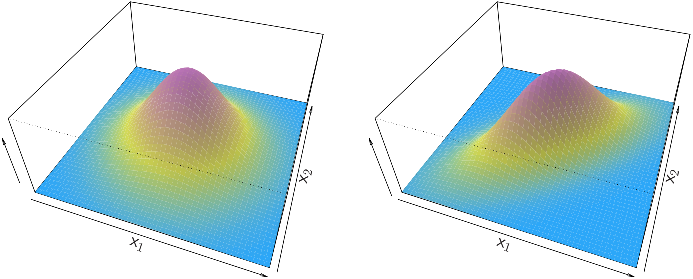
Linear Discriminant Analysis when $p > 1$

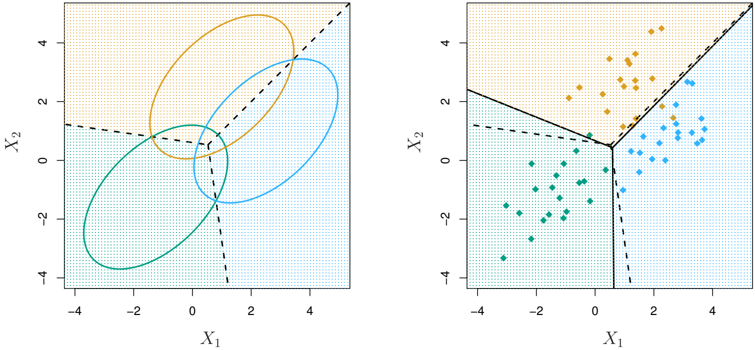


$$\text{Density: } f(x) = \frac{1}{(2\pi)^{p/2}|\boldsymbol{\Sigma}|^{1/2}} e^{-\frac{1}{2}(x-\mu)^T \boldsymbol{\Sigma}^{-1}(x-\mu)}$$

$$\text{Discriminant function: } \delta_k(x) = x^T \boldsymbol{\Sigma}^{-1}\mu_k - \frac{1}{2}\mu_k^T \boldsymbol{\Sigma}^{-1}\mu_k + \log \pi_k$$

Despite its complex form,
$\delta_k(x) = c_{k0} + c_{k1}x_1 + c_{k2}x_2 + \ldots + c_{kp}x_p$ — a linear function.

Illustration: $p = 2$ and $K = 3$ classes



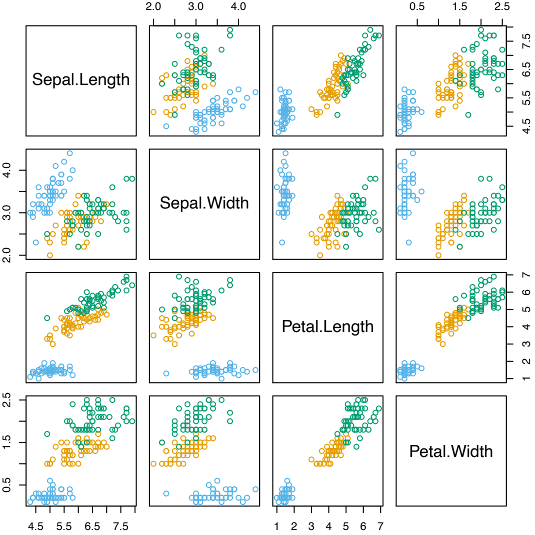
Here $\pi_1 = \pi_2 = \pi_3 = 1/3$.
The dashed lines are known as the *Bayes decision boundaries*.
Were they known, they would yield the fewest misclassification errors, among all possible classifiers.

Fisher's Iris Data

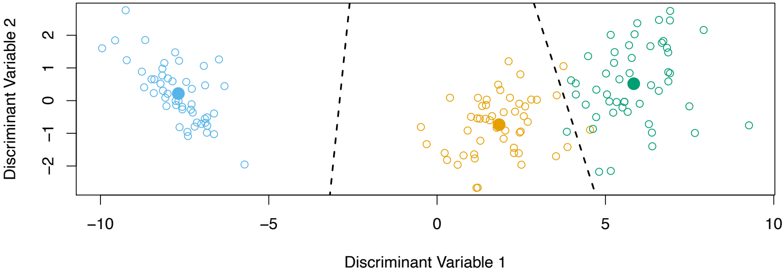
4 variables
3 species
50 samples/class

- Setosa
- Versicolor
- Virginica

LDA classifies all but 3 of the 150 training samples correctly.



Fisher's Discriminant Plot



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Why?

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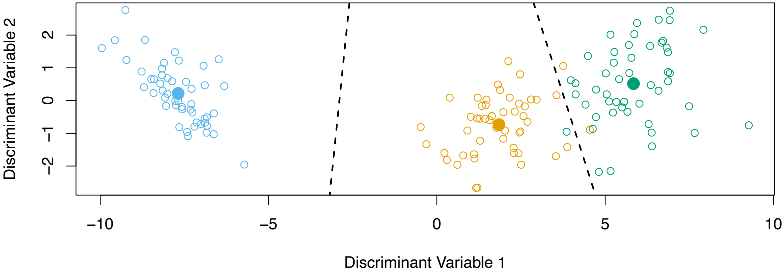

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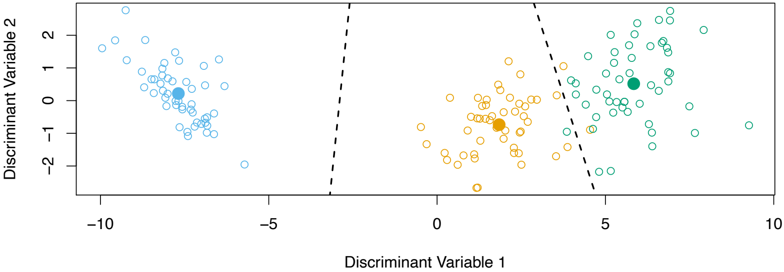

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Why? Because it essentially classifies to the closest centroid, and they span a $K-1$ dimensional plane.
Even when $K > 3$, we can find the "best" 2-dimensional plane for visualizing the discriminant rule.

From $\delta_k(x)$ to probabilities

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

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

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.

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When $K = 2$, we classify to class 2 if $\widehat{\Pr}(Y = 2|X = x) \geq 0.5$, else to class 1.

LDA on Credit Data

		True Default Status		
		No	Yes	Total
Predicted	No	9644	252	9896
Default Status	Yes	23	81	104
	Total	9667	333	10000

$(23 + 252)/10000$ errors — a 2.75% misclassification rate!

Some caveats:

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- If we classified to the prior — always to class `No` in this case — we would make 333/10000 errors, or only 3.33%.
- Of the true `No`'s, we make $23/9667 = 0.2\%$ errors; of the true `Yes`'s, we make $252/333 = 75.7\%$ errors!

Types of errors

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

False negative rate: The fraction of positive examples that are classified as negative — 75.7% in example.

We produced this table by classifying to class Yes if

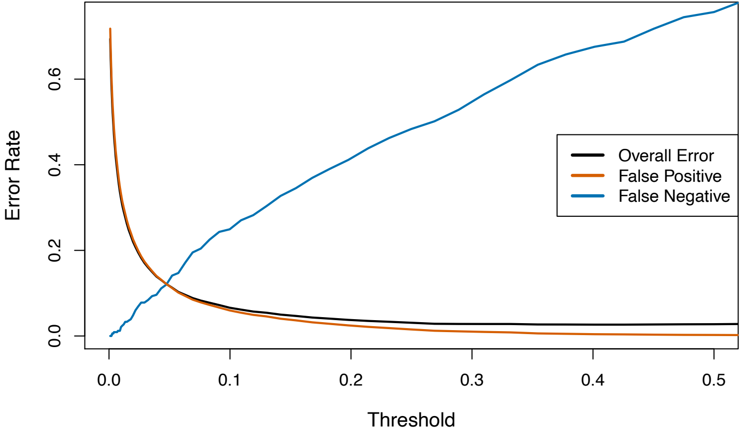
$$\widehat{\Pr}(\texttt{Default} = \texttt{Yes} | \texttt{Balance}, \texttt{Student}) \geq 0.5$$

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

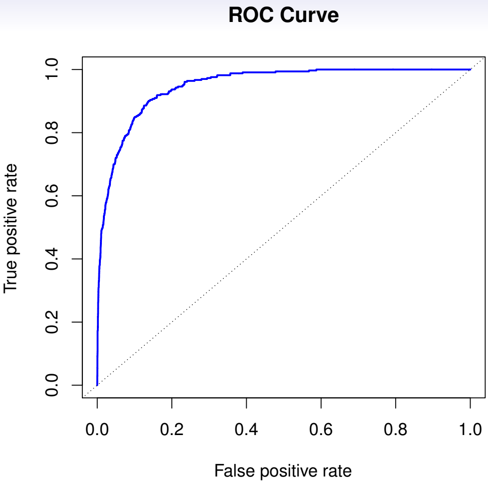
$$\widehat{\Pr}(\texttt{Default} = \texttt{Yes} | \texttt{Balance}, \texttt{Student}) \geq \textit{threshold},$$

and vary *threshold*.

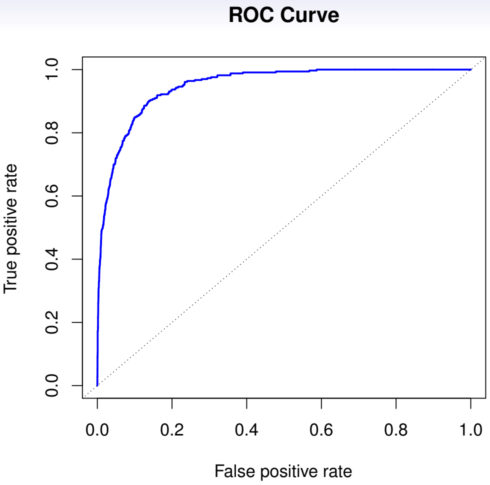
Varying the *threshold*



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



The *ROC plot* displays both simultaneously.



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Sometimes we use the *AUC* or *area under the curve* to summarize the overall performance. Higher *AUC* is good.

Other forms of Discriminant Analysis

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

When $f_k(x)$ are Gaussian densities, with the same covariance matrix $\mathbf{\Sigma}$ in each class, this leads to linear discriminant analysis. By altering the forms for $f_k(x)$, we get different classifiers.

- With Gaussians but different $\mathbf{\Sigma}_k$ in each class, we get *quadratic discriminant analysis*.

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- With $f_k(x) = \prod_{j=1}^{p} f_{jk}(x_j)$ (conditional independence model) in each class we get *naive Bayes*. For Gaussian this means the $\mathbf{\Sigma}_k$ are diagonal.

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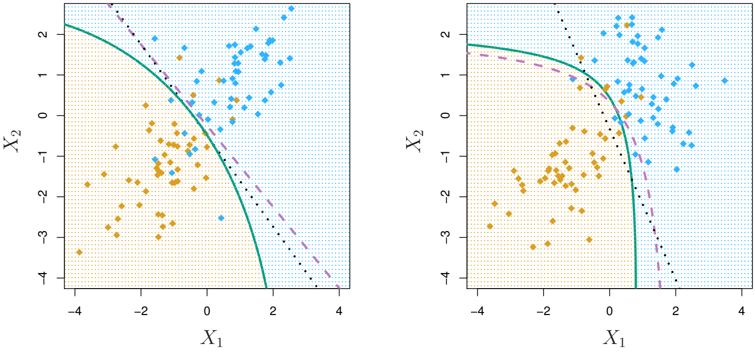
- With $f_k(x) = \prod_{j=1}^{p} f_{jk}(x_j)$ (conditional independence model) in each class we get *naive Bayes*. For Gaussian this means the $\mathbf{\Sigma}_k$ are diagonal.
- Many other forms, by proposing specific density models for $f_k(x)$, including nonparametric approaches.

Quadratic Discriminant Analysis



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

Because the $\mathbf{\Sigma}_k$ are different, the quadratic terms matter.

Naive Bayes

Assumes features are independent in each class.

Useful when p is large, and so multivariate methods like QDA and even LDA break down.

- Gaussian naive Bayes assumes each $\mathbf{\Sigma}_k$ is diagonal:

$$\begin{aligned}\delta_k(x) &\propto \log\left[\pi_k \prod_{j=1}^{p} f_{kj}(x_j)\right] \\ &= -\frac{1}{2}\sum_{j=1}^{p}\left[\frac{(x_j-\mu_{kj})^2}{\sigma_{kj}^2} + \log\sigma_{kj}^2\right] + \log\pi_k\end{aligned}$$

- can use for *mixed* feature vectors (qualitative and quantitative). If X_j is qualitative, replace $f_{kj}(x_j)$ with probability mass function (histogram) over discrete categories.

Despite strong assumptions, naive Bayes often produces good classification results.

Logistic Regression versus LDA

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

$$\log\left(\frac{p_1(x)}{1-p_1(x)}\right) = \log\left(\frac{p_1(x)}{p_2(x)}\right) = c_0 + c_1 x_1 + \ldots + c_p x_p$$

So it has the same form as logistic regression.

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- Logistic regression uses the conditional likelihood based on $\Pr(Y|X)$ (known as *discriminative learning*).
- LDA uses the full likelihood based on $\Pr(X, Y)$ (known as *generative learning*).
- Despite these differences, in practice the results are often very similar.