ESE 5420 Homework 4

Mohammed Raza Syed - Penn ID: 37486255

Problem 1

a) Likelihood Function for a Single Observation

The distribution of Y_i depends on a, b, σ , and x_i . Of these, only a and b are unknown. Since $Y_i \sim ax_i + b + \varepsilon_i$ and $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$, it follows that

$$Y_i \sim \mathcal{N}(ax_i + b, \sigma^2).$$

The probability density function for a normally distributed random variable Y_i with mean $\mu = ax_i + b$ and variance σ^2 is:

$$f(y_i|a, b, x_i, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_i - (ax_i + b))^2}{2\sigma^2}\right).$$

This is the likelihood function for a single observation y_i , given the parameters a, b, x_i , and σ .

b) Likelihood and Log-Likelihood for the Dataset

For the entire dataset $(x_1, y_1), \ldots, (x_n, y_n)$, the likelihood function is the product of the individual likelihoods for each observation, assuming independence:

$$L(a, b, \sigma) = \prod_{i=1}^{n} f(y_i | a, b, x_i, \sigma).$$

Substituting the expression for $f(y_i|a,b,x_i,\sigma)$ from part (a), we have:

$$L(a,b,\sigma) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_i - (ax_i + b))^2}{2\sigma^2}\right).$$

This simplifies to:

$$L(a,b,\sigma) = \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left(-\sum_{i=1}^{n} \frac{(y_i - (ax_i + b))^2}{2\sigma^2}\right).$$

The log-likelihood function, $\log L(a, b, \sigma)$, is obtained by taking the natural logarithm of the likelihood function:

$$\log L(a, b, \sigma) = -\frac{n}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - (ax_i + b))^2.$$

c) Maximum Likelihood Estimates for a and b

To find the maximum likelihood estimates for a and b, we need to maximize the log-likelihood function with respect to these parameters. Since σ is known and constant, maximizing $\log L(a,b,\sigma)$ is equivalent to minimizing the sum of squared residuals:

$$\sum_{i=1}^{n} (y_i - (ax_i + b))^2.$$

Partial Derivative with Respect to a The partial derivative of the sum of squared residuals with respect to a is:

$$\frac{\partial}{\partial a} \sum_{i=1}^{n} (y_i - (ax_i + b))^2 = -2 \sum_{i=1}^{n} x_i (y_i - (ax_i + b)) = 0.$$

This equation simplifies to:

$$\sum_{i=1}^{n} x_i y_i = a \sum_{i=1}^{n} x_i^2 + b \sum_{i=1}^{n} x_i.$$

Partial Derivative with Respect to b The partial derivative of the sum of squared residuals with respect to b is:

$$\frac{\partial}{\partial b} \sum_{i=1}^{n} (y_i - (ax_i + b))^2 = -2 \sum_{i=1}^{n} (y_i - (ax_i + b)) = 0.$$

This equation simplifies to:

$$\sum_{i=1}^{n} y_i = a \sum_{i=1}^{n} x_i + nb.$$

Solving for a **and** b Now we have two equations:

$$\sum_{i=1}^{n} x_i y_i = a \sum_{i=1}^{n} x_i^2 + b \sum_{i=1}^{n} x_i,$$

$$\sum_{i=1}^{n} y_i = a \sum_{i=1}^{n} x_i + nb.$$

To solve for a and b, we introduce the sample means:

$$\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$$
 and $\bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i$.

Using the second equation, we can rewrite it as:

$$\bar{y} = a\bar{x} + b.$$

Solving for b, we find:

$$b = \bar{y} - a\bar{x}.$$

Now, substitute $b = \bar{y} - a\bar{x}$ into the first equation:

$$\sum_{i=1}^{n} x_i y_i = a \sum_{i=1}^{n} x_i^2 + (\bar{y} - a\bar{x}) \cdot \sum_{i=1}^{n} x_i.$$

Expanding and simplifying, we get:

$$\sum_{i=1}^{n} x_i y_i - n\bar{y}\bar{x} = a \left(\sum_{i=1}^{n} x_i^2 - n\bar{x}^2 \right).$$

We can simplify each side as follows:

- For the left side, note that $\sum_{i=1}^{n} x_i y_i - n\bar{y}\bar{x}$ can be rewritten as:

$$\sum_{i=1}^{n} x_i y_i - n \bar{y} \bar{x} = \sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y}),$$

which represents the sum of the products of deviations of x and y from their means.

- For the right side, note that $\sum_{i=1}^n x_i^2 - n\bar{x}^2$ is the sum of squared deviations of x from its mean:

$$\sum_{i=1}^{n} x_i^2 - n\bar{x}^2 = \sum_{i=1}^{n} (x_i - \bar{x})^2.$$

Thus, our equation becomes:

$$\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y}) = a \sum_{i=1}^{n} (x_i - \bar{x})^2.$$

Now, solving for a gives:

$$a = \frac{\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n} (x_i - \bar{x})^2}.$$

Finally, we substitute a back to find b:

$$b = \bar{y} - a\bar{x}.$$

Therefore, the maximum likelihood estimates for a and b are:

$$a = \frac{\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n} (x_i - \bar{x})^2},$$

$$b = \bar{y} - a\bar{x}.$$

Problem 2

Given a set of points $\{(x_i, y_i)\}$ and the line equation $y = \beta_1 x + \beta_0$, we aim to minimize the sum of the squared perpendicular distances from these points to the line. This is formulated as minimizing:

$$L(\beta_0, \beta_1) = \sum_{i=1}^{n} \left(\frac{y_i - \beta_1 x_i - \beta_0}{\sqrt{1 + \beta_1^2}} \right)^2$$

Expanding the loss function for differentiation, we have:

$$L(\beta_0, \beta_1) = \frac{1}{1 + \beta_1^2} \sum_{i=1}^n (y_i - \beta_1 x_i - \beta_0)^2$$

The derivative of L with respect to β_0 while treating $\sqrt{1+\beta_1^2}$ as a constant with respect to β_0 is:

$$\frac{\partial L}{\partial \beta_0} = \frac{1}{1 + \beta_1^2} \cdot 2 \sum_{i=1}^{n} -1 \cdot (y_i - \beta_1 x_i - \beta_0)$$

Setting the derivative equal to zero for minimization:

$$\sum_{i=1}^{n} (y_i - \beta_1 x_i - \beta_0) = 0$$

$$n\beta_0 + \beta_1 \sum_{i=1}^n x_i = \sum_{i=1}^n y_i$$

$$\beta_0 = \frac{\sum_{i=1}^{n} y_i - \beta_1 \sum_{i=1}^{n} x_i}{n}$$

For β_1 , the derivative involves using the quotient rule:

$$\frac{\partial L}{\partial \beta_1} = \frac{(1+\beta_1^2) \cdot \frac{\partial}{\partial \beta_1} \left(\sum_{i=1}^n (y_i - \beta_1 x_i - \beta_0)^2 \right) - \sum_{i=1}^n (y_i - \beta_1 x_i - \beta_0)^2 \cdot 2\beta_1}{(1+\beta_1^2)^2}$$

Expanding the derivative of the sum squared:

$$\frac{\partial}{\partial \beta_1} \left(\sum_{i=1}^n (y_i - \beta_1 x_i - \beta_0)^2 \right) = -2 \sum_{i=1}^n x_i (y_i - \beta_1 x_i - \beta_0)$$

Substituting this back into the derivative formula and simplifying:

$$\frac{\partial L}{\partial \beta_1} = \frac{-2(1+\beta_1^2) \sum_{i=1}^n x_i (y_i - \beta_1 x_i - \beta_0) - 2\beta_1 \sum_{i=1}^n (y_i - \beta_1 x_i - \beta_0)^2}{(1+\beta_1^2)^2}$$

Setting the derivative to zero and rearranging leads to:

$$(1+\beta_1^2)\sum_{i=1}^n x_i(y_i-\beta_1x_i-\beta_0) + \beta_1\sum_{i=1}^n (y_i-\beta_1x_i-\beta_0)^2 = 0$$

Now, substituting $\beta_0 = \frac{\sum_{i=1}^n y_i - \beta_1 \sum_{i=1}^n x_i}{n}$ into this equation, we obtain:

$$(1+\beta_1^2)\sum_{i=1}^n x_i \left(y_i - \beta_1 x_i - \frac{\sum_{i=1}^n y_i - \beta_1 \sum_{i=1}^n x_i}{n}\right) + \beta_1 \sum_{i=1}^n \left(y_i - \beta_1 x_i - \frac{\sum_{i=1}^n y_i - \beta_1 \sum_{i=1}^n x_i}{n}\right)^2 = 0$$

This equation is now entirely in terms of β_1 , as desired. Solving for β_1 would typically require some complex methods

Problem 4

4.1

Since P(X = x, Y = y) = P(Y = y)P(X = x|Y = y), we can find P(X = x, Y = +1) and P(X = x, Y = -1) as follows:

For
$$P(X = x, Y = +1)$$
:

$$P(X = x, Y = +1) = P(Y = +1) \cdot P(X = x | Y = +1)$$

Substituting the given values:

$$= \frac{3}{4} \cdot \frac{1}{2} \exp(-|x - 2|)$$

Simplifying, we get:

$$P(X = x, Y = +1) = \frac{3}{8} \exp(-|x - 2|)$$

For P(X = x, Y = -1):

$$P(X = x, Y = -1) = P(Y = -1) \cdot P(X = x | Y = -1)$$

Substituting the given values:

$$= \frac{1}{4} \cdot \frac{1}{2} \exp(-|x+2|)$$

Simplifying, we get:

$$P(X = x, Y = -1) = \frac{1}{8} \exp(-|x + 2|)$$

Thus, the expressions for P(X = x, Y = y) are:

$$P(X = x, Y = +1) = \frac{3}{8} \exp(-|x - 2|),$$

$$P(X = x, Y = -1) = \frac{1}{8} \exp(-|x + 2|).$$

4.2

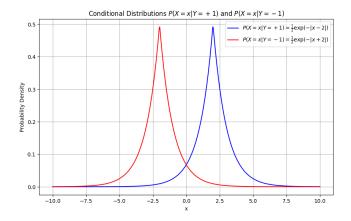


Figure 1: Conditional Distributions P(X = x | Y = +1) and P(X = x | Y = -1)

4.3

To find the Bayes optimal classification rule, we want to assign Y=+1 if P(Y=+1|X=x)>P(Y=-1|X=x) and Y=-1 otherwise.

Using Bayes' theorem, we have:

$$P(Y = +1|X = x) = \frac{P(X = x|Y = +1)P(Y = +1)}{P(X = x)}$$

$$P(Y = -1|X = x) = \frac{P(X = x|Y = -1)P(Y = -1)}{P(X = x)}$$

Since P(X = x) is the same in both cases, we only need to compare P(X = x|Y = +1)P(Y = +1) and P(X = x|Y = -1)P(Y = -1). This leads to the decision rule:

Assign
$$Y = +1$$
 if $P(X = x | Y = +1)P(Y = +1) > P(X = x | Y = -1)P(Y = -1)$.

Given:

$$P(X = x | Y = +1) = \frac{1}{2} \exp(-|x - 2|),$$

$$P(X = x | Y = -1) = \frac{1}{2} \exp(-|x + 2|),$$

$$P(Y = +1) = \frac{3}{4}, \quad P(Y = -1) = \frac{1}{4}.$$

Our inequality becomes:

$$\frac{1}{2}\exp(-|x-2|)\cdot\frac{3}{4} > \frac{1}{2}\exp(-|x+2|)\cdot\frac{1}{4}.$$

We can cancel the common terms $\frac{1}{2}$ from both sides, resulting in:

$$3\exp(-|x-2|) > \exp(-|x+2|).$$

Taking the natural logarithm on both sides gives:

$$ln(3) > |x - 2| - |x + 2|.$$

Solving the Inequality

To solve $\ln(3) > |x-2| - |x+2|$, we need to handle the absolute values by considering different cases for x.

Case 1: $x \ge 2$ In this case:

$$|x-2| = x-2$$
 and $|x+2| = x+2$.

Substituting into the inequality, we get:

$$ln(3) > (x-2) - (x+2).$$

Simplifying, we have:

$$ln(3) > -4.$$

Since $ln(3) \approx 1.0986$, this inequality is always true for $x \geq 2$.

Case 2: $-2 \le x < 2$ In this range:

$$|x-2| = 2-x$$
 and $|x+2| = x+2$.

Substituting, we get:

$$ln(3) > (2 - x) - (x + 2).$$

Simplifying, we have:

$$\ln(3) > -2x.$$

Dividing both sides by -2 (and reversing the inequality):

$$x > \frac{-\ln(3)}{2} \approx -0.5493.$$

Thus, for this case, the inequality holds when x > -0.5493.

Case 3: x < -2 In this range:

$$|x-2| = -x+2$$
 and $|x+2| = -x-2$.

Substituting, we get:

$$ln(3) > (-x+2) - (-x-2).$$

Simplifying, we have:

Since $ln(3) \approx 1.0986 < 4$, this inequality is never true for x < -2. Combining the Results For $x \ge 2$, the inequality is always true. For -0.5493 < x < 2, the inequality holds. For x < -0.5493, the inequality does not hold.

The threshold value that separates the two regions is approximately x = -0.5493. Therefore, the Bayes optimal classification rule is:

Classify as
$$Y = +1$$
 if $x > -0.5493$, and as $Y = -1$ if $x < -0.5493$.

Verification

To confirm this threshold, let us evaluate the inequality $\ln(3) > |x-2| - |x+2|$ at sample values around the threshold.

1. For x = -1:

$$|x-2| = 3$$
, $|x+2| = 1$
 $|x-2| - |x+2| = 3 - 1 = 2$

Since $ln(3) \approx 1.0986 < 2$, the inequality does not hold for x = -1.

2. For x = 0:

$$|x-2| = 2$$
, $|x+2| = 2$
 $|x-2| - |x+2| = 2 - 2 = 0$

Since ln(3) > 0, the inequality holds for x = 0.

3. For x = -0.6:

$$|x-2| = 2.6, |x+2| = 1.4$$

 $|x-2| - |x+2| = 2.6 - 1.4 = 1.2$

Since $ln(3) \approx 1.0986 < 1.2$, the inequality does not hold for x = -0.6.

4. For x = -0.5:

$$|x-2| = 2.5, \quad |x+2| = 1.5$$

 $|x-2| - |x+2| = 2.5 - 1.5 = 1.0$

Since ln(3) > 1.0, the inequality holds for x = -0.5.

These results confirm that the inequality holds for x > -0.5493 and does not hold for x < -0.5493. This verifies that the Bayes optimal classification rule is indeed:

- Classify as Y = +1 if x > -0.5493 - Classify as Y = -1 if x < -0.5493

4.4

The classification error is given by:

$$P(\text{error}) = P(X < -0.5493 \mid Y = +1) \cdot P(Y = +1) + P(X > -0.5493 \mid Y = -1) \cdot P(Y = -1)$$

Given:

$$P(X = x \mid Y = +1) = \frac{1}{2} \exp(-|x - 2|), \quad P(Y = +1) = \frac{3}{4}$$

$$P(X = x \mid Y = -1) = \frac{1}{2} \exp(-|x + 2|), \quad P(Y = -1) = \frac{1}{4}$$

The CDF for a Laplace distribution centered at μ with scale parameter b is given by:

$$F(x; \mu, b) = \begin{cases} \frac{1}{2} \exp\left(\frac{x-\mu}{b}\right) & \text{if } x < \mu \\ 1 - \frac{1}{2} \exp\left(-\frac{x-\mu}{b}\right) & \text{if } x \ge \mu \end{cases}$$

For Y = +1 (center $\mu = 2$):

$$P(X < -0.5493 \mid Y = +1) = \frac{1}{2} \exp\left(\frac{-0.5493 - 2}{1}\right)$$
$$-0.5493 - 2 = -2.5493$$
$$P(X < -0.5493 \mid Y = +1) = \frac{1}{2} \exp(-2.5493)$$

For Y = -1 (center $\mu = -2$):

$$P(X > -0.5493 \mid Y = -1) = 1 - P(X \le -0.5493 \mid Y = -1)$$

Since -0.5493 > -2,

$$\begin{split} P(X \leq -0.5493 \mid Y = -1) &= 1 - \frac{1}{2} \exp\left(-\frac{-0.5493 + 2}{1}\right) \\ &- 0.5493 + 2 = 1.4507 \\ P(X \leq -0.5493 \mid Y = -1) &= 1 - \frac{1}{2} \exp(-1.4507) \\ P(X > -0.5493 \mid Y = -1) &= \frac{1}{2} \exp(-1.4507) \end{split}$$

Substituting values:

$$P(\text{error}) = \left(\frac{1}{2}\exp(-2.5493)\right) \cdot \frac{3}{4} + \left(\frac{1}{2}\exp(-1.4507)\right) \cdot \frac{1}{4}$$

Calculating:

$$\exp(-2.5493) \approx 0.0781$$
, $\exp(-1.4507) \approx 0.2344$

$$P(\text{error}) = (0.03905) \cdot 0.75 + (0.1172) \cdot 0.25$$
$$= 0.0293 + 0.0293 = 0.0586$$

Therefore, the probability of classification error is approximately:

$$P(\text{error}) \approx 0.0586 \text{ or } 5.86\%$$

4.5

Quadratic Discriminant Analysis (QDA) offers a more flexible approach compared to Linear Discriminant Analysis (LDA) by allowing different classes to have their own covariance matrices. Here are the main steps involved in training a QDA model.

• Estimation of Parameters:

- Class Priors (π_k) : The prior probability of each class k is estimated as the proportion of training instances in that class. Mathematically:

$$\pi_k = \frac{N_k}{N}$$

where N_k is the number of instances in class k, and N is the total number of training instances.

- Class Means (μ_k): The mean vector for each class k represents the average feature values of instances in that class. It is calculated as:

$$\mu_k = \frac{1}{N_k} \sum_{i: y_i = k} x_i$$

where x_i are the feature vectors of instances that belong to class k.

- Covariance Matrices (Σ_k): Unlike LDA, QDA estimates a separate covariance matrix for each class k, allowing different variance and correlation structures for each class. The covariance matrix for class k is calculated as:

$$\Sigma_k = \frac{1}{N_k - 1} \sum_{i: u_i = k} (x_i - \mu_k) (x_i - \mu_k)^T$$

This matrix captures the spread and relationships between features within each class.

• Parametric Model: QDA assumes that each class k follows a multi-variate normal (Gaussian) distribution with its own mean vector μ_k and covariance matrix Σ_k . Thus, the likelihood of a feature vector x given class k is:

$$p(x|y=k) = \frac{1}{(2\pi)^{d/2} |\Sigma_k|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_k)^T \Sigma_k^{-1} (x-\mu_k)\right)$$

where d is the number of features, μ_k is the mean vector, and Σ_k is the covariance matrix for class k.

• **Discriminant Function**: In QDA, the decision rule is based on the log-likelihood ratio. The discriminant function for class k can be derived from

the log of the likelihood function for p(x|y=k), along with the prior π_k . For a given class k, the discriminant function is:

$$\delta_k(x) = -\frac{1}{2}\log|\Sigma_k| - \frac{1}{2}(x - \mu_k)^T \Sigma_k^{-1}(x - \mu_k) + \log \pi_k$$

This function combines the prior probability of each class and the fit of x under the class's Gaussian distribution.

• Classification Rule: To classify an observation x, QDA assigns it to the class k that maximizes the discriminant function $\delta_k(x)$. This is represented by:

$$\hat{y} = \arg\max_{k} \delta_k(x)$$

This rule selects the class k that gives the highest log-likelihood score for x, accounting for both the Gaussian distribution characteristics of each class and the class prior probabilities.

4.6

As $n \to \infty$, the parameters of the trained QDA model will converge to their true population values:

• Class Prior Probabilities:

$$P(Y = +1) = \frac{3}{4}, \quad P(Y = -1) = \frac{1}{4}$$

• Class Means:

$$\mu_{+1} = 2, \quad \mu_{-1} = -2$$

• Class Variances:

$$\sigma_{+1}^2 = 2, \quad \sigma_{-1}^2 = 2$$

Thus, the QDA model will accurately capture the underlying distributions for each class.

4.7

To simplify the QDA classifier using the provided discriminant function for onedimensional data, we proceed as follows:

The QDA classifier assigns an input x to class Y=k by maximizing the discriminant function:

$$\delta_k(x) = -\frac{1}{2}\log(\sigma_k^2) - \frac{(x-\mu_k)^2}{2\sigma_k^2} + \log(\pi_k)$$

where:

• μ_k is the mean of class k,

- σ_k^2 is the variance of class k,
- π_k is the prior probability of class k.

For this problem, we have two classes, Y = +1 and Y = -1, with:

- Means: $\mu_{+1} = 2$ and $\mu_{-1} = -2$,
- Variances: $\sigma_{+1}^2 = 2$ and $\sigma_{-1}^2 = 2$,
- Priors: $\pi_{+1} = \frac{3}{4}$ and $\pi_{-1} = \frac{1}{4}$.

We start by writing the discriminant functions for each class. For Y = +1:

$$\delta_{+1}(x) = -\frac{1}{2}\log(2) - \frac{(x-2)^2}{4} + \log\left(\frac{3}{4}\right)$$

For Y = -1:

$$\delta_{-1}(x) = -\frac{1}{2}\log(2) - \frac{(x+2)^2}{4} + \log\left(\frac{1}{4}\right)$$

The decision rule is to assign class Y = +1 if $\delta_{+1}(x) > \delta_{-1}(x)$. Substituting the expressions for $\delta_{+1}(x)$ and $\delta_{-1}(x)$ and simplifying gives:

$$-\frac{(x-2)^2}{4} + \log(3) > -\frac{(x+2)^2}{4}$$

We now expand the squared terms on each side. For the left side:

$$-\frac{(x-2)^2}{4} + \log(3) = -\frac{x^2 - 4x + 4}{4} + \log(3) = -\frac{x^2}{4} + x - 1 + \log(3)$$

For the right side:

$$-\frac{(x+2)^2}{4} = -\frac{x^2+4x+4}{4} = -\frac{x^2}{4} - x - 1$$

Substituting back, we get:

$$-\frac{x^2}{4} + x - 1 + \log(3) > -\frac{x^2}{4} - x - 1$$

$$x - 1 + \log(3) > -x - 1$$

$$x + \log(3) > -x$$

$$2x + \log(3) > 0$$

$$x > -\frac{\log(3)}{2}$$

Thus, the simplified classification rule is: - Classify as Y=+1 if $x>-\frac{\log(3)}{2}$, - Classify as Y=-1 if $x<-\frac{\log(3)}{2}$.

The decision boundary is at $x = -\frac{\log(3)}{2}$, which is approximately -0.5493. This threshold is derived based on maximizing the likelihood of each class given the discriminant function, resulting in a simple decision rule based on whether x is greater or less than this threshold.

- Classify as Y=+1 if x>-0.5493 - Classify as Y=-1 if x<-0.5493

4.8

In Part 7, the QDA classifier yielded a decision rule with a threshold at x=-0.5493, which matches the Bayes optimal decision boundary for this problem as computed in Q4.3

QDA performs optimally when we have many training data points, as the parameters estimated by QDA (class means, variances, and priors) converge to their true population values. Thus, with sufficient data, QDA approximates the Bayes optimal classifier closely.

In summary:

- QDA performs optimally when there are many training data points, as it captures the true class distributions accurately.
- In this problem, where the data distribution aligns with the QDA model assumptions, the QDA classifier achieves Bayes optimal performance even with finite data.