EE708, Assignment 4 Submission

Dhruv Gupta, Roll no: 240354

Problem 1

Question

A dataset contains 200 samples classified into two classes:

120 positive and 80 negatives.

- a Compute the Gini index before splitting.
- b If a split results in subsets:

Left: (50 positive, 10 negative) Right: (70 positive, 70 negative) Compute the weighted Gini index and determine whether the split improves purity

Answer

Formula for Gini Index is:

Gini-Index =
$$1 - \sum_{i=1}^{K} p(i)^2$$

Where p(i) represents the probability of the object being classified into a particular class out of K classes.

We have, p(positive) = 120/200 = 0.6 and p(negative) = 80/200 = 0.4 Hence, our Gini-Index before splitting can be written as:

$$GI_{initial} = 1 - (0.6^2 + 0.4^2) = 0.48$$

After the split happens:

$$p(\text{positive and left}) = 50/60 = 0.833$$
 $p(\text{positive and right}) = 70/140 = 0.5$

$$p(\text{negative and left}) = 10/60 = 0.167$$
 $p(\text{negative and right}) = 70/140 = 0.5$

$$GI_{left} = 1 - (0.833^2 + 0.167^2) = 0.278$$
 $GI_{right} = 1 - (0.5^2 + 0.5^2) = 0.5$

Weighted sum of Gini-Indices after the split can be written as:

$$GI_{final} = p(left) \cdot GI_{left} + p(right) \cdot GI_{right}$$

$$\implies GI_{final} = \frac{60}{200} \cdot 0.278 + \frac{140}{200} \cdot 0.5 = 0.43$$

So, we get: the final Gini-Index after splitting as 0.43, which is less than the initial GI, hence, **the split improves purity.**

Problem 2

Question

Consider the given dataset with two independent variables (x_1, x_2) and one dependent variable (y):

- a Use the sum of squared errors (SSE) to determine the best splitting point for x_1 .
- b Construct the first split of a regression tree using SSE as the impurity measure.

Answer

(a) Best Splitting Point for x_1 Using SSE

Calculate Total SSE Without Splitting: The mean of y is:

$$\bar{y} = \frac{10 + 12 + 15 + 18 + 21 + 25 + 28 + 30}{8} = 19.875$$

The total SSE is:

$$SSE = \sum (y_i - 19.875)^2 = 484.875$$

Evaluate Possible Splits for x_1 and Compute SSE:

For each split, we divide the data into left $(x_1 \leq k)$ and right $(x_1 > k)$ groups. The SSE for each group is calculated using the formula:

$$SSE = \sum (y_i - \bar{y})^2$$

After evaluating all possible splits, the split at $x_1 = 4.5$ results in the lowest SSE, making it the best choice.

(b) First Split Using SSE as the Impurity Measure

We can consider the first split from either x_1 or x_2 . On calculation, we see that the SSE is same for first split at either $x_1 = 4.5$ or $x_2 = 10$. At $x_1 = 4.5$:

$$\bar{y}_L = \frac{10 + 12 + 15 + 18}{4} = 13.75 \qquad \bar{y}_R = \frac{21 + 25 + 28 + 30}{4} = 26$$

$$SSE_R = (21 - 26)^2 + (25 - 26)^2 + (28 - 26)^2 + (30 - 26)^2 = 34$$

$$SSE_L = (10 - 13.75)^2 + (12 - 13.75)^2 + (15 - 13.75)^2 + (18 - 13.75)^2 = 21.5$$

Total SSE After Split:

$$SSE_{\text{split}} = 21.5 + 34 = 55.5$$

Thus, the first split is made at $x_1 = 4.5$ using SSE as the impurity measure.

Problem 3

Question

Consider a 2-dimensional feature space with a dataset of N=10 points. VQ system maps these points into K=3 clusters using a codebook. Given the following initial cluster centroids:

$$C_1 = (2,3)$$
 $C_2 = (5,8)$ $C_3 = (9,4)$

Assign the following data points to their closest centroid using squared Euclidean distance:

$$(1,2)$$
 $(3,4)$ $(6,7)$ $(8,3)$, $(5,5)$

- a Compute the new centroids after one iteration of vector quantization.
- b Show whether the distortion decreases after this iteration.

Answer

Computing distances: Given Centroids: Cluster Assignment Given the initial centroids:

$$C_1 = (2,3), \quad C_2 = (5,8), \quad C_3 = (9,4)$$

And the five data points:

$$P_1 = (1, 2), P_2 = (3, 4), P_3 = (6, 7), P_4 = (8, 3), P_5 = (5, 5)$$

We compute the squared Euclidean distance (distortion) for each data point to the centroids using the following formula:

$$d^{2} = (x_{1} - x_{2})^{2} + (y_{1} - y_{2})^{2}$$

Assigning clusters: For the first point, P_1 , we have the distances:

$$d^{2}(P_{1}, C_{1}) = 2$$
 $d^{2}(P_{1}, C_{1}) = 52$ $d^{2}(P_{1}, C_{1}) = 68$

Hence, P_1 belongs in cluster 1.

Similarly, following this process of assigning clusters, we get the following results:

$$(1,2) \to C_1, \quad (3,4) \to C_1,$$

 $(6,7) \to C_2, \quad (8,3) \to C_3, \quad (5,5) \to C_2$

Centroid Updates: New centroids are calculated as the mean of points in each cluster:

$$C'_1 = \frac{(1,2) + (3,4)}{2} = (2,3)$$
 $C'_2 = \frac{(6,7) + (5,5)}{2} = (5.5,6)$ $C'_3 = (8,3)$

This completes our first iteration of vector quantisation.

Answer continued

Distortion Comparison: The total distortion is calculated as:

$$D = \sum_{\text{all points}} d^2(\text{point, its centroid})$$

Initial distortion (with centroids C_i): $D_{\text{initial}} = 2 + 2 + 2 + 2 + 9 = 17$ Final distortion (with centroids C'_i): $D_{\text{final}} = 2 + 2 + 1.25 + 1.25 + 0 = 6.5$

Clearly, the distortion has decreased significantly after this iteration of VQ.

Problem 4

Question

$$E_Z[\ln p(X, Z|\mu, \Sigma, \pi)] = \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) (\ln \pi_k + \ln \mathcal{N}(x_n|\mu_k, \Sigma_k))$$

Show that if we maximize the first equation with respect to Σ_k and π_k while keeping the responsibilities $\gamma(z_{nk})$ fixed, we obtain the closed-form solutions given by the following equations:

$$\Sigma_{k} = \frac{1}{N_{k}} \sum_{n=1}^{N} \gamma(z_{nk}) (x_{n} - \mu_{k}) (x_{n} - \mu_{k})^{T} \qquad \pi_{k} = \frac{N_{k}}{N}$$

Answer

We perform the process of "Expectation Maximization"; we have to maximize the log-likelihood function with respect to Σ_k and π_k , hence we will partially differentiate it with respect to these parameters and set the equation equal to zero.

Gaussian Distribution: $\mathcal{N}(x_n|\mu_k, \Sigma_k)$ is a Gaussian distribution function given by:

$$\mathcal{N}(x|\mu_k, \Sigma_k) = \frac{1}{(2\pi)^{d/2} |\Sigma_k|^{1/2}} \exp\left(-\frac{1}{2} (x - \mu_k)^T \Sigma_k^{-1} (x - \mu_k)\right)$$

Logarithm of $\mathcal{N}(x_n|\mu_k, \Sigma_k)$ would be:

$$ln \mathcal{N}(x|\mu_k, \Sigma_k) = -\frac{1}{2}ln|\Sigma_k| - \left(\frac{1}{2}(x-\mu_k)^T \Sigma_k^{-1}(x-\mu_k)\right) + \text{constant}$$

We will use this result in further steps.

Answer continued

Maximization of expected log likelihood function: We substitute the calculated value of $\ln \mathcal{N}(x|\mu_k, \Sigma_k)$ into the equation:

$$E_Z[\ln p(X, Z|\mu, \Sigma, \pi)] = \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) (\ln \pi_k + \ln \mathcal{N}(x_n|\mu_k, \Sigma_k))$$

Note: We are keeping the responsibility $\gamma(z_{nk})$ constant here for all further calculations as mentioned in the question.

Maximize with respect to Σ_k : We differentiate the expected log likelihood with respect to Σ_k and set it equal to zero.

$$\frac{\partial}{\partial \Sigma_k} \sum_{n=1}^N \gamma(z_{nk}) \left(-\frac{1}{2} \ln |\Sigma_k| - \frac{1}{2} (x_n - \mu_k)^T \Sigma_k^{-1} (x_n - \mu_k) \right) = 0$$

Solving this results in the closed-form solution:

$$\Sigma_k = \frac{1}{\psi} \sum_{n=1}^{N} \gamma(z_{nk}) (x_n - \mu_k) (x_n - \mu_k)^T, \quad \text{where } \psi = \sum_{n=1}^{N} \gamma(z_{nk})$$

Maximize with respect to π_k : Here, π_k represents the mixing coefficients, so there is a constraint that $\sum_{k=1}^{K} \pi_k = 1$, this means we can use the method of Lagrange Multipliers and solve this.

We differentiate the Log-Likelihood wrt π_k and get:

$$\pi_k = \frac{\psi}{N}, \quad \text{where } \psi = \sum_{n=1}^N \gamma(z_{nk})$$

 ψ represents the effective number of points assigned to a specific cluster

Problem 5

Question

Consider a density model given by a mixture distribution

$$p(x) = \sum_{k=1}^{K} \pi_k p(x|k)$$

and suppose that we partition the vector x into two parts so that $x = (x_a, x_b)$. Show that the conditional density $p(x_b|x_a)$ is itself a mixture distribution and find expressions for the mixing coefficients and component densities.

Answer

Using Bayes' theorem:

$$p(x_b|x_a) = \frac{p(x_a, x_b)}{p(x_a)}$$

Now, $p(x) = p(x_a, x_b)$

$$p(x_b|x_a) = \frac{\sum_{i=1}^{K} \pi_i p(x_a, x_b|i)}{\sum_{j=1}^{K} \pi_j p(x_a|j)}$$

Now, $p(x_a, x_b|i) = p(x_a|i) \cdot p(x_b|x_a, i)$

$$p(x_b|x_a) = \frac{\sum_{i=1}^{K} \pi_i p(x_a|i) \cdot p(x_b|x_a, i)}{\sum_{j=1}^{K} \pi_j p(x_a|j)}$$

Define a new mixing component, $\gamma_i(x_a) = \frac{\pi_i p(x_a|i)}{\sum_{j=1}^K \pi_j p(x_a|j)}$

$$p(x_b|x_a) = \sum_{i=1}^K \gamma_i(x_a) \cdot p(x_b|x_a, i)$$

This proves that $p(x_b|x_a)$ is also in itself a mixture distribution.

Problem 6

Question

Consider a mixture of Gaussian distributions given by

$$p(x|\Theta) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x|\mu_k, \Sigma_k)$$

where:

K: Number of Gaussian components

 π_k : mixing coefficients such that $\sum_{k=1}^K \pi_k = 1$ and $\pi_k > 0$ $\mathcal{N}(x|\mu_k, \Sigma_k)$: Gaussian density with mean μ_k and covariance Σ_k

 $\Theta = \{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$: represents the parameters of the model.

- a Write down the complete log-likelihood function for a dataset $\{x_1, x_2...x_N\}$ assuming that the data points are drawn independently from the mixture
- b Derive the Maximum Likelihood Estimation (MLE) update rules for π_k, μ_k and Σ_k , assuming that the component that generated each data point is known.

Answer

To write the complete log-likelihood function, we will first find the likelihood function, $L(\Theta)$. Probability of x being modeled by Θ is the product of probabilities of each individual component x_n being modeled by Θ

$$p(x|\Theta) = \prod_{n=1}^{N} \sum_{k=1}^{K} p(x_n|\Theta) \implies L(\Theta) = \prod_{n=1}^{N} \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n|\mu_k, \Sigma_k)$$

So our log-likelihood function becomes:

$$lnL(\Theta) = \sum_{n=1}^{N} ln \left(\sum_{k=1}^{K} \pi_k \mathcal{N}(x_n | \mu_k, \Sigma_k) \right)$$

MLE Update Rules:

Since we're assuming we know which component each datapoint belongs to, we can introduce a latent variable, z_{nk} , where $z_{nk} = 1$ if the point x_n was generated by component k, otherwise zero. Hence, our log likelihood can be written as:

$$lnL(\Theta) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} \cdot ln\left(\pi_k \mathcal{N}(x_n | \mu_k, \Sigma_k)\right)$$

$$\implies lnL(\Theta) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} \cdot [ln\pi_k + ln\mathcal{N}(x_n | \mu_k, \Sigma_k)]$$

After performing Expectation Maximization on the log-liklihood function with latent variable introduced, we get the following update rules:

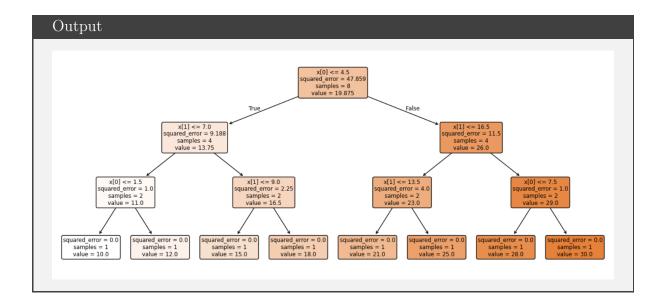
$$\pi_k = \frac{\sum_{n=1}^{N} z_{nk}}{N} \qquad \mu_k = \frac{\sum_{n=1}^{N} z_{nk} \cdot x_n}{\sum_{n=1}^{N} z_{nk}}$$

$$\Sigma_k = \frac{\sum_{n=1}^{N} z_{nk} \cdot (x_n - \mu_k)(x_n - \mu_k)^T}{\sum_{n=1}^{N} z_{nk}}$$

Problem 7

Question

Write a code to obtain a fully grown regression tree for the data given in Q2 and visualize the regression tree.



Problem 8

Question

Binary classification tree:

- a Train a fully grown binary classification tree based on Gini impurity using the dataset A4-train.csv and visualize it.
- b Compute the Sum of Squared Errors (SSE) on the test dataset (A4-test.csv) at each depth and plot the variation of SSE with depth.
- c Determine the optimal pruning depth by selecting the depth where SSE change is minimal.
- d Visualize the pruned tree.

