MATH 829: Introduction to Data Mining and Analysis
Linear Discriminant Analysis

Dominique Guillot

Departments of Mathematical Sciences
University of Delaware

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Linear discriminant analysis (LDA)

- Categorical data $Y$. Predictors $X_1, \ldots, X_p$. 

We saw how logistic regression can be used to predict $Y$ by modelling the log-odds

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\log \frac{P(Y = 1 | X = x)}{P(Y = 0 | X = x)} = x^T \beta.
$$

Now examine other models for $P(Y = i | X = x)$.

Recall: Bayes' theorem (Rev. Thomas Bayes, 1701–1761). Given two events $A, B$:

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P(A | B) = \frac{P(B | A) P(A)}{P(B)}.
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Going back to our prediction using Bayes’ theorem:

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P(Y = i | X = x) = \frac{P(X = x | Y = i)P(Y = i)}{P(X = x)}
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Using Bayes’ theorem

More precisely, suppose

- $Y \in \{1, \ldots, k\}$.
- $P(Y = i) = \pi_i \quad (i = 1, \ldots, k)$.
- $P(X = x | Y = i) \sim f_i(x) \quad (i = 1, \ldots, k)$. 

We can easily estimate $\pi_i$ using the proportion of observations in category $i$.

We need a model for $f_i(x)$. 

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= \frac{f_i(x)\pi_i}{\sum_{j=1}^{k} f_j(x)\pi_j}.
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- We can easily estimate $\pi_i$ using the proportion of observations in category $i$.
- We need a model for $f_i(x)$. 

Using Bayes’ theorem
Using a Gaussian model: LDA and QDA

A natural model for the $f_j$'s is the multivariate Gaussian distribution:

$$f_j(x) = \frac{1}{\sqrt{(2\pi)^p \det \Sigma_j}} e^{-\frac{1}{2} (x-\mu_j)^T \Sigma_j^{-1} (x-\mu_j)}.$$
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**Linear discriminant analysis (LDA):** We assume $\Sigma_j = \Sigma$ for all $j = 1, \ldots, k$.

**Quadratic discriminant analysis (QDA):** general case, i.e., $\Sigma_j$ can be distinct.
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Note: When $p$ is large, using QDA instead of LDA can dramatically increase the number of parameters to estimate.

In order to use LDA or QDA, we need:

- An estimate of the class probabilities $\pi_j$.
- An estimate of the mean vectors $\mu_j$.
- An estimate of the covariance matrices $\Sigma_j$ (or $\Sigma$ for LDA).
LDA: Suppose we have $N$ observations, and $N_j$ of these observations belong to the $j$ category ($j = 1, \ldots, k$). We use

- $\hat{\pi}_j = \frac{N_j}{N}$.
- $\hat{\mu}_j = \frac{1}{N_j} \sum_{y_i = j} x_i$ (average of $x$ over each category).
- $\hat{\Sigma} = \frac{1}{N-k} \sum_{j=1}^{k} \sum_{y_i = j} (x_i - \hat{\mu}_j)(x_i - \hat{\mu}_j)^T$. (Pooled variance.)
Estimating the parameters

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**FIGURE 4.5.** The left panel shows three Gaussian distributions, with the same covariance and different means. Included are the contours of constant density enclosing 95% of the probability in each case. The Bayes decision boundaries between each pair of classes are shown (broken straight lines), and the Bayes decision boundaries separating all three classes are the thicker solid lines (a subset of the former). On the right we see a sample of 30 drawn from each Gaussian distribution, and the fitted LDA decision boundaries.

ESL, Figure 4.5.
In the previous figure, we saw that the decision boundary is linear. Indeed, examining the log-odds:

\[ \log \frac{P(Y = l|X = x)}{P(Y = m|X = x)} = \log \frac{f_l(x)}{f_m(x)} + \log \frac{\pi_l}{\pi_m} \]

\[ = \log \frac{\pi_l}{\pi_m} - \frac{1}{2} (\mu_l + \mu_m)^T \Sigma^{-1} (\mu_l - \mu_m) + x^T \Sigma^{-1} (\mu_l - \mu_m) \]

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Note that the previous expression is *linear* in \(x\).
LDA: linearity of the decision boundary

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How is this different from LDA?

- In LDA, the parameters are more constrained and are not estimated the same way.
- Can lead to smaller variance if the Gaussian model is correct.
- In practice, logistic regression is considered safer and more robust.
- LDA and logistic regression often return similar results.
Let us now examining the log-odds for QDA: in that case no simplification occurs as before

\[
\log \frac{P(Y = l \mid X = x)}{P(Y = m \mid X = x)} = \log \frac{\pi_l}{\pi_m} + \frac{1}{2} \log \frac{\det \Sigma_m}{\det \Sigma_l} - \frac{1}{2} (x - \mu_l)^T \Sigma_l^{-1} (x - \mu_l) - \frac{1}{2} (x - \mu_m)^T \Sigma_l^{-1} (x - \mu_m).
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$$\log \frac{P(Y = l | X = x)}{P(Y = m | X = x)}$$

$$= \log \frac{\pi_l}{\pi_m} + \frac{1}{2} \log \frac{\det \Sigma_m}{\det \Sigma_l}$$

$$- \frac{1}{2} (x - \mu_l)^T \Sigma_l^{-1} (x - \mu_l) - \frac{1}{2} (x - \mu_m)^T \Sigma_l^{-1} (x - \mu_m).$$

**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 $X_1, X_2, X_1X_2, X_1^2, X_2^2$). The right plot shows the quadratic decision boundaries found by QDA. The differences are small, as is usually the case.

ESL, Figure 4.6.
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Problems when $n < p$:

- Estimating covariance matrices when $n$ is small compared to $p$ is challenging.
- The *sample covariance* (MLE for Gaussian)
  \[ S = \frac{1}{n-1} \sum_{j=1}^{n} (x_i - \hat{\mu})(x_i - \hat{\mu})^T \]
  has rank at most $\min(n, p)$ so is singular when $n < p$.
- This is a problem since $\Sigma$ needs to be inverted in LDA and QDA.
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  has rank at most \( \min(n, p) \)
  so is singular when \( n < p \).
- This is a problem since \( \Sigma \) needs to be inverted in LDA and QDA.

Many strategies exist to obtain better estimates of \( \Sigma \) (or \( \Sigma_j \)).

Among them:

- Regularization methods. E.g. \( \hat{\Sigma}(\lambda) = \hat{\Sigma} + \lambda I \).
- Graphical modelling (discussed later during the course).
LDA:

```python
from sklearn.lda import LDA
```

QDA:

```python
from sklearn.qda import QDA
```