Machine Learning

Homework Assignment 5

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Part (a)

To model the parameters of a Gaussian mixture model (GMM) using a multi-layer neural network for 1D i.i.d. data samples x, the network's output should represent:

1. Mixing Coefficients (π_k) :

- A softmax output to ensure $\sum_{k=1}^{K} \pi_k = 1$ and $\pi_k > 0$
- Size: K units (for K components)

2. Means (μ_k) :

- Linear output (unconstrained real values)
- Size: K units

3. Variances (σ_k^2) :

- Softplus/exp output to ensure positivity
- \bullet Size: K units (for diagonal covariance in 1D)

The network takes x as input and outputs all GMM parameters $(\pi_k, \mu_k, \sigma_k^2)$ simultaneously. For batch processing, outputs are structured as tensors with dimensions matching the number of components K.

Total Output Units: 3K (for K-component GMM)

Part (b)

Recommended Activation Functions for GMM Parameters in Neural Networks

For a neural network estimating Gaussian Mixture Model (GMM) parameters, the output layers should use the following activation functions to ensure valid parameter values:

1. Mixture Weights (π_k)

- Constraint: Must be probabilities $(0 \le \pi_k \le 1)$ summing to 1
- Activation: Softmax
 - Ensures $\sum \pi_k = 1$ and $\pi_k > 0$
 - Example: For 3 components, outputs [0.2, 0.5, 0.3]

2. Means (μ_k)

- Constraint: Can be any real number
- Activation: Linear (no activation)
 - Allows $\mu_k \in (-\infty, +\infty)$
 - Example: Outputs $\left[-1.2, 0.5, 3.1\right]$ for 3 components

3. Variances (σ_k^2)

- Constraint: Must be strictly positive
- Recommended Activations:
 - Softplus: $\sigma_k^2 = \log(1 + \exp(z))$ (Smooth, avoids exact zeros)
 - **Exponential:** $\sigma_k^2 = \exp(z)$ (More aggressive for small values)
 - Example: Converts network output [-0.3, 1.2] to [0.74, 3.32]

Special Cases

For full covariance matrices (multidimensional case):

- Use Cholesky decomposition with:
 - Linear activation for off-diagonal elements
 - Softplus/Exp for diagonal elements

Note

The network should output all parameters simultaneously in a vector of length 3K (for K components):

$$[\pi_1...\pi_K, \mu_1...\mu_K, \sigma_1^2...\sigma_K^2]$$

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These choices guarantee:

1. Valid probability distribution (π_k)

- 2. Unconstrained means
- 3. Positive-definite covariance

while remaining fully differentiable for backpropagation.

Part (c)

Loss Function for Neural Network Estimating GMM Parameters

For a neural network predicting Gaussian Mixture Model (GMM) parameters, the appropriate loss function is the negative log-likelihood (NLL) of the data under the predicted mixture distribution:

Mathematical Formulation

$$L = -\frac{1}{N} \sum_{i=1}^{N} \log \left(\sum_{k=1}^{K} \pi_k \cdot \mathcal{N}(x_i | \mu_k, \sigma_k^2) \right)$$

Where:

- π_k, μ_k, σ_k^2 are the network's outputs (after proper activations)
- $\mathcal{N}(x_i|\mu_k, \sigma_k^2)$ is the Gaussian PDF evaluated at x_i
- \bullet N is the number of samples in the batch

Key Properties

- Interpretation: Minimizing this loss is equivalent to maximizing the likelihood of the data.
- Numerical Stability:
 - Compute the log-sum-exp of component log-probabilities to avoid underflow:

$$\log \sum_{k=1}^{K} \exp(\log \pi_k + \log \mathcal{N}(x_i | \mu_k, \sigma_k^2))$$

• Gradient Flow: The loss is differentiable w.r.t. all parameters $(\pi_k, \mu_k, \sigma_k^2)$, enabling backpropagation.

Notice: The order of α and β is different from the one in the question, but it does not affect the solution.

Part (a)

We have a random variable x generated through a two-level hierarchical process involving two independent binary variables y and z.

Given:

- $P(y=1) = \beta$, $P(y=0) = 1 \beta$
- $P(z=1) = \alpha$, $P(z=0) = 1 \alpha$ (independent of y)

Steps of Solution

1. Joint Distribution Decomposition

The joint distribution factors as:

$$P(x, y, z) = P(x|y, z) \cdot P(z|y) \cdot P(y)$$

Since z is independent of y, P(z|y) = P(z)

2. Component Evaluation

- P(y): $P(y=1) = \beta$, $P(y=0) = 1 \beta$
- P(z): $P(z = 1) = \alpha$, $P(z = 0) = 1 \alpha$
- \bullet P(x|y,z):
 - For y = 0:

*
$$z = 0$$
: $x \sim \text{Exp}(\lambda_1) \to P(x|y = 0, z = 0) = \lambda_1 e^{-\lambda_1 x}$

*
$$z = 1$$
: $x \sim \text{Exp}(\lambda_2) \to P(x|y = 0, z = 1) = \lambda_2 e^{-\lambda_2 x}$

- For y = 1:

*
$$z = 0$$
: $x \sim N(\mu_1, 1) \to P(x|y = 1, z = 0) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(x-\mu_1)^2}{2}}$

*
$$z = 1$$
: $x \sim N(\mu_2, 1) \to P(x|y = 1, z = 1) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(x-\mu_2)^2}{2}}$

3. Final Joint Distribution

$$P(x,y,z) = \begin{cases} (1-\beta)(1-\alpha)\lambda_1 e^{-\lambda_1 x} & \text{if } y = 0, z = 0\\ (1-\beta)\alpha\lambda_2 e^{-\lambda_2 x} & \text{if } y = 0, z = 1\\ \beta(1-\alpha)\frac{1}{\sqrt{2\pi}}e^{-\frac{(x-\mu_1)^2}{2}} & \text{if } y = 1, z = 0\\ \beta\alpha\frac{1}{\sqrt{2\pi}}e^{-\frac{(x-\mu_2)^2}{2}} & \text{if } y = 1, z = 1 \end{cases}$$

Part (b)

Complete Data Log-Likelihood Derivation

1. Complete Data Likelihood

For N i.i.d. observations:

$$\mathcal{L}_{\text{complete}} = \prod_{i=1}^{N} P(x_i, y_i, z_i)$$

Expanding:

$$\mathcal{L}_{\text{complete}} = \prod_{i:y_i=0,z_i=0} \left[(1-\beta)(1-\alpha)\lambda_1 e^{-\lambda_1 x_i} \right]$$

$$\times \prod_{i:y_i=0,z_i=1} \left[(1-\beta)\alpha\lambda_2 e^{-\lambda_2 x_i} \right]$$

$$\times \prod_{i:y_i=1,z_i=0} \left[\beta(1-\alpha) \frac{1}{\sqrt{2\pi}} e^{-\frac{(x_i-\mu_1)^2}{2}} \right]$$

$$\times \prod_{i:y_i=1,z_i=1} \left[\beta\alpha \frac{1}{\sqrt{2\pi}} e^{-\frac{(x_i-\mu_2)^2}{2}} \right]$$

2. Log-Likelihood Derivation

Taking natural logarithm:

$$\ell_{\text{complete}} = \sum_{i:y_i = 0, z_i = 0} \left[\ln(1 - \beta) + \ln(1 - \alpha) + \ln \lambda_1 - \lambda_1 x_i \right]$$

$$+ \sum_{i:y_i = 0, z_i = 1} \left[\ln(1 - \beta) + \ln \alpha + \ln \lambda_2 - \lambda_2 x_i \right]$$

$$+ \sum_{i:y_i = 1, z_i = 0} \left[\ln \beta + \ln(1 - \alpha) - \frac{1}{2} \ln(2\pi) - \frac{(x_i - \mu_1)^2}{2} \right]$$

$$+ \sum_{i:y_i = 1, z_i = 1} \left[\ln \beta + \ln \alpha - \frac{1}{2} \ln(2\pi) - \frac{(x_i - \mu_2)^2}{2} \right]$$

3. Final Expression

Let $N_{ab} := \#\{i : y_i = a, z_i = b\}$. Then:

$$\ell_{\text{complete}} = N_{00} \left[\ln(1 - \beta) + \ln(1 - \alpha) + \ln \lambda_1 \right]$$

$$+ N_{01} \left[\ln(1 - \beta) + \ln \alpha + \ln \lambda_2 \right]$$

$$+ N_{10} \left[\ln \beta + \ln(1 - \alpha) - \frac{1}{2} \ln(2\pi) \right]$$

$$+ N_{11} \left[\ln \beta + \ln \alpha - \frac{1}{2} \ln(2\pi) \right]$$

$$- \lambda_1 \sum_{i:y_i=0,z_i=0} x_i - \lambda_2 \sum_{i:y_i=0,z_i=1} x_i$$

$$- \frac{1}{2} \sum_{i:y_i=1,z_i=0} (x_i - \mu_1)^2 - \frac{1}{2} \sum_{i:y_i=1,z_i=1} (x_i - \mu_2)^2$$

where "Group ab" denotes observations where y = a, z = b.

Part (c)

E-Step for Hidden Variables (y_i, z_i) in EM Algorithm

1. Goal of the E-Step

Compute posterior probabilities for each observation x_i :

- $\gamma_{i,00} = P(y_i = 0, z_i = 0 \mid x_i)$
- $\gamma_{i,01} = P(y_i = 0, z_i = 1 \mid x_i)$
- $\gamma_{i,10} = P(y_i = 1, z_i = 0 \mid x_i)$
- $\gamma_{i,11} = P(y_i = 1, z_i = 1 \mid x_i)$

2. Bayes' Rule Application

For each $(a, b) \in \{0, 1\}^2$:

$$\gamma_{i,ab} = \frac{P(x_i \mid y_i = a, z_i = b) \cdot P(y_i = a, z_i = b)}{P(x_i)}$$

where:

$$P(x_i) = \sum_{a,b} P(x_i \mid y_i = a, z_i = b) \cdot P(y_i = a, z_i = b)$$

3. Component Probabilities

Joint probabilities:

$$P(y_i = 0, z_i = 0) = (1 - \beta)(1 - \alpha)$$

$$P(y_i = 0, z_i = 1) = (1 - \beta)\alpha$$

$$P(y_i = 1, z_i = 0) = \beta(1 - \alpha)$$

$$P(y_i = 1, z_i = 1) = \beta\alpha$$

Conditional likelihoods:

$$P(x_i \mid y_i = 0, z_i = 0) = \lambda_1 e^{-\lambda_1 x_i}$$

$$P(x_i \mid y_i = 0, z_i = 1) = \lambda_2 e^{-\lambda_2 x_i}$$

$$P(x_i \mid y_i = 1, z_i = 0) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(x_i - \mu_1)^2}{2}}$$

$$P(x_i \mid y_i = 1, z_i = 1) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(x_i - \mu_2)^2}{2}}$$

4. Posterior Probabilities

$$\gamma_{i,00} = \frac{(1-\beta)(1-\alpha)\lambda_1 e^{-\lambda_1 x_i}}{P(x_i)}$$

$$\gamma_{i,01} = \frac{(1-\beta)\alpha\lambda_2 e^{-\lambda_2 x_i}}{P(x_i)}$$

$$\gamma_{i,10} = \frac{\beta(1-\alpha)\frac{1}{\sqrt{2\pi}}e^{-\frac{(x_i-\mu_1)^2}{2}}}{P(x_i)}$$

$$\gamma_{i,11} = \frac{\beta\alpha\frac{1}{\sqrt{2\pi}}e^{-\frac{(x_i-\mu_2)^2}{2}}}{P(x_i)}$$

where $P(x_i)$ is the sum of all numerators.

5. Expected Values Computation

Expected counts:

$$\mathbb{E}[N_{00}] = \sum_{i=1}^{N} \gamma_{i,00}$$

$$\mathbb{E}[N_{01}] = \sum_{i=1}^{N} \gamma_{i,01}$$

$$\mathbb{E}[N_{10}] = \sum_{i=1}^{N} \gamma_{i,10}$$

$$\mathbb{E}[N_{11}] = \sum_{i=1}^{N} \gamma_{i,11}$$

Auxiliary expected values:

$$\mathbb{E}\left[\sum_{i:y_i=0,z_i=0} x_i\right] = \sum_{i=1}^N \gamma_{i,00} x_i$$

$$\mathbb{E}\left[\sum_{i:y_i=0,z_i=1} x_i\right] = \sum_{i=1}^N \gamma_{i,01} x_i$$

$$\mathbb{E}\left[\sum_{i:y_i=1,z_i=0} (x_i - \mu_1)^2\right] = \sum_{i=1}^N \gamma_{i,10} (x_i - \mu_1)^2$$

$$\mathbb{E}\left[\sum_{i:y_i=1,z_i=1} (x_i - \mu_2)^2\right] = \sum_{i=1}^N \gamma_{i,11} (x_i - \mu_2)^2$$

Part (d)

M-Step: Updating Parameters β , μ_2 , and λ_2

1. Update Rule for β

Parameter β represents $P(y_i = 1)$.

Update Formula:

$$\beta^{\text{new}} = \frac{\mathbb{E}[N_{10} + N_{11}]}{N} = \frac{\sum_{i=1}^{N} (\gamma_{i,10} + \gamma_{i,11})}{N}$$

where:

- $\gamma_{i,10} = P(y_i = 1, z_i = 0 \mid x_i)$
- $\gamma_{i,11} = P(y_i = 1, z_i = 1 \mid x_i)$

Derivation: The update maximizes the expected complete-data log-likelihood with respect to β , representing the expected proportion of observations where $y_i = 1$.

2. Update Rule for μ_2

Parameter μ_2 is the mean of the Gaussian distribution when $(y_i = 1, z_i = 1)$.

Update Formula:

$$\mu_2^{\text{new}} = \frac{\sum_{i=1}^{N} \gamma_{i,11} x_i}{\sum_{i=1}^{N} \gamma_{i,11}}$$

Derivation: This update maximizes the Gaussian component of the log-likelihood, weighted by the responsibilities $\gamma_{i,11}$. It represents the weighted average of observations assigned to $(y_i = 1, z_i = 1)$.

3. Update Rule for λ_2

Parameter λ_2 is the rate of the exponential distribution when $(y_i = 0, z_i = 1)$.

Update Formula:

$$\lambda_2^{\text{new}} = \frac{\sum_{i=1}^{N} \gamma_{i,01}}{\sum_{i=1}^{N} \gamma_{i,01} x_i}$$

Derivation: This update maximizes the exponential component of the log-likelihood, weighted by the responsibilities $\gamma_{i,01}$. It is the inverse of the weighted mean of observations assigned to $(y_i = 0, z_i = 1)$.

Summary of Dependencies

- For β : Requires $\gamma_{i,10}$, $\gamma_{i,11}$ from E-step
- For μ_2 : Requires $\gamma_{i,11}$, x_i from data
- For λ_2 : Requires $\gamma_{i,01}$, x_i from data

Each update maximizes the corresponding term in the expected complete-data log-likelihood while keeping other parameters fixed.

Remark on Derivation

The update rules are derived by maximizing the expected complete-data log-likelihood:

$$Q(\theta|\theta^{\text{old}}) = \mathbb{E}_{y,z|x,\theta^{\text{old}}}[\log P(x,y,z|\theta)]$$

with respect to each parameter while holding others fixed.

1. Update Rule for β

Derivation: The term involving β in the expected log-likelihood is:

$$\sum_{i=1}^{N} \left[\gamma_{i,10} \ln \beta + \gamma_{i,11} \ln \beta + \gamma_{i,00} \ln(1-\beta) + \gamma_{i,01} \ln(1-\beta) \right]$$

Taking derivative with respect to β and setting to zero:

$$\frac{\sum_{i}(\gamma_{i,10} + \gamma_{i,11})}{\beta} - \frac{\sum_{i}(\gamma_{i,00} + \gamma_{i,01})}{1 - \beta} = 0$$

Solving yields:

$$\beta^{\text{new}} = \frac{\sum_{i=1}^{N} (\gamma_{i,10} + \gamma_{i,11})}{N}$$

2. Update Rule for μ_2

Derivation: The term involving μ_2 is:

$$\sum_{i=1}^{N} \gamma_{i,11} \left[-\frac{(x_i - \mu_2)^2}{2} \right]$$

Taking derivative and setting to zero:

$$\sum_{i} \gamma_{i,11}(x_i - \mu_2) = 0$$

Solving yields:

$$\mu_2^{\text{new}} = \frac{\sum_{i=1}^{N} \gamma_{i,11} x_i}{\sum_{i=1}^{N} \gamma_{i,11}}$$

3. Update Rule for λ_2

Derivation: The term involving λ_2 is:

$$\sum_{i=1}^{N} \gamma_{i,01} \left[\ln \lambda_2 - \lambda_2 x_i \right]$$

Taking derivative and setting to zero:

$$\frac{\sum_{i} \gamma_{i,01}}{\lambda_2} - \sum_{i} \gamma_{i,01} x_i = 0$$

Solving yields:

$$\lambda_2^{\text{new}} = \frac{\sum_{i=1}^{N} \gamma_{i,01}}{\sum_{i=1}^{N} \gamma_{i,01} x_i}$$

Part (a)

Computational Complexity Comparison

General Steps in Agglomerative Clustering

Both single linkage and complete linkage follow these steps:

1. Initial Distance Computation: $O(n^2)$ for n points

2. Cluster Initialization: O(n)

3. Iterative Merging: O(n) iterations

Linkage Definitions

• Single Linkage:

$$d(C_1, C_2) = \min_{x \in C_1, y \in C_2} d(x, y)$$

• Complete Linkage:

$$d(C_1, C_2) = \max_{x \in C_1, y \in C_2} d(x, y)$$

Complexity Analysis

1. Distance Matrix Updates:

• When merging clusters A and B into cluster AB:

Single:
$$d(AB, C) = \min(d(A, C), d(B, C))$$

Complete: $d(AB, C) = \max(d(A, C), d(B, C))$

• Both require O(1) per update

• Total updates: $O(n^2)$ over all iterations

2. Finding Closest Clusters:

 $\bullet\,$ Naive implementation: $O(n^2)$ per iteration

• Optimized (with priority queue): $O(n \log n)$ per iteration

• Total iterations: O(n)

Overall Complexity

• Space Complexity: $O(n^2)$ for distance matrix

• Time Complexity:

- Naive implementation: $O(n^3)$

- Optimized implementation: $O(n^2 \log n)$

Conclusion

Single linkage and complete linkage have identical asymptotic complexity:

• Both require $O(n^2)$ space

• Both require $O(n^3)$ time (naive) or $O(n^2 \log n)$ time (optimized)

• The only difference is in the min/max operation used in distance updates

Part (b)

Which method is more robust to outliers?

Complete linkage is more robust to outliers than single linkage.

Reasoning

1. Single Linkage

• Uses minimum distance between clusters:

$$d(C_1, C_2) = \min_{x \in C_1, y \in C_2} d(x, y)$$

• Weakness to Outliers:

- Susceptible to "chaining effect"

- Single outlier can cause premature cluster merging

- Only considers closest pair of points

2. Complete Linkage

• Uses maximum distance between clusters:

$$d(C_1, C_2) = \max_{x \in C_1, y \in C_2} d(x, y)$$

• Robustness to Outliers:

- Considers worst-case separation

- Requires all points to be relatively close for merging

- Individual outliers cannot force cluster merging

Therefore, when dealing with datasets containing potential outliers, complete linkage is the more reliable choice.

Part (c)

Complete Linkage Hierarchical Clustering

Given Points:

- A(0, 0.5)
- B(0.5, 0)
- C(3, 1)
- D(3.5, 1)
- E(3, 0.5)
- F(2, 2)

Pairwise Euclidean Distances:

	A	В	\mathbf{C}	D	${ m E}$	\mathbf{F}
A	0	0.71	3.04	3.54	3.04	2.06
В	0.71	0	2.92	3.43	2.55	2.50
\mathbf{C}	3.04	2.92	0	0.5	0.5	1.41
D	3.54	3.43	0.5	0	0.71	1.80
\mathbf{E}	3.04	2.55	0.5	0.71	0	1.80
F	2.06	0.71 0 2.92 3.43 2.55 2.50	1.41	1.80	1.80	0

Clustering Steps:

- 1. First Merge: C, E (d = 0.5)
 - \bullet Clusters: {A}, {B}, {C,E}, {D}, {F}
 - Updated distances:

$$d(\{C, E\}, D) = \max(0.5, 0.71) = 0.71$$

$$d(\{C, E\}, F) = \max(1.41, 1.80) = 1.80$$

$$d(\{C, E\}, A) = \max(3.04, 3.04) = 3.04$$

$$d(\{C, E\}, B) = \max(2.92, 2.55) = 2.92$$

- 2. Second Merge: $\{C,E\}$, D (d = 0.71)
 - \bullet Clusters: {A}, {B}, {C,E,D}, {F}
 - Updated distances:

$$d({C, E, D}, F) = \max(1.41, 1.80, 1.80) = 1.80$$

$$d({C, E, D}, A) = \max(3.04, 3.04, 3.54) = 3.54$$

$$d({C, E, D}, B) = \max(2.92, 2.55, 3.43) = 3.43$$

3. **Third Merge:** A, B (d = 0.71)

• Clusters: {A,B}, {C,E,D}, {F}

4. Fourth Merge: $\{C,E,D\}$, F (d = 1.80)

• Clusters: {A,B}, {C,E,D,F}

5. Final Merge: $\{A,B\}$, $\{C,E,D,F\}$ (d = 3.54)

Merge Summary:

Step	Merge	Distance
1	C, E	0.5
2	(C,E), D	0.71
3	A, B	0.71
4	(C,E,D), F	1.80
5	(A,B), (C,E,D,F)	3.54

Dendrogram:

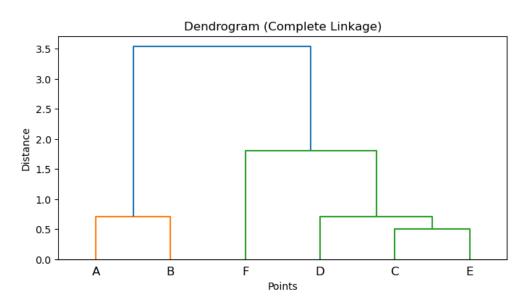


Figure 3.1: Hierarchical Clustering Dendrogram

Part (a)

When is choosing the right ϵ value more challenging?

Choosing ϵ in DBSCAN is particularly challenging in two main scenarios:

1. Data with Varying Densities

- Challenge: DBSCAN uses a single ϵ value globally
- Problems:
 - Small ϵ : May correctly identifies dense clusters but misses sparse ones (breaking them into noise).
 - Large ϵ : Merges distinct dense clusters or includes noise
- **Reasoning:** Fixed density threshold (ϵ , MinPts) cannot accommodate naturally varying cluster densities

2. High-Dimensional Data

- Challenge: Curse of dimensionality affects distance metrics
- Problems:
 - Too small ϵ : Most points become noise
 - Too large ϵ : All points merge into one cluster
- Reasoning: Euclidean distances become less meaningful in high dimensions, making ϵ harder to interpret

Part (b)

Given MinPts = 3, which plot requires larger ϵ to produce two clusters? Plot 2 requires a larger ϵ value.

Reasoning

• Plot 1:

- Both inner and outer clusters are dense
- Smaller ϵ sufficient to form clusters

• Plot 2:

- Inner points are sparsely distributed
- Outer circle is dense
- Larger ϵ needed to connect sparse inner points into a cluster

Conclusion: Plot 2 needs larger ϵ to connect the sparse inner points while the dense outer circle forms naturally.

Part (c)

How will ϵ change when MinPts = 1 compared to part (b)?

General Effect of MinPts = 1

With MinPts = 1:

- Each point needs only one neighbor to be a core point
- Much smaller ϵ sufficient for cluster formation
- Can form single-point clusters

Analysis by Plot

Plot 1:

- Dense clusters in both regions
- ϵ will decrease significantly
- Only needs to connect nearest neighbors

Plot 2:

- Dense outer circle: very small distances between points
- Sparse inner points: can form individual clusters
- ϵ will decrease very much compared to part (b)

Conclusion

 ϵ will be much smaller in both plots because:

- Only needs to connect nearest neighbor pairs
- No requirement to form large connected components
- Especially significant decrease in Plot 2 where previously large ϵ was needed to connect sparse inner points

Part (d)

Using ϵ from part (b), which plot will have more black points labeled as noise? Plot 1 will have more black points labeled as noise.

Reasoning

• Plot 1:

- Smaller ϵ due to dense clusters
- Smaller neighborhood radius for black points
- Less likely to have sufficient neighbors within ϵ
- Most black points will be labeled as noise

• Plot 2:

- Larger ϵ due to sparse inner points
- Larger neighborhood radius for black points
- More likely to capture enough neighbors from dense outer ring
- Fewer black points will be labeled as noise

Conclusion

Plot 1 will identify more black points as noise because:

- \bullet Smaller ϵ means smaller neighborhoods
- Black points less likely to meet MinPts requirement
- \bullet Contrast with Plot 2 where larger ϵ increases chance of cluster inclusion