Lecture 10 Linear Discriminant Analysis II

ECE 625: Data Analysis and Knowledge Discovery

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Outline

From discriminant rule to probabilities

- Once we have estimates $\hat{\delta}_k(x)$, we can turn these into estimates for class probabilities:

$$\widehat{\Pr}(Y = k|X = x) = \frac{e^{\hat{\delta}_k(x)}}{\sum_{l=1}^{K} e^{\hat{\delta}_l(x)}}.$$

softmax

- So classifying to the largest $\hat{\delta}_k(x)$ amounts to classifying to the class for which $\widehat{\Pr}(Y = k|X = x)$ is largest.
- When $K = 2$, we classify to class 2 if $\widehat{\Pr}(Y = k|X = x) > 0.5$ or else to class 1.

For two classes, there is a single number
that sets the boundary
It is important you know how to derive the decision boundary

LDA on credit data

How do we evaluate the accuracy of a classification method?

```
> table(default.pred$class,defaultData$default)

       No  Yes
  No  9645  254
  Yes   22   79
> 22/9667
[1] 0.002275784
> 254/333
[1] 0.7627628
```

FN FNR = 254/(254+79) = FN/sum of its column

FP FPR = 22/(9645+22) = FP/sum of its column

- $(22 + 254)/10000$ errors — 2.76% misclassification rate!
- However, this is training error, and we may be over fitting. Not a big concern here since $n = 10000$ and $p = 3$.
- If we classified ~~to the prior —~~ always to class `No` in this case — we would make $333/10000 = 3.33\%$ errors.
- Of the true `No` 's, we make $22/9667 = 0.2\%$ errors, of the true `Yes` 's, we make $254/333 = 76.3\%$ errors.

Types of errors

Predict positive but negative

- False positive rate: The fraction of negative examples that are classified as positive 0.2% in example.

Predict negative but positive

- False negative rate: The fraction of positive examples that are classified as negative 76.3% in example. Method Failed!
- We produced this table by classifying to class `Yes` if

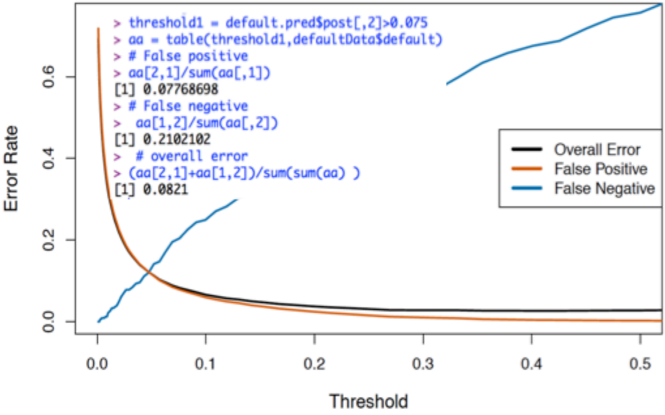
$$\widehat{\Pr}(\texttt{Default=Yes}|\texttt{Balance, Incoming, Student}) \geq 0.5.$$

- We can change the two error rates by changing the threshold from 0.5 to some other value in $[0, 1]$:

$$\widehat{\Pr}(\texttt{Default=Yes}|\texttt{Balance, Incoming, Student}) \geq \textit{threshold}.$$

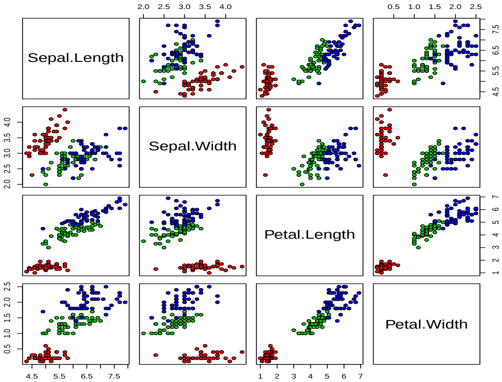
and vary *threshold*.

Varying the threshold



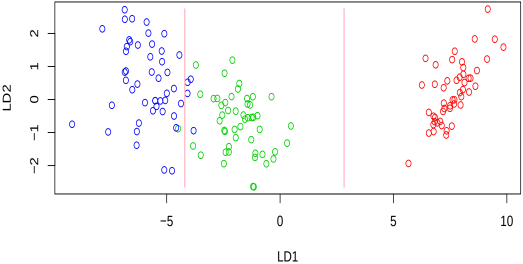
In order to reduce the false negative rate, we may want to reduce the threshold to 0.1 or less.

Fisher's Iris Data



- 4 variables, 3 species, and 50 samples per class
- Blue - Setosa, Orange - Versicolor, and Green Virginica
- LDA classifies all but 3 of the 150 training samples correctly.

Fisher's Iris Data



- When there are K classes, linear discriminant analysis can be viewed exactly in a $K-1$ dimensional plot.
- Why? Because it essentially classifies to the closest centroid, and they span a $K-1$ dimensional plane.
- Even when $K > 3$, we can find the best 2-dimensional plane for vizualizing the discriminant rule.

Other forms of Discriminant Analysis

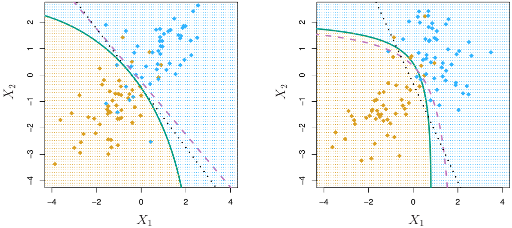
- When $f_k(x)$ are Gaussian densities, with the same covariance matrix Σ in each class, the Bayes Theorem

$$\Pr(Y = k|X = x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{K} \pi_l f_l(x)},$$

this leads to linear discriminant analysis.

- By altering the forms for $f_k(x)$, we get different classifiers.
  - With Gaussians but different Σ_k in each class, we get quadratic discriminant analysis.
  - With $f_k(x) = \Pi_{j=1}^{p} f_{jk}(x_j)$ (conditional independence model) in each class we get naive Bayes. For Gaussian this means the Σ_k are diagonal.
  - Many other forms, by proposing specific density models for $f_k(x)$, including nonparametric approaches.

Quadratic Discriminant Analysis



- As in the following Σ_k are different, so in QDA quadratic term matters

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

- Black dotted: LDA boundary; Purple dashed: Bayes' boundary; Green solid: QDA boundary
- Left: variances of the classes are equal (LDA is better fit)
- Right: variances of the classes are not equal (QDA is better fit)

QDA versus LDA

- Since QDA allows for different variances among classes, the resulting boundaries become quadratic.
- QDA will work best when the variances are very different between classes and we have enough observations to accurately estimate the variances.
- LDA will work best when the variances are similar among classes or we don't have enough data to accurately estimate the variances.

Logistic Regression versus LDA

- For a two-class problem, one can show that for LDA

$$\log\left(\frac{p_1(x)}{1-p_1(x)}\right) = \log\left(\frac{p_1(x)}{p_2(x)}\right) = c_0 + c_1x_1 + \cdots + c_px_p(x).$$

- So it has the same form as logistic regression. The difference is in how the parameters are estimated.
- Logistic regression uses the conditional likelihood based on $\Pr(Y|X)$ (aka discriminative learning).
- LDA uses the full likelihood based on $\Pr(X|Y)$ (aka generative learning).
- Despite these difference, in practice the results are often very similar.
- Same connection between LDA and logistic regression also holds for multidimensional data with $p > 1$.

Comparison of Different Methods Learned so far

- Logistics Regression (LR): linear decision boundary; can be better if observations are non-Gaussian.
- LDA: linear decision boundary; can be better if the Gaussian assumption is true.
- K-nearest neighbours (KNN): checking which class your K nearest neighbors belong to; non-parametric; dominate when decision boundary is highly non-linear; low interpretability; doesn't work in cases with limited training samples.
- QDA: nonlinear decision boundary; a compromise between KNN and linear methods (LR, LDA) in cases with limited training samples.

Summary and Remarks

- Linear Discriminant Analysis for $p > 1$
- From discriminant rule to probabilities
- Quadratic Discriminant Analysis
- Read textbook Chapter 4 and R code
- Do R lab