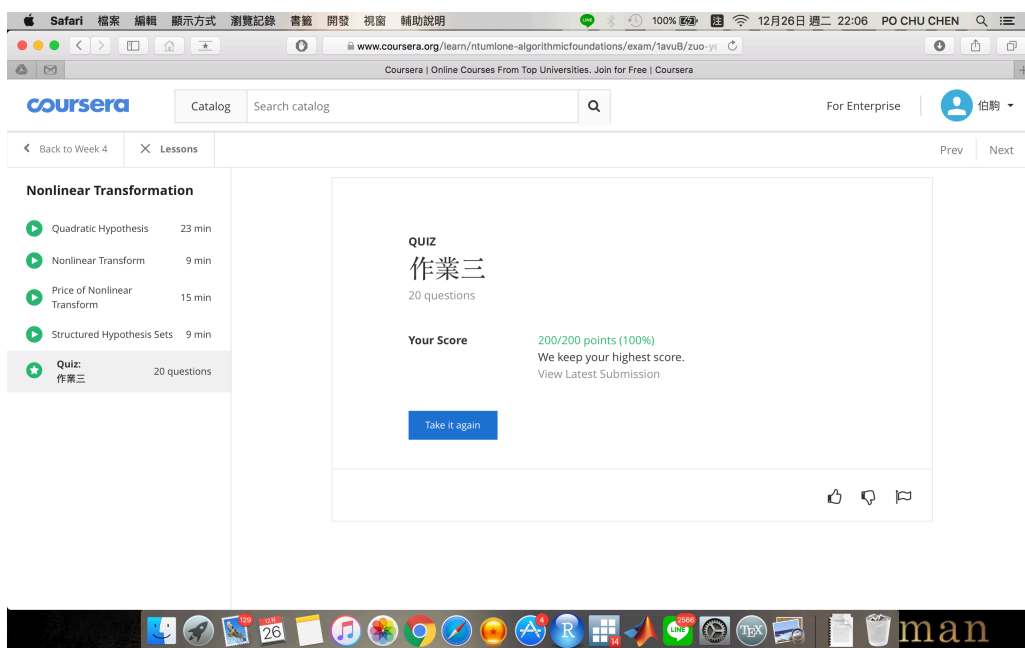
Home Work 3

Machine Learning Foundations

R04323050

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1.



2.

Claim: $(I - H)$ is idempotent. i.e $(I - H)^2 = (I - H)$, where $H = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T$

$$\begin{aligned}
H &= \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T, \quad H \cdot H = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \cdot \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \\
&= \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} (\mathbf{X}^T \mathbf{X}) (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \\
&= \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} I \mathbf{X}^T \\
&= \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T = H
\end{aligned}$$

$$\begin{aligned}
\text{Hence, } (I - H)^2 &= (I - H) \cdot (I - H) \\
&= I(I - H) - H(I - H) = I - H - H + H \cdot H \\
&= I - 2H + H = I - H
\end{aligned}$$

3.

$err(\mathbf{w}) = \max(0, -y\mathbf{w}^T \mathbf{x})$, W.L.O.G. let $y = 1$

① $\mathbf{w}^T \mathbf{x} < 0$, $err(\mathbf{w}) = -y\mathbf{w}^T \mathbf{x}$, $\nabla_{\mathbf{w}} err(\mathbf{w}) = -y\mathbf{x}$, $y \neq \text{sgn}(\mathbf{w}^T \mathbf{x})$

② $\mathbf{w}^T \mathbf{x} > 0$, $err(\mathbf{w}) = 0$, $\nabla_{\mathbf{w}} err(\mathbf{w}) = 0$, $y = \text{sgn}(\mathbf{w}^T \mathbf{x})$

Plugging the formula of SGD: $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + \eta \cdot (-\nabla_{\mathbf{w}} err(\mathbf{w}))$

Let $\eta = 1$, then $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \nabla_{\mathbf{w}} err(\mathbf{w}) = \mathbf{w}_t + \llbracket y \neq \text{sgn}(\mathbf{w}^T \mathbf{x}) \rrbracket \cdot (y\mathbf{x})$

It's obvious that the above result is a PLA iteration in P.11 of slides 11.

4.

Given $\widehat{E}_2(\Delta u, \Delta v)$ is the second-order Taylor's expansion of $E(u, v)$.

$$\widehat{E}_2(\Delta u, \Delta v) = E(u, v) + \begin{bmatrix} \frac{\partial E}{\partial u} & \frac{\partial E}{\partial v} \end{bmatrix} \begin{bmatrix} \Delta u \\ \Delta v \end{bmatrix} + \frac{1}{2} \begin{bmatrix} \Delta u & \Delta v \end{bmatrix} \begin{bmatrix} \frac{\partial^2 E}{\partial u^2} & \frac{\partial^2 E}{\partial v \partial u} \\ \frac{\partial^2 E}{\partial u \partial v} & \frac{\partial^2 E}{\partial v^2} \end{bmatrix} \begin{bmatrix} \Delta u \\ \Delta v \end{bmatrix}, \text{ where we}$$

$$\text{let } \mathbf{z} = \begin{bmatrix} \Delta u \\ \Delta v \end{bmatrix}, \quad \nabla E(u, v) = \begin{bmatrix} \frac{\partial E}{\partial u} & \frac{\partial E}{\partial v} \end{bmatrix}, \quad \nabla^2 E(u, v) = \begin{bmatrix} \frac{\partial^2 E}{\partial u^2} & \frac{\partial^2 E}{\partial v \partial u} \\ \frac{\partial^2 E}{\partial u \partial v} & \frac{\partial^2 E}{\partial v^2} \end{bmatrix}.$$

Hence, $\widehat{E}_2(\nabla u, \nabla v) = E(u, v) + \nabla E(u, v) \mathbf{z} + \frac{1}{2} \mathbf{z}^T \nabla^2 E(u, v) \mathbf{z}$

F.O.C. $\frac{\partial \widehat{E}_2}{\partial \mathbf{z}} = \nabla E(u, v) + \nabla^2 E(u, v) \mathbf{z} = 0 \Rightarrow \mathbf{z}^* = \frac{-\nabla E(u, v)}{\nabla^2 E(u, v)} = -(\nabla^2 E(u, v))^{-1} \nabla E(u, v)$

S.O.C. $\frac{\partial^2 \widehat{E}_2}{\partial \mathbf{z}^2} = \nabla^2 E(u, v)$, which is a positive definite matrix given by question. Thus, we know \mathbf{z}^* can achieve a minimum solution.

5.

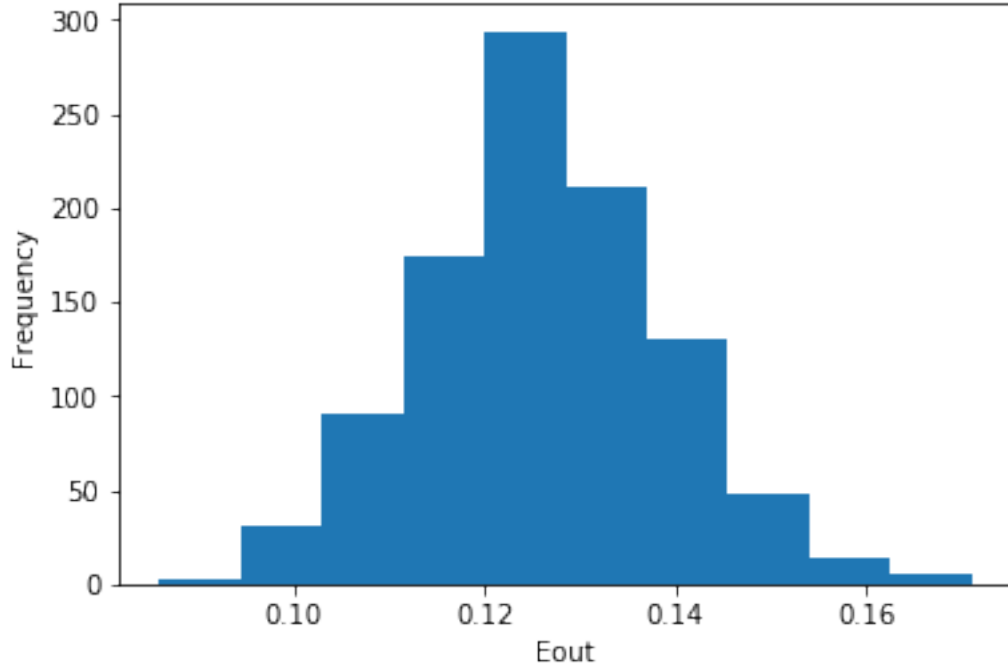
$$\begin{aligned}
\max_{\mathbf{w}} \text{likelihood}(\mathbf{w}) &\propto \prod_{n=1}^N h_y(x_n) \\
&\Leftrightarrow \max_{\mathbf{w}} \ln \prod_{n=1}^N \frac{\exp(\mathbf{w}_{y_n}^T x_n)}{\sum_{i=1}^K \exp(\mathbf{w}_i^T x_n)} = \max_{\mathbf{w}} \sum_{n=1}^N \ln \frac{\exp(\mathbf{w}_{y_n}^T x_n)}{\sum_{i=1}^K \exp(\mathbf{w}_i^T x_n)} \\
&\Leftrightarrow \min_{\mathbf{w}} \frac{1}{N} \sum_{n=1}^N -\ln \frac{\exp(\mathbf{w}_{y_n}^T x_n)}{\sum_{i=1}^K \exp(\mathbf{w}_i^T x_n)}.
\end{aligned}$$

Thus, $E_{in} = \frac{1}{N} \sum_{n=1}^N \left[\ln \left(\sum_{k=1}^K \exp(\mathbf{w}_k^T x_n) \right) - \mathbf{w}_{y_n}^T x_n \right]$

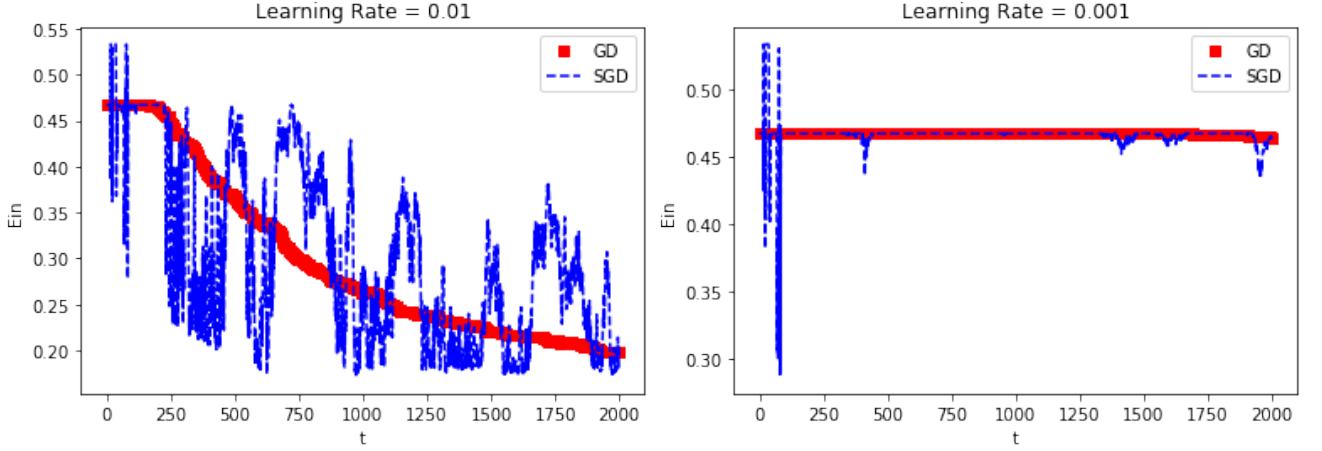
6.

$$\frac{\partial E_{in}}{\partial \mathbf{w}_i} = \frac{1}{N} \sum_{n=1}^N \left\{ \frac{\exp(\mathbf{w}_i^T x_n)}{\sum_{i=1}^K \exp(\mathbf{w}_i^T x_n)} x_n - \mathbb{I}[y_n = i] x_n \right\} = \frac{1}{N} \sum_{n=1}^N ((h_i(x_n) - \mathbb{I}[y_n = i]) x_n)$$

7.

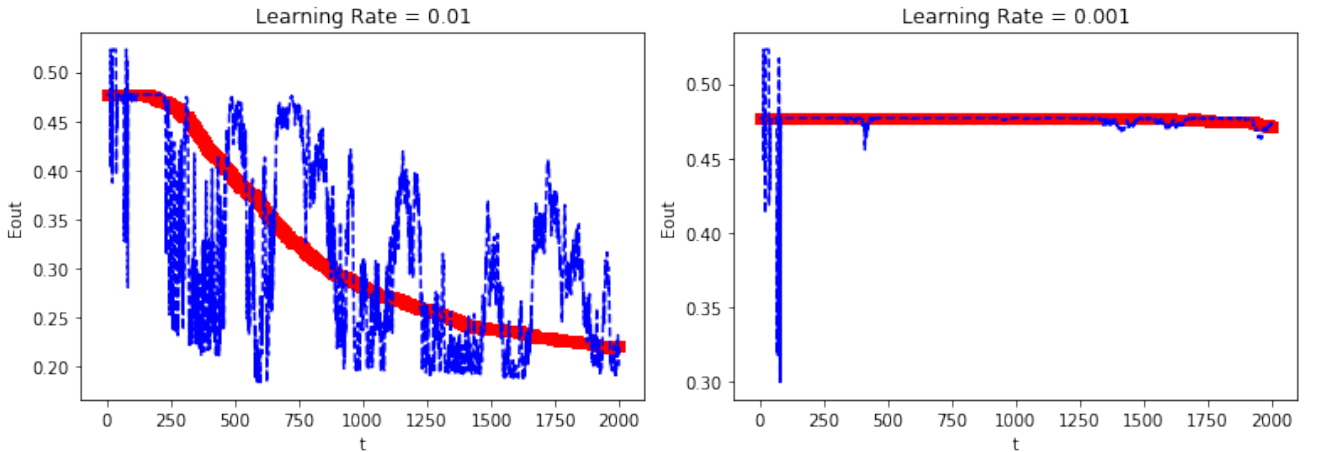


8.



Comparing the GD with SGD version, we can observe that the descent of error rate for GD version is more stable than SGD one's, though after 2000 iterations, their error rate could be almost the same. Moreover, it seems the fixed learning rate = 0.01 is more suitable than 0.001 since it decrease the error rate to a lower level after iterations, implying that $\eta = 0.001$ may be too low steps for learning.

9.



We can find that the trend in figure E_{in} and E_{out} are almost same, which highly corresponds to what we expect: $E_{in} \approx E_{out}$. Combining with the result in previous question, we find that this algorithm achieves the learning goal.

10.

(a). We can consider the problem as solving: $\mathbf{X} \cdot \mathbf{w}_{LIN} \approx \mathbf{y}$

We want to find a vector \mathbf{w}_{LIN} such that $\|\mathbf{X} \cdot \mathbf{w}_{LIN} - \mathbf{y}\| \leq \|\mathbf{X} \cdot \mathbf{u} - \mathbf{y}\|, \forall \mathbf{u} \in \mathbb{R}^N$

In P.15 of slides 9, we know $\|\mathbf{X} \cdot \mathbf{w}_{LIN} - \mathbf{y}\| \Leftrightarrow \mathbf{X} \cdot \mathbf{w}_{LIN} = \mathbf{H} \cdot \mathbf{y}$, where \mathbf{H} is a orthogonal projection matrix for $Col(\mathbf{X})$.

Claim: \mathbf{X} is a $N \times (d + 1)$ matrix with $rank(\mathbf{X}) = \rho$, and the SVD of \mathbf{X} is $\mathbf{X} = U\Gamma V^T$ given in question setting, then $\mathbf{H} = UU^T$.

Let $UU^T = P$, we can observe that $P^2 = P^T = P$. By theorem¹, we know P is a orthogonal projection matrix of $Col(P)$. We want to show $Col(P) = Col(\mathbf{X})$, then $P = \mathbf{H} = UU^T$.

First, we modify matrix Γ by defining :

$$\Gamma^\dagger = \begin{bmatrix} \frac{1}{\gamma_1} & 0 & 0 & \cdots & 0 \\ 0 & \frac{1}{\gamma_2} & 0 & \cdots & 0 \\ 0 & 0 & \frac{1}{\gamma_3} & \cdots & 0 \\ 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & \cdots & \frac{1}{\gamma_\rho} \end{bmatrix}, \text{ where we know } \Gamma = \begin{bmatrix} \gamma_1 & 0 & 0 & \cdots & 0 \\ 0 & \gamma_2 & 0 & \cdots & 0 \\ 0 & 0 & \gamma_3 & \cdots & 0 \\ 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & \cdots & \gamma_\rho \end{bmatrix}, \gamma_1, \gamma_2, \dots, \gamma_\rho > 0$$

It's actually easy to observe that $\Gamma^\dagger = \Gamma^{-1}$, then

$$\begin{aligned} \mathbf{X}(V\Gamma^{-1}U^T) &= U\Gamma V^T V\Gamma^{-1}U^T \\ &= U\Gamma\Gamma^{-1}U^T \\ &= UU^T = P \end{aligned}$$

Therefore, for any vector $\mathbf{v} \in \mathbb{R}^N$, we have $P \cdot \mathbf{v} = \mathbf{X} \cdot \mathbf{z}$, where $\mathbf{z} = (V\Gamma^{-1}U^T)\mathbf{v}$, meaning $P \cdot \mathbf{v}$ is in $Col(\mathbf{X})$, i.e $Col(P)$ is a subspace of $Col(\mathbf{X})$. Also, $rank(P) = {}^2\rho$, i.e $dim(Col(P)) = \rho$, then by theorem³, $Col(P) = Col(\mathbf{X})$, hence $P = \mathbf{H} = UU^T$.

¹Suppose P is a $n \times n$ matrix such that $P^2 = P^T = P$, then P is a orthogonal projection matrix for $Col(P)$. The detailed proof can be checked in Lawrence and Stephen, *Elementary Linear Algebra: A Matrix Approach*.

²By the property of Gramian Matrix, for any real matrix $A_{m \times n}$, $rank(A) = rank(AA^T) = rank(A^T A)$. Thus, in this question, we have $rank(U) = rank(U^T U) = rank(UU^T) = rank(I_\rho) = rank(P) = \rho$

³If V and W are both the subspace of \mathbb{R}^n , and $dim(V) = dim(W)$, then $V = W$. The detailed proof can be checked in Lawrence and Stephen, *Elementary Linear Algebra: A Matrix Approach*

For the vector \mathbf{w}_{LIN} such that $\|\mathbf{X} \cdot \mathbf{u} - \mathbf{y}\|$ is minimum, we let $\mathbf{w}_{LIN} = V\Gamma^{-1}U^T\mathbf{y}$, then $\mathbf{X} \cdot \mathbf{w}_{LIN} = \mathbf{X}(V\Gamma^{-1}U^T)\mathbf{y} = \mathbf{H} \cdot \mathbf{y}$, i.e $\mathbf{w}_{LIN} = V\Gamma^{-1}U^T\mathbf{y}$ is a solution.

(b). Suppose there is another vector $\mathbf{s} \in \mathbb{R}^{d+1}$ can also minimize $\|\mathbf{X} \cdot \mathbf{u} - \mathbf{y}\|$ and $\mathbf{s} \neq \mathbf{w}_{LIN}$. Let $\mathbf{t} = \mathbf{s} - \mathbf{w}_{LIN} (\neq \mathbf{0})$, then

$$\mathbf{X} \cdot \mathbf{t} = \mathbf{X}(\mathbf{s} - \mathbf{w}) = \mathbf{H} \cdot \mathbf{y} - \mathbf{H} \cdot \mathbf{y} = \mathbf{0}$$

Plugging SVD for \mathbf{X} , besides U and Γ are invertible, we have

$$\begin{aligned} U\Gamma V^T \mathbf{t} &= \mathbf{0} \\ \Rightarrow \Gamma V^T \mathbf{t} &= \mathbf{0} \\ \Rightarrow V^T \mathbf{t} &= \mathbf{0} \end{aligned}$$

Also, we know V^T is a orthogonal matrix, it will reserve the inner-product.

$$\therefore \mathbf{t} \cdot \mathbf{w} = (V^T \mathbf{t}) \cdot (V^T \mathbf{w}) = 0$$

Now by $\mathbf{s} = \mathbf{t} + \mathbf{w}_{LIN}$, $\|\mathbf{s}\|^2 = \|\mathbf{t} + \mathbf{w}_{LIN}\|^2 = \|\mathbf{t}\|^2 + \|\mathbf{w}_{LIN}\|^2 > \|\mathbf{w}_{LIN}\|^2$, i.e \mathbf{w}_{LIN} has the least norm(shortest).