MathDNN Homework 1

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Problem 1

(a) Let
$$X_i = \begin{bmatrix} x_{i1} \\ \vdots \\ x_{ip} \end{bmatrix}$$
 and $\theta = \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_p \end{bmatrix}$, then for $j = 1, \dots, p$,
$$\frac{\partial}{\partial \theta_j} l_i(\theta) = \frac{\partial}{\partial \theta_j} \left[\frac{1}{2} (X_i^{\mathsf{T}} \theta - Y_i)^2 \right]$$

$$= \frac{\partial}{\partial \theta_j} \left[\frac{1}{2} (x_{i1} \theta_1 + \dots + x_{ip} \theta_p - Y_i)^2 \right]$$

$$= (x_{i1} \theta_1 + \dots + x_{ip} \theta_p - Y_i) x_{ij}$$

$$= (X_i^{\mathsf{T}} \theta - Y_i) x_{ij}.$$

Therefore

$$\nabla_{\theta} l_{i}(\theta) = \begin{bmatrix} \frac{\partial}{\partial \theta_{1}} l_{i}(\theta) \\ \vdots \\ \frac{\partial}{\partial \theta_{p}} l_{i}(\theta) \end{bmatrix}$$

$$= \begin{bmatrix} (X_{i}^{\mathsf{T}} \theta - Y_{i}) x_{i1} \\ \vdots \\ (X_{i}^{\mathsf{T}} \theta - Y_{i}) x_{ip} \end{bmatrix} = (X_{i}^{\mathsf{T}} \theta - Y_{i}) \begin{bmatrix} x_{i1} \\ \vdots \\ x_{ip} \end{bmatrix}$$

$$= (X_{i}^{\mathsf{T}} \theta - Y_{i}) X_{i}.$$

(b) Let
$$X_{i} = \begin{bmatrix} x_{i1} \\ \vdots \\ x_{ip} \end{bmatrix}$$
 and $\theta = \begin{bmatrix} \theta_{1} \\ \vdots \\ \theta_{p} \end{bmatrix}$, then for $j = 1, \dots, p$,
$$\frac{\partial}{\partial \theta_{j}} \mathcal{L}(\theta) = \frac{\partial}{\partial \theta_{j}} \left[\frac{1}{2} \| X \theta - Y \|^{2} \right]$$

$$= \frac{\partial}{\partial \theta_{j}} \left[\frac{1}{2} \left\| \begin{bmatrix} X_{1}^{\mathsf{T}} \theta - Y_{1} \\ \vdots \\ X_{N}^{\mathsf{T}} \theta - Y_{N} \end{bmatrix} \right|^{2} \right] = \frac{\partial}{\partial \theta_{j}} \left[\sum_{i=1}^{N} \frac{1}{2} (X_{i}^{\mathsf{T}} \theta - Y_{i})^{2} \right] = \frac{\partial}{\partial \theta_{j}} \left[\sum_{i=1}^{N} l_{i}(\theta) \right]$$

$$= \sum_{i=1}^{N} \frac{\partial}{\partial \theta_{i}} l_{i}(\theta) = \sum_{i=1}^{N} (X_{i}^{\mathsf{T}} \theta - Y_{i}) x_{ij}.$$

Therefore

$$\nabla_{\theta} \mathcal{L}(\theta) = \begin{bmatrix} \sum_{i=1}^{N} (X_{i}^{\mathsf{T}} \theta - Y_{i}) x_{i1} \\ \vdots \\ \sum_{i=1}^{N} (X_{i}^{\mathsf{T}} \theta - Y_{i}) x_{ip} \end{bmatrix}$$

$$= \begin{bmatrix} (X_{1}^{\mathsf{T}} \theta - Y_{1}) x_{11} + (X_{2}^{\mathsf{T}} \theta - Y_{2}) x_{21} + \dots + (X_{N}^{\mathsf{T}} \theta - Y_{N}) x_{N1} \\ \vdots \\ (X_{1}^{\mathsf{T}} \theta - Y_{1}) x_{1p} + (X_{2}^{\mathsf{T}} \theta - Y_{2}) x_{2p} + \dots + (X_{N}^{\mathsf{T}} \theta - Y_{N}) x_{Np} \end{bmatrix}$$

$$= \sum_{i=1}^{N} X_{i} (X_{i}^{\mathsf{T}} \theta - Y_{i}) = \sum_{i=1}^{N} (X^{\mathsf{T}})_{:,i} (X \theta - Y)_{i}$$

$$= X^{\mathsf{T}} (X \theta - Y).$$

Problem 2

Since $f(\theta) = \theta^2/2$, we can get $f'(\theta) = \theta$ and the iteration equation can be written as

$$\theta^{k+1} = (1 - \alpha)\theta^k.$$

Thus the nth iteration gives

$$\theta^n = (1 - \alpha)\theta^{n-1} = \dots = (1 - \alpha)^n \theta^0.$$

Therefore if $\alpha > 2$ and $\theta^0 \neq 0$, θ^n diverges since it is a geometric sequence where its ratio is less than -1.

Problem 3

Since $f(\theta) = \frac{1}{2} \|X\theta - Y\|^2$, we can get $\nabla f(\theta) = X^{\intercal}(X\theta - Y)$ and the iteration equation can be written as

$$\theta^{k+1} = \theta^k - \alpha X^{\mathsf{T}} (X \theta^k - Y).$$

Assume $X^\intercal X$ is invertible and let $\theta^* = (X^\intercal X)^{-1} X^\intercal Y$, then

$$\begin{split} \theta^{k+1} - \theta^* &= \theta^k - \alpha X^\intercal \big(X \theta^k - Y \big) - (X^\intercal X)^{-1} X^\intercal Y \\ &= \theta^k - \alpha X^\intercal X \theta^k + \alpha X^\intercal Y - (X^\intercal X)^{-1} X^\intercal Y \\ &= (I - \alpha X^\intercal X) \theta^k + (\alpha X^\intercal X - I) (X^\intercal X)^{-1} X^\intercal Y = (I - \alpha X^\intercal X) \theta^k + (\alpha X^\intercal X - I) \theta^* \\ &= (I - \alpha X^\intercal X) (\theta^k - \theta^*) \end{split}$$

where $I \in \mathbb{R}^{p \times p}$ is an identity matrix. Thus the *n*th iteration gives

$$\theta^n - \theta^* = (I - \alpha X^{\mathsf{T}} X) (\theta^{n-1} - \theta^*) = \dots = (I - \alpha X^{\mathsf{T}} X)^n (\theta^0 - \theta^*).$$

Since $X^{\intercal}X$ is a symmetric matrix and a positive matrix, it has p real positive eigenvalues and is diagonalizable by them. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p \geq 0$ the eigenvalues and M the matrix with the eigenvectors as its columns, then

$$M^{-1}X^{\mathsf{T}}XM = \operatorname{diag}(\lambda_1, \cdots, \lambda_p), \ X^{\mathsf{T}}X \sim \operatorname{diag}(\lambda_1, \cdots, \lambda_p)$$

and gradually

$$\begin{split} I - \alpha X^{\intercal} X &= I - \alpha M \mathrm{diag}(\lambda_1, \cdots, \lambda_p) M^{-1} \\ &= M I M^{-1} - M (\alpha \, \mathrm{diag}(\lambda_1, \cdots, \lambda_p)) M^{-1} \\ &= M (I - \alpha \, \mathrm{diag}(\lambda_1, \cdots, \lambda_p)) M^1 = M \mathrm{diag}(1 - \alpha \lambda_1, \cdots, 1 - \alpha \lambda_p) M^{-1} \end{split}$$

so $I - \alpha X^{\intercal}X \sim \text{diag}(1 - \alpha \lambda_1, \dots, 1 - \alpha \lambda_p)$. Therefore

$$(I - \alpha X^{\mathsf{T}} X)^n = M \operatorname{diag}(1 - \alpha \lambda_1, \cdots, 1 - \alpha \lambda_p)^n M^{-1}$$
$$= M \operatorname{diag}((1 - \alpha \lambda_1)^n, \cdots, (1 - \alpha \lambda_p)^n) M^{-1}.$$

If $\alpha > 2/\rho(X^{\mathsf{T}}X)$, we can obtain $1 - \alpha\lambda_1 < -1$ since $\rho(X^TX) = \lambda_1 \ge 0$. Therefore $(1 - \alpha\lambda_1)^n$ diverges, and consequently $(I - \alpha X^{\mathsf{T}}X)^n$, $\theta^n - \theta^*$, and θ^n also diverge.