CS545: Linear Models for Classification

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Outline

**Linear Least Squares for Classification**
- Indicator Variables
- Masking Problem
- Example

**Generative Models for Classification**
- QDA
- Fitting the Generative Distributions to Data
- Overfitting
- LDA
- Example
To classify a sample as being a member of 1 of 3 different classes, we could use integers 1, 2, and 3 as target outputs.
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Linear function of $x$ seems to match data fairly well. Why is this not a good idea?
We must convert the continuous y-axis value to discrete integers 1, 2, or 3. Without adding more parameters, we are forced to use the general solution of splitting at 1.5 and 2.5.
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Rats! Boundaries are not where we want them.
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Let the output be $y = (y_1, y_2, y_3)$. Convert these values to a class by picking the maximum value.

$$\text{class} = \arg\max_i y_i$$
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- Targets
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Can plot the three output components on three separate graphs. What linear functions will each one learn?

Overlay them to see which one is the maximum for each \( x \) value.
See any potential problems?
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What if the green line is too low?
See any potential problems?

What if the green line is too low?

What could cause this?
Too few samples from Class 2.

There may be no values of \( x \) for which the second output, \( y_2 \), of our linear model is larger than the other two. Class 2 has become masked by the other classes. What other shape of function response would work better for this data? Hold that thought, while we try an example.
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Application: Parkinsons Data Set from UCI ML Archive

- 147 samples from subjects with Parkinsons, 48 samples from healthy subjects
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- Each sample composed of 21 numerical features extracted from voice recordings
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- 147 samples from subjects with Parkinsons, 48 samples from healthy subjects
- Each sample composed of 21 numerical features extracted from voice recordings
- from collaboration with the University of Oxford and the National Center for Voice and Speech in Denver.
Read and Prepare the Data

```r
# data <- read.table("parkinsons.data", header=TRUE, sep=" ", )
# remove name and make numeric
# data <- as.matrix(data[, -1])
# randomly rearrange data
# data <- data[sample(nrow(data)),]
# status is 0 for healthy, 1 for Parkinsons
# status <- data[, "status"]
# remove status column from data
# data <- data[, -which(colnames(data) == "status")]

dataHealthy <- data[status == 0,]
dataParks <- data[status == 1,]
nHealthy <- nrow(dataHealthy)
nParks <- nrow(dataParks)
```

---

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```

- **Look at the data**

```r
> data[1:2,]
[1,]  223.361  263.872  87.638  0.00352  2e-05
[2,] 136.926  159.866 131.276  0.00293  2e-05
   MDVP.RAP MDVP.PPQ Jitter.DDP MDVP.Shimmer MDVP.Shimmer.dB. Shimmer.APQ3
[1,] 0.00169 0.00188 0.00506 0.02536  0.225  0.01379
[2,] 0.00118 0.00153 0.00355 0.01259  0.112  0.00656
   Shimmer.APQ5 MDVP.APQ Shimmer.DDA NHR HNR RPDE DFA
[1,]  0.01478  0.01909  0.04137  0.01493 20.366 0.566849 0.574282
[2,]  0.00717  0.01140  0.01968  0.00581 25.703 0.460600 0.646846
   spread1 spread2 D2 PPE
[1,]  5.456811  0.345238 2.840556 0.232861
[2,]  6.547148  0.152813 2.041277 0.138512
```
Make Train and Test Partitions

- For small sample size or very uneven number of samples from each class, force equal sampling proportions of two classes when building train, test partitions.
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- Two indicator variables is equivalent to using single variable. We will use values 1 and 2 to indicate Class 1 (healthy) and Class 2 (Parkinsons).
Make Train and Test Partitions

- For small sample size or very uneven number of samples from each class, force equal sampling proportions of two classes when building train, test partitions.
- Two indicator variables is equivalent to using single variable. We will use values 1 and 2 to indicate Class 1 (healthy) and Class 2 (Parkinsons).

```r
trainf <- 0.8
Xtrain <- rbind(dataHealthy[1:floor(trainf*nHealthy)],
                 dataParks[1:floor(trainf*nParks)])
Ttrain <- matrix(c(rep(1,floor(trainf*nHealthy)),
                     rep(2,floor(trainf*nParks))))
Xtest <- rbind(dataHealthy[-(1:floor(trainf*nHealthy))],
                dataParks[-(1:floor(trainf*nParks))])
Ttest <- matrix(c(rep(1,nHealthy-floor(trainf*nHealthy)),
                  rep(2,nParks-floor(trainf*nParks))))
```
Calculate Linear Least Squares Solution

- Standardize

```r
standardize <- makeStandardizeF(Xtrain)
Xtrain1 <- cbind(1, standardize(Xtrain))
```

Test it.

```r
TtrainPredicted <- Xtrain1 %*% w
TtestPredicted <- cbind(1, standardize(Xtest)) %*% w
pCorrectTrain <- sum(apply(abs(cbind(TtrainPredicted - 1, TtrainPredicted - 2)), 1, which.min) == Ttrain) / length(Ttrain) * 100
pCorrectTest <- sum(apply(abs(cbind(TtestPredicted - 1, TtestPredicted - 2)), 1, which.min) == Ttest) / length(Ttest) * 100
```

```
Training data 93.54839 percent correct
Testing data 80 percent correct
```

Repeating it all, gives

```
Training data 90.32258 percent correct
Testing data 95 percent correct
```
Calculate Linear Least Squares Solution

- **Standardize**
  
  ```r
  standardize <- makeStandardizeF(Xtrain)
  Xtrain1 <- cbind(1, standardize(Xtrain))
  ```

- **Calculate \( w \)**
  
  ```r
  w <- solve(t(Xtrain1) %*% Xtrain1, t(Xtrain1) %*% Ttrain)
  ```
Calculate Linear Least Squares Solution

- **Standardize**

  \[
  \text{standardize} \leftarrow \text{makeStandardizeF}(X\text{train}) \\
  X\text{train1} \leftarrow \text{cbind}(1, \text{standardize}(X\text{train}))
  \]

- **Calculate } w\]

  \[
  w \leftarrow \text{solve}(t(X\text{train1}) \ast X\text{train1}, t(X\text{train1}) \ast T\text{train})
  \]

- **Test it.**

  \[
  T\text{trainPredicted} \leftarrow X\text{train1} \ast w \\
  T\text{testPredicted} \leftarrow \text{cbind}(1, \text{standardize}(X\text{test})) \ast w \\
  p\text{CorrectTrain} \leftarrow \text{sum}(\text{apply}(\text{abs}(\text{cbind}(T\text{trainPredicted} - 1, T\text{trainPredicted} - 2)), 1, \text{which.min} == T\text{train}) / \text{length}(T\text{train}) \ast 100.0 \\
  p\text{CorrectTest} \leftarrow \text{sum}(\text{apply}(\text{abs}(\text{cbind}(T\text{testPredicted} - 1, T\text{testPredicted} - 2)), 1, \text{which.min} == T\text{test}) / \text{length}(T\text{test}) \ast 100.0 \\
  \text{cat}("\text{Training data}, p\text{CorrectTrain}," \ \text{percent correct} \ \text{\n")} \\
  \text{cat}("\text{Testing data}, p\text{CorrectTest}," \ \text{percent correct} \ \text{\n")}
  \]

results in

Training **data** 93.54839 percent correct
Testing **data** 80 percent correct
Calculate Linear Least Squares Solution

- **Standardize**
  
  ```r
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- **Calculate w**
  
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  w <- solve(t(Xtrain1)%*%Xtrain1,t(Xtrain1)%*%Ttrain)
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  ```r
  TtrainPredicted <- Xtrain1 %*% w
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  pCorrectTrain <- sum(apply(abs(cbind(TtrainPredicted-1, TtrainPredicted-2)),
                             1, which.min) == Ttrain) / length(Ttrain) * 100.0
  pCorrectTest <- sum(apply(abs(cbind(TtestPredicted-1, TtestPredicted-2)),
                             1, which.min) == Ttest) / length(Ttest) * 100.0
  cat("Training data", pCorrectTrain," percent correct \n")
  cat("Testing data", pCorrectTest," percent correct \n")
  ```

results in

- Training data 93.54839 percent correct
- Testing data 80 percent correct

- **Repeating it all, gives**

  - Training data 90.32258 percent correct
  - Testing data 95 percent correct
Plot it

- What visualization would you use to check the results?
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- Let’s plot the true class with the output of the model for each training sample, then each testing sample.
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- Let’s plot the true class with the output of the model for each training sample, then each testing sample.

```r
par(mfrow=c(1,2),bty="n")
matplot(cbind(Ttrain, TtrainPredicted ), type="b",pch=1,lty=1, xlab="Sample",ylab="True and Predicted Class",main="Train Data")
matplot(cbind(Ttest,TtestPredicted ), type="b",pch=1,lty=1, xlab="Sample",ylab="True and Predicted Class",main="Test Data")
par(p)
```
Outline

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  Overfitting
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  Example
Back to that Masking Problem

What function shape were you thinking of that might fix the masking problem?
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- Radial basis function? Good choice! But, remember what a radial basis function resembles?
- Right again! A Gaussian distribution.
- This leads us into our discussion of generative models for classification. A very common generative model is the use of one Gaussian distribution to model data from each class. This is “generative”, because we are assuming that the Gaussian distribution is the underlying process that generates the data samples.
Using Generative Model to Classify

- So, let’s say we come up with the generative distribution, such as a Gaussian distribution, for Class $k$, called $p(x|\text{Class} = k)$, or $p(x|C = k)$. How do we use it to classify?
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- Ultimately we would like to know $p(C = k|x)$. How do we get this from $p(x|C = k)$?
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- Ultimately we would like to know $p(C = k|x)$. How do we get this from $p(x|C = k)$?

- Remember that

$$p(C = k, x) = p(C = k|x)p(x) = p(x|C = k)p(C = k)$$
Bayes’ Rule for Classification

\[ p(C = k|x) = \frac{p(x|C = k)p(C = k)}{p(x)} \]
Bayes’ Rule for Classification

\[ p(C = k | x) = \frac{p(x | C = k)p(C = k)}{p(x)} \]
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\[ p(C = k | x) = \frac{p(x | C = k)p(C = k)}{p(x)} \]

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Bayes’ Rule for Classification

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Simplify to just Two Classes

- For two classes, \( k \in \{1, 2\} \). We will classify a sample \( x \) as Class 2 if \( p(C = 2|x) > p(C = 1|x) \). Now expand and simplify...
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\[
p(C = 2|x) > p(C = 1|x)
\]

\[
\frac{p(x|C = 2)p(C = 2)}{p(x)} > \frac{p(x|C = 1)p(C = 1)}{p(x)}
\]

\[
p(x|C = 2)p(C = 2) > p(x|C = 1)p(C = 1)
\]
Use our Gaussian Assumption

Using our assumption that the generative distribution for each class is a Gaussian distribution,

\[ p(x|C = 2)p(C = 2) > p(x|C = 1)p(C = 1) \]

\[
\frac{1}{(2\pi)^{d/2} |\Sigma_2|^{1/2}} e^{-\frac{1}{2}(x-\mu_2)^T \Sigma_2^{-1}(x-\mu_2)} p(C = 2) > \frac{1}{(2\pi)^{d/2} |\Sigma_1|^{1/2}} e^{-\frac{1}{2}(x-\mu_1)^T \Sigma_1^{-1}(x-\mu_1)} p(C = 1)
\]

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|\Sigma_2|^{-\frac{1}{2}} e^{-\frac{1}{2}(x-\mu_2)^T \Sigma_2^{-1}(x-\mu_2)} p(C = 2) > |\Sigma_1|^{-\frac{1}{2}} e^{-\frac{1}{2}(x-\mu_1)^T \Sigma_1^{-1}(x-\mu_1)} p(C = 1)
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|\Sigma_2|^{-\frac{1}{2}} e^{-\frac{1}{2}(x-\mu_2)^T\Sigma_2^{-1}(x-\mu_2)} p(C = 2) > |\Sigma_1|^{-\frac{1}{2}} e^{-\frac{1}{2}(x-\mu_1)^T\Sigma_1^{-1}(x-\mu_1)} p(C = 1)
\]

- Hey, there are multiplications and exponentials here. Let’s use logarithms.
\[ |\Sigma_2| \cdot \frac{1}{2} e^{-\frac{1}{2}(x-\mu_2)^T \Sigma_2^{-1}(x-\mu_2)} p(C = 2) \]
\[ > |\Sigma_1| \cdot \frac{1}{2} e^{-\frac{1}{2}(x-\mu_1)^T \Sigma_1^{-1}(x-\mu_1)} p(C = 1) \]

\[ -\frac{1}{2} \ln |\Sigma_2| + -\frac{1}{2} (x - \mu_2)^T \Sigma_2^{-1}(x - \mu_2) + \ln p(C = 2) \]
\[ > -\frac{1}{2} \ln |\Sigma_1| + -\frac{1}{2} (x - \mu_1)^T \Sigma_1^{-1}(x - \mu_1) + \ln p(C = 1) \]

- If we define each side of this last inequality as a discriminant function, \( \delta_k(x) \) for Class \( k \), then

\[ \delta_k(x) = -\frac{1}{2} \ln |\Sigma_k| + \frac{1}{2} (x - \mu_k)^T \Sigma_k^{-1}(x - \mu_k) + \ln P(C = k) \]

and the class of a new sample \( x \) is \( \text{argmax}_k \delta_k(x) \).
\[
|\Sigma_2|^{\frac{1}{2}} e^{-\frac{1}{2}(x-\mu_2)^T \Sigma_2^{-1}(x-\mu_2)} p(C = 2) > |\Sigma_1|^{\frac{1}{2}} e^{-\frac{1}{2}(x-\mu_1)^T \Sigma_1^{-1}(x-\mu_1)} p(C = 1)
\]

\[
-\frac{1}{2} \ln |\Sigma_2| - \frac{1}{2} (x - \mu_2)^T \Sigma_2^{-1} (x - \mu_2) + \ln p(C = 2) > -\frac{1}{2} \ln |\Sigma_1| - \frac{1}{2} (x - \mu_1)^T \Sigma_1^{-1} (x - \mu_1) + \ln p(C = 1)
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- If we define each side of this last inequality as a discriminant function, \( \delta_k(x) \) for Class \( k \), then
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  \delta_k(x) = -\frac{1}{2} \ln |\Sigma_k| - \frac{1}{2} (x - \mu_k)^T \Sigma_k^{-1} (x - \mu_k) + \ln P(C = k)
  \]
  and the class of a new sample \( x \) is argmax\(_k\) \( \delta_k(x) \).
- The boundary between Class 1 and Class 2 is the set of points \( x \) for which \( \delta_2(x) = \delta_1(x) \). This equation is quadratic in \( x \), meaning that the boundary between Class 1 and 2 is quadratic. We have just defined Quadratic Discriminant Analysis, or QDA.
Fitting the Generative Distributions to Data

Let’s use the maximum likelihood solution for a Gaussian distribution.

\[ \mu_k = \frac{1}{N_k} \sum_{x \in X_k} x \]

\[ \Sigma_k = \frac{1}{N_k - 1} \sum_{x \in X_k} (x - \mu_k)(x - \mu_k)^T \]

What about \( p(C = k) \), which is the a priori probability distribution of Class \( k \)? If we have no prior belief that one class is more likely than any other, \( p(C = k) = \frac{N_k}{N} \) where \( N \) is the total number of samples from all classes.
Fitting the Generative Distributions to Data

- Let’s use the maximum likelihood solution for a Gaussian distribution.
- Let $X_k$ be the set of training samples from Class $k$, and $N_k$ be the number of training samples from Class $k$.

$$
\mu_k = \frac{1}{N_k} \sum_{x \in X_k} x
$$

$$
\Sigma_k = \frac{1}{N_k - 1} \sum_{x \in X_k} (x - \mu_k)(x - \mu_k)^T
$$

Where $\mu_k$ is the mean and $\Sigma_k$ is the covariance matrix for Class $k$. $p(C = k)$, which is the a priori probability distribution of Class $k$, is equal to $\frac{N_k}{N}$ where $N$ is the total number of samples from all classes.

Fitting the Generative Distributions to Data

- Let’s use the maximum likelihood solution for a Gaussian distribution.
- Let $X_k$ be the set of training samples from Class $k$, and $N_k$ be the number of training samples from Class $k$.

\[
\begin{align*}
\mu_k &= \frac{1}{N_k} \sum_{x \in X_k} x \\
\Sigma_k &= \frac{1}{N_k - 1} \sum_{x \in X_k} (x - \mu_k)(x - \mu_k)^T
\end{align*}
\]

- What about $p(C = k)$, which is the a priori probability distribution of Class $k$? If we have no prior belief that one class is more likely than any other,

\[
p(C = k) = \frac{N_k}{N}
\]

where $N$ is the total number of samples from all classes.
Two Classes for Two-Dimensional Samples

- Given samples from two classes, calculate $\mu_1$ and $\Sigma_1$ and $\mu_2$ and $\Sigma_2$. 

Class 1

Class 2

Points with probability 0.5

$\mu_1$

$\mu_2$
Can QDA Overfit

- Assuming single Gaussian as model of data from each class does not seem to lead to an exceedingly complex model. But, how many parameters are there in the mean and covariance matrix, if data is $d$-dimensional?

- Mean has $d$ components.
- Covariance matrix has $d^2$ components. If $d = 100$, the covariance matrix has 100,000 parameters. Whoa!
- Actually the covariance matrix is symmetric, so it only has $d(d+1)/2$ unique values. Still a lot. And we have one for each class, so total number of parameters, including mean, is $K(d(d+1)/2)$. 

- What if the data distribution is under-sampled?
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- Actually the covariance matrix is symmetric, so it only has $\frac{d^2}{2} + \frac{d}{2} = \frac{d(d+1)}{2}$ unique values. Still a lot. And we have one for each class, so total number of parameters, including mean, is $K\left(d + \frac{d(d+1)}{2}\right)$.
Can QDA Overfit

- Assuming single Gaussian as model of data from each class does not seem to lead to an exceedingly complex model. But, how many parameters are there in the mean and covariance matrix, if data is $d$-dimensional?
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- What if the data distribution is under-sampled?
Gaussian for Class 1 is far from correct. Class boundary will now lead to many errors.
How to Reduce Overfitting?

- Need to remove flexibility from the Gaussian model. How?
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How to Reduce Overfitting?

- Need to remove flexibility from the Gaussian model. How?
- Could restrict all covariance matrices to be diagonal. The ellipses would be parallel to the axes. Wouldn’t work well if features are correlated.
- Could force all classes to have the same covariance matrix by averaging the covariance matrices from every class.
- Seems like a bad idea, but at least we are using all of the data samples to come up with a covariance matrix.
Averaging Covariance Matrices from Every Class

- Covariance matrix for each class is now the average of covariance matrix for each class, weighted by the fraction of samples from that class.

![Diagram showing averaging covariance matrices for two classes.](Image)

Points with probability 0.5

Class 1

Class 2

Better result than using unique covariance matrices. Notice the boundary. It is now linear, not the quadratic curve we had before. Why?
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LDA

- Remember our discriminant function.

\[ \delta_k(x) = -\frac{1}{2} \ln |\Sigma_k| - \frac{1}{2} (x - \mu_k)^T \Sigma_k^{-1} (x - \mu_k) + \ln P(C = k) \]
LDA

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- When we compare discriminant functions, \( \delta_2(x) > \delta_1(x) \), and use the same covariance matrix \( \Sigma \) for every class, we get
  \[
  -\frac{1}{2} \ln |\Sigma| + -\frac{1}{2} (x - \mu_2)^T \Sigma^{-1} (x - \mu_2) + \ln p(C = 2) \\
  > -\frac{1}{2} \ln |\Sigma| + -\frac{1}{2} (x - \mu_1)^T \Sigma^{-1} (x - \mu_1) + \ln p(C = 1)
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LDA

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  \]

- which can be simplified to
  \[
  -\frac{1}{2} (x - \mu_2)^T \Sigma^{-1} (x - \mu_2) + \ln p(C = 2)
  > -\frac{1}{2} (x - \mu_1)^T \Sigma^{-1} (x - \mu_1) + \ln p(C = 1)
  \]

  and
  \[
  x^T \Sigma^{-1} \mu_1 - \frac{1}{2} \mu_1^T \Sigma^{-1} \mu_1 + \log P(C = 1)
  > x^T \Sigma^{-1} \mu_2 - \frac{1}{2} \mu_2^T \Sigma^{-1} \mu_2 + \log P(C = 2)
  \]
From previous slide

\[ x^T \Sigma^{-1} \mu_1 - \frac{1}{2} \mu_1^T \Sigma^{-1} \mu_1 + \log P(C = 1) \]
\[
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\]

So, our discriminant function has become

\[
\delta_k(w) = x^T \Sigma^{-1} \mu_k - \frac{1}{2} \mu_k^T \Sigma^{-1} \mu_k + \log P(C = k)
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$$x^T \Sigma^{-1} \mu_1 - \frac{1}{2} \mu_1^T \Sigma^{-1} \mu_1 + \log P(C = 1)$$
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This is linear in $x$, hence and can be written as

$$\delta_k(w) = x^T w_k + \text{constant}_k$$
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\[
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\]

\[
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This is linear in \(x\), hence and can be written as

\[
\delta_k(w) = x^T w_k + \text{constant}_k
\]

or, if we add a constant 1 to \(x\) and include constant\(_k\) in \(w\)

\[
\delta_k(w) = x^T w_k
\]
So, using Gaussian distributions as generative models and restricting the covariance matrices to all be the weighted average of class covariance matrices, results in a linear boundary. This approach is called Linear Discriminant Analysis (LDA).
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Both QDA and LDA are based on Gaussian distributions for modeling the data samples in each class.
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Undersampled data
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• Undersampled data
  • Small number of samples
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QDA is more flexible, but LDA often works better in practice. When?

Undersampled data
  - Small number of samples
  - High dimensional data
Parkinsons Data, with QDA

- Calculate means and covariance matrices

```r
Xtrains <- standardize(Xtrain)
Xtests  <- standardize(Xtest)
mean1  <- colMeans(Xtrains[Ttrain==1,])
cov1   <- cov(Xtrains[Ttrain==1,])
mean2  <- colMeans(Xtrains[Ttrain==2,])
cov2   <- cov(Xtrains[Ttrain==2,])
```

Form the QDA discriminant functions.

```r
makeQDADiscF <- function(mean, sigma, prior)
{
  sigmaInv <- solve(sigma)
  function(X)
  {
    diff <- X - matrix(mean, nrow(X), ncol(X), byrow=TRUE) - 0.5 * log(det(sigma)) - 0.5 * rowSums(diff %*% sigmaInv * diff) + log(prior)
  }
}
qdadisc1 <- makeQDADiscF(mean1, cov1, nHealthy/(nHealthy+nParks))
qdadisc2 <- makeQDADiscF(mean2, cov2, nParks/(nHealthy+nParks))
```

Apply them to the train and test data.

```r
TtrainPredicted <- apply(cbind(qdadisc1(Xtrains),qdadiscs2(Xtrains)),1,which.max)
TtestPredicted <- apply(cbind(qdadisc1(Xtests),qdadisc2(Xtests)),1,which.max)
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```
Results

Training data 100 percent correct
Testing data 90 percent correct
How about LDA?

- Same as QDA, but form one covariance matrix. Can reuse `makeQDADiscF`.

```r
N <- nHealthy + nParks
covavg <- cov1 * nHealthy/N + cov2 * nParks/N
ldadisc1 <- makeQDADiscF(mean1,covavg,nHealthy/(nHealthy+nParks))
ldadisc2 <- makeQDADiscF(mean2,covavg,nParks/(nHealthy+nParks))
```
How about LDA?

- Same as QDA, but form one covariance matrix. Can reuse `makeQDADiscF`.

\[
\begin{align*}
N &< - \text{nHealthy} + \text{nParks} \\
\text{covavg} &< - \text{cov1} \times \text{nHealthy}/N + \text{cov2} \times \text{nParks}/N \\
\text{ldadisc1} &< - \text{makeQDADiscF} (\text{mean1}, \text{covavg}, \text{nHealthy}/(\text{nHealthy}+\text{nParks})) \\
\text{ldadisc2} &< - \text{makeQDADiscF} (\text{mean2}, \text{covavg}, \text{nParks}/(\text{nHealthy}+\text{nParks}))
\end{align*}
\]

- Results are

  Training data 100 percent correct
  Testing data 82.5 percent correct