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1. (1%) 解釋什麼樣的 **data preprocessing** 可以 **improve** 你的 **training/testing accuracy**, e.g., 你怎麼挑掉你覺得不適合的 **data points**。請提供數據(例如 **kaggle public score RMSE**)以佐證你的想法。

計算各個 **feature** 與 **PM2.5** 的相關係數，只選擇相關係數絕對值大於 0.5 的 **feature** 放入模型中，分別為 **CO**, **NO**, **NOx**, **PM10**，與放入前 8 個 **feature** 的模型在相同條件下比較，可發現前者表現較好。(上圖為挑選過 **feature**, 下圖為直接使用前 8 個 **feature**)

| | | | |
|---|---------|---------|-------------------------------------|
|  my_sol (3).csv Complete · 2d ago | 3.88222 | 3.25476 | <input checked="" type="checkbox"/> |
|  my_sol (6).csv Complete (after deadline) · 12s ago | 5.89725 | 6.14305 | <input type="checkbox"/> |

2. (1%) 請實作 **2nd-order polynomial regression model** (不用考慮交互項)。

a. 貼上 **polynomial regression** 版本的 **Gradient descent code** 內容

```
import numpy as np
import math

def minibatch(x, y, config):

    # Randomize the data in minibatch
    index = np.arange(x.shape[0])
    np.random.shuffle(index)
    x = x[index]
    y = y[index]

    # Initialization
    batch_size = config.batch_size
    lr = config.lr
    lam = config.lam
    epoch = config.epoch

    beta_1 = 0.9
    beta_2 = 0.99
```

```

# Polynomial regression: three parameters (z, w, b)
z = np.full(x[0].shape, 0.1).reshape(-1, 1)
w = np.full(x[0].shape, 0.1).reshape(-1, 1)
bias = 0.1

m_t_z = np.zeros(z.shape)
v_t_z = np.zeros(z.shape)
m_t_w = np.zeros(w.shape)
v_t_w = np.zeros(w.shape)
m_t_b = 0.0
v_t_b = 0.0
t = 0
epsilon = 1e-8

# Training loop
for num in range(epoch):
    for b in range(int(x.shape[0] / batch_size)):
        t += 1
        x_batch = x[b * batch_size:(b + 1) * batch_size]
        y_batch = y[b * batch_size:(b + 1) *
batch_size].reshape(-1, 1)

        # Prediction of polynomial regression
        pred = np.dot(x_batch ** 2, z) + np.dot(x_batch, w) +
bias

        # Loss
        loss = y_batch - pred

        # Compute gradients
        g_t_z = -2 * np.dot(np.square(x_batch).T, loss)
        g_t_w = -2 * np.dot(x_batch.T, loss)
        g_t_b = -2 * loss.sum()

        m_t_z = beta_1 * m_t_z + (1 - beta_1) * g_t_z
        v_t_z = beta_2 * v_t_z + (1 - beta_2) * (g_t_z ** 2)
        m_cap_z = m_t_z / (1 - (beta_1 ** t))
        v_cap_z = v_t_z / (1 - (beta_2 ** t))

```

```

m_t_w = beta_1 * m_t_w + (1 - beta_1) * g_t_w
v_t_w = beta_2 * v_t_w + (1 - beta_2) * (g_t_w ** 2)
m_cap_w = m_t_w / (1 - (beta_1 ** t))
v_cap_w = v_t_w / (1 - (beta_2 ** t))

m_t_b = 0.9 * m_t_b + (1 - 0.9) * g_t_b
v_t_b = 0.99 * v_t_b + (1 - 0.99) * (g_t_b ** 2)
m_cap_b = m_t_b / (1 - (0.9 ** t))
v_cap_b = v_t_b / (1 - (0.99 ** t))

# Update parameters
z -= ((lr * m_cap_z) / (np.sqrt(v_cap_z) +
epsilon)).reshape(-1, 1)
w -= ((lr * m_cap_w) / (np.sqrt(v_cap_w) +
epsilon)).reshape(-1, 1)
bias -= (lr * m_cap_b) / (math.sqrt(v_cap_b) +
epsilon)

return z, w, bias

```

b. 在只使用 NO 數值作為 **feature** 的情況下，紀錄該 **model** 所訓練出的 **parameter** 數值 (**w2**, **w1**, **b**) 以及 **kaggle public score**.
 在如下圖的設定，**random seed = 9487**，最後得到的結果為所附的 **kaggle public score**.

```

train_config = Namespace(
    batch_size = 512,
    lr = 1e-1,
    lam = 0.001,
    epoch = 1,
)

feats = [2]

```



my_sol_test_no.csv
 Complete (after deadline) · now

12.99882

21.00481



平方項係數 (**w2**) 為[[0.0324149],[-0.10955948],[-0.01614332],[0.09518239],
 [-0.051995],[0.0658696],[-0.07257947],[0.08801479]] (8*1 的矩陣)
 一次項係數 (**w1**) 為[[0.38487713],[0.27877768],[0.26185372],[0.24145826],
 [0.22826823],[0.29885901],[0.26746609],[0.36222515]] (8*1 的矩陣)
 常數 (**b**) 為 0.7981775406162891

Problem 1.

(a) apply first order approximation

$$f(w + \Delta w) = f(w) + (\Delta w)^T \cdot \nabla_w f(w)$$

$$f(w) = w^T A w$$

$$f(w + \Delta w) = (w + \Delta w)^T A (w + \Delta w)$$

$$= (w^T + \Delta w^T) A (w + \Delta w)$$

$$= w^T A w + w^T A \Delta w + \Delta w^T A w$$

$$\text{since } \Delta w \rightarrow 0, \Delta w^T A \Delta w \rightarrow 0$$

$$f(w + \Delta w) = w^T A w + w^T A \Delta w + \Delta w^T A w$$

$$\text{since } w^T A \Delta w \in \mathbb{R}^{1 \times 1}, w^T A \Delta w = (w^T A \Delta w)^T = \Delta w^T A^T w$$

$$f(w + \Delta w) = f(w) + \Delta w^T A^T w + \Delta w^T A w$$

$$= f(w) + \Delta w^T (A^T w + A w)$$

$$= f(w) + \Delta w^T \cdot \nabla_w f(w)$$

$$\nabla_w f(w) = A^T w + A w, \text{ if } A \text{ is symmetric}$$

$$A^T = A$$

$$\nabla_w f(w) = 2Aw$$

$$(b) \text{ let } A = \begin{bmatrix} A_1 \\ A_2 \\ \vdots \\ A_m \end{bmatrix}, B = [B_1 B_2 \dots B_m]$$

$$A_i \in \mathbb{R}^{1 \times m}$$

$$B_i \in \mathbb{R}^{m \times 1}$$

$$(AB)_{ij} = A_i \cdot B_j$$

$$\text{tr}(AB) = \sum_{i=1}^m \sum_{j=1}^m A_{ij} B_{ji}$$

$$\frac{\partial \text{tr}(AB)}{\partial A_{ij}} = \frac{\sum_{k=1}^m \sum_{w=1}^m A_{kw} B_{kw}}{\partial A_{ij}} = A_{ij} B_{ji} + \sum_{k=1}^m \sum_{w=1}^m A_{kw} B_{kw} \quad \begin{matrix} \text{when } k=i \\ \text{and } w=j \end{matrix}$$

$$= B_{ji} = B_{ji}$$

1- (c) we have $X^{-1} = \frac{1}{\det A} (\text{adj } A)$, $\text{adj } A = (C_A)^T$

by cofactor expansion

$$\det A = \sum_{k=1}^n a_{ik} C_{ik}$$

$$\frac{\partial \det A}{\partial a_{ij}} = \sum_{k=1}^n \left(\frac{\partial a_{ik}}{\partial a_{ij}} C_{ik} + a_{ik} \frac{\partial C_{ik}}{\partial a_{ij}} \right)$$

If $k=j$, $\frac{\partial a_{ik}}{\partial a_{ij}} = 1$, $k \neq j$, $\frac{\partial a_{ik}}{\partial a_{ij}} = 0$

C_{ik} does not affect by a_{ij} , $\frac{\partial C_{ik}}{\partial a_{ij}} = 0$

$$\frac{\partial \det A}{\partial a_{ij}} = C_{ij}$$

$$\frac{\partial \ln(\det A)}{\partial a_{ij}} = \frac{1}{\det A} \cdot C_{ij} = \frac{1}{\det A} (\text{adj } A)^T_{ij}$$

$$= (A^{-1})^T_{ij} = e_j^T A^{-1} e_i$$

Reference

<https://statisticaloddsandends.wordpress.com/2018/05/24/derivative-of-log-det-x/>

2. (a) 不失一般性, 设 $y_1 \sim y_j \in c_1$, $y_j \sim y_n \in c_2$

$$(i) L(\theta) = \prod_{i=1}^n P_{\theta}[X=x_i, Y=y_i]$$

$$= \prod_{i=1}^j P_{(\pi_1, \mu_1, \Sigma_1)}[X=x_i, Y=y_i] \times \prod_{i=j+1}^n P_{(\pi_2, \mu_2, \Sigma_2)}[X=x_i, Y=y_i]$$

$$= \prod_{i=1}^j \pi_1 \frac{\exp(-\frac{1}{2}(x_i - \mu_1)^T \Sigma_1^{-1}(x_i - \mu_1))}{\sqrt{(2\pi)^d |\Sigma_1|}} \times \prod_{i=j+1}^n \pi_2 \frac{\exp(-\frac{1}{2}(x_i - \mu_2)^T \Sigma_2^{-1}(x_i - \mu_2))}{\sqrt{(2\pi)^d |\Sigma_2|}}$$

$$= (\pi_1)^j (2\pi)^{-\frac{dj}{2}} |\Sigma_1|^{-\frac{j}{2}} \cdot \exp\left(-\frac{1}{2} \sum_{i=1}^j (x_i - \mu_1)^T \Sigma_1^{-1} (x_i - \mu_1)\right) \cdot (\pi_2)^{n-j} (2\pi)^{-\frac{d(n-j)}{2}} |\Sigma_2|^{-\frac{n-j}{2}} \cdot \exp\left(-\frac{1}{2} \sum_{i=j+1}^n (x_i - \mu_2)^T \Sigma_2^{-1} (x_i - \mu_2)\right)$$

$$(ii) \text{ maximize } L(\theta) \Rightarrow \text{ maximize } \ln(L(\theta))$$

$$\ln(L(\theta)) = j \ln(\pi_1) - \frac{dj}{2} \ln(2\pi) - \frac{j}{2} \ln(|\Sigma_1|) - \frac{1}{2} \left(\sum_{i=1}^j (x_i - \mu_1)^T \Sigma_1^{-1} (x_i - \mu_1) \right) + (n-j) \ln(\pi_2) - \frac{d(n-j)}{2} \ln(2\pi) - \frac{(n-j)}{2} \ln(|\Sigma_2|) - \frac{1}{2} \sum_{i=j+1}^n (x_i - \mu_2)^T \Sigma_2^{-1} (x_i - \mu_2)$$

Since d, j, π are constant
maximize $\ln(L(\theta))$ means

$$\text{maximize } j \ln(\pi_1) + (n-j) \ln(\pi_2) - \frac{1}{2} \left(j \ln(|\Sigma_1|) + \sum_{i=1}^j (x_i - \mu_1)^T \Sigma_1^{-1} (x_i - \mu_1) \right) - \frac{1}{2} \left((n-j) \ln(|\Sigma_2|) + \sum_{i=j+1}^n (x_i - \mu_2)^T \Sigma_2^{-1} (x_i - \mu_2) \right)$$

to maximize $j \ln(\pi_1) + (n-j) \ln(\pi_2)$, we knew $\pi_1 + \pi_2 = 1$
because sum of probability = 1,

$$\frac{d}{d\pi_1} (j \ln(\pi_1) + (n-j) \ln(1-\pi_1)) = j \cdot \frac{1}{\pi_1} + (j-n) \cdot \frac{1}{1-\pi_1} = 0$$

$$\pi_1^* = \frac{j}{n}, \quad \pi_2^* = \frac{n-j}{n}$$

$\frac{1}{2} \times 2. (a)$
 (ii) maximize $-\frac{1}{2} (j \cdot \ln |\Sigma_1| + \sum_{i=1}^j (x_i - \mu_1)^T \Sigma_1^{-1} (x_i - \mu_1))$
 we already know $\nabla_A \ln(\det(A)) = (A^{-1})^T \nabla_A \text{tr}(BA) = B^T$
 $\nabla_X (X^T A X) = 2AX$ when A is symmetric
 Σ_1 is symmetric
 $\nabla_{\mu_1} \left(-\frac{1}{2} (j \cdot \ln |\Sigma_1| + \sum_{i=1}^j (x_i - \mu_1)^T \Sigma_1^{-1} (x_i - \mu_1)) \right)$
 $= -\frac{1}{2} \left(0 + \sum_{i=1}^j 2 \Sigma_1^{-1} (x_i - \mu_1) \right)$
 $= -\sum_{i=1}^j \Sigma_1^{-1} (x_i - \mu_1) = -\Sigma_1^{-1} \left(\sum_{i=1}^j (x_i) - j \mu_1 \right)$
 since Σ_1 is non-singular $-\Sigma_1^{-1} \left(\sum_{i=1}^j (x_i) - j \mu_1 \right) = 0$
 only when $\sum_{i=1}^j x_i - j \mu_1 = 0 \Rightarrow \mu_1^* = \frac{1}{j} \sum_{i=1}^j x_i$
 $|\Sigma_1| = \frac{1}{|\Sigma_1^{-1}|}$
 $\rightarrow -\frac{1}{2} (j \cdot \ln |\Sigma_1|) - \frac{1}{2} \sum_{i=1}^j (x_i - \mu_1)^T \Sigma_1^{-1} (x_i - \mu_1)$
 $= -\frac{1}{2} j \cdot \ln |\Sigma_1| - \frac{1}{2} \sum_{i=1}^j (x_i - \mu_1)^T \Sigma_1^{-1} (x_i - \mu_1)$
 $\nabla_{\Sigma_1} \left(-\frac{1}{2} (j \cdot \ln |\Sigma_1| - \sum_{i=1}^j (x_i - \mu_1)^T \Sigma_1^{-1} (x_i - \mu_1)) \right)$
 $= \frac{1}{2} (j \cdot \Sigma_1^{-T} - \nabla_{\Sigma_1} \left(\sum_{i=1}^j \text{tr}((x_i - \mu_1)^T \Sigma_1^{-1} (x_i - \mu_1)) \right))$
 if c is scalar, $\text{tr}(c) = c$
 $\text{tr}(AB) = \text{tr}(BA)$
 $= \frac{j}{2} \Sigma_1^{-T} - \frac{1}{2} \sum_{i=1}^j \nabla_{\Sigma_1} (\text{tr}((x_i - \mu_1)(x_i - \mu_1)^T \Sigma_1^{-1}))$
 $= \frac{j}{2} \Sigma_1^{-T} - \frac{1}{2} \sum_{i=1}^j ((x_i - \mu_1)(x_i - \mu_1)^T \Sigma_1^{-1})^T = 0$
 $j \Sigma_1 = \sum_{i=1}^j (x_i - \mu_1)(x_i - \mu_1)^T$
 $\Sigma_1^* = \frac{1}{j} \sum_{i=1}^j (x_i - \mu_1)(x_i - \mu_1)^T$
 since Σ_1 and μ_1 does not interfere Σ_2 and μ_2 , by the same
 steps we can find $\mu_2^* = \frac{1}{n-j} \sum_{i=j+1}^n x_i$, $\Sigma_2^* = \frac{1}{n-j} \sum_{i=j+1}^n (x_i - \mu_2)(x_i - \mu_2)^T$

Reference

<https://www.statlect.com/fundamentals-of-statistics/multivariate-normal-distribution-maximum-likelihood>

2. (a)

$$(iii) P_{\theta}[Y=C_1 | X=x] = \frac{P_{\theta}(X=x, Y=C_1)}{P_{\theta}(X=x, Y=C_1) + P_{\theta}(X=x, Y=C_2)}$$

(when $X=x$, the probability of $Y=C_1$)

$$= \frac{\pi_1 \cdot \frac{\exp(-\frac{1}{2}(x-\mu_1)^T \Sigma_1^{-1}(x-\mu_1))}{\sqrt{(2\pi)^d |\Sigma_1|}}}{\pi_1 \cdot \frac{\exp(-\frac{1}{2}(x-\mu_1)^T \Sigma_1^{-1}(x-\mu_1))}{\sqrt{(2\pi)^d |\Sigma_1|}} + \pi_2 \cdot \frac{\exp(-\frac{1}{2}(x-\mu_2)^T \Sigma_2^{-1}(x-\mu_2))}{\sqrt{(2\pi)^d |\Sigma_2|}}}$$

$$P_{\theta}[X=x | Y=C_1]$$

(when $Y=C_1$, the probability of $X=x$)

$$= \frac{P_{\theta}(X=x, Y=C_1)}{P_{\theta}(X=x, Y=C_1) + P_{\theta}(X=x, Y=C_2)}$$

recall $\pi_1^* = \frac{j}{n}$, $P_{\theta}[X=x | Y=C_1] = \frac{\exp(-\frac{1}{2}(x-\mu_1)^T \Sigma_1^{-1}(x-\mu_1))}{\sqrt{(2\pi)^d |\Sigma_1|}}$

2. (a)

$$(iv) P_{\theta}[Y=C_1 | X=x] = \frac{P_{\theta}(X=x, Y=C_1)}{P_{\theta}(X=x, Y=C_1) + P_{\theta}(X=x, Y=C_2)}$$

$$= \frac{1}{1 + \frac{P(X=x, Y=C_2)}{P(X=x, Y=C_1)}} = \sigma(z) = \frac{1}{1 + \exp(-z)}$$

$$z = \ln \frac{P(X=x, Y=C_1)}{P(X=x, Y=C_2)} = \ln \frac{P(X|C_1)}{P(X|C_2)} + \ln \frac{\pi_1}{\pi_2}$$

(in a. (iii), we know $P(X|C_1)$)

$$\ln \frac{P(X|C_1)}{P(X|C_2)} = \ln \frac{\frac{1}{\sqrt{|\Sigma_2|}} \exp\{-\frac{1}{2}(x-\mu_1)^T \Sigma_1^{-1}(x-\mu_1) + \frac{1}{2}(x-\mu_2)^T \Sigma_2^{-1}(x-\mu_2)\}}{\frac{1}{\sqrt{|\Sigma_1|}}}$$

$$= \ln \frac{\sqrt{|\Sigma_2|}}{\sqrt{|\Sigma_1|}} - \frac{1}{2}[(x-\mu_1)^T \Sigma_1^{-1}(x-\mu_1) - (x-\mu_2)^T \Sigma_2^{-1}(x-\mu_2)]$$

$$\begin{aligned}
 2. (a) \quad Z &= \ln \frac{\pi_1}{\pi_2} + \ln \frac{\sqrt{|\Sigma_2|}}{\sqrt{|\Sigma_1|}} - \frac{1}{2} [(x-\mu_1)^T \Sigma_1^{-1} (x-\mu_1) - (x-\mu_2)^T \Sigma_2^{-1} (x-\mu_2)] \\
 (iv) \quad & (x-\mu_1)^T \Sigma_1^{-1} (x-\mu_1) \\
 &= (x^T \Sigma_1^{-1} + \mu_1^T \Sigma_1^{-1}) (x-\mu_1) \\
 &= x^T \Sigma_1^{-1} x - \underbrace{x^T \Sigma_1^{-1} \mu_1}_{\text{same}} - \mu_1^T \Sigma_1^{-1} x + \mu_1^T \Sigma_1^{-1} \mu_1 \\
 &= x^T \Sigma_1^{-1} x - 2 \mu_1^T \Sigma_1^{-1} x + \mu_1^T \Sigma_1^{-1} \mu_1 \\
 & \text{and so is } (x-\mu_2)^T \Sigma_2^{-1} (x-\mu_2) \\
 &= x^T \Sigma_2^{-1} x - 2 \mu_2^T \Sigma_2^{-1} x + \mu_2^T \Sigma_2^{-1} \mu_2 \\
 \downarrow \\
 Z &= \ln \frac{\pi_1}{\pi_2} + \ln \frac{\sqrt{|\Sigma_2|}}{\sqrt{|\Sigma_1|}} - \frac{1}{2} x^T \Sigma_1^{-1} x + \mu_1^T \Sigma_1^{-1} x \\
 &\quad - \frac{1}{2} \mu_1^T \Sigma_1^{-1} \mu_1 + \frac{1}{2} x^T \Sigma_2^{-1} x - \mu_2^T \Sigma_2^{-1} x + \frac{1}{2} \mu_2^T \Sigma_2^{-1} \mu_2
 \end{aligned}$$

2. (b) rewrite $\ln(L(\theta)) = (n-j)\ln(\pi_2) + j\ln\pi_1$
 $-\frac{1}{2} [j\ln|\Sigma| + \sum_{i=1}^j (x_i - \mu_1)^T \Sigma^{-1} (x_i - \mu_1) + (n-j)\ln|\Sigma| + \sum_{i=j+1}^n (x_i - \mu_2)^T \Sigma^{-1} (x_i - \mu_2)]$
 π_1, π_2 are not affected by Σ , have the same result
 $\pi_1^* = \frac{j}{n} \quad \pi_2^* = \frac{n-j}{n}$

$\nabla_{\mu_1} \ln(L(\theta)) = -\frac{1}{2} \nabla_{\mu_1} \left(\sum_{i=1}^j (x_i - \mu_1)^T \Sigma^{-1} (x_i - \mu_1) \right)$
 $= -\frac{1}{2} \sum_{i=1}^j \Sigma^{-1} (x_i - \mu_1) = 0$ Σ^{-1} are symmetric
 $\sum_{i=1}^j \Sigma^{-1} (x_i - \mu_1) = 0, \quad \sum_{i=1}^j (x_i - \mu_1) = 0$
 $\mu_1^* = \frac{1}{j} \sum_{i=1}^j x_i, \quad \text{同理 } \mu_2^* = \frac{1}{n-j} \sum_{i=j+1}^n x_i$

$\nabla_{\Sigma^{-1}} \ln(L(\theta)) = \frac{1}{2} \nabla_{\Sigma^{-1}} \ln|\Sigma^{-1}| - \frac{1}{2} \nabla_{\Sigma^{-1}} \sum_{i=1}^j (x_i - \mu_1)^T \Sigma^{-1} (x_i - \mu_1)$
 $= \frac{n}{2} \Sigma^{-1} - \frac{1}{2} \nabla_{\Sigma^{-1}} \left(\sum_{i=1}^j (x_i - \mu_1)^T \Sigma^{-1} (x_i - \mu_1) \right)$
 $= \frac{n}{2} \Sigma^{-1} - \frac{1}{2} \nabla_{\Sigma^{-1}} \left(\sum_{i=1}^j (x_i - \mu_2)^T \Sigma^{-1} (x_i - \mu_2) \right)$

(by the same computation in 2. (a). (ii))
 $\rightarrow = \frac{n}{2} \Sigma^{-1} - \frac{1}{2} \left(\sum_{i=1}^j (x_i - \mu_1)(x_i - \mu_2)^T + \sum_{i=j+1}^n (x_i - \mu_2)(x_i - \mu_2)^T \right)$
 $\Sigma^* = \frac{\sum_{i=1}^j (x_i - \mu_1)(x_i - \mu_1)^T + \sum_{i=j+1}^n (x_i - \mu_2)(x_i - \mu_2)^T}{n}$

Math 3

Let $c2 = \text{class } 0$ in the dataset

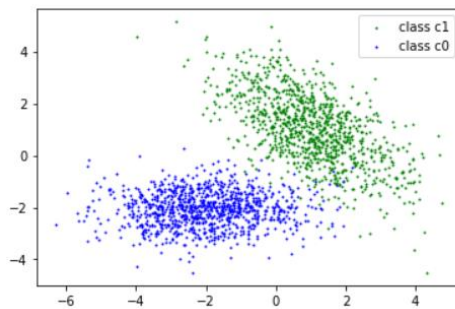
a.

$$\vartheta^* = (\pi_1^*, \pi_2^*, \mu_1^*, \mu_2^*, \Sigma^*) = (0.5, 0.5, [1.011436374828497, 1.004931936779685], [-2.025716971154811, -2.0461950110868674], [[1.85889712, -0.51610136], [-0.51610136, 1.14373928]])$$

b.

$$\vartheta^* = (\pi_1^*, \pi_2^*, \mu_1^*, \mu_2^*, \Sigma_1^*, \Sigma_2^*) = (0.5, 0.5, [1.011436374828497, 1.004931936779685], [-2.025716971154811, -2.0461950110868674], [[1.70649036, -1.06606724], [-1.06606724, 1.82770502]], [[2.0133172, 0.03389842], [0.03389842, 0.46023378]])$$

c. I would choose the method in (a) because we can simply draw a straight line to distinguish class 1 and class 0.



4. (a) rewrite $\sum_i k_i (y_i - x_i^T \theta)^2 + \lambda \sum_j w_j^2, \lambda > 0$
 as $(y - X\theta)^T K (y - X\theta) + \lambda \|\theta\|_2^2$

$$= (y - X\theta)^T K (y - X\theta) + \lambda \cdot \theta^T \cdot \theta$$

$$\nabla_{\theta} ((y - X\theta)^T K (y - X\theta) + \lambda \cdot \theta^T \theta)$$

$$= \lambda \mathbf{I} \cdot 2\theta - 2 X^T K (y - X\theta) = 0$$

$$- X^T K y + (X^T K X \theta + \lambda \mathbf{I} \theta) = 0$$

$$(\lambda \mathbf{I} + X^T K X) \theta = X^T K y$$

$$\theta^* = (X^T K X + \lambda \mathbf{I})^{-1} X^T K y$$

$$(\theta + \Delta\theta)^T (\theta + \Delta\theta) - \theta^T \theta = (\Delta\theta)^T \cdot \nabla (\theta^T \theta)$$

$$= (\theta^T + \Delta\theta^T) (\theta + \Delta\theta) - \theta^T \theta$$

$$= \theta^T \theta + 2(\Delta\theta)^T \theta + (\Delta\theta)^T \Delta\theta - \theta^T \theta$$

$$= (\Delta\theta)^T \cdot 2\theta + (\Delta\theta)^T \cdot \Delta\theta$$

$$(y - X(\theta + \Delta\theta))^T K (y - X(\theta + \Delta\theta)) - (y - X\theta)^T K (y - X\theta)$$

$$= (y^T - \theta^T X^T - (\Delta\theta)^T X^T) K (y - X\theta - X\Delta\theta)$$

$$= (y - X\theta)^T K (y - X\theta) -$$

$$= (y - X\theta)^T K (-X\Delta\theta) - (\Delta\theta)^T X^T K (y - X\theta)$$

$$+ (\Delta\theta)^T X^T K X \Delta\theta \quad \Delta\theta \rightarrow 0$$

$$= -(\Delta\theta)^T X^T K^T (y - X\theta) - (\Delta\theta)^T X^T K (y - X\theta)$$

$$K^T = K \text{ since } K \text{ is diagonal} = -(\Delta\theta)^T 2 X^T K (y - X\theta)$$

4. (b)

$$L = \sum_i k_i (y_i - x_i \theta)^2 + \lambda \sum_j w_j^2$$

$$= (\mathbf{y} - \mathbf{X}\theta)^T \mathbf{K} (\mathbf{y} - \mathbf{X}\theta) + \lambda \|\mathbf{w}\|_2^2$$

$$\theta = \begin{bmatrix} \mathbf{w} \\ b \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} \tilde{\mathbf{X}} & \mathbf{1} \end{bmatrix} \quad \begin{array}{l} \text{below the } \mathbf{X} \text{ has} \\ \text{become } \tilde{\mathbf{X}} \end{array}$$

$$= (\mathbf{y} - [\tilde{\mathbf{X}}, \mathbf{1}] \begin{bmatrix} \mathbf{w} \\ b \end{bmatrix})^T \mathbf{K} (\mathbf{y} - [\tilde{\mathbf{X}}, \mathbf{1}] \begin{bmatrix} \mathbf{w} \\ b \end{bmatrix}) + \lambda \|\mathbf{w}\|_2^2 + \lambda b^2$$

$$= (\mathbf{y} - \tilde{\mathbf{X}}\mathbf{w} - b\mathbf{e})^T \mathbf{K} (\mathbf{y} - \tilde{\mathbf{X}}\mathbf{w} - b\mathbf{e})$$

$$\text{let } \mathbf{B} = b\mathbf{e} = \begin{bmatrix} b \\ b \\ \vdots \\ b \end{bmatrix} \quad + \lambda \|\mathbf{w}\|_2^2 + \lambda b^2$$

$$= (\mathbf{y}^T - \mathbf{w}^T \tilde{\mathbf{X}}^T - \mathbf{B}^T) \mathbf{K} (\mathbf{y} - \tilde{\mathbf{X}}\mathbf{w} - \mathbf{B})$$

$$= (\mathbf{y}^T \mathbf{K} - \mathbf{w}^T \tilde{\mathbf{X}}^T \mathbf{K} - \mathbf{B}^T \mathbf{K}) (\mathbf{y} - \tilde{\mathbf{X}}\mathbf{w} - \mathbf{B}) + \lambda \mathbf{w}^T \mathbf{w} + \lambda b^2$$

$$= \mathbf{y}^T \mathbf{K} \mathbf{y} - \mathbf{y}^T \mathbf{K} \tilde{\mathbf{X}} \mathbf{w} - \mathbf{y}^T \mathbf{K} \mathbf{B} - \mathbf{w}^T \tilde{\mathbf{X}}^T \mathbf{K} \mathbf{y} + \mathbf{w}^T \tilde{\mathbf{X}}^T \mathbf{K} \tilde{\mathbf{X}} \mathbf{w} + \mathbf{w}^T \tilde{\mathbf{X}}^T \mathbf{K} \mathbf{B} - \mathbf{B}^T \mathbf{K} \mathbf{y} + \mathbf{B}^T \mathbf{K} \tilde{\mathbf{X}} \mathbf{w} + \mathbf{B}^T \mathbf{K} \mathbf{B} + \lambda \mathbf{w}^T \mathbf{w} + \lambda b^2$$

$$= \mathbf{y}^T \mathbf{K} \mathbf{y} - 2 \mathbf{y}^T \mathbf{K} \tilde{\mathbf{X}} \mathbf{w} - 2 \mathbf{y}^T \mathbf{K} \mathbf{B} + 2 \mathbf{B}^T \mathbf{K} \tilde{\mathbf{X}} \mathbf{w} + \mathbf{w}^T \tilde{\mathbf{X}}^T \mathbf{K} \tilde{\mathbf{X}} \mathbf{w} + \mathbf{B}^T \mathbf{K} \mathbf{B} + \lambda \mathbf{w}^T \mathbf{w} + \lambda b^2$$

$$\begin{aligned} \nabla_b L &= 2b \operatorname{tr}(\mathbf{K}) - 2(\mathbf{y}_1 k_1 + \mathbf{y}_2 k_2 + \dots + \mathbf{y}_n k_n) \quad \frac{\partial \mathbf{y}^T \mathbf{K} \mathbf{B}}{\partial b} \\ &\quad + 2((\tilde{\mathbf{X}} \mathbf{w})_1 k_1 + (\tilde{\mathbf{X}} \mathbf{w})_2 k_2 + \dots + (\tilde{\mathbf{X}} \mathbf{w})_n k_n) \\ &= 2b \operatorname{tr}(\mathbf{K}) - 2 \mathbf{e}^T \mathbf{K} \mathbf{y} + 2 \mathbf{e}^T \mathbf{K} \tilde{\mathbf{X}} \mathbf{w} \quad \frac{\partial \mathbf{B}^T \mathbf{K} \tilde{\mathbf{X}} \mathbf{w}}{\partial b} \\ &= 0 \quad b^* = \frac{(\mathbf{e}^T \mathbf{K} \mathbf{y} - \mathbf{e}^T \mathbf{K} \tilde{\mathbf{X}} \mathbf{w})}{\operatorname{tr}(\mathbf{K})} \end{aligned}$$

$$\nabla_w L = -2 \frac{\partial \tilde{y}^T K \tilde{x} w}{\partial w} + 2 \frac{\partial B^T K \tilde{x} w}{\partial w} + \lambda \frac{w^T w}{\partial w} + \frac{w^T \tilde{x}^T K \tilde{x} w}{\partial w}$$

$$= -2 \tilde{x}^T K \tilde{y} + 2 \tilde{x}^T K B + 2 \lambda w + 2 \tilde{x}^T K \tilde{x} w$$

$$4-b) = 0 \quad -\tilde{x}^T K \tilde{y} + \tilde{x}^T K B + \lambda I w + \tilde{x}^T K \tilde{x} w = 0$$

$$(\tilde{x}^T K \tilde{x} + \lambda I) w = \tilde{x}^T K (\tilde{y} - B)$$

$$B = \left[\begin{array}{c} \frac{e^T K \tilde{y} - e^T K \tilde{x} w}{\text{tr}(K)} \\ \vdots \\ \frac{e^T K \tilde{y} - e^T K \tilde{x} w}{\text{tr}(K)} \end{array} \right] \quad e^n = e \frac{e^T K \tilde{y} - e^T K \tilde{x} w}{\text{tr}(K)}$$

$$(\tilde{x}^T K \tilde{x} + \lambda I) w = \tilde{x}^T K \left(\tilde{y} - e \frac{e^T K \tilde{y} - e^T K \tilde{x} w}{\text{tr}(K)} \right)$$

$$(\tilde{x}^T K \tilde{x} + \lambda I) w = \tilde{x}^T K \left(\tilde{y} - \frac{e e^T K \tilde{x} w}{\text{tr}(K)} \right)$$

$$= \tilde{x}^T K \left(\tilde{y} - \frac{e e^T K \tilde{y}}{\text{tr}(K)} \right)$$

$$\left(\tilde{x}^T K \tilde{x} + \lambda I - \frac{\tilde{x}^T K e e^T K \tilde{x}}{\text{tr}(K)} \right) w = \tilde{x}^T K \left(\tilde{y} - \frac{e e^T K \tilde{y}}{\text{tr}(K)} \right)$$

$$W^* = \left(\tilde{x}^T K \tilde{x} + \lambda I - \frac{\tilde{x}^T K e e^T K \tilde{x}}{\text{tr}(K)} \right)^{-1} \tilde{x}^T K \left(\tilde{y} - \frac{e e^T K \tilde{y}}{\text{tr}(K)} \right)$$

$$\begin{aligned}
5. \quad f_{w,b}(x) &= w^T x + b \\
\hat{L}_{ss}(w,b) &= \mathbb{E} \left[\frac{1}{2N} \sum_{i=1}^N (f_{w,b}(x_i + \eta_i) - y_i)^2 \right] \\
&= \frac{1}{2N} \mathbb{E} \left[\sum_{i=1}^N (f_{w,b}(x_i + \eta_i) - y_i)^2 \right] \\
&= \frac{1}{2N} \sum_{i=1}^N \mathbb{E} [(w^T(x_i + \eta_i) - y_i)^2] \\
&= \frac{1}{2N} \sum_{i=1}^N \mathbb{E} [(w^T x_i - y_i + w^T \eta_i)^2] \\
&= \frac{1}{2N} \sum_{i=1}^N \mathbb{E} [(f_{w,b}(x_i) - y_i + w^T \eta_i)^2] \\
&= \frac{1}{2N} \sum_{i=1}^N \left((f_{w,b}(x_i) - y_i)^2 + 2(f_{w,b}(x_i) - y_i) \mathbb{E}(w^T \eta_i) + \mathbb{E}(w^T \eta_i)^2 \right) \\
&= \frac{1}{2N} \sum_{i=1}^N (f_{w,b}(x_i) - y_i)^2 + \frac{1}{2N} \sum_{i=1}^N 2(f_{w,b}(x_i) - y_i) \cdot w^T \mathbb{E}(\eta_i) \\
&\quad + \frac{1}{2N} \sum_{i=1}^N \|w\|^2 \cdot \mathbb{E}[\eta_i^2] \quad , \text{ since } \mathbb{E}[\eta_i] = 0 \\
&\quad \mathbb{E}[x^2] = E(x)^2 + \text{Var}(x) \\
&= \frac{1}{2N} \sum_{i=1}^N (f_{w,b}(x_i) - y_i)^2 + 0 + \frac{1}{2N} \sum_{i=1}^N \|w\|^2 \cdot (\mathbb{E}(\eta_i)^2 + \sigma^2) \\
&= \frac{1}{2N} \sum_{i=1}^N (f_{w,b}(x_i) - y_i)^2 + \frac{1}{2N} \sum_{i=1}^N \|w\|^2 \cdot (0 + \sigma^2) \\
&= \frac{1}{2N} \sum_{i=1}^N (f_{w,b}(x_i) - y_i)^2 + \frac{\sigma^2}{2N} \cdot N \cdot \|w\|^2 \\
&= \frac{1}{2N} \sum_{i=1}^N (f_{w,b}(x_i) - y_i)^2 + \frac{\sigma^2}{2} \|w\|^2
\end{aligned}$$