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These are each obtained by solving the partial score equations for μ_j or Σ, assuming the other is known. The full maximum-likelihood solution requires their simultaneous solution, and suggests iteration. However, the solution is easier. We plug the estimated means (18) (using W for Σ), into (20) which gives

$$\begin{aligned}
\hat{\Sigma} &= W + \sum_{j=1}^{J} \frac{N_j}{N}(\bar{x}_j - \hat{\mu}_j)(\bar{x}_j - \hat{\mu}_j)^T \\
&= W + B - \hat{B}_{(K)} \\
&= W + B - WVV^TBVV^TW \\
&= W + WV_\perp V_\perp^T BV_\perp V_\perp^T W
\end{aligned} \tag{21}$$

where $V_\perp^T WV = 0$ and $V_\perp^T$ spans the complementary $p-K$ dimensional subspace of R^p. To complete the proof, we show that the same V is optimal using the new metric $\hat{\Sigma}$.

First of all note that

1. $V^T\hat{\Sigma}V = V^TWV + 0 = I_K$, and
2. $BV = WVD_K = \hat{\Sigma}VD_K$, where the first equality is the definition of V, and $D_K = \text{diag}(\gamma_1, ..., \gamma_K)$.

We have thus established that V is also an eigen-matrix of B with respect to $\hat{\Sigma}$; we have still to show that it has remained optimal.

Note that

$$\begin{aligned}
V_\perp^T\hat{\Sigma}V_\perp &= I_{p-K} + V_\perp^T BV_\perp \\
&= I_{p-K} + D_{p-K}
\end{aligned} \tag{22}$$

where D_{p-K} are the eigenvalues of B corresponding to $V_\perp$ and W. So in the metric $\hat{\Sigma}$, the columns of V are orthonormal eigenvectors of B, $V_\perp$ is orthogonal and orthogonal to V. Thus the columns of $V_\perp$ remain eigenvectors of B wrt $\hat{\Sigma}$, with eigenvalues $(I_{p-K} + D_{p-K})^{-1}D_{p-K} \leq D_{p-K}$, and thus the order does not change.

This shows that the constrained maximum-likelihood estimated means coincide with the rank-K LDA means. Using the fact that $\hat{\Sigma}^{-1} = VV^T + V_\perp(D_{p-K}^{-1}(I_{p-K} + D_{p-K})V_\perp^T$, is not hard to show that *relative* Mahalanobis distances $(x - \hat{\mu_j})^T\hat{\Sigma}^{-1}(x - \hat{\mu_j}) - (x - \hat{\mu_\ell})^T\hat{\Sigma}^{-1}(x - \hat{\mu_\ell})$ coincide with relative Euclidean distances in the reduced LDA space, and hence classification based on the fitted constrained Gaussian model and LDA coincide.

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report comes with this package, and is also available from
`ftp:netlib.att.com/netlib/att/stat/doc/94/6.ps`.

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A Appendix

A.1 Reduced rank models

In proposition 1 in section 3 we claimed that maximising the log-likelihood (8):

$$2\ell(\mu_j, \Sigma, K) = -\sum_{j=1}^{J} \sum_{g_i = j} (x_i - \mu_j)^T \Sigma^{-1} (x_i - \mu_j) - N \log |\Sigma|$$

subject to rank$\{\mu_j\} = K$

is equivalent to reduced rank LDA. In the following outline of a proof, we draw heavily on Mardia et al. (1979, hereafter MKB) for some basic multivariate statistics results. Let B be the between-class covariance matrix, and for fixed Σ, let V denote the matrix of leading K eigenvectors of $\Sigma^{-1}B$.

Σ known, μ_j unknown In section 12.5.2 (page 338) of MKB a solution to (8) is given, assuming Σ is known. This has the form of the usual LDA solution, except with W replaced by Σ. One can write the estimated means as

$$\hat{\mu}_j = \Sigma V V^T (\bar{x}_j - \bar{x}) + \bar{x} \tag{18}$$

and thus the *estimated* (rank-K) between matrix as

$$\hat{B}_{(K)} = \Sigma V V^T B V V^T \Sigma. \tag{19}$$

μ_j known, Σ unknown Although this case is not explicitly stated in MKB, one deduces (and easily checks) from their equation (4.2.7) on page 104 that

$$\hat{\Sigma} = W + \sum_{j=1}^{J} \frac{N_j}{N} (\bar{x}_j - \mu_j)(\bar{x}_j - \mu_j)^T \tag{20}$$

- This allows natural generalisations by replacing the linear regression by more exotic forms:
  - Adaptive nonparametric regressions enrich the procedure by expanding and transforming the predictor set;
  - Penalised regressions regularise the coefficients in cases where the predictors are sampled analogue signals over some spatial domain.
- We can shrink the between-subclass variability relative to the between class variability. This often leads to more sensible low dimensional views, and is a natural way to regularise in the presence of many subclasses.
- Our procedure provides a smooth enhancement to the LVQ algorithm, and in fact uses LVQ for initialisation.

In the longer version of this paper (Hastie & Tibshirani 1993) we illustrate the MDA procedure on a number of simulated examples; it performed favourably against a range of competitors, including neural networks. Further comparisons with other discrimination techniques, in a variety of different problems, would be useful future work.

Software

We have written a set of functions for fitting FDA, PDA and MDA models in the S/Splus language (Becker, Chambers & Wilks 1988, Chambers & Hastie 1991). The function `fda()` fits FDA and PDA models. A `method` argument allows the user to specify the multi-response regression method to be used; the default is linear regression and thus Fisher's LDA. Other regression methods provided for FDA are polynomial regression, ridge regression, BRUTO, and MARS. For PDA a generalised form of ridge regression is included. Users supply a penalty matrix and target *df*, and the procedure derives the appropriate penalty constant. The `mda()` function has additional arguments for controlling the number of subclasses, their initialisation, and *df* parameters to control the shrinkage.

The software is reasonably efficient for moderately sized data sets, although ultimately is limited by the data management strategies in S. For example the digit classification problem has 1756 training observations with 256 variables (pixels); a 12 subclass model took roughly 1 minute on a SGI Indigo workstation. The main computational burden is the large regression. For smaller problems computation time is no issue, and typically less than 10 EM steps are required.

A variety of functions is provided for making predictions of varying types from these models (class predictions, posterior probability estimates, canonical coordinates), based on models of specified dimensions. Other functions are provided for producing plots, misclassification (confusion) matrices, and for extracting coefficients. The software is publicly available from the statistics archive at Carnegie-Mellon University — `lib.stat.cmu.edu`. Either send the email message `send fda-mda from S` to `statlib@lib.stat.cmu.edu`, or else login to `statlib` via ftp and `cd S`. The technical

7.3 MDA and penalised optimal scoring

In general steps 1-4 of the MDA/FDA or MDA/PDA optimal scoring algorithm can be seen to minimise

$$\sum_{k=1}^{K}\left[\sum_{j=1}^{J}\sum_{g_i=j}\sum_{r=1}^{R_j} p(c_{jr}|x_i,j)(\theta_k(c_{rk})-\eta_k(x_i))^2+\lambda J(\eta_k)\right] \tag{17}$$

where $\eta_k(x)=x^T\beta_k$, $J(\eta_k)=\beta_k^T\Omega\beta_k$, Ω is a penalty matrix, and the scoring functions θ_k are suitable normalised. Here x might represent the original predictors, and the penalty enforces smoothness of the coefficients vectors β_k themselves, or else might be a basis expansion of the original predictors, and the penalty ensures that the composition $\eta_k(x)$ is smooth in the original domain.

A reasonable goal, consistent with our approach so far, would be to derive this penalised optimal scoring criterion as the M-step of a suitably regularised Gaussian (mixture) likelihood. Since in the unpenalised case these β_k are scaled versions of the right eigenvectors v_k in (16)(Hastie et al. 1994*a*), it might seem natural to maximise the mixture likelihood subject to an appropriate penalty on the v_k. This was the approach taken by Kiiveri (1989) in the context of penalised LDA.

We first analyse the simpler case of penalised LDA via a penalised Gaussian likelihood. Unfortunately, it does not lead to a simple (non-iterative) MLE if Σ is unknown, and if Σ is assumed known and equal to W, it still differs from the optimal scoring procedure. Hastie et al. (1994*a*) show that optimal scoring corresponds to LDA with a fixed, penalised within-class covariance $W+\Omega$. In other words, Gaussian maximum-likelihood for the rank-reduced means with Σ assumed known and equal to $W+\Omega$. This is also the approach taken by Leurgans, Moyeed & Silverman (1993).

For MDA, things get more complicated since the corresponding version of W is a weighted within-covariance, which changes at each iteration. We are thus unable to write down an explicit likelihood criterion. We nevertheless use the penalised MDA optimal scoring algorithm, which corresponds to using $W+\Omega$ in place of W in the M-step.

8 Discussion

Classification by Gaussian mixtures is not a new idea. In this paper we have added to the functionality of this approach:

- Reduced rank versions allow valuable low dimensional views of the data, even in the two class case, and provide a natural means for regularisation.
- The M-step of the EM algorithm can be solved via a weighted optimal scoring algorithm, which amounts to a multiple linear regression of a blurred response matrix Z.

For lack of space we omit the proof, which is given in a longer version of this paper (Hastie & Tibshirani 1993) and is available from the authors or via ftp.

The form of the penalty in (13)-(15) requires some explanation. The modelled mean matrix U has R rows for subclasses, and p columns for predictors. Our penalty matrix Q works on individual columns of U; any composite penalty has to add these up in a sensible way, since the predictors are correlated. The rank-K mean model can be written

$$U = U_0 + \Phi V^T \Sigma \tag{16}$$

with $\Phi_{R\times K}$ and $V_{p\times K}$ ($V^T\Sigma V = I_K$) to be determined. This is the form in which the unshrunken solutions emerge. Now $\mathrm{tr}(\Sigma^{-1}U^TQU) = \mathrm{tr}(\Phi^TQ\Phi)$, where $\Phi = (U - U_0)V$, the projection of the means onto the subspace spanned by the Σ-orthonormal basis V. Hence we simply add the penalties for the uncorrelated columns of Φ, which is equivalent to adding the Σ^{-1}-weighted penalties for the columns of U.

From the form of Q, it is clear that as the γ_j get large, the only vectors permitted will be constant within a class, and the problem will degenerate to the standard LDA model.

7.2 Choosing the amount of shrinking

In practice it is difficult to guess suitable values for γ_j. One strategy is to let $\gamma_j = \gamma\,\forall j$ and then choose γ in some objective way, for example by cross-validation or evaluation on a test data set. Here we describe a strategy that helps the analyst choose γ_j in a more subjective way.

In the proof of proposition 3, it emerges that the shrunken means $\tilde{M} = (D_p + Q_\gamma)^{-1}D_pM$ are used in the subsequent LDA. The shrinkage operator $S = (D_p+Q_\gamma)^{-1}D_p$ is like a smoother, and it makes sense to use its trace as the effective number of parameters after the shrinking (Hastie & Tibshirani 1990). Given D_p, it is easy to work backwards and derive γ such that $\mathrm{tr}(S) = df$ for some nominal value of df. A subjective strategy is to select a (possibly large) number of subclass centres R_j for each class, and then fit the shrunken model such that:

- The effective overall number of centres is df, with $J \le df \le R = \sum_j R_j$; or
- The effective number of centres per class is df_j, with $1 \le df_j \le R_j$. Here we use the fact that Q and hence S is block diagonal, so one can compute df_j for each class.

Figure 6 illustrates the former case, where we shrunk from a total of 12 centres to an effective total of 8. Notice how the leading two eigenvectors focus more on between-class separation (than for the unshrunk case), while the third starts picking up within-subclass variation.

then $Q = \text{diag}(\gamma_1 Q_1, \gamma_2 Q_2, \ldots, \gamma_J Q_J)$ is an appropriate, composite penalty matrix for penalising the sub-components of an R-vector for deviations about their class means. The relative strengths of the penalties on the diagonal can be controlled by the parameters γ_j.

We now consider maximising a penalised version of (11):

Definition 1 *Let U be the $R \times p$ rank-K matrix of means for the rank-K MDA problem. The shrunken MDA estimate of rank K maximises the penalised mixture log-likelihood:*

$$\ell_Q^{mix}(U, \Sigma, \pi_{jr}) = \ell^{mix}(U, \Sigma, \pi_{jr}) - tr(\Sigma^{-1} U^T Q U)/2 \tag{13}$$

subject to rank$(U) = K$.

Our use in (13) of Σ^{-1} to weight the components of the penalty is explained in proposition 3 below.

An EM algorithm emerges just as in the unshrunk case, and the M-step corresponds to a penalised, reduced rank, augmented and weighted R class Gaussian log-likelihood analogous to that in proposition 2:

$$2\ell_Q^{weight}(\mu_{rj}, \Sigma) = -\sum_{j=1}^{J} \sum_{g_i=j} \sum_{r=1}^{R_j} p(c_{jr}|x_i, j) D(x, \mu_{jr}) - N \log|\Sigma| - \text{tr}(\Sigma^{-1} U^T Q U) \tag{14}$$

subject to rank$(U) = K$. Unfortunately, the maximiser of (14) does not have a simple solution like the unshrunk version. The solution is characterised by an expression for the means and covariance just as in (18) and (20) in appendix A.1. But unlike there, the solution now requires iteration between the mean and the covariance estimators. Apart from the added computational complexity, this destroys the valuable link with optimal scoring.

We prefer to use a restricted version (REML), where we fix the estimated covariance at the weighted, pooled within-subclass covariance W as in (6). For this restricted case we have:

Proposition 3 *Consider maximising the restricted, M-step, penalised log-likelihood:*

$$2\ell_Q^{weight}(\mu_{rj}|W) = -\sum_{j=1}^{J} \sum_{g_i=j} \sum_{r=1}^{R_j} p(c_{jr}|x_i, j) D(x, \mu_{jr}) - tr(W^{-1} U^T Q U) \tag{15}$$

subject to rank$(U) = K$. Here $D(\cdot, \cdot)$ is defined in terms of W. The solution corresponds to a shrunken LDA. If M is the $R \times p$ weighted subclass centroid matrix, and D_p the diagonal weight matrix with rth element the sum of the weights for the rth subclass, then the shrunken LDA is based on the shrunken between-subclass matrix

$$B_Q = M D_p (D_p + Q)^{-1} D_p M.$$

This shrunken LDA can be fit using a modified MDA algorithm, in which the only change is that $Z^T \hat{Z}$ is decomposed with normalisation $\Theta^T (D_p + Q) \Theta = I_K$.

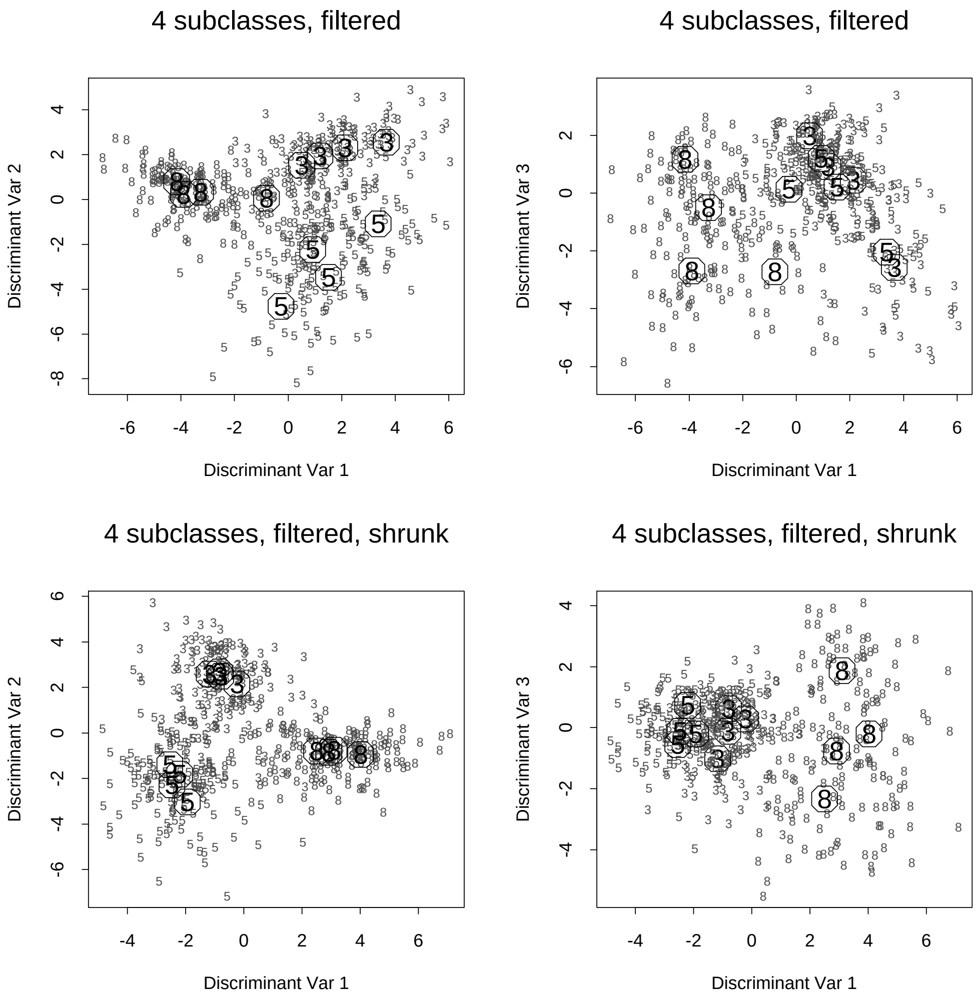

Figure 6: *The top two panels show the the first 3 discriminant coordinates for the MDA fit, with the centroids indicated. The lower two panels show the corresponding coordinates for the shrunken MDA model. We see that in the latter case, the leading two coordinates concentrate on group separation, while separation in the subclass centroids plays a stronger role for the 3s in the 3rd coordinate. For the top left plot, subclass separation is given as much weight as class separation, and we see more class overlap.*

The inputs are highly correlated because of their spatial arrangement, and some kind of smoothing or filtering always helps. We used an M-dimensional orthonormal basis of smooth functions on the 16×16 spatial domain of the image. These were derived from the roughness penalty matrix of a two-dimensional, 3rd degree thin-plate spline smoother; they are the M trailing eigenvectors, which are the smoothest and penalised the least. Given this $256 \times M$ basis matrix P, an input pixel vector x is replaced by $x^* = P^T x$. The performance of LDA improved by nearly 20% because of the filtering alone, with $M = 64$. MDA with four subclasses per digit gave no better performance, but further regularisation helped:

- reducing M from 64 to 49 yielded a 12% improvement;
- with $M = 64$, and shrinking to a total of 8 effective centres yielded a 20% improvement.

We tried other shrinking strategies, such as using 7 subclasses per class and shrinking down to 8 as above; the test errors were 6.6%. Shrinking down to 18 gave 6.4% errors. An empirical conclusion we draw is that a small amount of shrinking helps by smoothing the decision boundaries; a large amount of shrinking can hurt by losing the flexibility of having different centres.

Figure 5 displays the fitted subclass centroids as images: some spatial differences are apparent within a class. Figure 6 illustrates the effect of shrinkage on the eigenvectors, discussed further in section 7.

7 Shrinking and Penalisation

In this section we make precise our notion of shrinking the sub-class centres, as well as the interpretation of penalised optimal scoring in the context of the present model.

7.1 MDA with centroid shrinking

The subspace reduced model in proposition 2 is fitted iteratively using weighted LDA, which essentially treats all classes and subclasses interchangeably. Our proposal here is to bias this decomposition, and the positions of the means themselves, in such a way that within each class the variance of the subclass centroids is damped relative to between-class variance. This will have the effect of pulling the centroids away from the decision boundaries, and hence making them smoother. We do this by penalising the mixture likelihood for between-subclass variability. In the limit (infinite penalty), we expect the standard single-Gaussian-per-class LDA model to emerge.

Let $\pi_j = \{\pi_{jk}\}$ be the vector of R_j subclass probabilities for the Jth class (summing to 1), and $\Delta_j = (I - 1\pi_j^T)$, where I is the identity matrix and 1 is a column vector of ones. For any vector u with R_j elements, $\Delta_j u$ is a vector of deviations of the elements of u about their weighted mean, and likewise $u^T \Delta_j^T \Delta_j u$ is a positive, scalar measure of the spread of u about its mean. If $Q_j = \Delta_j^T \Delta_j$ is the corresponding penalty matrix,

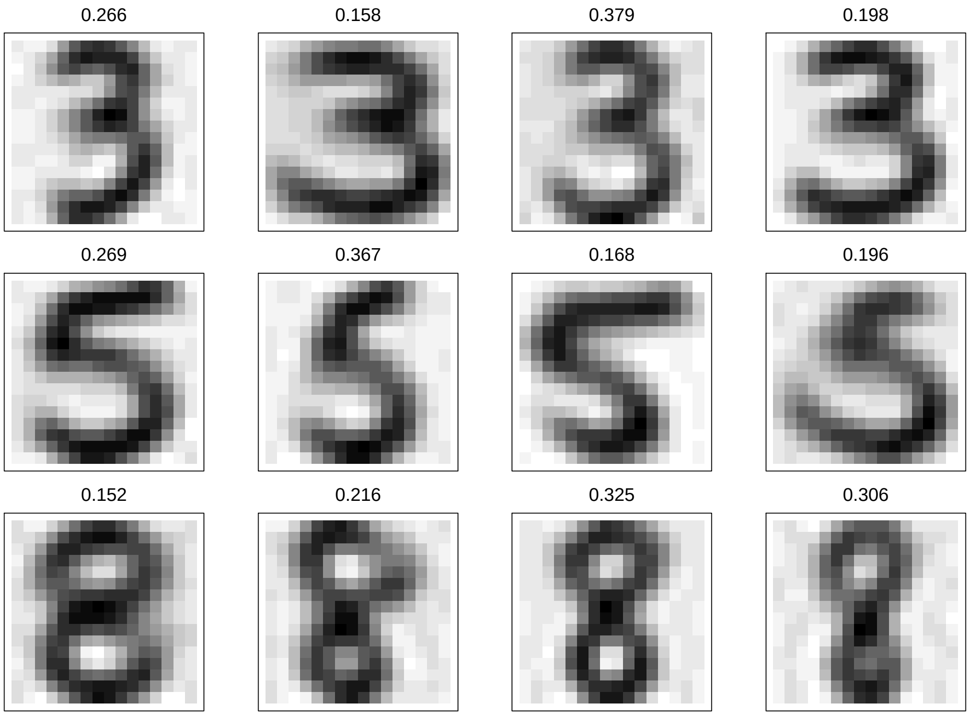

Figure 5: *The subclass centroids for the filtered MDA fit, displayed in unfiltered form. Above each image, the within-class mixing parameter* π_{jr} *is indicated. Not all the centroids are very different, which suggests that different numbers of subclasses could be used with different classes.*

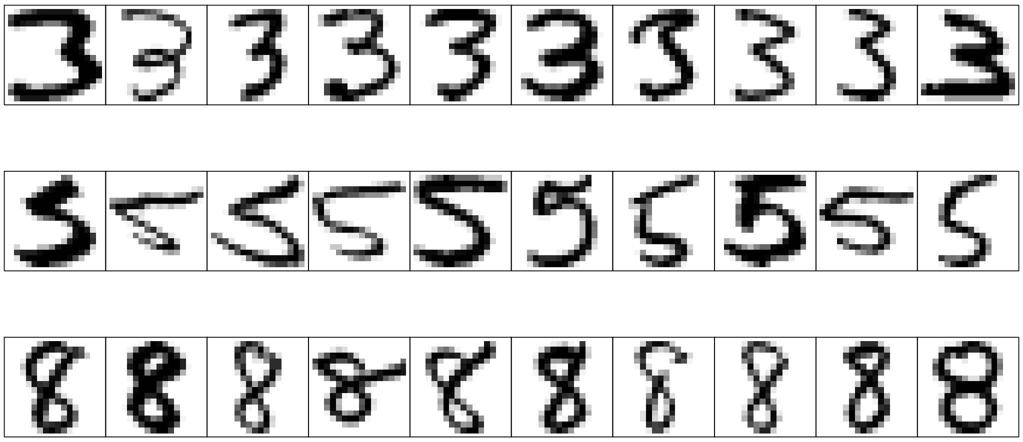

Figure 4: *A random selection of digitised handwritten 3s, 5s and 8s. Each image is a 8 bit, greyscale version of the original binary image, size and orientation normalised to* 16×16 *pixels.*

Table 2: *Digit classification results — 3s, 5s and 8s. The filtered models correspond to a hierarchical basis of smooth two-dimensional functions, derived from the thin-plate smoothing-spline penalty functional. The shrunken MDA model shrunk the 12 centroids to an effective total of 8.*

Technique	Error rates (%)	
	Training	Test
LDA	1.6	8.7
LDA (filtered – 64df)	3.1	7.1
LDA (filtered – 49df)	3.6	7.7
MDA (filtered – 64df, 4 subclasses)	2.7	7.1
MDA (filtered – 49df, 4 subclasses)	2.3	6.3
MDA (filtered – 64df, 4 subclasses, shrunk)	2.7	5.8

- if too few centres are provided, nonlinearities can compensate;
- extreme nonlinearities, which are costly in terms of fitted degrees of freedom, can be avoided by using mixtures.

- the adaptive aspect of FDA plays the role of a variable selector, and it is convenient having a regression procedure play this role.

The PDA extension to MDA is justified in exactly the same way as for PDA itself. Two of our examples support penalisation:

- The waveform predictors in section 4 represent noisy functions sampled at 21 evenly spaced abscissae. The discriminant coefficients were penalised using a 2nd-derivative roughness penalty, reducing the effective number of parameters from 21 down to 4, and gave on average an 8% improvement in the classification performance. Figure 3 shows the fitted penalised discriminant functions $(\hat{\Sigma}+\Omega)^{-1}\hat{\mu}_{jr}$ for each subclass — and compares them to the unpenalised versions. We see that penalisation plays two roles:
  - Variance reduction: the unpenalised MDA discriminant functions appear unnecessarily wiggly, for which we pay a price in generalisation errors.
  - Interpretation: by superimposing the known generating functions, we see that the discriminant functions are appropriately placed for picking out the peaks and valley of the mixture distribution for each class. It would be much harder and less convincing to attempt the same interpretations using the unpenalised discriminant functions.
- The handwritten digit example in the next section is a natural for both mixture models and for penalisation:
  - There are several characteristic ways for writing each digit, calling for a mixture model;
  - pixel greyscale values have strong spatial correlation, calling for regularisation for the same reasons as given in the waveform example.

6 Example: Handwritten Digit Recognition

In Hastie et al. (1994*a*) we illustrated PDA on a handwritten digit recognition task. Here we focus on a difficult sub-task, that of distinguishing handwritten 3s, 5s and 8s. We use the same training data as Le Cun et al. (1990), who normalised binary images for size and orientation, resulting in 8-bit, 16×16 greyscale images. We have 658 threes, 556 fives and 542 eights in our training set, and roughly a quarter the number of test examples. Figure 4 shows some examples from each.

Although we tried some preliminary experiments on the larger 10 class problem (roughly 8,000 observations, 256 predictors, 40 subclasses), the compute time in our current S implementation encouraged us to focus on this smaller subset of the data.

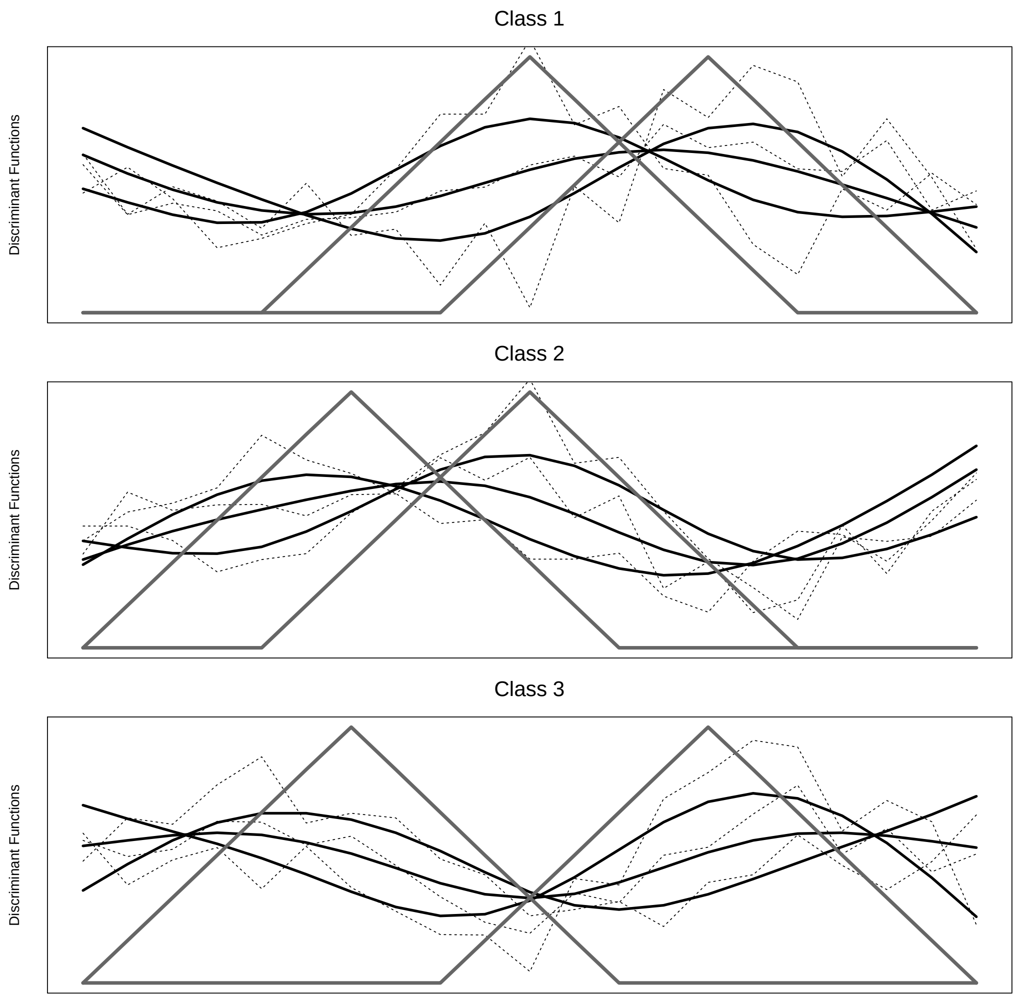

Figure 3: *Discriminant functions for the subclasses in the waveform example; each panel represents the subclasses for a single class. The smooth functions are* $(\hat{\Sigma} + \Omega)^{-1}\hat{\mu}_{jr}$*, produced by the MDA algorithm using a penalised regression method. The wiggly functions are the unpenalised versions* $\hat{\Sigma}^{-1}\hat{\mu}_{jr}$*. Superimposed on the figures are the generating waveforms, shifted and scaled to fit into the plots.*

analysis. For lack of space we omit the proof, which is given in a longer version of this paper (Hastie & Tibshirani 1993) and is available from the authors or via ftp.

We don't actually obtain estimates of the means and covariance from this MDA algorithm. The K-dimensional fit $\eta(x)$ produced by the algorithm is actually the coordinate of the discriminant projection of x onto the subspace spanned by the reduced-rank subclass centroids (up to known scale factors). Relative Euclidean distances in this subspace are Mahalanobis distances in the implicitly estimated covariance. The projected means themselves are scaled rows of Θ. Since relative distances are all that are needed in (3) and (7), we have all the ingredients needed for fitting the model, and for classification. Details of these equivalences are given in Hastie et al (1992a, b).

One advantage of this approach is immediately clear: the M-step in proposition 2 involved a weighted LDA of $\sum_j N_j R_j$ observations, while here we only have N observations!

There is an even more compelling reason for using optimal scoring to fit LDA and MDA models. By expressing the problem as a multiple regression of a response matrix Y or Z, we can immediately generalise it by using in step 2 regression methods more exotic than linear regression. Two classes of such generalisations emerge:

FDA: Here multivariate adaptive nonlinear regression replaces the linear regression, and the linear map $\eta(X)$ becomes a nonlinear map. Hastie et al. (1994*b*) describe the class of nonlinear regression methods that can be used, including adaptive additive models, the multivariate adaptive regression spline (MARS) model of Friedman (1991), projection pursuit regression, and neural networks. They call the resulting procedure "FDA" for flexible discriminant analysis. These procedures amount to expanding the original predictors x in an adaptive way into a set of transformed predictors $h(x)$, and then performing LDA or MDA in the new space. In some cases the nonparametric regressions consist of a basis expansion followed by a penalised regression (e.g. additive splines). In this case the transformed space $h(x)$ is large, and the penalised regression translates into a penalised version of LDA or MDA.

PDA: Here we fit a more restrictive linear map via penalised least squares (Hastie et al. 1994*a*). The idea is that the feature vectors x_i arise as digitised analogue signals, and are spatially correlated (pixels in an image, log-spectra at different frequencies). The penalisation amounts to regularising the large, near singular, covariance matrix $\hat{\Sigma}$ by adding a penalty: $\hat{\Sigma} + \Omega$, which in turn ensures that the coefficients v_k are spatially smooth (and hence borrow strength from neighbouring values.)

Our experience in many examples and simulations (Hastie & Tibshirani 1993) in using this FDA extension of MDA suggests:

- Both FDA and standard MDA are capable of producing non-linear decision boundaries. Adding the non-linear capabilities of FDA to MDA puts these components in competition with each other, and typically does not yield a much improved decision boundary. Figure 1 supports this claim. One can imagine that in difficult situations the two components can support each other:

computational advantages and facilitates some useful generalisations of both techniques.

Consider first the LDA model. If $Y_{N\times J}$ is an *indicator response matrix* representing the classes, then we can regress Y against the predictor matrix X to get fitted values $\hat{Y} = HY$. This is followed by a suitably normalised eigen-decomposition of $Y^THY = Y^T\hat{Y}$, which contains all the ingredients for an LDA of any rank (Breiman & Ihaka (1984), Hastie et al. (1994*b*)).

This simple procedure carries over to the M-step of the MDA algorithm. Instead of using a response indicator matrix Y, we use a *blurred* response matrix $Z_{N\times R}$, whose rows consist of the current subclass probabilities for each observation. At each M-step, this Z is used in a multiple linear regression followed by an eigen-decomposition, just as in the LDA case above.

Hastie et al. (1994*b*) called this procedure optimal scoring, which we now describe in more detail for MDA.

Mixture Discriminant Analysis by Optimal Scoring: MDA

Iinitialise: Start with a set of R_j subclasses c_{jr} for each class, and associated subclass probabilities $\hat{p}(c_{jr}|x_i, j)$. These can be derived, for example, from a LVQ or K-means preprocessing of the data. Let $R = \sum R_j$.

Iterate:

1. *Compute Blurred Response:* Define the blurred response matrix $Z_{N\times R}$ as follows: if $g_i = j$, then fill the jth block of R_j entries in the ith row with the values $\hat{p}(c_{jr}|x_i, j)$, $r = 1, \ldots, R_j$, and the rest with zeros. Z is the mixture analogue of an indicator-response matrix, except observations can belong to several (sub-)classes with associated probabilities.
2. *Multivariate linear regression:* Fit a multi-response, linear regression of Z on X. Let $\hat{Z}$ be the fitted values, and $\eta(x)$ be the vector of fitted regression functions.
3. *Optimal scores:* Let Θ be the largest K nontrivial eigenvectors of $Z^T\hat{Z}$, with normalisation $\Theta^T D_p \Theta = I_K$. Here D_p is a diagonal $R \times R$ matrix of weights, with rth entry the sum of the elements of the rth column of Z (the total weight for subclass r).
4. *Update* the fitted model from step 2 using the optimal scores: $\eta(x) \leftarrow \Theta^T\eta(x)$.
5. *Update* $\hat{p}(c_{jr}|x_i, j)$ and $\hat{\pi}_{jr}$ using formulas (3) and (4).

To show that this MDA algorithm corresponds to the EM algorithm in proposition 2, we need to show that steps 1–4 fit the augmented and weighted rank-K discriminant

Table 1: *Results for waveform data. The values are averages over 10 simulations, with the standard error of the average in parentheses. The five entries above the line are taken from Hastie et al. (1994*b*). The first model below the line is MDA with 3 subclasses per class. The next line is the same, except that the discriminant coefficients are penalised via a roughness penalty to effectively 4df. The third is the corresponding penalised LDA or PDA model.*

Technique	Error Rates	
	Training	Test
LDA	0.121(.006)	0.191(.006)
QDA	0.039(.004)	0.205(.006)
CART	0.072(.003)	0.289(.004)
FDA/MARS (degree = 1)	0.100(.006)	0.191(.006)
FDA/MARS (degree = 2)	0.068(.004)	0.215(.002)
MDA (3 subclasses)	0.087(.005)	0.169(.006)
MDA (3 subclasses, penalised 4df)	0.137(.006)	0.157(.005)
PDA (penalised 4df)	0.150(.005)	0.171(.005)

where $i = 1, 2, \ldots 21$, u is uniform on $(0, 1)$, ϵ_i are standard normal variates, and the h_i are the shifted triangular waveforms: $h_1(i) = \max(6 - |i - 11|, 0)$, $h_2(i) = h_1(i - 4)$ and $h_3(i) = h_1(i + 4)$.

Table 1 extends a simulation of Hastie et al. (1994*b*) to include the methods discussed here. Each training sample has 300 observations, and equal priors were used, so there are roughly 100 observations in each class. We used test samples of size 500. The two MDA models are described in the caption. More details on the penalisation are given in section 7.

Figure 2 shows the leading canonical variates for the penalised MDA model, evaluated at the test data. As we might have guessed, the classes appear to lie on the edges of a triangle. This is because the $h_j(i)$ are represented by 3 points in 21-space, thereby forming vertices of a triangle, and each class is represented as a convex combination of a pair of vertices, and hence lie on an edge. Also it is clear visually that all the information lies in the first two dimensions; the percent of variance explained by the first two coordinates is 99.8%, and we would lose nothing by truncating the solution thus. The Bayes risk for this problem is about 0.14 (Breiman et al. 1984); MDA comes close to the optimal rate, which is not surprising since the structure of the MDA model is similar to the generating model.

5 MDA by optimal scoring

One can use "optimal scoring" — multiple linear regression followed by an eigen analysis— to fit both the LDA and MDA models, as we show in this section. This has significant

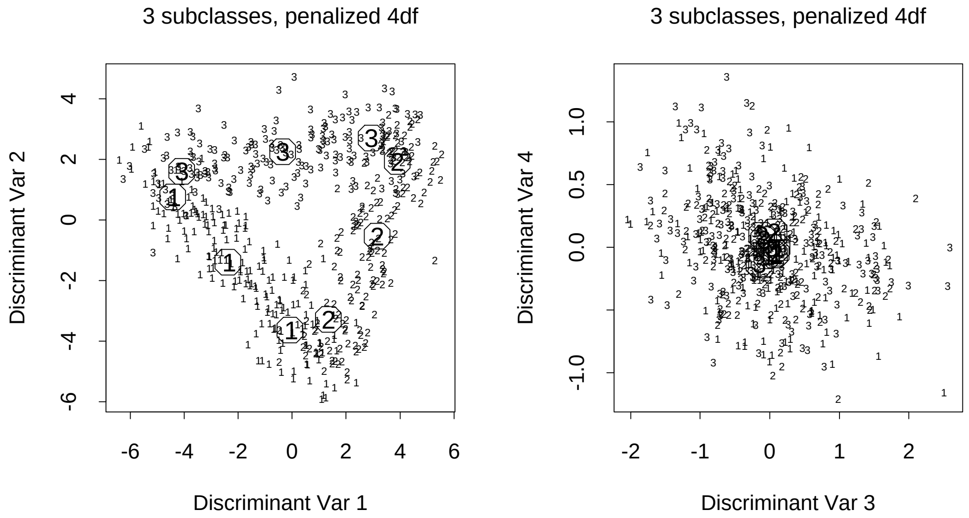

Figure 2: *Some two dimensional views of the MDA model fitted to a sample of the waveform model. The points are independent test data, projected onto the leading two canonical coordinates (left panel), and the third and forth (right panel). The subclass centres are indicated.*

- Step (3) of the EM algorithm requires only *differences* in Mahalanobis distances from the estimated centres. This is convenient, since weighted LDA will only supply distances in the K dimensional subspace of span$\{\mu_{jr}\}$.

- The solution to this problem *cannot* be obtained by a simple reduction of the full rank mixture solution. We need to perform a reduced rank weighted LDA at each of the iterations of the EM algorithm. The reason is that the weights computed in step (3) should depend on the reduced-rank rather than the full-rank solution.

We collect these results in the following.

Proposition 2 *Consider maximisation of the constrained mixture density log-likelihood*

$$\ell^{mix}(\mu_{jr}, \Sigma, \pi_{jr}) \propto \sum_{j=1}^{J} \sum_{g_i=j} \log \sum_{r=1}^{R_j} \pi_{jr} e^{-D(x,\mu_{jr})/2} - \frac{N}{2} \log |\Sigma| \tag{11}$$

subject to rank$\{\mu_{jr}\} = K$*. This is achieved by an EM algorithm analogous to that defined in (3)-(6), with steps (5)-(6) replaced by the equations for maximising the weighted and augmented log-likelihood:*

$$2\ell^{weight}(\mu_{rj}, \Sigma) \propto -\sum_{j=1}^{J} \sum_{g_i=j} \sum_{r=1}^{R_j} p(c_{jr}|x_i, j) D(x, \mu_{jr}) - N \log |\Sigma|$$

subject to rank$\{\mu_{jr}\} = K$*. This latter maximisation can be achieved via a similarly augmented and weighted rank-*K *LDA.*

The lower left panel in figure 1 shows the effect of rank reduction on this simple example. Practically speaking, the approximate reduced-rank solution — obtained by a weighted rank reduction of the full mixture solution — is more attractive than the exact reduced rank solution described above. This is because the latter requires one to fit the model iteratively for each dimension K of interest. We have found in a simulation experiment (not shown here) that the two approaches tend to agree quite well.

4 Example: waveform data

We now illustrate some of these ideas on a popular simulated example, taken from Breiman et al. (1984, pg 49-55), and used in Hastie et al. (1994*b*) and elsewhere. It is a three class problem with 21 variables, and is considered to be a difficult pattern recognition problem. The predictors are defined by

$$\begin{aligned} x_i &= uh_1(i) + (1-u)h_2(i) + \epsilon_i \qquad \text{Class 1} \\ x_i &= uh_1(i) + (1-u)h_3(i) + \epsilon_i \qquad \text{Class 2} \\ x_i &= uh_2(i) + (1-u)h_3(i) + \epsilon_i \qquad \text{Class 3} \end{aligned} \tag{12}$$

performance. This standard Fisher-Rao decomposition (Mardia, Kent & Bibby 1979, for example) is derived by successively maximising the ratio of between- to within-group variance of linear combinations of the variables: $v^T Bv/v^T Wv$, where B is the between class covariance (of the class centroids) and W the pooled within-class covariance. In this section we show that reduced rank LDA can be viewed as a restricted Gaussian maximum likelihood solution, and then extend this concept to the mixture model.

Proposition 1 *Consider maximising the Gaussian log-likelihood*

$$2\ell(\mu_j, \Sigma, d) = -\sum_{j=1}^{J} \sum_{g_i=j} (x_i - \mu_j)^T \Sigma^{-1} (x_i - \mu_j) - N \log |\Sigma| \tag{8}$$

subject to the constraints $\mathrm{rank}\{\mu_j\}_{j=1}^J = K \le \min(J-1, p)$. *The solution is*

$$\begin{aligned} \hat{\mu}_j &= WVV^T(\bar{x}_j - \bar{x}) + \bar{x} & (9) \\ \hat{\Sigma} &= W + \sum_{j=1}^{J} \frac{N_j}{N} (\bar{x}_j - \hat{\mu}_j)(\bar{x}_j - \hat{\mu}_j)^T \\ &= W + WV_\perp V_\perp^T B V_\perp V_\perp^T W & (10) \end{aligned}$$

where V is a matrix consisting of the leading K eigenvectors of $W^{-1}B$. This solution effectively coincides with the reduced rank LDA solution:

- *$\hat{\mu}_j$ is the projection of the jth sample mean onto the discriminant subspace of rank K.*
- *classification based on $(x - \hat{\mu}_j)^T \hat{\Sigma}^{-1} (x - \hat{\mu}_j)$ is equivalent to the reduced linear discriminant rule of rank K.*

Much of this result was proved by Campbell (1984), although he appears to have overlooked the last claim — we outline a simple proof in Appendix A.1.

Now consider a reduced rank version of the mixture model. We take the Gaussian mixture log-likelihood ℓ^{mix} (equation 2) and maximise it subject to the rank K constraint on the subclass means: $\mathrm{rank}\{\mu_{rj}\} = K$.

How might we achieve this maximisation? Once again we can use the EM algorithm. Steps (3) and (4) remain the same, and are conditional on the current (reduced rank) versions of the centres and the corresponding pooled covariance estimate. Steps (5) and (6) can be viewed as weighted mean and pooled-covariance maximum-likelihood estimates in a *weighted* and *augmented* R-class problem. We augment the data by replicating the N_j observations in class j R_j times, with the ℓth such replication having observation weights $p(c_{j\ell}|x_i, j)$. This is done for each of the J classes, resulting in an augmented and weighted training set of $\sum_{j=1}^J N_j R_j$ observations. Note that the sum of all the weights is N. We now impose the rank restriction. By analogy with the early part of this section, this can be achieved by a weighted version of LDA. We postpone the details of how this final step is carried out until section 5. Two details are worth noting right away:

only difference is that the subclass indicator is replaced $\hat{p}(c_{jr}|x_i, j)$, the estimated probability that observation i falls in subclass c_{jr} given that it is observed to fall into class j. Since $\hat{p}(c_{jr}|x_i, j)$ is a function of $\hat{\mu}_{jr}$ and $\hat{\Sigma}$, the equations (3–6) must be iterated.

The posterior class probabilities are (by Bayes theorem)

$$P(G = j|X = x) \sim \Pi_j \, \mathrm{Prob}(x|j) \sim \Pi_j \sum_{r=1}^{R_j} \pi_{jr} e^{-D(x,\mu_{jr})/2} \tag{7}$$

normalised so that $\sum_{j=1}^{J} P(G = j|X = x) = 1$. The classification rule chooses j to maximise $p(j|x)$. Notice that this does not have the same form as a linear discriminant rule for the R subclasses, and in particular is likely to be nonlinear.

2.1 Cluster sizes and starting values

The EM iteration above requires a choice of cluster sizes R_j, and starting values for the means μ_{jr}, the covariance matrix Σ and the cluster probabilities $p(c_{jr}|x, j)$. We currently use two different strategies:

K-means: We choose a fixed number of clusters (say r) for each class, and then use a k-means clustering algorithm to estimate a set of r subclass centroids $\hat{\mu}_{jr}$ for each class. Then for all observations in class j, $\hat{p}(c_{jr}|x_i, j)$ is set to 1 if $\hat{\mu}_{jr}$ is the closest centroid to x_i, and 0 otherwise.

LVQ: We run the LVQ algorithm on the training data, and let it select the R_j and $\hat{\mu}_{jr}$ (we supply R). As in the previous case we use the output to produce $\hat{p}(c_{jr}|x_i, j)$.

In either case these within class weights determine a new set of $\hat{\mu}_{jr}$s from (5) and $\hat{\Sigma}$ from (6), and the iterations go from there.

Both k-means and LVQ require starting centres, which are typically randomly selected x_i. It is known (Pal, Bezdek & Tsao 1993, for example) that both these procedures suffer from variability due to random starting values. Our strategy is to try a number (10) of different starts, and choose the best. We use either a likelihood based criterion, or more cheaply, training sample misclassification, to guide the choice. Our experience has been that MDA *always* outperforms the starting procedure (LVQ or kmeans) with respect to classification of the training data.

We have no automatic way for selecting the R_j or in the case of LVQ, the total R. We treat these as meta-parameters, and hope for a validation set on which to try different values.

3 Reduced rank discrimination

In linear discriminant analysis with J classes, one can choose a subspace of rank $r < J$ that maximally separates the class centroids. This is mainly useful for descriptive purposes, but is also a form of regularisation and often leads to improved classification mixture model, for example, one could allow each subclass to have a different covariance matrix, or force the subclasses within a given class to have the same covariance matrix. The particular model chosen here is attractive because it keeps the total number of parameters under control, and as we will see, it has the right structure to permit the other generalisations we have in mind.

Let Π_j be the prior for class j, and within class j let π_{jr} be the mixing probability for the rth subclass, $\sum_{r=1}^{R_j} \pi_{jr} = 1$. Note that while often the Π_j are known or easily estimated from the training data, the π_{jr} are unknown model parameters. Let $D(x, \mu) = (x-\mu)^T \Sigma^{-1}(x-\mu)$ be the Mahalanobis distance between x and μ.

The mixture density for class j is

$$\begin{aligned} m_j(x) &= P(X = x | G = j) \\ &= |2\pi\Sigma|^{-1/2} \sum_{r=1}^{R_j} \pi_{jr} e^{-D(x,\mu_{jr})/2}, \end{aligned} \tag{1}$$

and the conditional log-likelihood for the data is

$$\ell^{mix}(\mu_{rj}, \Sigma, \pi_{jr}) = \sum_{i=1}^{N} \log m_{g_i}(x_i) \tag{2}$$

The EM algorithm provides a convenient method for maximising $\ell^{mix}(\theta)$. The EM steps are:

$$\begin{aligned} \hat{p}(c_{jr}|x, j) &= \text{Prob}(x \in r\text{th subclass of class } j \,|x, j) \\ &= \frac{\pi_{jr} e^{-D(x,\mu_{jr})/2}}{\sum_{k=1}^{R_j} \pi_{jk} e^{-D(x,\mu_{jk})/2}} \end{aligned} \tag{3}$$

$$\hat{\pi}_{jr} \propto \sum_{g_i=j} p(c_{jr}|x_i, j), \qquad \sum_{r=1}^{R_j} \hat{\pi}_{jr} = 1 \tag{4}$$

$$\hat{\mu}_{jr} = \frac{\sum_{g_i=j} x_i p(c_{jr}|x_i, j)}{\sum_{g_i=j} p(c_{jr}|x_i, j)} \tag{5}$$

$$\hat{\Sigma} = (1/N) \sum_{j=1}^{J} \sum_{g_i=j} \sum_{r=1}^{R_j} p(c_{jr}|x_i, j)(x_i - \mu_{jr})(x_i - \mu_{jr})^T \tag{6}$$

The notation $\sum_{g_i=j}$ means summing over all observations belonging to the jth class.

In the above (3) and (4) are the *Estimation* step, while (5) and (6) are the *Maximisation* step. These are a straightforward generalisation of the EM algorithm for estimating normal mixtures (e.g. Titterington, Smith and Makov, 1985, page 86-87). (5) and (6) have the same appearance as the maximum-likelihood estimate for the complete normal discriminant problem, i.e., the situation where we observe the subclass membership. The by downweighting "rough" directions relative to "smooth" directions in this enlarged space, when computing Mahalanobis distances. PDA (Hastie, Buja & Tibshirani 1994*a*) is a closely related technique for classifying digitised analogue signals. PDA starts with a high dimensional feature set, such as pixels from a digitised image, or spectral values on a grid of frequencies. Again a penalised discriminant analysis is used, but here to ensure spatial smoothness of the discriminant coefficients. Both of these techniques adapt naturally to MDA: in the (enlarged) feature space, we use a mixture of Gaussians rather than a single one per class, and still use a penalised metric when computing distances.

Figure 1 illustrates some of these techniques with a simple example. Not surprisingly the MDA technique has the most satisfactory boundary (the problem is a setup for MDA), and hence its boundary is close to optimal. The LVQ boundary seems unnecessarily biased and wiggly. The FDA boundary is a reasonable approximation to the optimal boundary. The lower-left panel shows a rank-1 version of the MDA fit, which also does acceptably well. The lower right panel shows the result of MDA combined with the nonlinear transformations of FDA — there is no noticeable improvement.

To summarise then, our proposal for MDA has the following features:

- The classes are modelled as mixtures of Gaussians, rather than a single Gaussian as in LDA;
- Optimal subspace identification is possible as in LDA, with added functionality;
- We can shrink the subclass centres, for example towards a common centre;
- The flexibility of FDA and PDA is easily and naturally accommodated.

The paper is organised as follows. In section 2 we discuss the normal mixture model and an EM algorithm for its estimation. In section 3 we discuss reduced rank versions of the procedures, which we demonstrate in section 4 on the well-known waveform example of Breiman, Friedman, Olshen & Stone (1984). In section 5 we show how the MDA algorithm can be expressed as a repeated-regression procedure using optimal scoring (Hastie et al. 1994*b*), which in turn allows useful nonparametric extensions. Section 6 further illustrates these techniques on a handwritten digit-recognition problem. Section 7 is about the centroid shrinking.

2 Extending LDA by normal mixtures

The approach to classification taken here is to model the class densities of the predictors $P(X\,|\,G)$ by Gaussian mixture models. These are flipped around via Bayes theorem and class priors to give models for the class posterior probabilities $P(G\,|\,X)$ — a basic ingredient for classification.

Suppose we have training data $(x_i, g_i) \in R^p \times \mathcal{J},\ i = 1, 2, \ldots N$. We divide each class j into R_j artificial subclasses, denoted by c_{jr}, $r = 1, 2, \ldots R_j$ and define $R = \sum_{j=1}^{J} R_j$. Our model assumes that each subclass has a multivariate normal distribution with its own mean vector μ_{jr} and common covariance matrix Σ. This is not the only possible

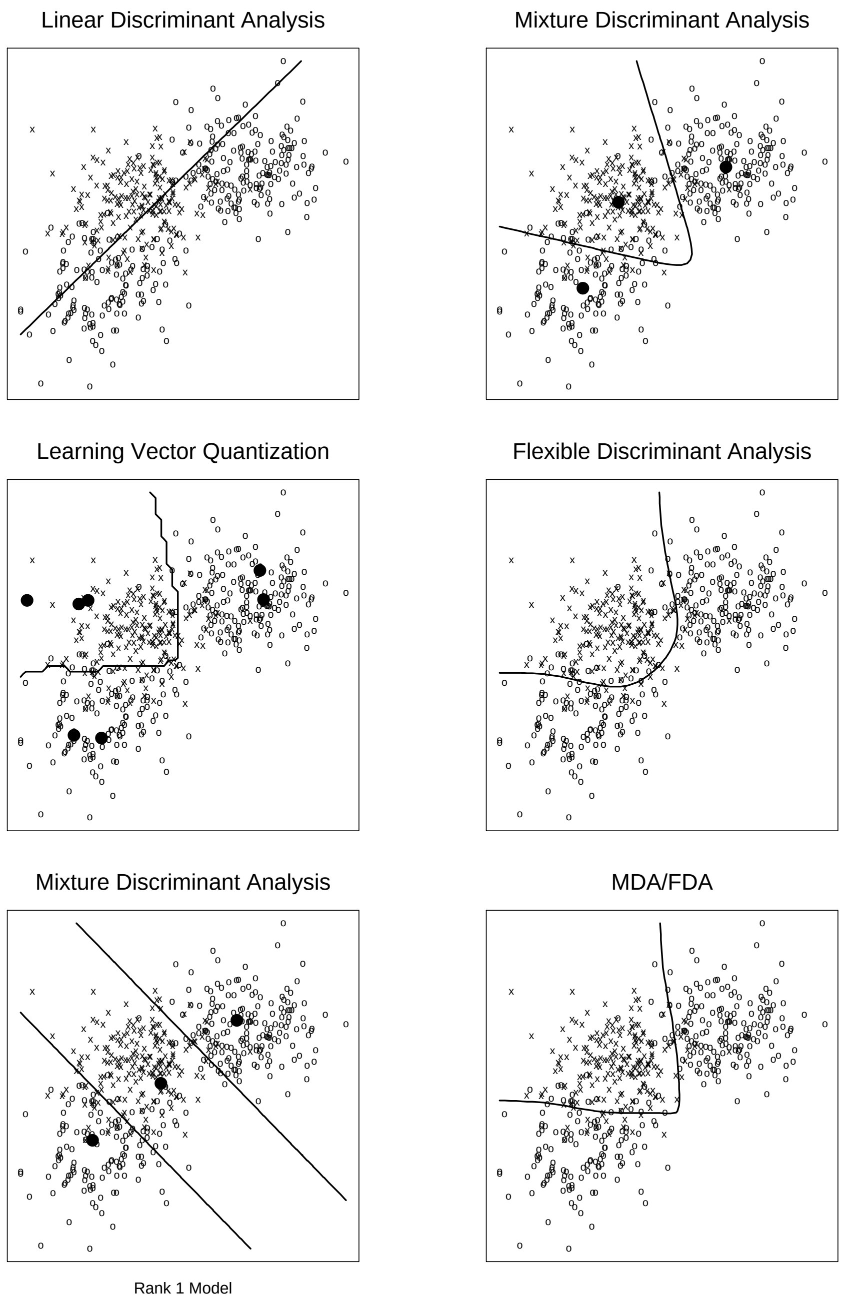

Figure 1: *A two class problem in which one of the classes occurs in two separated circular clouds. The panels are labled according to the technique that produced the decision boundary.*

discriminant analysis (LDA) and multiple logistic regression, nearest neighbour methods and classification trees. Neural network classifiers have become a powerful alternative, with the ability to incorporate a very large number of features in an adaptive nonlinear model. Ripley (1994) gives an informative review from a statistician's viewpoint.

LDA can be derived as the maximum likelihood method for normal populations with different means and common covariance matrix. It is natural therefore to generalise LDA by assuming that each observed class is in fact a mixture of unobserved normally distributed subclasses. This approach is sometimes mentioned in the statistical literature (McLachlan 1992, Cheng & Titterington 1994, for example) and more often in the pattern recognition literature (Taxt, Hjort & Eikvil 1991), but does not seem to have generated much attention. Particular neural network models using Gaussian radial basis functions can be derived from a Gaussian mixture modelling formulation (Tresp, Hollatz & Ahmad 1995).

In this paper we develop the mixture approach to discrimination in a number of interesting and useful directions. For brevity we refer to this mixture discriminant analysis technique as MDA.

LDA is not only a classification procedure, but also a data-reduction tool. We can represent multi-class data in low dimensional projections or plots that highlight their class differences. Our MDA procedure has this feature as well — we can produce a hierarchy of coordinates in terms of their abilities to separate the classes (and subclasses). An interesting twist occurs here: for two-class data, LDA produces a (not so interesting) single coordinate, while MDA will produce up to one less than the number of subclasses in the mixture representation.

A technique known as *Learning Vector Quantisation* or LVQ has received a lot of attention in the pattern recognition literature (Kohonen 1989); MDA can be viewed as a smooth version of LVQ. LVQ finds a *set* of cluster centres for each class; classification is performed by finding the closest centre, and assigning the associated class. The online learning algorithms for LVQ are similar to the k-means algorithm, with biases built in to encourage good classification. While LVQ generalises clustering to classification problems, MDA generalises mixture density estimation to classification problems.

An additional feature of our model is *subclass shrinkage*: we can regulate the within-class spread of the mixture centres relative to their between-class spread. This emphasises our bias towards classification, much like LVQ biases clustering techniques towards classification. A small amount of shrinkage tends to smooth the decision boundaries, and is a form of regularisation. It also allows us to use many subclass centres per class, and shrink them until the *effective number* of centres is a required smaller amount.

Other methods have been proposed to generalise LDA to allow nonlinear decision boundaries. In Hastie, Tibshirani & Buja (1994*b*), this is achieved by using adaptive, nonparametric regression methods. The link between nonparametric regression and discriminant analysis is provided by the *optimal scoring* approach, first suggested by Breiman & Ihaka (1984). Hastie et al. (1994*b*) call this procedure *Flexible Discriminant analysis* (FDA). The generic version of FDA based on smoothing splines operates by expanding the predictors into a large (adaptively selected) basis set, and then performing a *penalised* discriminant analysis in the enlarged space. Intuitively the penalisation works

Discriminant Analysis by Gaussian Mixtures

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Abstract

Fisher-Rao linear discriminant analysis (LDA) is a valuable tool for multigroup classification. LDA is equivalent to maximum likelihood classification assuming Gaussian distributions for each class. In this paper, we fitted Gaussian mixtures to each class to facilitate effective classification in non-normal settings, especially when the classes are clustered. Low dimensional views are an important by-product of LDA—our new techniques inherit this feature. We are able to control the within-class spread of the subclass centres relative to the between-class spread. Our technique for fitting these models permits a natural blend with nonparametric versions of LDA.

Keywords: Classification, Pattern Recognition, Clustering, Nonparametric Regression, Radial Basis Functions.

1 Introduction

In the generic classification or discrimination problem, the outcome of interest G falls into J unordered classes, which for convenience we denote by the set $\mathcal{J} = \{1, 2, 3, \cdots J\}$. We wish to build a rule for predicting the class membership of an item based on p measurements of predictors or features $X \in R^p$. Our training sample consists of the class membership and predictors for N items. This is an important practical problem with applications in many fields. Traditional statistical methods for this problem include linear