ML2024 Fall Homework Assignment 1
Handwritten

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Problem 1 (Preliminary) (1 pt)

In this problem, you need to find the derivative of 2-norm or a scalar with respect to a vector or a matrix. For (b) and (c), you may start by considering

$$\frac{\partial y}{\partial \mathbf{X}} = \begin{bmatrix} \frac{\partial y}{\partial x_{11}} & \cdots & \frac{\partial y}{\partial x_{1n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial y}{\partial x_{n1}} & \cdots & \frac{\partial y}{\partial x_{nn}} \end{bmatrix}.$$

(Hint: Find a partial derivative with respect to the (i,j)-th component and sort out the vector or matrix form.)

(a) (0.2 pts)

(i) (0.1 pts) Given $\mathbf{x}, \mathbf{a} \in \mathbb{R}^n$. Show that

$$\frac{\partial \|\mathbf{x}-\mathbf{a}\|_2}{\partial \mathbf{x}} = \frac{\mathbf{x}-\mathbf{a}}{\|\mathbf{x}-\mathbf{a}\|_2}.$$

(ii) (0.1 pts) Given $\mathbf{a} \in \mathbb{R}^m$, $\mathbf{X} \in \mathbb{R}^{m\times n}$, $\mathbf{b} \in \mathbb{R}^n$. Show that

$$\frac{\partial \mathbf{a}^\mathsf{T}\mathbf{X}\mathbf{b}}{\partial \mathbf{X}} = \mathbf{a}\mathbf{b}^\mathsf{T}.$$

(b) (0.2 pts) Let $\mathbf{X} \in \mathbb{R}^{n\times n}$. Show that

$$\frac{\partial \det(\mathbf{X})}{\partial \mathbf{X}} = \det(\mathbf{X}) \left(\mathbf{X}^{-1}\right)^\mathsf{T}.$$

Hint: Recall the cofactor matrix

$$\mathbf{C} = \begin{bmatrix} C_{11} & \cdots & C_{1n} \\ \vdots & \ddots & \vdots \\ C_{n1} & \cdots & C_{nn} \end{bmatrix}$$

where $C_{ij} = (-1)^{i+j} M_{ij}$ and $M_{ij} = \det\left((x_{mn})_{m\neq i, n\neq j}\right)$. The adjoint matrix is the transpose of the cofactor matrix

$$\operatorname{adj}(\mathbf{X}) = \mathbf{C}^\mathsf{T}.$$

We have an identity

$$\mathbf{X}\operatorname{adj}(\mathbf{X}) = \det(\mathbf{X})\mathbf{I}.$$

You may check Wikipedia for more details.

(c) (0.6 pts) Prove that

$$\frac{\partial \log(\det(\mathbf{A}))}{\partial a_{ij}} = \mathbf{e}_j^\mathsf{T} \mathbf{A}^{-1} \mathbf{e}_i, \tag{1}$$

where $\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mm} \end{bmatrix} \in \mathbb{R}^{m\times m}$ is a (non-singular) matrix, and $\mathbf{e}_j$ is the unit vector along the j-th axis (e.g. $\mathbf{e}_3 = [0, 0, 1, 0, ..., 0]^T$). It is common to write (1) as

$$\frac{\partial \log(\det(\mathbf{A}))}{\partial \mathbf{A}} = \left(\mathbf{A}^{-1}\right)^\mathsf{T}$$

Hint: Same as (b).

Problem 2 (Classification with Gaussian Mixture Model) (2.4 pts)

In this question, we tackle the binary classification problem through the generative approach, where we assume the data point X (viewed as a $\mathbb{R}^d$-valued r.v.) and its label Y (viewed as a $\{\mathcal{C}_1, \mathcal{C}_2\}$-valued r.v.) are generated according to the generative model (paramerized by θ) as follows:

$$\mathbb{P}_\theta[X = \mathbf{x}, Y = \mathcal{C}_k] = \pi_k f_{\boldsymbol{\mu}_k, \Sigma_k}(\mathbf{x}) \quad (k \in \{1, 2\}) \tag{2}$$

where $\theta = (\pi_1, \pi_2, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \Sigma_1, \Sigma_2)$ for which

$$f_{\boldsymbol{\mu}_k, \Sigma_k}(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}} \frac{1}{|\Sigma_k|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_k)^\mathsf{T} \Sigma_k^{-1} (\mathbf{x} - \boldsymbol{\mu}_k)\right).$$

Now suppose we observe data points $\mathbf{x}_1, ..., \mathbf{x}_N$ and their corresponding labels $y_1, ..., y_N$, and $\pi_1 + \pi_2 = 1$.

(a) (1.2 pt)

(i) (0.3 pt) Please write down the likelihood function $L(\theta)$ that describes how likely the generative model would generate the observed data $\{(\mathbf{x}_i, y_i)\}_{i=1}^N$ in terms of $\theta = (\pi_1, \pi_2, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \Sigma_1, \Sigma_2)$.

(ii) (0.3 pt) Find the maximum likelihood estimate $\theta^* = (\pi_1^*, \pi_2^*, \boldsymbol{\mu}_1^*, \boldsymbol{\mu}_2^*, \Sigma_1^*, \Sigma_2^*)$ that maximizes the likelihood function $L(\theta)$.

(iii) (0.3 pt) Write down $\mathbb{P}_\theta[Y = \mathcal{C}_1 | X = \mathbf{x}]$ and $\mathbb{P}_\theta[X = \mathbf{x} | Y = \mathcal{C}_1]$ in terms of $\theta = (\pi_1, \pi_2, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \Sigma_1, \Sigma_2)$. What are the physical meaning of the aforementioned quantities?

(iv) (0.3 pt) Express $\mathbb{P}_\theta[Y = \mathcal{C}_1 | X = \mathbf{x}]$ in the form of $\sigma(z)$, where $\sigma(\cdot)$ denotes the sigmoid function, and express z in terms of $\theta = (\pi_1, \pi_2, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \Sigma_1, \Sigma_2)$ and x.

(b) (1.2 pt) Suppose we pose an additional constraint that the covariance matrices of the two Gaussian distributions are identical, namely $\Sigma_1 = \Sigma_2 = \Sigma$, in which the generative model is parameterized by $\vartheta = (\pi_1, \pi_2, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \Sigma)$. Redo questions (a) under such setting.

Problem 3 (Closed-Form Linear Regression Solution) (1 pts + Bonus 1.5 pts)

Consider the linear regression model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\theta} + \boldsymbol{\epsilon},$$

where $\mathbf{y} \in \mathbb{R}^n, \mathbf{X} \in \mathbb{R}^{n\times d}, \boldsymbol{\theta} \in \mathbb{R}^d$ and $\boldsymbol{\epsilon} \in \mathbb{R}^n$. Denote $\mathbf{X}_i \in \mathbb{R}^{1\times d}$ as the i-th row of $\mathbf{X}$, with the following interpretations:

- If the linear model has the bias term, then write $\boldsymbol{\theta} = [w_1, \cdots, w_m, b]^\mathsf{T}$ and $\mathbf{X}_i = [x_{i,1}, x_{i,2}, \cdots, x_{i,m}, 1]$, namely $d = m + 1$.

- If the linear model has no bias term, then write $\boldsymbol{\theta} = [w_1, \cdots, w_d]^T$ and $\mathbf{X}_i = [x_{i,1}, x_{i,2}, \cdots, x_{i,m}]$, namely $d = m$.

(a) Without the bias term, consider the L^2-regularized loss function:

$$\sum_i \kappa_i \left(y_i - \boldsymbol{X}_{\mathrm{i}}\boldsymbol{\theta}\right)^2 + \lambda \sum_j w_j^2, \quad \lambda > 0,\ \kappa_i > 0 \text{ for all } i.$$

Show that the optimal solution that minimizes the loss function is $\boldsymbol{\theta}^{*} = \left(\boldsymbol{X}^T\boldsymbol{K}\boldsymbol{X} + \lambda\boldsymbol{I}\right)^{-1}\boldsymbol{X}^T\boldsymbol{K}\boldsymbol{y}$, where

$$\boldsymbol{K} = \begin{bmatrix} \kappa_1 & & 0 \\ & \ddots & \\ 0 & & \kappa_n \end{bmatrix}$$

is a diagonal matrix and $\boldsymbol{I}$ is the $d \times d$ identical matrix.

(b) (Bonus, 1.5 pts) With the bias term, the L^2-regularized loss function becomes

$$\sum_i \kappa_i \left(y_i - \boldsymbol{X}_{\mathrm{i}}\boldsymbol{\theta}\right)^2 + \lambda \sum_j w_j^2, \quad \lambda > 0,\ \kappa_i > 0 \text{ for all } i.$$

Show that the optimal solution that minimizes the loss function is $\boldsymbol{\theta}^{*} = [\boldsymbol{w}^{\star T}, b^{\star}]^T$, where

$$\boldsymbol{w}^{\star} = \left(\tilde{\boldsymbol{X}}^T\boldsymbol{K}\tilde{\boldsymbol{X}} + \lambda\boldsymbol{I} - \frac{1}{\mathrm{Tr}\left(\boldsymbol{K}\right)}\tilde{\boldsymbol{X}}^T\boldsymbol{K}\boldsymbol{e}\boldsymbol{e}^T\boldsymbol{K}\tilde{\boldsymbol{X}}\right)^{-1}\tilde{\boldsymbol{X}}^T\boldsymbol{K}\left(\boldsymbol{y} - \frac{1}{\mathrm{Tr}\left(\boldsymbol{K}\right)}\boldsymbol{e}\boldsymbol{e}^T\boldsymbol{K}\boldsymbol{y}\right),$$

$$b^{\star} = \frac{1}{\mathrm{Tr}\left(\boldsymbol{K}\right)}\left(\boldsymbol{e}^T\boldsymbol{K}\boldsymbol{y} - \boldsymbol{e}^T\boldsymbol{K}\tilde{\boldsymbol{X}}\boldsymbol{w}^{\star}\right)$$

for which $\boldsymbol{e} = [1\ ...\ 1]^T$ denotes the all one vector, $\boldsymbol{X} = [\tilde{\boldsymbol{X}}\boldsymbol{e}]$, $\mathrm{Tr}\left(\boldsymbol{K}\right)$ is the trace of the matrix $\boldsymbol{K}$, and that $\mathbf{K}$ and $\mathbf{I}$ are defined as in (a).

Problem 4 (Noise and Regularization) (1 pts)

Consider the linear model $f_{\mathbf{w},b} : \mathbb{R}^k \to \mathbb{R}$, where $\mathbf{w} \in \mathbb{R}^k$ and $b \in \mathbb{R}$, defined as

$$f_{\mathbf{w},b}(x) = \mathbf{w}^T\mathbf{x} + b$$

Given dataset $S = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$, if the inputs $\mathbf{x}_i \in \mathbb{R}^k$ are contaminated with input noise $\boldsymbol{\eta}_i \in \mathbb{R}^k$, we may consider the expected sum-of-squares loss in the presence of input noise as

$$\tilde{L}_{ss}(\mathbf{w}, b) = \mathbb{E}\left[\frac{1}{2N}\sum_{i=1}^N \left(f_{\mathbf{w},b}(\mathbf{x}_i + \boldsymbol{\eta}_i) - y_i\right)^2\right]$$

where the expectation is taken over the randomness of input noises $\boldsymbol{\eta}_1, ..., \boldsymbol{\eta}_N$. Additionally, the inputs $(\mathbf{x}_i)$ and the input noise $(\boldsymbol{\eta}_i)$ are independent.

Now assume the input noises $\eta_i = [\eta_{i,1}, \eta_{i,2}, ..., \eta_{i,k}]^T$ are random vectors with zero mean $\mathbb{E}[\eta_{i,j}] = 0$, and the covariance between components is given by

$$\mathbb{E}[\eta_{i,j}\eta_{i',j'}] = \delta_{i,i'}\delta_{j,j'}\sigma^2$$

where $\delta_{i,i'} = \begin{cases} 1 & \text{, if } i = i' \\ 0 & \text{, otherwise.} \end{cases}$ denotes the Kronecker delta.

Please show that

$$\tilde{L}_{ss}(\mathbf{w}, b) = \frac{1}{2N}\sum_{i=1}^N \left(f_{\mathbf{w},b}(\mathbf{x}_i) - y_i\right)^2 + \frac{\sigma^2}{2}\|\mathbf{w}\|^2$$

That is, minimizing the expected sum-of-squares loss in the presence of input noise is equivalent to minimizing noise-free sum-of-squares loss with the addition of a L^2-regularization term on the weights. (Hint: $\|\mathbf{x}\|^{\mathbf{2}} = \mathbf{x}^{\mathbf{T}}\mathbf{x} = \mathbf{tr}(\mathbf{x}\mathbf{x}^{\mathbf{T}})$ and the square of a vector is dot product with itself)

Problem 5 (Gradient descent for Logistic Regression with Vectorized Feature) (0.6 pts)

This problem is related to the appendix of W2_Logistic_Regression.pdf. Consider the following optimization problem

$$\min_{\mathbf{w}} \ell(\mathbf{w}), \tag{3}$$

where

$$\ell(\mathbf{w}) = \frac{1}{d}\sum_{n=1}^{d} \ell^{(n)}(\mathbf{w}), \quad \ell^{(n)}(\mathbf{w}) = \ln\left(1 + \exp\left(-y_n\left(\mathbf{w}^\mathsf{T}\mathbf{x}_n\right)\right)\right).$$

Assume that there are d training data, $\mathbf{x}_n$ is the n-th training data, and the label $y_n = \pm 1$.

(a) (0.2 pts) Prove that $\frac{1}{\ln 2}\ell^{(n)}(\mathbf{w})$ is an upper bound of $\mathbb{1}\{\text{sign}\left(\mathbf{w}^\mathsf{T}\mathbf{x}_n\right) \neq y_n\}$ for any $\mathbf{w}$, where $\mathbb{1}\{\cdot\}$ is the indicator function. Do not use graph calculator for the arguments.

(b) (0.2 pts) For a given $(\mathbf{x}_n, y_n)$, derive its gradient $\nabla\ell^{(n)}(\mathbf{w})$.

(c) (0.2 pts) Prove that the optimization problem 3 is equivalent to minimizing the following objective function

$$\mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{d}\left(\frac{1+y_n}{2}\ln\frac{1+\tanh\left(\frac{1}{2}\mathbf{w}^\mathsf{T}\mathbf{x}_n\right)}{2} + \frac{1-y_n}{2}\ln\frac{1-\tanh\left(\frac{1}{2}\mathbf{w}^\mathsf{T}\mathbf{x}_n\right)}{2}\right).$$

Problem 6 (Mathematical Background) (0 pt)

Please click the following link `https://www.cs.cmu.edu/~mgormley/courses/10601/homework/hw1.zip` to download the Homework 1 from CMU 2023 Machine Learning Website. You are encouraged to practice Section 3 to Section 6 of this homework to brush up some of the mathematical background that will be useful for this course. **This problem will not be graded**. However, you are encouraged to consult TA by joining TA hour if you find any questions.

Some Tools You Need to Know

1. Orthogonal Matrix
2. Positive Definite, Semipositive Definite
3. Eigenvalue Decomposition, Singular value decomposition
4. Lagrange Multiplier
5. Trace

You can find the definition and the usage by yourself. It is also welcome to discuss with TA in TA hour.