Clustering Singular and Non-Singular Covariance Matrices for Classification

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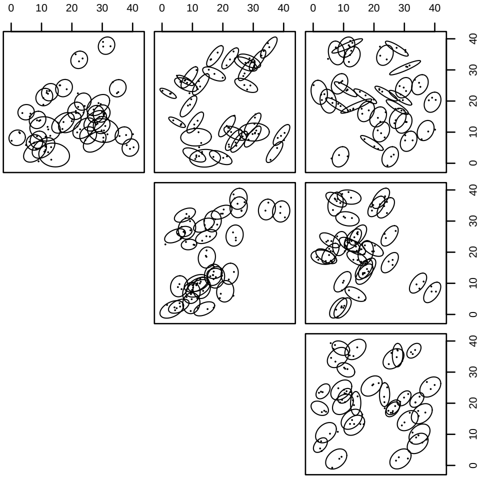
Motivating Example

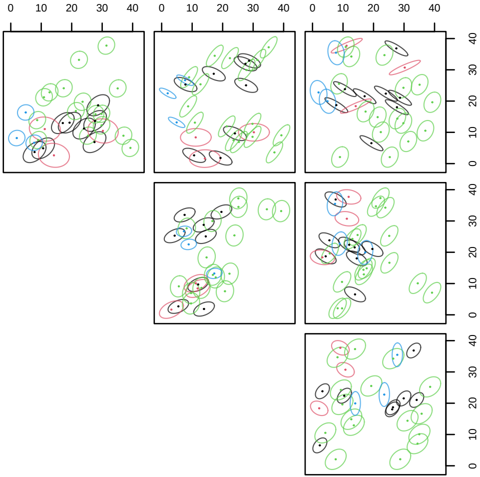
Consider a high dimensional space with with many classes and few observations per class which often appears is forensic identification of source problems.

- This example has 30 classes and 3 observations per class which follow multivariate normal distributions in a 4 dimensional space
- Quadratic Discriminant Analysis (QDA) will yield singular covariance matrices
- One would then need to use Linear Discriminant Analysis (LDA)



Motivating Example

- Assuming a shared covariance matrix is a strong assumption to make
- There may be clusters of covariance matrices shared between all classes
- **Goal:** Can we cluster common covariance matrices and pool with clusters
- This will increase the discrimination power between classes by providing stable estimates of the covariance matrices



Models

Let X_{ij} be a random vector of length p which is the *jth* observation from the *ith* class for $i \in \{1, 2, \dots, C\}$ and $j \in \{1, 2, \dots, n_i\}$.

Models

Linear Discriminant Analysis (LDA)

$$X_{ij} \sim N_p(\mu_i, \mathbf{\Sigma}),\ \hat{z} = \text{argmax}_i \phi(x; \mu_i, \mathbf{\Sigma})$$

Quadratic Discriminant Analysis (QDA)

$$X_{ij} \sim N_p(\mu_i, \mathbf{\Sigma}_i),\ \hat{z} = \text{argmax}_i \phi(x; \mu_i, \mathbf{\Sigma}_i)$$

Proposed Model: Latent Covariance Discriminant Analysis (LCDA)

$$X_{ij} | Z_i = k \sim N_p(\mu_i, \mathbf{\Sigma}_k) \text{ where } Z_i \sim \mathit{Categorical}(\pi_1, \dots \pi_K),\ \hat{z} = \text{argmax}_i \phi(x; \mu_i, \mathbf{\Sigma}_k)$$

Expectation Maximization Algorithm

The Expectation Maximization (EM) A. P. Dempster et al. algorithm is an iterative method which finds MLEs in situations where latent variables exist

E-step

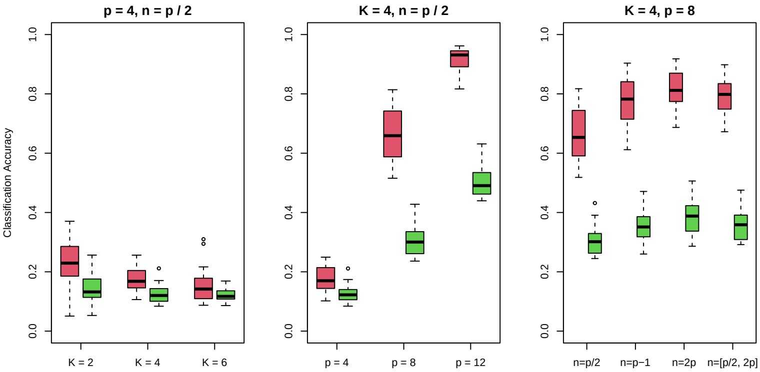
$$\tau_{ik} = \frac{\pi_k |\boldsymbol{\Sigma}_k|^{-\frac{n_i}{2}} e^{-\frac{1}{2} tr(\boldsymbol{\Sigma}_k^{-1} S_i)}}{\sum_{k'=1}^{K} \pi_{k'} |\boldsymbol{\Sigma}_{k'}|^{-\frac{n_i}{2}} e^{-\frac{1}{2} tr(\boldsymbol{\Sigma}_{k'}^{-1} S_i)}} \text{ where } S_i = \sum_{j=1}^{n_i} (x_{ij} - \mu_i)(x_{ij} - \mu_i)^T$$

M-step

$$\hat{\pi}_k = \frac{1}{C} \sum_{i=1}^{C} \tau_{ik}, \; \hat{\mu}_{\mathbf{i}} = \frac{1}{n_i} \sum_{j=1}^{n_i} x_{ij}, \text{ and } \hat{\boldsymbol{\Sigma}}_k = \frac{\sum_{i=1}^{C} \tau_{ik} S_i}{\sum_{i=1}^{C} \tau_{ik} n_i}$$

Simulation Study

A stimulation study is performed in order to understand the performance of the model by looking at the out-of-sample classification rate (**LDA: Green, LCDA: Red**)

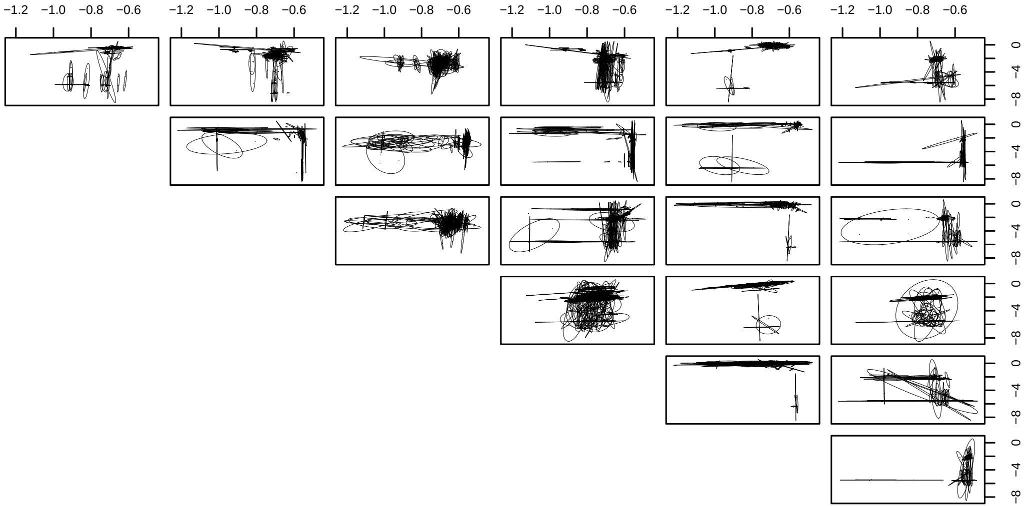


Glass Dataset Description

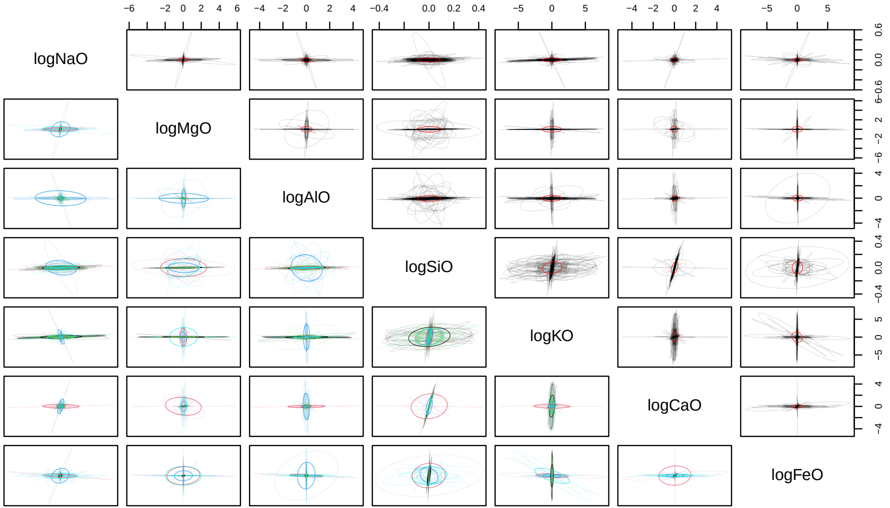
The LCDA and LDA are applied to the Zadora glass dataset Aitken et al. [2007]

- 200 Windows (classes)
- 4 fragments from each window (observations per class)
- Each measured 3 times (mean is taken)
- 7 trace elements are measured
- Ratios of Sodium, Magnesium, Aluminium, Silicon, Potassium, Calcium and Iron to Oxygen

Glass Contour Plots



Glass Results



LDA: 43%

LCDA: **57%**

Conclusion

- LDA has strong assumptions
- QDA leads to unstable or degenerate densities
- LCDA assumes there is a finite number of latent covariance matrices shared between all classes
- LCDA showed large improvements in terms of classification accuracy over LDA in situations where QDA is not even possible

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Thank you!