Lecture 14: Discriminant Analysis

CS109A Introduction to Data Science
Pavlos Protopapas and Kevin Rader
Lecture Outline

- Discriminant Analysis
  - LDA for one predictor
  - LDA for $p > 1$
  - QDA
- Comparison of Classification Methods (so far)
Recall the Heart Data (for classification)

<table>
<thead>
<tr>
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<th>Fbs</th>
<th>RestECG</th>
<th>MaxHR</th>
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<th>Oldpeak</th>
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<td>normal</td>
<td>No</td>
</tr>
</tbody>
</table>

response variable $Y$ is Yes/No
Discriminant Analysis for Classification
Linear Discriminant Analysis (LDA)

Linear discriminant analysis (LDA) takes a different approach to classification than logistic regression. Rather than attempting to model the conditional distribution of $Y$ given $X$, $P(Y = k|X = x)$, LDA models the distribution of the predictors $X$ given the different categories that $Y$ takes on, $P(X = x|Y = k)$.

In order to flip these distributions around to model $P(X = x|Y = k)$ an analyst uses Bayes' theorem.

In this setting with one feature ($X$), Bayes' theorem can then be written as:

$$P(Y = k|X = x) = \frac{f_k(x)\pi_k}{\sum_{j=1}^{K} f_j(x)\pi_j}$$

What does this mean?
LDA (cont.)

The left hand side, \( P(Y = k | X = x) \), is called the *posterior* probability and gives the probability that the observation is in the \( k^{th} \) category given the feature, \( X \), takes on a specific value, \( x \). The numerator on the right is conditional distribution of the feature within category \( k \), \( \pi_k \), times the *prior* probability that observation is in the \( k^{th} \) category.

The *Bayes' classifier* is then selected. That is the observation assigned to the group for which the posterior probability is the largest.
Inventor of LDA: R.A. Fisher

The 'Father' of Statistics. More famous for work in genetics (statistically concluded that Mendel's genetic experiments were 'massaged').

Novel statistical work includes:

- Experimental Design
- ANOVA
- $F$-test (why do you think it's called the $F$-test?)
- Exact test for 2 x 2 tables
- Maximum Likelihood Theory
- Use of $\alpha = 0.05$ significance level: “The value for which $P = .05$, or 1 in 20, is 1.96 or nearly 2; it is convenient to take this point as a limit in judging whether a deviation is to be considered significant or not”.
- And so much more...
LDA for one predictor

LDA has the simplest form when there is just one predictor/feature ($p = 1$). In order to estimate $f_k(x)$, we have to assume it comes from a specific distribution. If $X$ is quantitative, what distribution do you think we should use?

One common assumption is that $f_k(x)$ comes from a Normal distribution:

$$f_k(x) = \frac{1}{\sqrt{2\pi\sigma_k^2}} \exp\left(-\frac{(x - \mu_k)^2}{2\sigma_k^2}\right)$$

In shorthand notation, this is often written as $X \mid Y = k \sim N(\mu_k, \sigma_k^2)$, meaning, the distribution of the feature $X$ within category $k$ is Normally distributed with mean $\mu_k$ and variance $\sigma_k^2$. 
An extra assumption that the variances are equal, 
\[ \sigma_{\downarrow 1 \uparrow 2} = \sigma_{\downarrow 2 \uparrow 2} = \cdots = \sigma_{\downarrow K \uparrow 2} \] will simplify our lives.

Plugging this assumed likelihood into the Bayes' formula (to get the posterior) results in:

\[
P(Y = k | X = x) = \frac{\pi_k \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left( -\frac{(x - \mu_k)^2}{2\sigma^2} \right)}{\sum_{j=1}^{K} \pi_j \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left( -\frac{(x - \mu_j)^2}{2\sigma^2} \right)}
\]

The Bayes classifier will be the one that maximizes this over all values chosen for \( x \). How should we maximize?

So we take the log of this expression and rearrange to simplify our maximization...
LDA for one predictor (cont.)

So we maximize the following simplified expression:

$$\delta_k(x) = x \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log \pi_k$$

How does this simplify if we have just two classes ($K = 2$) and if we set our prior probabilities to be equal?

This is equivalent to choosing a decision boundary for $x$ for which

$$x = \frac{\mu_1^2 - \mu_2^2}{2(\mu_1 - \mu_2)} = \frac{\mu_1 + \mu_2}{2}$$

Intuitively, why does this expression make sense? What do we use in practice?
In practice we don’t know the true mean, variance, and prior. So we estimate them with the classical estimates, and plug-them into the expression:

\[
\hat{\mu}_k = \frac{1}{n_k} \sum_{i:y_i=k} x_i
\]

and

\[
\hat{\sigma}^2 = \frac{1}{n - K} \sum_{k=1}^{K} \sum_{i:y_i=k} (x_i - \hat{\mu}_k)^2
\]

where \( n \) is the total sample size and \( n_k \) is the sample size within class \( k \) (thus, \( n = \sum n_k \)).
LDA for one predictor (cont.)

This classifier works great if the classes are about equal in proportion, but can easily be extended to unequal class sizes.

Instead of assuming all priors are equal, we instead set the priors to match the 'prevalence' in the data set:

$$\hat{\pi}_k = \hat{n}_k / n$$

Note: we can use a prior probability from knowledge of the subject as well; for example, if we expect the test set to have a different prevalence than the training set.

How could we do this in the Dem. vs. Rep. data set?
LDA for one predictor (cont.)

Plugging all of these estimates back into the original logged maximization formula we get:

\[ \hat{\delta}_k(x) = x \frac{\hat{\mu}_k}{\hat{\sigma}^2} - \frac{\hat{\mu}_k^2}{2\hat{\sigma}^2} + \log \hat{\pi}_k \]

Thus this classifier is called the linear discriminant classifier: this discriminant function is a linear function of \( x \).
Illustration of LDA when $p = 1$
LDA when $p > 1$
LDA when $p > 1$

LDA generalizes 'nicely' to the case when there is more than one predictor.

Instead of assuming the one predictor is Normally distributed, it assumes that the set of predictors for each class is 'multivariate normal distributed' (shorthand: MVN). What does that mean?

This means that the vector of $X$ for an observation has a multidimensional normal distribution with a mean vector, $\mu$, and a covariance matrix, $\Sigma$. 

Multivariate Normal Distribution

Here is a visualization of the Multivariate Normal distribution with 2 variables:
The joint PDF of the Multivariate Normal distribution, 
\( \vec{X} \sim MVN(\vec{\mu}, \Sigma) \), is:

\[
f(\vec{x}) = \frac{1}{2\pi^{p/2}|\Sigma|^{1/2}} \exp \left( -\frac{1}{2}(\vec{x} - \vec{\mu})^T \Sigma^{-1}(\vec{x} - \vec{\mu}) \right)
\]

where \( \vec{X} \) is a \( p \) dimensional vector and \( |\Sigma| \) is the determinant of the \( p \times p \) covariance matrix.

Let's do a quick dimension analysis sanity check...

What do \( \vec{X} \) and \( \Sigma \) look like?
LDA when $p > 1$

Discriminant analysis in the multiple predictor case assumes the set of predictors for each class is then multivariate $\mathbf{X} \sim MN(\mathbf{\mu}, \Sigma)$.

Just like with LDA for one predictor, we make an extra assumption that the covariances are equal in each group, $\Sigma_{\downarrow 1} = \Sigma_{\downarrow 2} = \ldots = \Sigma_{\downarrow K}$. in order to simplify our lives.

Now plugging this assumed likelihood into the Bayes’ formula (to get the posterior) results in:

$$P(Y = k | \mathbf{X} = \mathbf{x}) = \frac{\pi_k \frac{1}{2^{p/2} |\Sigma|^{1/2}} \exp \left( -\frac{1}{2} (\mathbf{x} - \mathbf{\mu}_k)^T \Sigma^{-1} (\mathbf{x} - \mathbf{\mu}_k) \right)}{\sum_{j=1}^K \frac{1}{2^{p/2} |\Sigma|^{1/2}} \exp \left( -\frac{1}{2} (\mathbf{x} - \mathbf{\mu}_j)^T \Sigma^{-1} (\mathbf{x} - \mathbf{\mu}_j) \right)}$$
LDA when $p > 1$ (cont.)

Then doing the same steps as before (taking log and maximizing), we see that the classification will for an observation based on its predictors, $x$, will be the one that maximizes (maximum of $K$ of these $\delta\downarrow k (x)$):

$$\delta_k(x) = \bar{x}^T \Sigma^{-1} \bar{\mu}_k - \frac{1}{2} \bar{\mu}_k^T \Sigma^{-1} \bar{\mu}_k + \log \pi_k$$

Note: this is just the vector-matrix version of the formula we saw earlier in lecture:

$$\delta_k(x) = x \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2 \sigma^2} + \log \pi_k$$

What do we have to estimate now with the vector-matrix version? How many parameters are there?

There are $pK$ means, $pK$ variances, $K$ prior proportions, and $(p@2) = p(p-1)/2$ covariances to estimate.
LDA when $K > 2$

The linear discriminant nature of LDA still holds not only when $p > 1$, but also when $K > 2$ for that matter as well. A picture can be very illustrative:
Quadratic Discriminant Analysis (QDA)
A generalization to linear discriminant analysis is quadratic discriminant analysis (QDA).

Why do you suppose the choice in name?

The implementation is just a slight variation on LDA. Instead of assuming the covariances of the MVN distributions within classes are equal, we instead allow them to be different.

This relaxation of an assumption completely changes the picture...
QDA in a picture

A picture can be very illustrative:
QDA (cont.)

When performing QDA, performing classification for an observation based on its predictors $x$ is equivalent to maximizing the following over the $K$ classes:

$$\delta_k(x) = -\frac{1}{2} x^T \Sigma_k^{-1} x + x^T \Sigma_k^{-1} \mu_k - \frac{1}{2} \mu_k^T \Sigma_k^{-1} \mu_k - \frac{1}{2} \log |\Sigma_k| + \log \pi_k$$

Notice the `quadratic form' of this expression. Hence the name QDA.

Now how many parameters are there to be estimated?

There are $pK$ means, $pK$ variances, $K$ prior proportions, and $(\frac{p(p-1)}{2})K$ covariances to estimate. This could slow us down very much if $K$ is large...
Discriminant Analysis in Python

LDA is already implemented in Python via the sklearn.discriminant_analysis package through the LinearDiscriminantAnalysis function.

QDA is in the same package and is the QuadraticDiscriminantAnalysis function.

It's very easy to use. Let's see how this works
Discriminant Analysis in Python (cont.)

```python
# read in the GSS data
gssdata = pd.read_csv("gsspartyid.csv")
print(gssdata[1:5])

<table>
<thead>
<tr>
<th>politicalparty</th>
<th>income</th>
<th>educ</th>
<th>abortion</th>
<th>republican</th>
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</thead>
<tbody>
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<td>906</td>
<td>6</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>Democrat</td>
<td>1373</td>
<td>6</td>
<td>0</td>
<td>0</td>
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<tr>
<td>Democrat</td>
<td>1941</td>
<td>4</td>
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<td>0</td>
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<tr>
<td>Democrat</td>
<td>355</td>
<td>7</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

LDA = da.LinearDiscriminantAnalysis()
X = gssdata["income", "educ", "abortion"]
model_LDA = LDA.fit(X, gssdata['republican'])
print("Specificity is",np.mean(model_LDA.predict(X[gssdata["republican"]]==0)))
print("Sensitivity is",1-np.mean(model_LDA.predict(X[gssdata["republican"]]==1)))
print("False positive rate is",np.mean(gssdata['republican'][model_LDA.predict(X)==1]))
print("False negative rate is",1-np.mean(gssdata['republican'][model_LDA.predict(X)==0]))

Specificity is 0.388387096774
Sensitivity is 0.374060150376
False positive rate is 0.5252365930595369
False negative rate is 0.7043090638930163
```
QDA vs. LDA

So both QDA and LDA take a similar approach to solving this classification problem: they use Bayes' rule to flip the conditional probability statement and assume observations within each class are multivariate Normal (MVN) distributed.

QDA differs in that it does not assume a common covariance across classes for these MVNs. What advantage does this have? What disadvantage does this have?
QDA vs. LDA (cont.)

So generally speaking, when should QDA be used over LDA? LDA over QDA?

The extra covariance parameters that need to be estimated in QDA not only slow us down, but also allow for another opportunity for overfitting. Thus if your training set is small, LDA should perform better for out-of-sample prediction, aka, predicting future observations (how do we mimic this process?)
Comparison of Classification Methods (so far)
Quadratic Discriminant Analysis (QDA)

We have seen 3 major methods for doing classification:

• Logistic Regression
• $k$-NN
• Discriminant Analysis (LDA and QDA)

For a specific problem, which approach should be used?

Well of course, it depends on the nature of the data. So how should we decide?

Visualize the data!
Six Classification Models We'll Compare

Let's investigate which method will work the best (as measured by lowest overall classification error rate), by considering 6 different models for 4 different data sets (each data set as a pair of predictors...you can think of them as the first 2 PCA components...to come later in the lecture). The 6 models to consider are:

• A logistic regression with only 'linear' main effects
• A logistic regression with only 'linear' and 'quadratic' effects
• LDA
• QDA
• $k$-NN where $k = 3$
• $k$-NN where $k = 25$

What else will also be important to measure (besides error rate)?
Which method should perform better? #1

\[ n = 20,000, \ p = 2, \ K = 2, \ \pi_1 = \pi_2 = \]

<table>
<thead>
<tr>
<th>method</th>
<th>misclass rate</th>
<th>run time (ms)</th>
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<tbody>
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<td>logit1</td>
<td>0.04410</td>
<td>417.95</td>
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<tr>
<td>logit2</td>
<td>0.04405</td>
<td>229.71</td>
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<tr>
<td>lda</td>
<td>0.04425</td>
<td>50.63</td>
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<tr>
<td>qda</td>
<td>0.04410</td>
<td>49.08</td>
</tr>
<tr>
<td>knn3</td>
<td>0.05225</td>
<td>1856.11</td>
</tr>
<tr>
<td>knn25</td>
<td>0.04500</td>
<td>2166.57</td>
</tr>
</tbody>
</table>

Notice anything fishy about our answers? What did Kevin do? What should he have done?
Easy to implement in Python

```python
lda = da.LinearDiscriminantAnalysis()
qda = da.QuadraticDiscriminantAnalysis()
lda.fit(X,y)
qda.fit(X,y)
logit2 = sk.linear_model.LogisticRegression(C = 1000000)
logit1 = sk.linear_model.LogisticRegression(C = 1000000)
logit1.fit(X,y)
logit2.fit(X2,y)

print("Overall misclassification rate of Logit1 is",(1-logit1.score(X,y)))
print("Overall misclassification rate of Logit2 is",(1-logit2.score(X2,y)))
print("Overall misclassification rate of LDA is",(1-lda.score(X,y)))
print("Overall misclassification rate of QDA is",(1-qda.score(X,y)))
```

Overall misclassification rate of Logit1 is 0.0441
Overall misclassification rate of Logit2 is 0.0441
Overall misclassification rate of LDA is 0.04425
Overall misclassification rate of QDA is 0.0441
Which method should perform better? #2

\[ n = 20,000, \ p = 2, \ K = 2, \ \pi_1 = \pi_2 = 0.5 \]

<table>
<thead>
<tr>
<th>method</th>
<th>misclass rate</th>
<th>run time (ms)</th>
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</thead>
<tbody>
<tr>
<td>logit1</td>
<td>0.12230</td>
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<td>logit2</td>
<td>0.11860</td>
<td>196.42</td>
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<tr>
<td>lda</td>
<td>0.12215</td>
<td>47.93</td>
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<td>qda</td>
<td>0.11445</td>
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<td>knn3</td>
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<td>0.12015</td>
<td>2223.13</td>
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</tbody>
</table>
Which method should perform better? #3

\[ n = 20,000, \ p = 2, \ K = 2, \ \pi_1 = \pi_2 = 0.5 \]

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<td>logit2</td>
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<td>0.20270</td>
<td>2166.77</td>
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</table>
Which method should perform better? #4

\[ n = 20,000, \ p = 2, \ K = 2, \ \pi_1 = \pi_2 = 0.5 \]

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<td>2126.38</td>
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Summary of Results

Generally speaking:

- LDA outperforms Logistic Regression if the distribution of predictors is reasonably MVN (with constant covariance).
- QDA outperforms LDA if the covariances are not the same in the groups.
- k-NN outperforms the others if the decision boundary is extremely non-linear.
- Of course, we can always adapt our models (logistic and LDA/QDA) to include polynomial terms, interaction terms, etc... to improve classification (watch out for overfitting!)
- In order of **computational speed** (generally speaking, it depends on $K$, $p$, and $n$ of course):

  LDA > QDA > Logistic > $k$-NN