Lecture 9: Multiclass Classification (II)

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Outline

1. Nonlinear Discriminant Analysis
   - Quadratic discriminant analysis (QDA)
   - Regularized discriminant analysis (RDA)
2. Visualization of LDA

How to Fit a Quadratic Boundary

There are two popular ways:

1. Use LDA in the enlarged space containing quadratic polynomials
   - If $d = 2$, fit LDA in five-dimensional space spanned by

$$\{X_1, X_2, X_1X_2, X_1^2, X_2^2\}.$$

2. Use Quadratic Discriminant Analysis (QDA)

In practice, these two methods often give similar results.

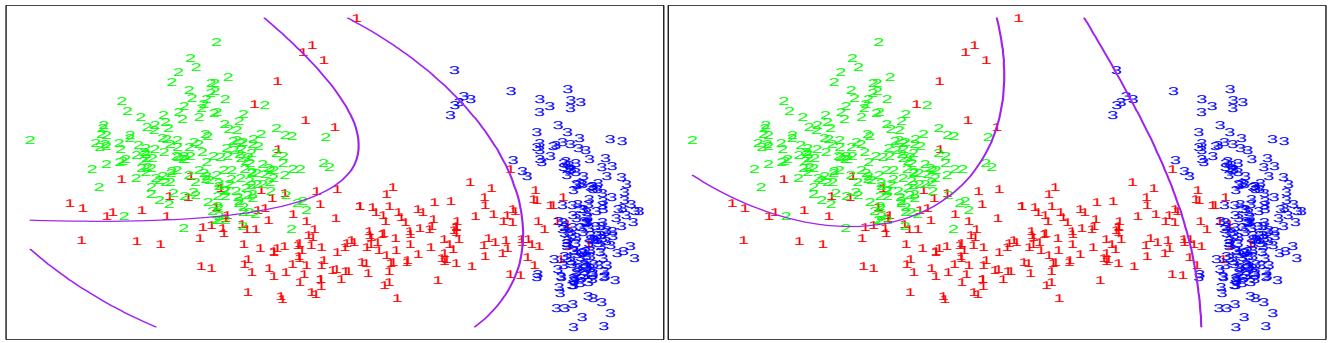


Figure 4.6: *Two methods for fitting quadratic boundaries. The left plot shows the quadratic decision boundaries for the data in Figure 4.1 (obtained using LDA in the five-dimensional space* $x_1, x_2, x_{12}, x_1^2, x_2^2$*). The right plot shows the quadratic decision boundaries found by QDA. The differences are small, as is usually the case.*

Quadratic Linear Discriminant Analysis

Model Setup: recall that

- $\pi_k = P(Y = k)$ for $k = 1, \cdots, K$
- $g_k(\mathbf{x})$ is the class-conditional densities of X in class k.

QDA Model Assumptions:

- Assume each class density is multivariate Gaussian, i.e.,

$$\mathbf{X}|Y = k \sim N(\boldsymbol{\mu}_k, \Sigma_k), \quad k = 1, \cdots, K$$

- Allow unequal covariances across classes.

Multivariate Normal Distribution

If $\mathbf{X} = (X_1, \cdots, X_d) \sim N_d(\boldsymbol{\mu}, \Sigma)$, then its density has the form

$$f(\mathbf{x}|\boldsymbol{\mu}, \Sigma) = (2\pi)^{-d/2}|\Sigma|^{-1/2} \exp\{-(\mathbf{x}-\boldsymbol{\mu})^T\Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu})/2\},$$

where $\boldsymbol{\mu}$ is the mean, and Σ is the covariance matrix.

- Contour of constant density for $N_d(\boldsymbol{\mu}, \Sigma)$ are ellipsoids defined by $\mathbf{x}$ such that

$$(\mathbf{x}-\boldsymbol{\mu})^T\Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu}) = c^2.$$

- These ellipsoids are centered at $\boldsymbol{\mu}$ and have axes $\pm c\sqrt{\lambda_j}\mathbf{e}_j$, where

$$\Sigma\mathbf{e}_j = \lambda_j\mathbf{e}_j, \quad j = 1, \cdots, d.$$

  Here $(\lambda_j, \mathbf{e}_j), j = 1, \cdots, p$ are the eigenvalue-eigenvector pairs of Σ.

Property of Multivariate Normal Distribution

Assume $\mathbf{X} \sim N_d(\boldsymbol{\mu}, \Sigma)$. Then

- Let χ^2_d denote the chi-square distribution with d degrees of freedom.

$$(\mathbf{X} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{X} - \boldsymbol{\mu}) \sim \chi^2_d.$$

- The $N_d(\boldsymbol{\mu}, \Sigma)$ distribution assigns probability $(1 - \alpha)$ to the solid ellipsoid

$$\{\mathbf{x} : (\mathbf{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) \leq \chi^2_d(\alpha)\},$$

where $\chi^2_d(\alpha)$ denotes the upper $(100\alpha\%)$th percentile of the χ^2_d distribution.

QDA Decision Rule

Under Gaussian assumption, the log-ratio of class k ad class l is:

$$\begin{aligned} \log \frac{\Pr(Y=k|\mathbf{X}=\mathbf{x})}{\Pr(Y=l|\mathbf{X}=\mathbf{x})} &= \log \frac{\pi_k \phi(\mathbf{x};\boldsymbol{\mu}_k,\Sigma_k)}{\pi_j \phi(\mathbf{x};\boldsymbol{\mu}_l,\Sigma_l)} \\ &= f_k(\mathbf{x}) - f_l(\mathbf{x}), \end{aligned}$$

where the discriminant functions (score) f_k is given by

$$f_k(\mathbf{x}) = -\frac{1}{2}\log|\Sigma_k| - \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^T\Sigma_k^{-1}(\mathbf{x}-\boldsymbol{\mu}_k) + \log\pi_k, \quad k = 1,\cdots,K.$$

The decision boundary between each pair of classes k and l is

$$\{\mathbf{x} : f_k(\mathbf{x}) = f_l(\mathbf{x})\}.$$

The decision rule is

$$f(\mathbf{x}) = \text{argmax}_{k=1,\ldots,K} f_k(\mathbf{x}).$$

More About QDA Decision Boundary

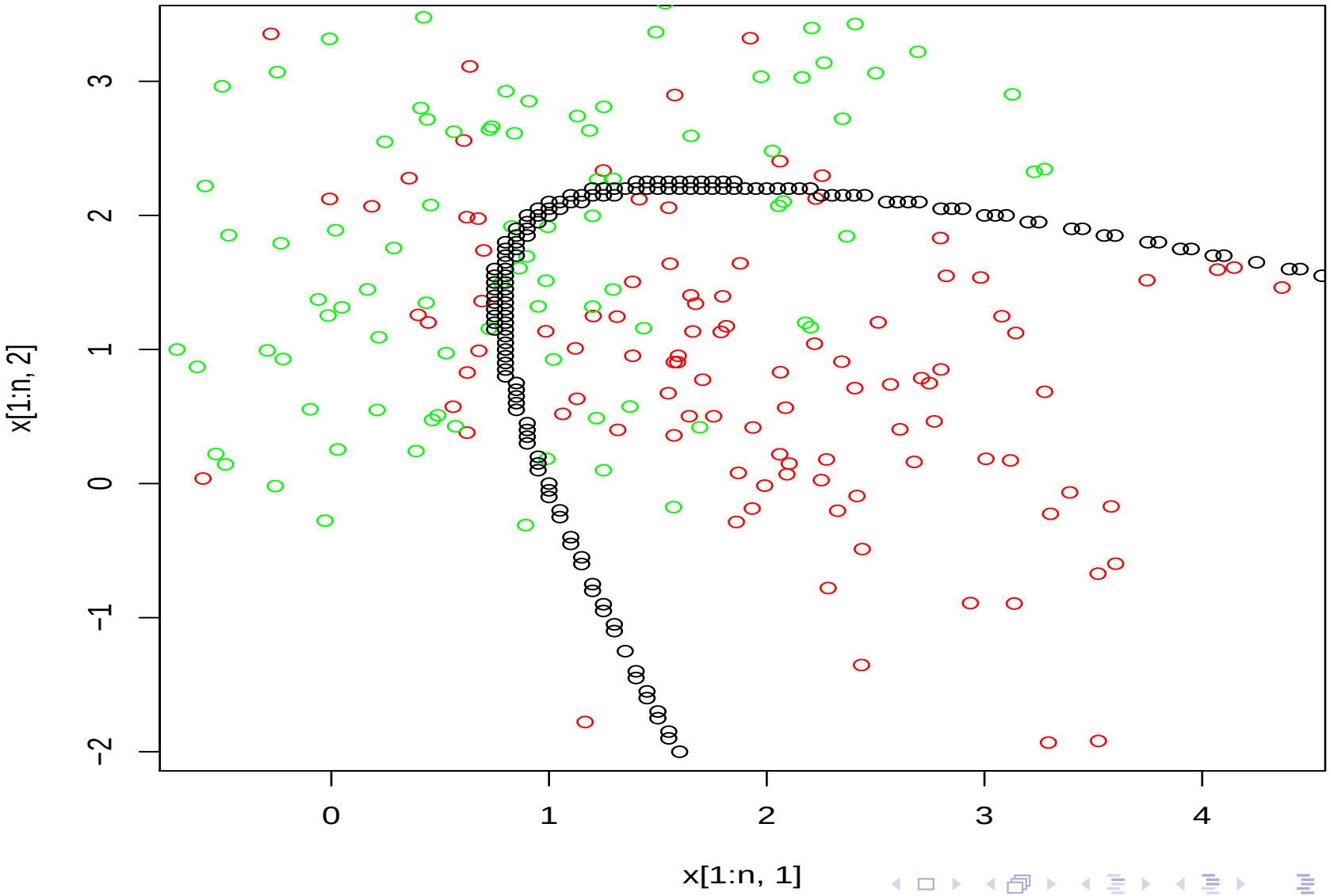
The discrimination function are quadratic in $\mathbf{x}$,

$$f_k(\mathbf{x}) = \mathbf{x}^T W_k \mathbf{x} + \boldsymbol{\beta}_{1k}^T \mathbf{x} + \beta_{0k}, \quad k = 1, \cdots, K.$$

The decision boundary between class k and class l is also quadratic

$$\{\mathbf{x} : \mathbf{x}^T (W_k - W_l)\mathbf{x} + (\boldsymbol{\beta}_{1k} - \boldsymbol{\beta}_{1l})^T \mathbf{x} + (\beta_{0k} - \beta_{0l}) = 0\}.$$

- QDA needs to estimate more parameters than LDA, and the difference is large when d is large.
  - Fitting LDA needs to estimate $(K-1) \times (d+1)$ parameters
  - Fitting QDA needs to estimate $(K-1) \times (d(d+3)/2+1)$ parameters


x[1:n, 2]
x[1:n, 1]
3
2
1
0
−1
−2
0
1
2
3
4

Interpretation of QDA

The discriminant function f_k depends on three factors:

- the generalized variance $|\Sigma_k|$
- the prior probability π_k
- the squared Mahalanobis distance from $\mathbf{x}$ to the population mean $\boldsymbol{\mu}_k$.

Here, a different distance function, with a different orientation and size of the constant-distance ellipsoid, is used for each class.

Parameter Estimation in QDA

In practice, we estimate the parameters from the training data

- $\hat{\pi}_k = n_k/n$, where n_k is the number of observations in class k for $k = 1, \cdots, K$.
- $\hat{\boldsymbol{\mu}}_k = \sum_{Y_i=k} \mathbf{x}_i/n_k$ for $k = 1, \cdots, K$.
- The within-class sample covariance

$$\hat{\Sigma}_k = \frac{1}{n_k - 1} \sum_{Y_i=k} (\mathbf{x}_i - \hat{\boldsymbol{\mu}}_k)(\mathbf{x}_i - \hat{\boldsymbol{\mu}}_k)^T.$$

The implementation of QDA is computationally intensive, since

- we need to conduct matrix inversion multiple times: compute $\hat{\Sigma}_k$ for $k = 1, \cdots, K$.

Speed Up QDA Computation

Idea: Diagonalizing $\hat{\Sigma}_k$ (with eigen-decomposition)

$$\hat{\Sigma}_k = U_k D_k U_k^T,$$

where U_k orthonormal and D_k diagonal with positive eigenvalues.

- $$\begin{aligned}(\mathbf{x}-\boldsymbol{\mu}_k)^T \Sigma_k^{-1}(\mathbf{x}-\boldsymbol{\mu}_k) &= [U_k^T(\mathbf{x}-\boldsymbol{\mu}_k)]^T D_k^{-1}[U_k^T(\mathbf{x}-\boldsymbol{\mu}_k)] \\ &= [D_k^{-\frac{1}{2}} U_k^T(\mathbf{x}-\boldsymbol{\mu}_k)]^T [D_k^{-\frac{1}{2}}[U_k^T(\mathbf{x}-\boldsymbol{\mu}_k)]\end{aligned}$$
- $\log|\hat{\Sigma}_k| = \sum_{l=1}^{K} \log d_{kl}$

R code for QDA Fitting (I)

There are two ways to call the function "qda". The first way is to use a formula and an optional data frame.

```
library(MASS)
qda(formula, data, subset)
```

Arguments:

- *formula*: the form "groups $\sim x_1 + x_2 + \ldots$", where the response is the grouping factor and the right hand side specifies the (non-factor) discriminators.
- *data*: data frame from which variables specified
- *subset*: An index vector specifying the cases to be used in the training sample.

Output:

- an object of class "qda" with multiple components

R code for QDA Fitting (II)

The second way is to use a matrix and group factor as the first two arguments.

```
library(MASS)
qda(x, grouping, prior = proportions, CV = FALSE)
```

Arguments:

- *x*: a matrix or data frame or Matrix containing predictors.
- *grouping*: a factor specifying the class for each observation.
- *prior*: the prior probabilities of class membership. If unspecified, the class proportions for the training set are used.

Output:

- If CV = TRUE, the return value is a list with components "class" (the MAP classification, a factor) and "posterior" (posterior probabilities for the classes).

R code for QDA Prediction

We use the "predict" or "predict.qda" function to classify multivariate observations with qda

```
predict(object, newdata, ...)
```

Arguments:

- *object*: object of class "qda"
- *newdata*: data frame of cases to be classified or, if "object" has a formula, a data frame with columns of the same names as the variables used.

Output:

- a list with the components "class" (the MAP classification, a factor) and "posterior" (posterior probabilities for the classes)

Illustration 1

```
Iris <- data.frame(rbind(iris3[,,1], iris3[,,2],
   iris3[,,3]), Sp = rep(c("s","c","v"), rep(50,3)))
train <- sample(1:150, 75)
table(Iris$Sp[train])
z <- qda(Sp ~ ., Iris, prior = c(1,1,1)/3, subset = train)
ypred <- predict(z, Iris[-train, ])$class
ytest <- Iris$Sp[-train]
testerr <- mean(ypred!=ytest)
```

Illustration 2

```
tr <- sample(1:50, 25)
train <- rbind(iris3[tr,,1], iris3[tr,,2], iris3[tr,,3])
test <- rbind(iris3[-tr,,1], iris3[-tr,,2], iris3[-tr,,3])
cl <- factor(c(rep("s",25), rep("c",25), rep("v",25)))
z <- qda(train, cl)
trainerr <- mean(predict(z,train)$class!=cl)
testerr <- mean(predict(z,test)$class!=cl)
```

Choice of LDA between QDA

Both LDA and QDA perform well on real classification problems.

- In STATLOG project (Michie et al. 1994), the LDA was among top 3 classifiers for 7 datasets; the QDA among top 3 for 4 datasets (totally 22 datasets)

Regularized Discriminant Analysis (RDA)

Friedman (1989) proposed a comprise between QDA and LDA:

- shrinking the separate covariances of QDA toward a common covariance in LDA.

The regularized covariance matrices are

$$\hat{\Sigma}_k(\alpha) = \alpha\hat{\Sigma}_k + (1-\alpha)\hat{\Sigma}, \quad \hat{\Sigma} \text{ pooled sample covariance matrix}$$

- $\alpha \in [0, 1]$, a continuum of models (compromise) between LDA and QDA. What if α is close to 1 (or 0)?
- In practice, choose α with validation data or CV.

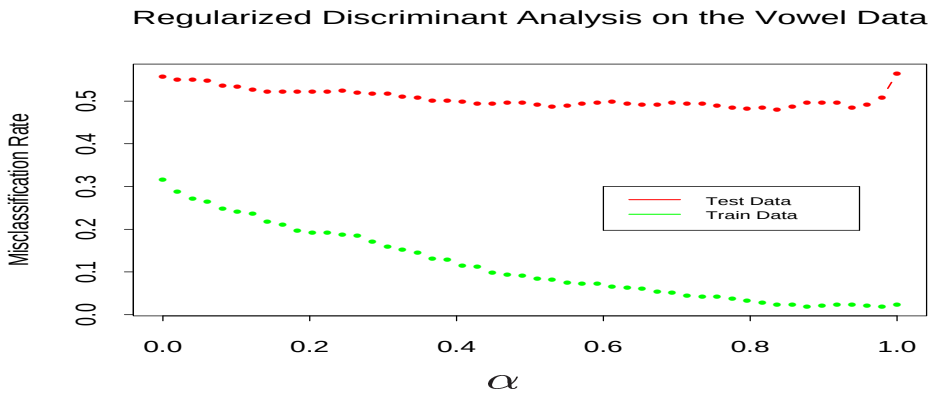


Figure 4.7: *Test and training errors for the vowel data, using regularized discriminant analysis with a series of values of* $\alpha \in [0, 1]$. *The optimum for the test data occurs around* $\alpha = 0.9$, *close to quadratic discriminant analysis.*

More on Regularized DA

Other regularized methods:

- For LDA, we can shrink $\hat{\Sigma}$ toward the scalar covariance, $\gamma \in [0, 1]$

$$\hat{\Sigma}(\gamma) = \gamma\hat{\Sigma} + (1-\gamma)\hat{\sigma}^2 I.$$

- A more general families of regularized QDA is indexed by (α, γ):

$$\hat{\Sigma}_k(\alpha, \gamma) = \alpha\hat{\Sigma}_k + (1-\alpha)\gamma\hat{\Sigma} + (1-\alpha)(1-\gamma)\hat{\sigma}^2 I.$$

Generalizing Linear Discriminant Analysis

More flexible, more complex decision boundaries (Chapter 12)

- FDA: *flexible* discriminant analysis
  - allow nonlinear boundary: recast the LDA problem as a linear regression problem and then use basis expansions to do discrimination
- PDA: *penalized* discriminant analysis
  - select variables: penalize the coefficients to be smooth or sparse, which is more interpretable
- MDA: *mixture* discriminant analysis
  - allow each class by a mixture of two or more Gaussian with different centroids, but each component Gaussian (within and between classes) shares the same covariance matrix.

Interpretation of LDA

Consider the eigen-decomposition of $\Sigma = UDU^T$. Then for each k,

$$\begin{aligned}(\mathbf{x}-\boldsymbol{\mu}_k)^T\Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu}_k) &= [U^T(\mathbf{x}-\mu_k)]^T D^{-1}[U^T(\mathbf{x}-\boldsymbol{\mu}_k)] \\ &= [D^{-\frac{1}{2}}U^T(\mathbf{x}-\boldsymbol{\mu}_k)]^T[D^{-\frac{1}{2}}U^T(\mathbf{x}-\boldsymbol{\mu}_k)].\end{aligned}$$

If we sphere the data with respect to Σ by

$$X^* \longleftarrow D^{-\frac{1}{2}}U^T X, \quad \boldsymbol{\mu}_k^* \longleftarrow D^{-\frac{1}{2}}U^T\boldsymbol{\mu}_k, \quad k = 1, \cdots, K$$

Then

$$(\mathbf{x}-\boldsymbol{\mu}_k)^T\Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu}_k) = (\mathbf{x}^*-\boldsymbol{\mu}_k^*)^T(\mathbf{x}^*-\boldsymbol{\mu}_k^*).$$

Note $Cov(X^*) = I_d$. Classify to the closest centroid (Enclidean distance) in the transformed space, adjusting π_0 and π_1.

Dimension Reduction in LDA

LDA allows us to visualize informative low-dimensional projections of data

- The K centroids in d-dimensional input space span a subspace H, with $dim(H) \leq K-1$
- Project $\mathbf{x}^*$ onto H and make a distance comparison there.
- We can ignore the distances orthogonal to H, since they will contribute equally to each class.

Data can be viewed in H without losing any information. When $K \ll d$, dimension reduction!

- When $K = 3$, we can view the data in a two-dimensional plot
- When $K > 3$, we might to find a subspace $H_L \subset H$ optimal for LDA in some sense.

Subspace Optimality

Fisher's Optimality for H_L:
the projected centroids are spread out as much as possible in terms of variance.

- This amounts to: finding principal components subspaces of the centroids.
- These principal components are called *discriminant coordinates or canonical variates*.
- Pick up the top-ranked discriminant coordinates. The lower rank, the centroids are less spread out.

For visualization:
we project the data onto the principal components of the K centroids.

Finding Optimal Subspace

- Compute the $K \times d$ matrix of class centroid $\mathbf{M}$
- Compute the common covariance matrix $\mathbf{W}$ (this is *within-class* covariance, pooled variance about the means)
- Compute $\mathbf{M}^* = \mathbf{M}\mathbf{W}^{-\frac{1}{2}}$ ($\mathbf{W}^{-\frac{1}{2}}$ is found using eigen-decomposition of $\mathbf{W}$)
- Compute $\mathbf{B}^*$, the covariance matrix of $\mathbf{M}^*$ (this is *between-class* covariance matrix)
- Compute eigen-decomposition of $\mathbf{B}^* = \mathbf{V}^* \mathbf{D}_B \mathbf{V}^{*T}$.
- The columns v_l^* of $\mathbf{V}^*$ in sequence from first to last define the coordinates of the optimal subspaces.

The lth discriminant variable is

$$Z_l = v_l^T X, \quad \text{where} \quad v_l = \mathbf{W}^{-\frac{1}{2}} v_l^*.$$

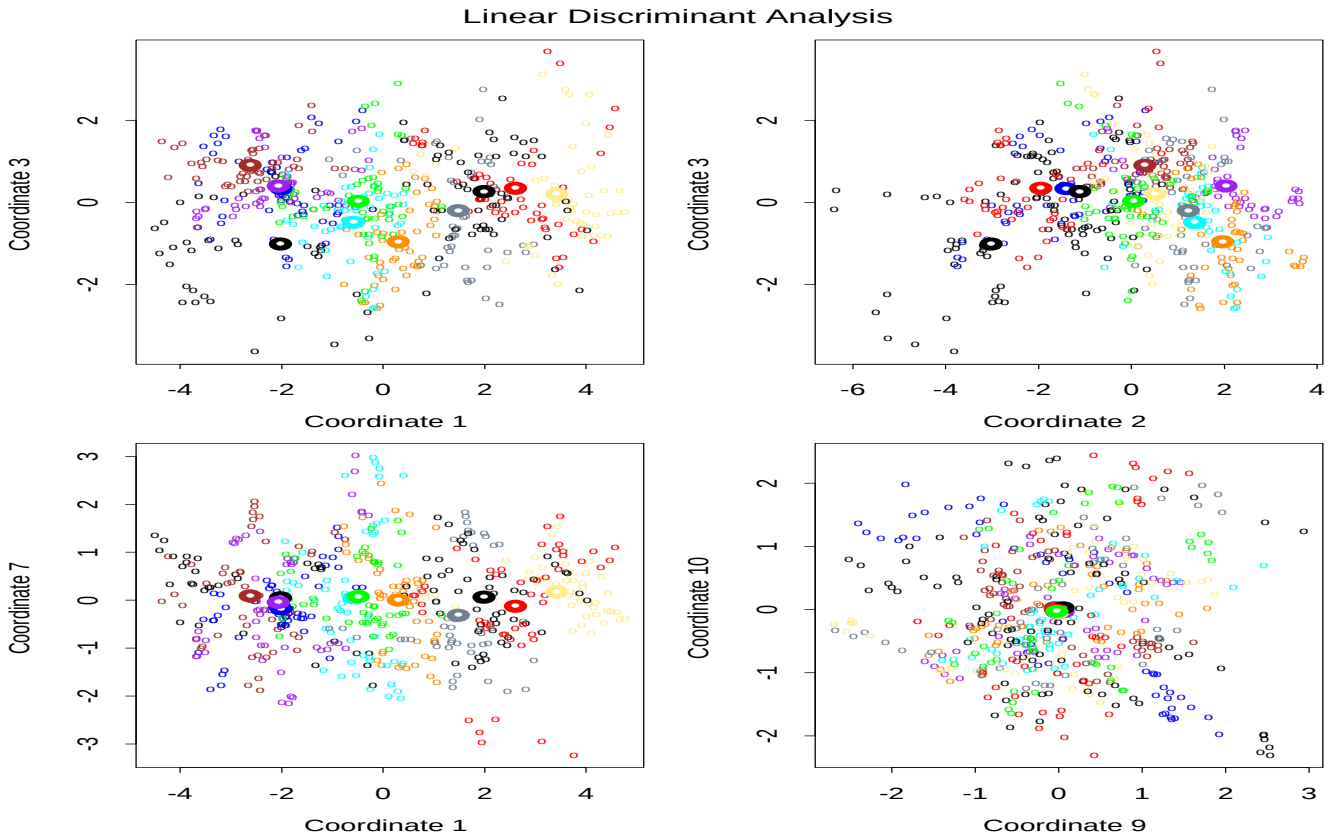


Figure 4.8: *Four projections onto pairs of canonical variates. Notice that as the rank of the canonical variates increases, the centroids become less spread out. In the lower right panel they appear to be superimposed, and the classes most confused.*

An Alternative View

Find the linear combination $Z = a^T X$ such that the between-class variance is maximized relative to the within-class variance.

- The first discriminant coordinate: $\max_{a_1} \frac{a_1^T \mathbf{B} a_1}{a_1^T \mathbf{W} a_1}$, where $\mathbf{B}$ is the covariance matrix of the class centroid matrix $\mathbf{M}$ ($\mathbf{M}$ is of size $K \times d$), and $\mathbf{W}$ is the within-class covariance.
- The other discriminant coordinates: $\max_{a_\ell} \frac{a_\ell^T \mathbf{B} a_\ell}{a_\ell^T \mathbf{W} a_\ell}$ subject to $a_\ell^T \mathbf{W} a_j = 0; j = 1, \ldots, \ell - 1$.
- The solution can be obtained by the eigen-decomposition of $\mathbf{W}^{-1}\mathbf{B}$.

We can show that $a_l = v_l$ for all $l = 1, \cdots, L$.

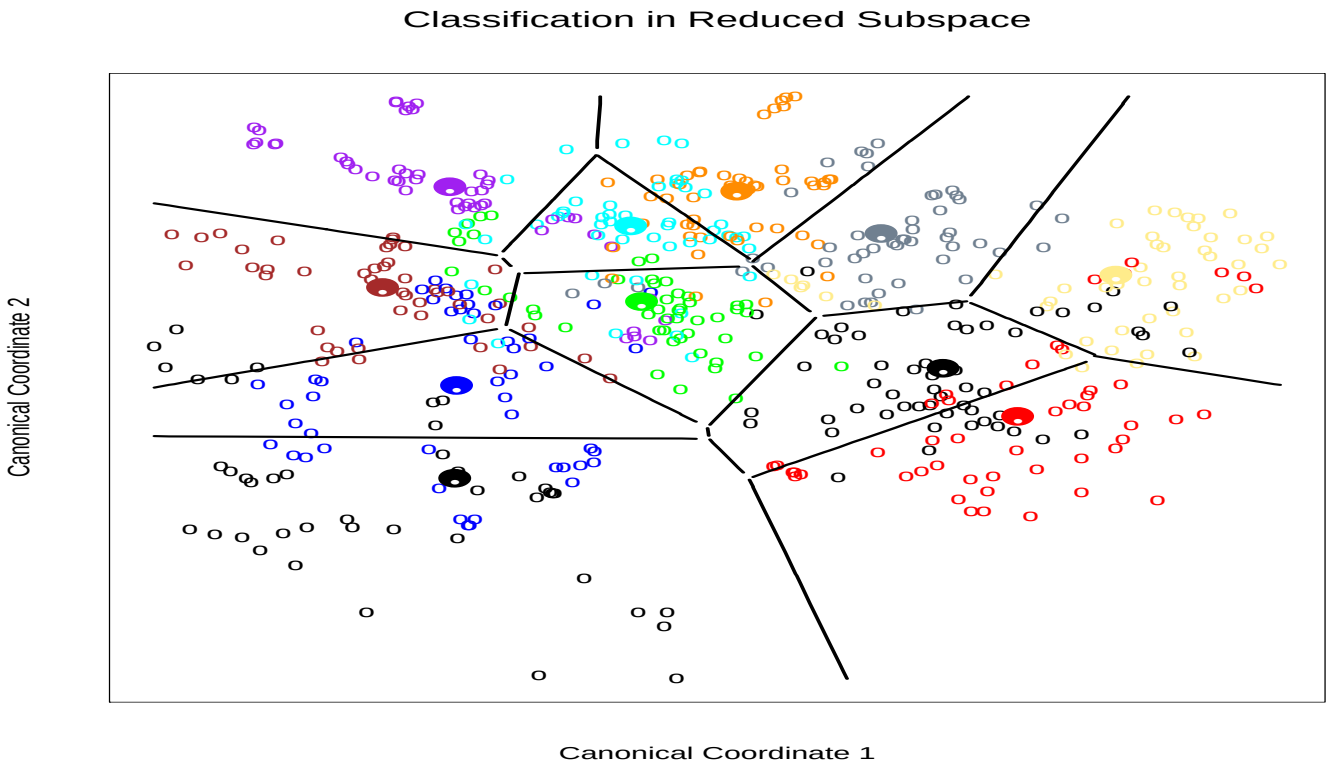


Figure 4.11: *Decision boundaries for the vowel training data, in the two-dimensional subspace spanned by the first two canonical variates. Note that in any higher-dimensional subspace, the decision boundaries are higher-dimensional affine planes, and could not be represented as lines.*