

Pattern Recognition
ECSE 4410/6410 CAPA
Spring 2021

LDA +

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Please Check the 2021 Syllabus

OVERVIEW

LDA +

- The limitations of logistic regression and the need for linear discriminant analysis
- The representation of the model that is learned from data and can be saved to file
- How the model is estimated from your data
- How to make predictions from a learned LDA model
- How to prepare your data to get the most from the LDA model
- The assumptions made by LDA about your training data
- How to calculate statistics required by the LDA model from your data
- How to make predictions using the learned LDA model

Linear Regression: Limitations

- LR → Simple and useful linear classification algorithm
- LR has limitations → thus, there is a need for alternate linear classification algorithms

LIMITATIONS

- Better used on 2-Class Problems:
 - It is intended for 2-class or binary classification problems
 - It can be extended for multiclass classification → downside: rarely used for this purpose
- Unstable when working with Well Separated Classes
 - Logistic regression can become unstable when the classes are well separated
- Unstable with Few Examples
 - With only a few examples from which to estimate the model parameters

Linear Regression: Limitations

LR - Unstable model →

- The LR model may converge on a set of coefficients but the outcome is "Poor Results" → poor performance
- The LR model may **not** reliably converge on a set of coefficients

LDA – potential solution:

- Address the above limitations
- It is the go-to linear method for multiclass classification problems
- Even with binary-classification problems, it is a good idea to try both LR and LDA

LDA Model Representation

The representation of LDA:

- It consists of statistical properties of our data
- These properties are calculated for each class
- For a **single input variable (x)** → this is the mean and the variance of the variable for each class
- For **multiple variables** \rightarrow the same properties calculated over the multivariate Gaussian, i.e. the means and the covariance matrix Σ (multi-dimensional generalization of variance)

Process:

- 1. Compute statistical properties estimated from our data
- 2. Plug the statistical properties into the LDA equation
- 3. Make predictions

LDA Models - Learning

- LDA makes simplifying assumptions about our data:
 - That our data is Gaussian shaped
 - That each variable is shaped like a bell curve when plotted
 - That each attribute has the same variance
 - That values of each variable vary around the mean by the same amount on average.

With these assumptions, the **LDA model estimates** the **mean** and **variance** *from our data* <u>for each class</u>

LDA Models - Learning

For each input (x) and for each class (k)

The mean (mean) value can be estimated by dividing the sum of values by the total number of values $\max_{i \in \mathbf{k}} mean_k = \frac{1}{n_k} \times \sum_{i=1}^n x_i$

- $mean_k$ = mean value of x for the class k
- = number of instances with class k

The variance is calculated across all classes as the average squared difference of each value from the mean:

$$sigma^{2} = \frac{1}{n-K} \times \sum_{i=1}^{n} (x_{i} - mean_{k})^{2}$$

- o sigma² = the variance across all inputs (x)
- = number of instances
- = number of classes
- = mean of x for the class to which xi belongs mean₁

LDA: Making Predictions

- LDA makes predictions by estimating the probability that a new set of inputs belongs to each class
- The class that gets the highest probability is the output class and a prediction is made.

The Bayes Theorem can be used to estimate the probability of the **output class** (k) **given the input** (x) <u>using:</u>

- 1. The probability of each class and
- 2. The probability of the data belonging to each class:

$$P(Y = k|X = x) = \frac{P(k) \times P(x|k)}{\sum_{l=1}^{K} P(l) \times P(x|l)}$$

LDA: Making Predictions

$$P(Y=k|X=x) = \frac{P(k) \times P(x|k)}{\sum_{l=1}^K P(l) \times P(x|l)}$$

- P(Y = k / X = x)
 - ightharpoonup Probability of the class Y = k given the input data x.
- P(R)
 - Base probability of a given class k we are considering (Y = k), e.g. the ratio of instances with this class in the training dataset.
- P(x/k)
 - Estimated probability of x, given that its is belonging the class k.
- The denominator normalizes across for each class l, e.g. the probability of the class P(l) and the probability of the input given the class P(x / l)

LDA: Making Predictions

A Gaussian distribution function can be used to estimate P(x / k).

Plugging the Gaussian into the above equation and simplifying we end up with:

$$D_k(x) = x \times \frac{mean_k}{sigma^2} - \frac{mean_k^2}{2 \times sigma^2} + ln(P(k))$$

It is no longer a probability as we discard some terms. Instead, it is called a discriminate function for class $k \rightarrow$

- It is calculated for each class k and
- The class that has the **largest discriminant value** will make the output classification (Y = k):

Dk(x) is the discriminate function for class k given input x

LDA: Preparing Data

Suggestions to consider when preparing data for use with LDA

- Classification Problems
 - LDA is intended for classification problems where the output variable is categorical.
 - LDA supports both binary and multiclass classification
- Gaussian Distribution
 - The standard LDA model assumes input variables are Gaussian
 - <u>Suggestion</u>: **review** the univariate distributions of each attribute → use transforms to *make them more Gaussian-looking* (e.g. **log** and **root** for **EXP distributions** and **Box-Cox** for **skewed distributions**).

LDA: Preparing Data Cont.

Suggestions to consider when preparing data for use with LDA

Remove Outliers

• Outliers need to be removed \rightarrow can skew the basic statistics (μ , σ) used to separate classes in LDA.

Same Variance

- LDA assumes that each input variable has the same variance.
- Standardize data (normalization) before using LDA so that mean=0
 and standard deviation=1.

LDA-based Method Extensions

- LDA → simple and effective method for classification → there are many extensions and variations to the method:
- Quadratic Discriminant Analysis: Each class uses its own estimate of variance
- Flexible Discriminant Analysis: nonlinear combination of inputs is used (e.g. splines)
- Regularized Discriminant Analysis: regularization is used into the estimate of the variance (or covariance) → this adjusts the influence of different LDA variables

LDA Step by Step (simplest case)

How to calculate an LDA model for simple dataset with 1 input and 1 output variable

We will show:

- 1. Dataset: what we are going to use for training and testing
- 2. Learning the LDA Model: learn all statistics needed to make predictions
- **3. Making Predictions**: use the learned LDA model to make predictions for each instance in the training dataset

DATASET

- LDA data assumptions :
- Input variables → have a Gaussian distribution
- The variance <u>calculated for</u> <u>each input variable</u> by class grouping - is the same
- The mix of classes in the training set is representative of the problem



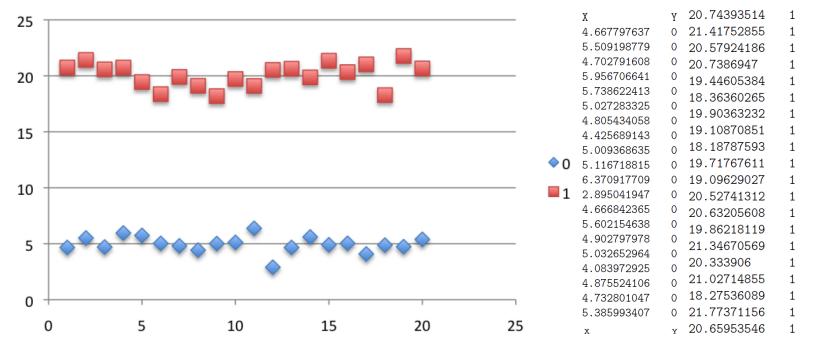
Dataset

Let's have a simple 2D dataset:

- Variables: X, Y; I/O
- X values: drawn from a Gaussian distribution
- Y = 0 or 1
- Class 0: All instances drawn from a Gaussian distribution with a μ =5, σ =1
- Class 1: same Gaussian,
 μ=20, σ=1
- The classes should be separable with a linear model like LDA







Learning the LDA Model

It requires the estimation of the following statistics from the training data **for each Class**:

- Mean per class
- Probability of an instance belong to the class
- Covariance for the input data





$$mean(x) = \frac{1}{n} \times \sum_{i=1}^{n} x_i$$

STEP 1 - MEAN

Y = 0: 4.975415507

Y = 1: 20.08706292

STEP 2 — Calculate Class Probabilities

$$P(y=0) = \frac{count(y=0)}{count(y=0) + count(y=1)}$$

$$P(y=1) = \frac{count(y=1)}{count(y=0) + count(y=1)}$$

$$P(y=0) = \frac{20}{20 + 20}$$
$$P(y=1) = \frac{20}{20 + 20}$$

- This is 0.5 for each class, as expected when creating the dataset.
- It is a good idea to work through each step of the model learning process.

STEP 3 - Variance

We need to calculate the <u>variance</u> for **the input variable** for **each class**

Variance = the difference of each instance from the mean

We can calculate the variance for our dataset in two steps:

- Calculate the squared difference for each input variable from the group mean
- 2. Calculate the mean of the squared difference
- Dataset is divided into 2 groups/classes as per the Y={0,1}
- Then, calculate the difference for each input value X from the mean from each class.

STEP 3 - Variance

We can calculate the difference of each input value from the mean using:

$$SquaredDifference = (x - mean_k)^2$$

X	Υ	(x-mean_k)^2				
4.668	0	0.0946	20.744	1	0.4315	
5.509	0	0.2849	21.418	1	1.7701	
4.703	0	0.0743	20.579	1	0.2422	
5.957	0	0.9629	20.739	1	0.4246	
5.739	0	0.5825	19.446	1	0.4109	
5.027	0	0.0027	18.364	1	2.9703	
4.805	0	0.0289	19.904	1	0.0336	
4.426	0	0.3022	19.109	1	0.9572	
5.009	0	0.0012	18.188	1	3.6069	
5.117	0	0.0200	19.718	1	0.1364	
6.371	0	1.9474	19.096	1	0.9816	
2.895	0	4.3280	20.527	1	0.1939	
4.667	0	0.0952	20.632	1	0.2970	
5.602	0	0.3928	19.862	1	0.0506	
4.903	0	0.0053	21.347	1	1.5867	
5.033	0	0.0033	20.334	1	0.0609	
4.084	0	0.7947	21.027	1	0.8838	
4.876	0	0.0100	18.275	1	3.2823	
4.733	0	0.0589	21.774	1	2.8448	
5.386	0 0.1686		20.660	1	0.3277	

	M		
STEP 1	Mean Y=0	Mean Y=1	
	4.975	20.087	
	VARI		
STEP 2	P(Y=0)	P(Y=1)	
	0.5	0.5	
	Σ((x-mean_k=0)^2)	Σ((x-mean_k=1)^2)	k= Class 0 or 1
STEP 3	10.1582	21.4932	



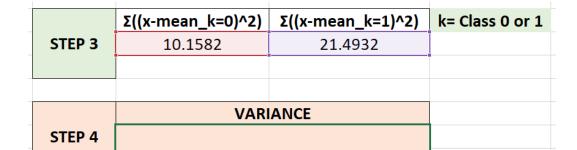
STEP 3 - Variance

Next, we can calculate the variance as the average squared difference from the mean as:

Х	Υ	(x-mean_k)^2		
4.668	0	0.0946		
5.509	0	0.2849		
4.703	0	0.0743		
5.957	0	0.9629		
5.739	0	0.5825		
5.027	0	0.0027		
4.805	0	0.0289		
4.426	0	0.3022		
5.009	0	0.0012		
5.117	0	0.0200		
6.371	0	1.9474		
2.895	0	4.3280		
4.667	0	0.0952		
5.602	0	0.3928		
4.903	0	0.0053		
5.033	0	0.0033		
4.084	0	0.7947		
4.876	0	0.0100		
4.733	0	0.0589		
5.386	0	0.1686		
20.744	1	0.4315		
21.418	1	1.7701		
20.579	1	0.2422		
20.739	1	0.4246		
19.446	1	0.4109		
18.364	1	2.9703		
19.904	1	0.0336		
19.109	1	0.9572		
18.188	1	3.6069		
19.718	1	0.1364		
19.096	1	0.9816		
20.527	1	0.1939		
20.632	1	0.2970		
19.862	1	0.0506		
21.347	1	1.5867		
20.334	1	0.0609		
21.027	1	0.8838		
18.275	1	3.2823		
21.774	1	2.8448		
20.660	1	0.3277		

$variance = \frac{1}{40 - 2} \times (10.15823013 + 21.49316708)$
variance = 0.832931506

Class 1 Class sample count 20



 $variance = \frac{1}{count(x) - count(classes)} \times \sum_{i=1}^{n} SquaredDifference(x_i)$

Class sample count 20

VARIANCE						
	0.832931506					

=1/(COUNT(E2:E41)-2)*(L10+M10)

STEP 4 - Predictions

 The discriminant function for a class given an input (x) is calculated using:

$$discriminant(x) = x \times \frac{mean}{variance} - \frac{mean^2}{2 \times variance} + ln(probability)$$

- x is the input value
- mean, variance and probability are calculated above for the class we are discriminating

Predictions are made by calculating the **discriminant function** for each class and predicting the class with the **largest value**.

STEP 4 - Calculations

Let's step through the calculation of the discriminate	Υ	(x-mean_k)^2				
value of each class for the 1 st instance.	4.668	0	0.0946			
	5.509	0	0.2849			
The 1 st instance in the dataset is:	4.703	0	0.0743			
X = 4:667797637 and Y = 0.	5.957	0	0.9629			
7 1.007737037 and 1 0.	5.739	0	0.5825			
The discriminate street, for V. Ois calculated as	5.027	0	0.0027			
The discriminant value for Y = 0 is calculated as	4.805	0	0.0289			
follows:	4.426	0	0.3022			
	5 000	0	0.0012			
$discriminant(Y = 0 x) = 4.667797637 \times \frac{4.975415507}{0.832931506} - \frac{4.97541550}{2 \times 0.832931}$	$\frac{7^2}{1} + ln(0)$	<u>5)</u> 0	0.0200			
	.506	0	1.9474			
discriminant(Y=0 x) = 12.3293558		0	4.3280			
We can also calculate the discriminant value for $V=1$:	0	0.0952				
we can also calculate the discriminant value for $T=1$.	We can also calculate the discriminant value for $Y = 1$:					
	0	0	0.0053			
$discriminant(Y = 1 x) = 4.667797637 \times \frac{20.08706292}{0.832931506} - \frac{20.08706292}{2 \times 0.832931}$	$\frac{2^2}{2} + ln(0.5)$	<u>5)</u> 0	0.0033			
	506	0	0.7947			
discriminant(Y = 1 x) = -130.3349038		0	0.0100			
	4.733	0	0.0589			
	0	0.1686				

STEP 4 – Decision Making

$$discriminant(Y=0|x) = 4.667797637 \times \frac{4.975415507}{0.832931506} - \frac{4.975415507^2}{2 \times 0.832931506} + ln(0.5) + ln$$

We can also calculate the discriminant value for Y = 1:

$$discriminant(Y=1|x) = 4.667797637 \times \frac{20.08706292}{0.832931506} - \frac{20.08706292^2}{2 \times 0.832931506} + ln(0.5)$$

$$discriminant(Y=1|x) = -130.3349038$$

The discriminant value for Y = 0 (12.3293558)

> (LARGER)

The discriminate value for Y = 1 (-130.3349038)

Thus, the model predicts Y = 0

CORRECT (as we already know)

STEP 4 – Repeat for ALL instances

We need to proceed to calculate the Y values for each instance in the dataset, as follows:

1						ı					
Х	Υ	(x-mean_k)^2	DISCRIMINANT Y=0	DISCRIMINANT Y=1	PREDICTION						
4.668	0	0.0946	12.3293558	-130.2836105	0	20.744	1	0.4315	108.3582168	257.4101954	1
5.509	0	0.2849	17.35536365	-109.992293	0	21.418	1	1.7701	112.3818455	273.6546443	1
4.703	0	0.0743	12.53838805	-129.4396923	0	20.579	1	0.2422	107.3744415	253.4384351	1
5.957	0	0.9629	20.02849769	-99.20014678	0	20.739	1	0.4246	108.3269137	257.2838164	1
5.739	0	0.5825	18.72579795	1252.345751	1	19.446	1	0.4109	100.60548	226.1103549	1
5.027	0	0.0027	14.47670003	-121.6142162	0	18.364	1	2.9703	94.1395889	200.0058493	1
4.805	0	0.0289	13.15151029	-126.9643563	0	19.904	1	0.0336	103.3387697	237.1453651	1
4.426	0	0.3022	10.88315002	-136.1223242	0	19.109	1	0.9572	98.59038855	217.9748998	1
5.009	0	0.0012	14.3696888	-122.0462488	0	18.188	1	3.6069	93.08990662	195.7680054	1
5.117	0	0.0200	15.0109321	-119.4573807	0	19.718	1	0.1364	102.2279828	232.6608258	1
6.371	0	1.9474	22.50273735	-89.21098953	0	19.096	1	0.9816	98.5162097	217.6754202	1
2.895	0	4.3280	1.740014309	-173.0355713	0	20.527	1	0.1939	107.0648488	252.1885279	1
4.667	0	0.0952	12.3236496	-130.306648	0	20.632	1	0.2970	107.6899208	254.7121084	1
5.602	0	0.3928	17.91062422	-107.7505598	0	19.862	1	0.0506	103.0911664	236.1457254	1
4.903	0	0.0053	13.73310188	-124.6163178	0	21.347	1	1.5867	111.9587938	271.9466728	1
5.033	0	0.0033	14.50877492	-121.4847215	0	20.334	1	0.0609	105.9089574	247.52189	1
4.084	0	0.7947	8.841949563	-144.3631881	0	21.027	1	0.8838	110.0499579	264.2401995	1
4.876	0	0.0100	13.57018471	-125.2740574	0	18.275	1	3.2823	93.61248743	197.8778018	1
4.733	0	0.0589	12.7176458	-128.7159815	0	21.774	1	2.8448	114.5094616	282.2443908	1
5.386	0	0.1686	16.61941128	-112.9635266	0	20.660	1	0.3277	20.02849769	255.374804	1
					7						
i											

- LDA has achieved an accuracy of 100% (no errors)
- This is not surprising given that the dataset was contrived so that the groups for Y = 0 and Y = 1 were clearly separable.

Create and Visualize Discriminant Analysis

Classifier

This example shows how to perform linear and quadratic classification of Fisher iris data.

```
load fisheriris
```

The column vector, species, consists of iris flowers of three different species, setosa, versicolor, virginica. The double matrix meas consists of four types of measurements on the flowers, the length and width of sepals and petals in centimeters, respectively.

Use petal length (third column in meas) and petal width (fourth column in meas) measurements. Save these as variables PL and PW, respectively.

```
PL = meas(:,3);
PW = meas(:,4);
```

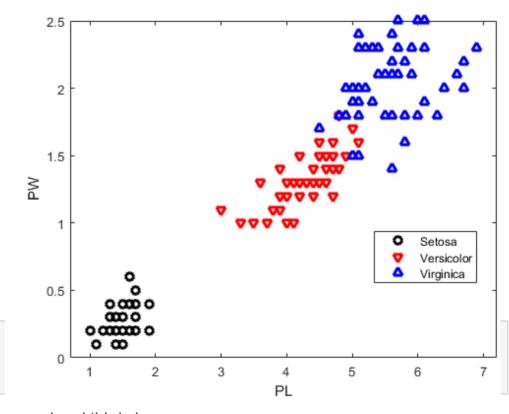
Plot the data, showing the classification, that is, create a scatter plot of the measurements, grouped by species.

```
h1 = gscatter(PL,PW,species,'krb','ov^',[],'off');
h1(1).LineWidth = 2;
h1(2).LineWidth = 2;
h1(3).LineWidth = 2;
legend('Setosa','Versicolor','Virginica','Location','best')
hold on
```

Create and Visualize Discriminant Analysis Classifier

Create a linear classifier.

```
X = [PL,PW];
MdlLinear = fitcdiscr(X,species);
```



Retrieve the coefficients for the linear boundary between the second and third classes.

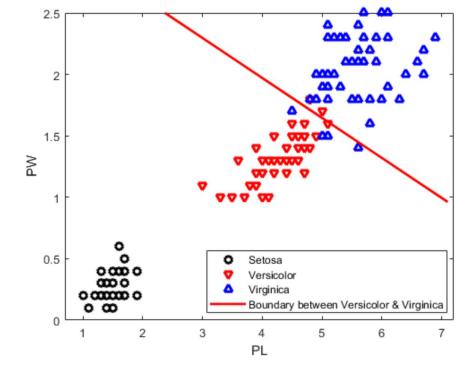
```
MdlLinear.ClassNames([2 3])

ans = 2x1 cell
```

```
ans = 2x1 cell
{'versicolor'}
{'virginica' }
```

```
K = MdlLinear.Coeffs(2,3).Const;
L = MdlLinear.Coeffs(2,3).Linear;
```

Create and Visualize Discriminant Analysis Classifier



Plot the curve that separates the second and third classes

$$K + \begin{bmatrix} x_1 & x_2 \end{bmatrix} L = 0.$$

```
f = @(x1,x2) K + L(1)*x1 + L(2)*x2;
h2 = fimplicit(f,[.9 7.1 0 2.5]);
h2.Color = 'r';
h2.LineWidth = 2;
h2.DisplayName = 'Boundary between Versicolor & Virginica';
```

Create and Visualize Discriminant Analysis Classifier

Retrieve the coefficients for the linear boundary between the first and second classes.

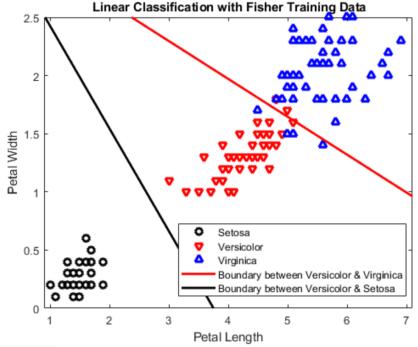
```
MdlLinear.ClassNames([1 2])

ans = 2x1 cell
   {'setosa' }
   {'versicolor'}
```

```
K = MdlLinear.Coeffs(1,2).Const;
L = MdlLinear.Coeffs(1,2).Linear;
```

Plot the curve that separates the first and second classes.

```
f = @(x1,x2) K + L(1)*x1 + L(2)*x2;
h3 = fimplicit(f,[.9 7.1 0 2.5]);
h3.Color = 'k';
h3.LineWidth = 2;
h3.DisplayName = 'Boundary between Versicolor & Setosa';
axis([.9 7.1 0 2.5])
xlabel('Petal Length')
ylabel('Petal Width')
title('{\bf Linear Classification with Fisher Training Data}')
```



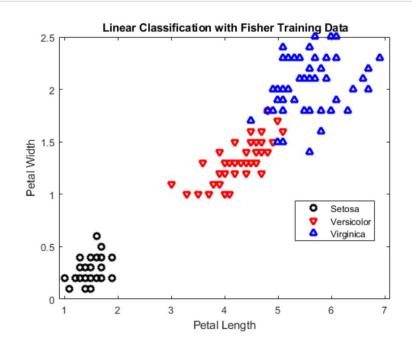
Create and Visualize Discriminant Analysis Classifier

Create a quadratic discriminant classifier.

```
MdlQuadratic = fitcdiscr(X,species,'DiscrimType','quadratic');
```

Remove the linear boundaries from the plot.

```
delete(h2);
delete(h3);
```



Retrieve the coefficients for the quadratic boundary between the second and third classes.

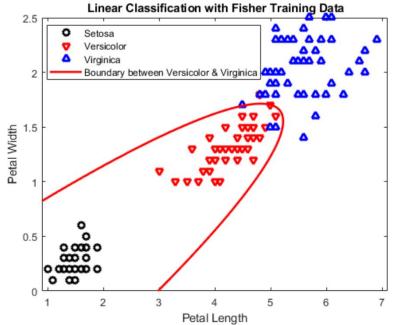
```
MdlQuadratic.ClassNames([2 3])
ans = 2x1 cell
{'versicolor'}
```

```
K = MdlQuadratic.Coeffs(2,3).Const;
L = MdlQuadratic.Coeffs(2,3).Linear;
Q = MdlQuadratic.Coeffs(2,3).Quadratic;
```

Plot the curve that separates the second and third classes

$$K + \begin{bmatrix} x_1 & x_2 \end{bmatrix} L + \begin{bmatrix} x_1 & x_2 \end{bmatrix} Q \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = 0.$$

{'virginica' }



Create and Visualize Discriminant Analysis Classifier

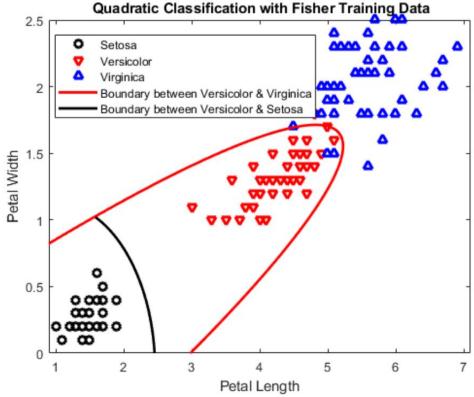
Retrieve the coefficients for the quadratic boundary between the first and second classes.

```
MdlQuadratic.ClassNames([1 2])

ans = 2x1 cell
   {'setosa' }
   {'versicolor'}
```

```
K = MdlQuadratic.Coeffs(1,2).Const;
L = MdlQuadratic.Coeffs(1,2).Linear;
Q = MdlQuadratic.Coeffs(1,2).Quadratic;
```

Plot the curve that separates the first and second and classes.



Discriminant Analysis Classification

Discriminant analysis is a classification method. It assumes that different classes generate data based on different Gaussian distributions.

- To train (create) a classifier, the fitting function estimates the parameters of a Gaussian distribution for each class (see <u>Creating Discriminant Analysis Model</u>).
- To predict the classes of new data, the trained classifier finds the class with the smallest misclassification cost (see <u>Prediction Using Discriminant Analysis Models</u>)
- Linear discriminant analysis is also known as the Fisher discriminant, named for its inventor, Sir R. A. Fisher [1].

Discriminant Analysis Classification

Create Discriminant Analysis Classifiers

This example shows how to train a basic discriminant analysis classifier to classify irises in Fisher's iris data.

Load the data.

```
load fisheriris
```

Create a default (linear) discriminant analysis classifier.

```
MdlLinear = fitcdiscr(meas, species);
```

To visualize the classification boundaries of a 2-D linear classification of the data, see Create and Visualize Discriminant Analysis Classifier.

Classify an iris with average measurements.

{'versicolor'}

```
meanmeas = mean(meas);
meanclass = predict(MdlLinear, meanmeas)

meanclass = 1x1 cell array
```

Discriminant Analysis Classification

Create a quadratic classifier.

```
MdlQuadratic = fitcdiscr(meas, species, 'DiscrimType', 'quadratic');
```

To visualize the classification boundaries of a 2-D quadratic classification of the data, see Create and Visualize Discriminant Analysis Classifier.

Classify an iris with average measurements using the quadratic classifier.

```
meanclass2 = predict(MdlQuadratic, meanmeas)

meanclass2 = 1x1 cell array
   {'versicolor'}
```

References

[1] Fisher, R. A. The Use of Multiple Measurements in Taxonomic Problems. Annals of Eugenics, Vol. 7, pp. 179–188, 1936. Available at https://digital.library.adelaide.edu.au/dspace/handle/2440/15227.

See Also → Functions → fitcdiscr

LDA – Face Recognition Solution

https://www.mathworks.com/matlabcentral/mlc-downloads/downloads/submissions/35106/versions/1/previews/PhD_tool/features/perform_lda_PhD.m/index.html

-- Homework --

Use code and Celebrity Face Dataset > after face normalization



What have we learned

- The model representation for LDA and what is distinct about a learned model
- How the parameters of the LDA model can be estimated from training data
- How the model can be used to make predictions on new data
- How to prepare your data to get the most from the method
- How to calculate the statistics from your dataset required by the LDA model
- How to use the LDA model to calculate a discriminant value for each class and make a prediction.
- MATLAB Examples

Questions?

