

NYCU Introduction to Machine Learning, Homework 2

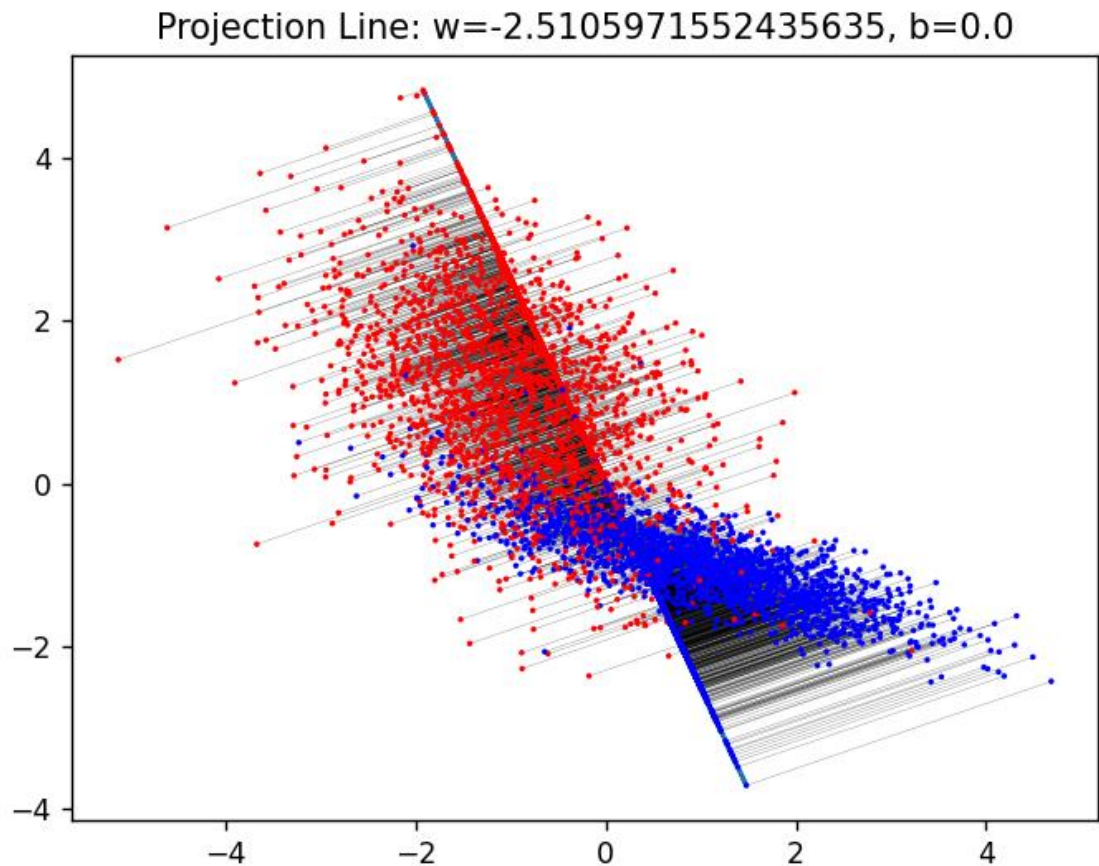
109550136 邱弘竣

Part. 1, Coding (60%):

1. (5%) Compute the mean vectors m_i ($i=1, 2$) of each 2 classes on training data
2. (5%) Compute the within-class scatter matrix S_W on training data
3. (5%) Compute the between-class scatter matrix S_B on training data
4. (5%) Compute the Fisher's linear discriminant w on training data
5. (20%) Project the testing data by Fisher's linear discriminant to get the class prediction by K-Nearest-Neighbor rule and report the accuracy score on testing data with K values from 1 to 5 (you should get accuracy over **0.88**)

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mean vector of class 1: [ 0.99253136 -0.99115481] mean vector of class 2: [-0.9888012  1.00522778]
Within-class scatter matrix SW: [[ 4337.38546493 -1795.55656547]
 [-1795.55656547  2834.75834886]]
Between-class scatter matrix SB: [[ 3.92567873 -3.95549783]
 [-3.95549783  3.98554344]]
Fisher's linear discriminant: [-0.37003809  0.92901658]
For K=1, Accuracy of test-set 0.8648
For K=2, Accuracy of test-set 0.8808
For K=3, Accuracy of test-set 0.88
For K=4, Accuracy of test-set 0.8896
For K=5, Accuracy of test-set 0.9
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6. (20%) Plot the 1) **best projection line** on the training data and show the slope and intercept on the title (you can choose any value of *intercept* for better visualization)
2) **colorize the data** with each class 3) project all data points on your projection line. Your result should look like the below image (This image is for reference, not the answer)



Part. 2, Questions (40%):

(10%) 1. What's the difference between the Principle Component Analysis and Fisher's Linear Discriminant?

LDA is supervised and attempts to find a feature subspace that maximizes class separability. PCA is unsupervised and is a technique that finds the directions of maximal variance.

(10%) 2. Please explain in detail how to extend the 2-class FLD into multi-class FLD (the number of classes is greater than two).

2. 2 class

$$J(w) = \frac{w^T S_B w}{w^T S_W w}$$

$$S_B = (m_2 - m_1)(m_2 - m_1)^T$$

$$S_W = \sum_{n \in C_1} (x_n - m_1)(x_n - m_1)^T + \sum_{n \in C_2} (x_n - m_2)(x_n - m_2)^T$$

$$\frac{\partial}{\partial w} J(w) = 0 \Rightarrow w \propto S_W^{-1} (m_2 - m_1)$$

K classes

$$S_B = \sum_{k=1}^K N_k (m_k - m)(m_k - m)^T \text{ where } m = \frac{1}{N} \sum_{n=1}^N x_n$$

$$S_W = \sum_{k=1}^K S_k \text{ where } \sum_{n \in C_k} (x_n - m_k)(x_n - m_k)^T, m_k = \frac{1}{N_k} \sum_{n \in C_k} x_n$$

$$J(w) = \frac{w^T S_B w}{w^T S_W w}$$

the optimal w is the eigenvector of $S_W^{-1} S_B$ that corresponds to the largest eigenvalue

(6%) 3. By making use of Eq (1) ~ Eq (5), show that the Fisher criterion Eq (6) can be written in the form Eq (7).

$$y = \mathbf{w}^T \mathbf{x} \quad \text{Eq (1)}$$

$$\mathbf{m}_1 = \frac{1}{N_1} \sum_{n \in C_1} \mathbf{x}_n \quad \mathbf{m}_2 = \frac{1}{N_2} \sum_{n \in C_2} \mathbf{x}_n \quad \text{Eq (2)}$$

$$m_2 - m_1 = \mathbf{w}^T (\mathbf{m}_2 - \mathbf{m}_1) \quad \text{Eq (3)}$$

$$m_k = \mathbf{w}^T \mathbf{m}_k \quad \text{Eq (4)}$$

$$s_k^2 = \sum_{n \in C_k} (y_n - m_k)^2 \quad \text{Eq (5)}$$

$$J(\mathbf{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2} \quad \text{Eq (6)}$$

$$J(\mathbf{w}) = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}} \quad \text{Eq (7)}$$

3.

$$\begin{aligned}
 \sum_k^2 &= \sum_{n \in C_k} (y_n - m_k)^2 \\
 &= \sum_{n \in C_k} (W^T x_n - W^T m_k)^2 \\
 &= \sum_{n \in C_k} W^T (x_n - m_k) (x_n - m_k)^T W \\
 &= W^T \sum_k W \\
 \sum_1^2 + \sum_2^2 &= W^T \sum_1 W + W^T \sum_2 W = W^T \sum W W \quad \text{--- ①}
 \end{aligned}$$

$$\begin{aligned}
 m_2 - m_1 &= W^T (m_2 - m_1) \\
 (m_2 - m_1)^2 &= W^T (m_2 - m_1) (m_2 - m_1)^T W \\
 &= W^T \sum W W \quad \text{--- ②}
 \end{aligned}$$

From ①, ②

$$J(W) = \frac{(m_2 - m_1)^2}{\sum_1^2 + \sum_2^2} = \frac{W^T \sum W W}{W^T \sum W W}$$

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(7%) 4. Show the derivative of the error function Eq (8) with respect to the activation a_k for an output unit having a logistic sigmoid activation function satisfies Eq (9).

$$E(\mathbf{w}) = - \sum_{n=1}^N \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\} \quad \text{Eq (8)}$$

$$\frac{\partial E}{\partial a_k} = y_k - t_k \quad \text{Eq (9)}$$

4.

$$\begin{aligned}
 \frac{\partial E}{\partial a_k} &= \frac{\partial E}{\partial y} \frac{\partial y}{\partial a} \\
 &= \left(\frac{-t_k}{y_k} + \frac{1-t_k}{1-y_k} \right) y_k (1-y_k) \\
 &= y_k - t_k
 \end{aligned}$$

#

$$\begin{aligned}
 \frac{\partial E}{\partial y} &= \frac{\partial}{\partial y} (t_k \ln y_k) + \frac{\partial}{\partial y} ((1-t_k) \ln(1-y_k)) \\
 &= \frac{-t_k}{y_k} + \frac{1-t_k}{1-y_k} \\
 \frac{\partial y}{\partial a} &= \frac{\partial}{\partial a} \left(\frac{1}{1+e^{-a}} \right) = \frac{-(-e^{-a})}{(1+e^{-a})^2} \\
 &= \frac{1+e^{-a}}{(1+e^{-a})^2} - \frac{1}{(1+e^{-a})^2} \\
 &= \frac{1}{1+e^{-a}} \left(1 - \frac{1}{1+e^{-a}} \right) \\
 &= y(1-y)
 \end{aligned}$$

(7%) 5. Show that maximizing likelihood for a multiclass neural network model in which the network outputs have the interpretation $y_k(\mathbf{x}, \mathbf{w}) = p(t_k = \mathbf{1} | \mathbf{x})$ is equivalent to the minimization

of the cross-entropy error function Eq (10).

$$E(\mathbf{w}) = - \sum_{n=1}^N \sum_{k=1}^K t_{kn} \ln y_k(\mathbf{x}_n, \mathbf{w}) \quad \text{Eq (10)}$$

5.

2-class

$$\mathcal{P}(t|w) = \prod_{n=1}^N y_n^{t_n} (1 - y_n)^{1-t_n} \quad \text{where } t = (t_1, \dots, t_N)^T, y_n = \mathcal{P}(t_n|w_n)$$

multiclass

$$\mathcal{P}(T|w_1, \dots, w_K) = \prod_{n=1}^N \prod_{k=1}^K \mathcal{P}(t_{nk}|w_k) = \prod_{n=1}^N \prod_{k=1}^K y_{nk}^{t_{nk}}$$

$$E(w_1, \dots, w_K) = -\ln \mathcal{P}(T|w_1, \dots, w_K) = -\sum_{n=1}^N \sum_{k=1}^K t_{nk} \ln y_{nk} \quad \#$$