DS 4400

Machine Learning and Data Mining I

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October 20 2020

Announcements

- HW 3 is out
  – Due on Thu, Oct. 29
- Project proposal
  – Due on Monday, Nov. 2
  – Team of 2
  – Resources and example projects on Piazza

Project Proposal

- Project Title
- Project Team
- Problem Description
  - What is the prediction problem you are trying to solve?
- Dataset
  - Link to data, brief description, number of records, feature dimensionality (at least 10K records)
- Approach and methodology
  - Normalization
  - Feature selection
  - Machine learning models you will try
  - Splitting into training and testing, cross validation
  - Language and packages you plan to use
- Metrics (how you will evaluate your models)
- References
  - How did you find out about the dataset, did anyone else used the data for a similar prediction task

Outline

- Generative vs Discriminative Models
- Linear Discriminant Analysis (LDA)
  - LDA is a linear classifier
  - LDA vs Logistic Regression
  - Lab
- Density Estimation
- Naïve Bayes classifier

Generative vs Discriminative

- Generative model
  - Given X and Y, learns the joint probability $P(X, Y)$
  - Can generate more examples from distribution
  - Examples: LDA, Naïve Bayes, language models (GPT-2)

- Discriminative model
  - Given X and Y, learns a decision function for classification
  - Examples: logistic regression, kNN

LDA

- Classify to one of k classes
- Logistic regression computes directly
  - $\mathrm{P}[Y = 1|X = x]$
  - Assume sigmoid function
- LDA uses Bayes Theorem to estimate it

LDA

Assume $f_k(x)$ is Gaussian!
Unidimensional case (d=1)

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

Continuous Random Variables

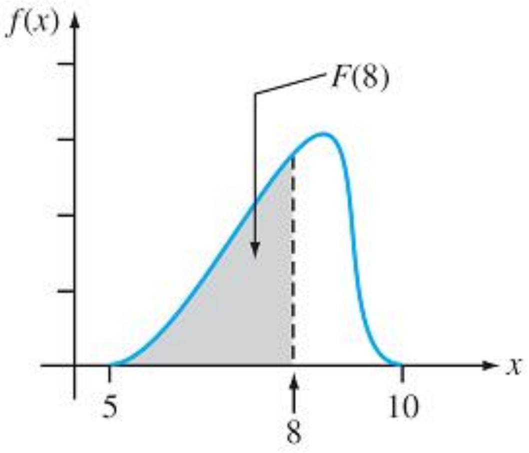
- X:U⟶V is continuous RV if it takes infinite number of values
- The **cumulative distribution function CDF** *F: R* ⟶ {0,1} for *X* is defined for every value *x* by:

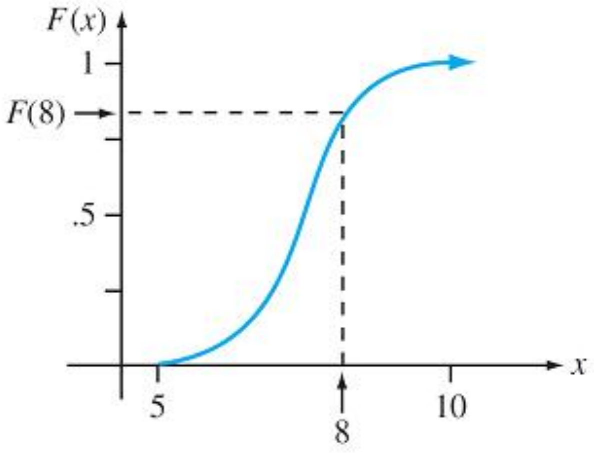
$$F(x) = \Pr(X \leq x)$$

- The **probability distribution function PDF** *f*(*x*) for *X is*

$$f(x) = dF(x)/dx$$

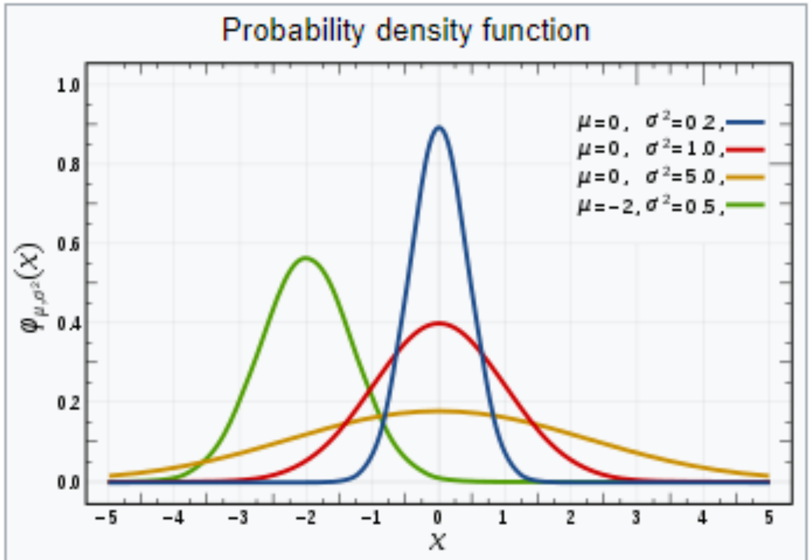
Increasing



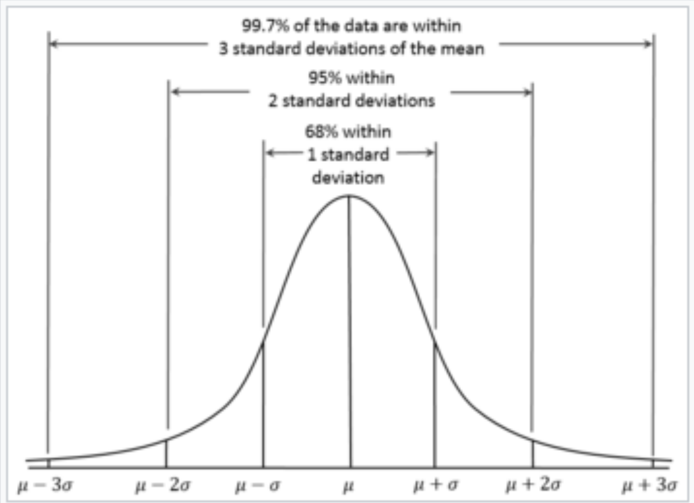


Gaussian Distribution

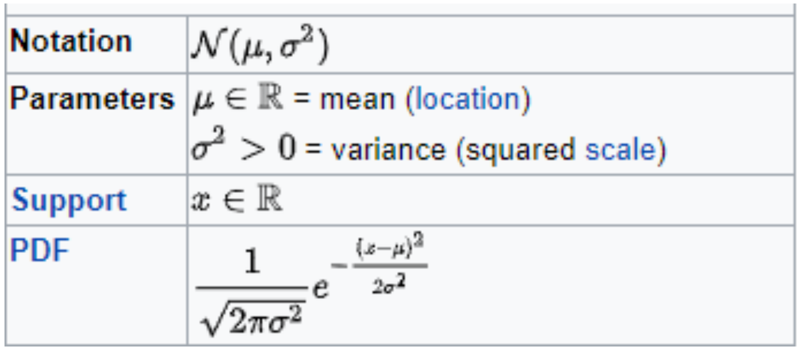
Normal Distribution



The red curve is the *standard normal distribution*


99.7% of the data are within 3 standard deviations of the mean
95% within 2 standard deviations
68% within 1 standard deviation
$\mu-3\sigma$
$\mu-2\sigma$
$\mu-\sigma$
μ
$\mu+\sigma$
$\mu+2\sigma$
$\mu+3\sigma$

For the normal distribution, the values less than one standard deviation away from the mean account for 68.27% of the set; while two standard deviations from the mean account for 95.45%; and three standard deviations account for 99.73%.



Notation	$\mathcal{N}(\mu, \sigma^2)$
Parameters	$\mu \in \mathbb{R}$ = mean (location) $\sigma^2 > 0$ = variance (squared scale)
Support	$x \in \mathbb{R}$
PDF	$\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$

LDA

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

Assume $f_k(x)$ is Gaussian!
Unidimensional case (d=1)

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

$$p_k(x) = \frac{\pi_k \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x - \mu_k)^2\right)}{\sum_{l=1}^{K} \pi_l \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x - \mu_l)^2\right)}.$$

Assumption: $\sigma_1 = \ \dots \sigma_k = \ \sigma$

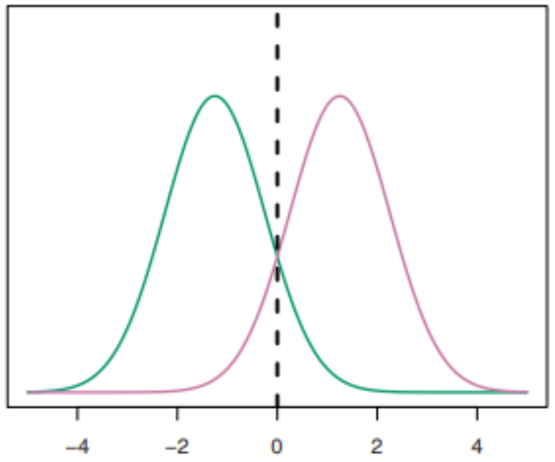
LDA decision boundary

Pick class k to maximize

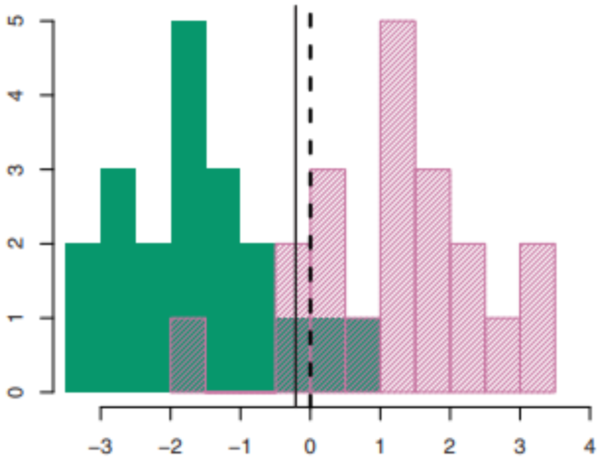
$$\delta_k(x) = x \cdot \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log(\pi_k)$$

Example: $k = 2, \pi_1 = \pi_2$

Classify as class 1 if $x > \frac{\mu_1+\mu_2}{2\sigma}$



True decision boundary



Estimated decision boundary

LDA in practice

Given training data $(x_i, y_i), i = 1, \dots, n, y_i \in \{1, \dots, K\}$

1. Estimate mean and variance

$$\boxed{\begin{aligned} \hat{\mu}_k &= \frac{1}{n_k} \sum_{i: y_i = k} x_i \\ \hat{\sigma}^2 &= \frac{1}{n-K} \sum_{k=1}^{K} \sum_{i: y_i = k} (x_i - \hat{\mu}_k)^2 \end{aligned}}$$

2. Estimate prior

$$\boxed{\hat{\pi}_k = n_k / n.}$$

Given testing point x, predict k that maximizes:

$$\boxed{\hat{\delta}_k(x) = x \cdot \frac{\hat{\mu}_k}{\hat{\sigma}^2} - \frac{\hat{\mu}_k^2}{2\hat{\sigma}^2} + \log(\hat{\pi}_k)}$$

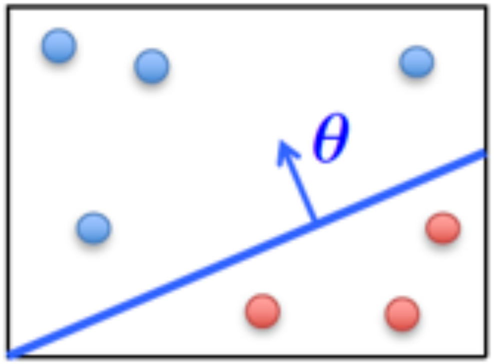
Linear models

- Perceptron

$$h(\boldsymbol{x}) = \operatorname{sign}(\boldsymbol{\theta}^\intercal \boldsymbol{x})$$

- Logistic regression

$$\boxed{h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^\intercal \boldsymbol{x}}}}$$



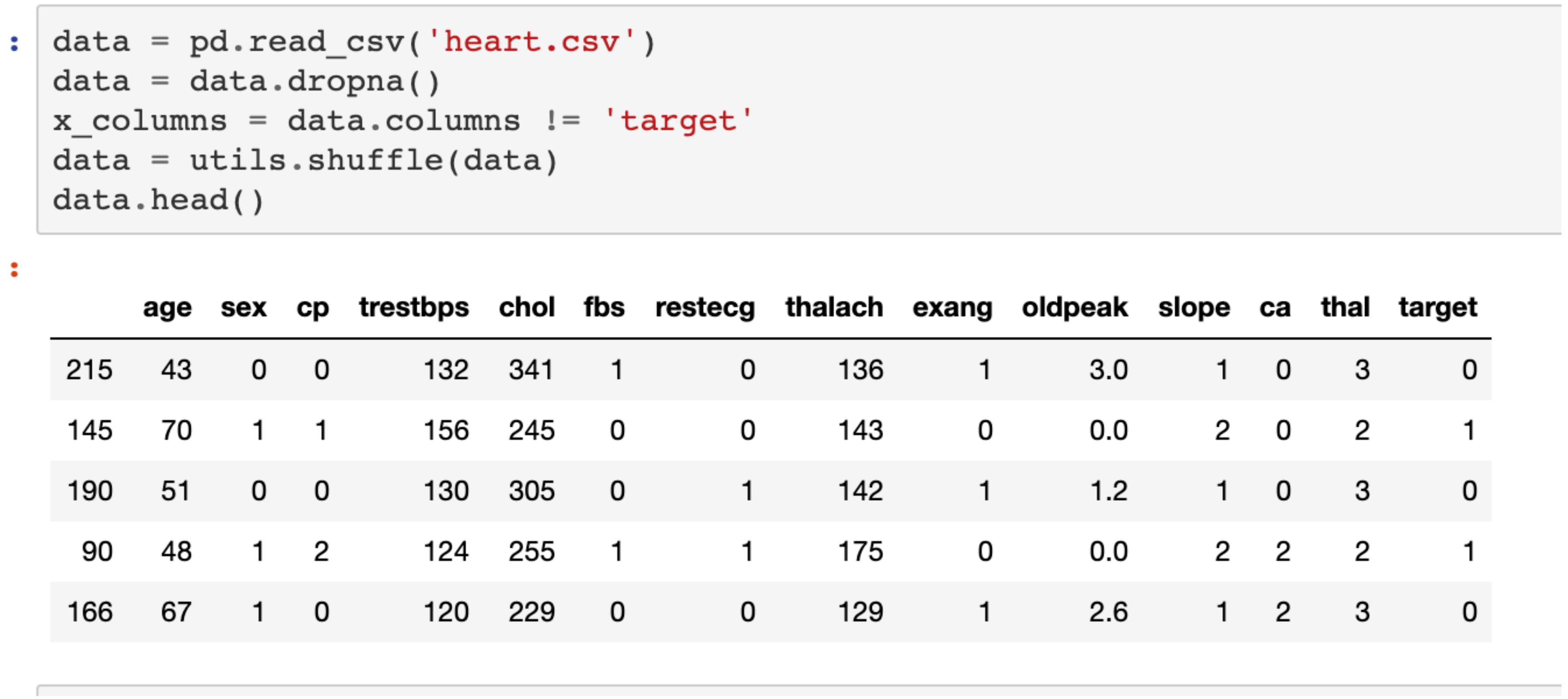
- LDA

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

LDA vs Logistic Regression

- Logistic regression computes directly $\Pr[Y = 1|X = x]$ by assuming sigmoid function
  - Uses Maximum Likelihood Estimation
  - Discriminative Model
- LDA uses Bayes Theorem to estimate it
  - Estimates mean, co-variance, and prior from training data
  - Generative model
  - Assumes Gaussian distribution for $f_k(x) = \Pr[X = x|Y = k]$
- Which one is better?
  - LDA can be sensitive to outliers
  - LDA works well for Gaussian distribution
  - Logistic regression is more complex to solve, but more expressive

Linear Classifier Lab

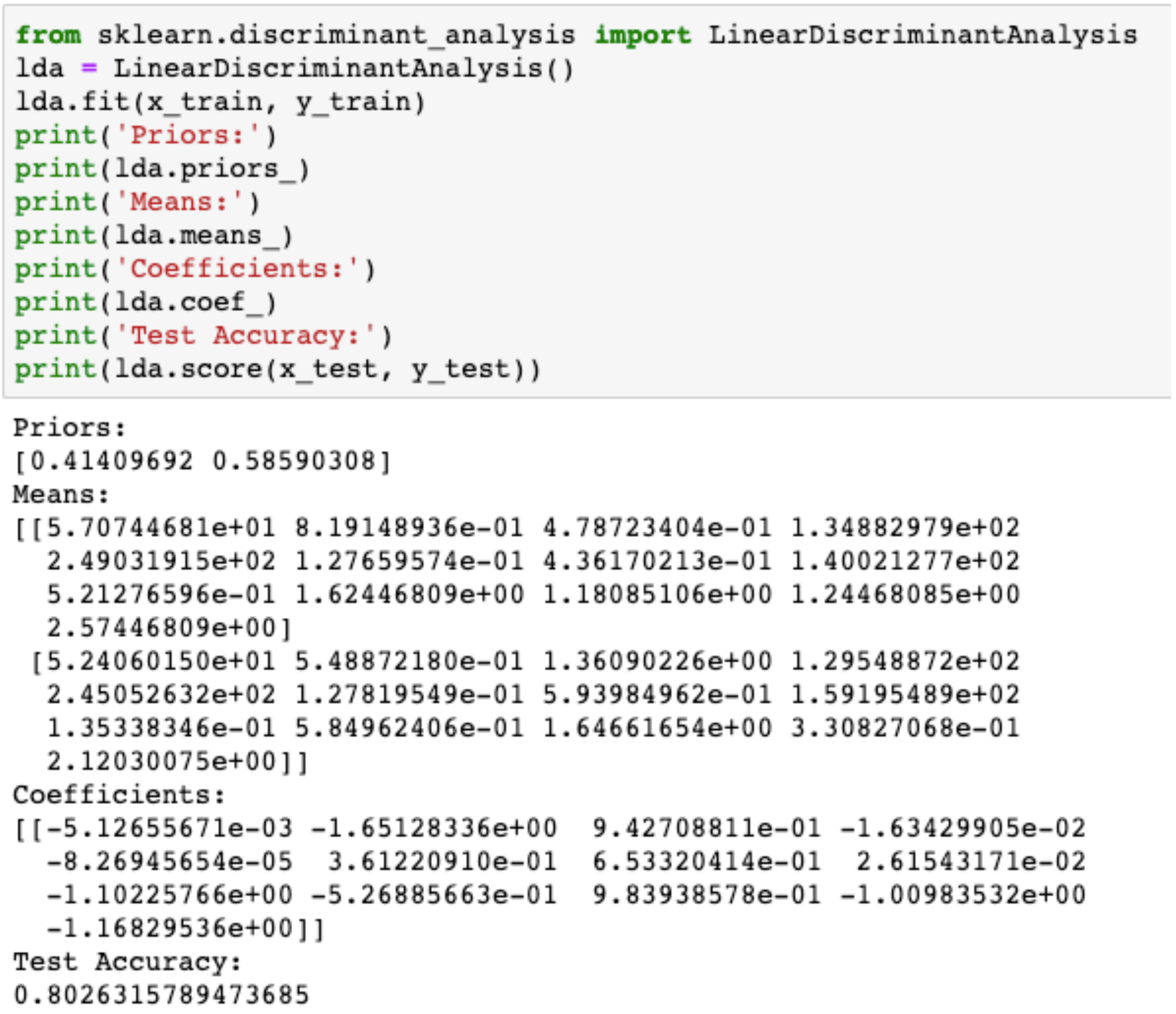


```
data = pd.read_csv('heart.csv')
data = data.dropna()
x_columns = data.columns != 'target'
data = utils.shuffle(data)
data.head()
```

	age	sex	cp	trestbps	chol	fbs	restecg	thalach	exang	oldpeak	slope	ca	thal	target
215	43	0	0	132	341	1	0	136	1	3.0	1	0	3	0
145	70	1	1	156	245	0	0	143	0	0.0	2	0	2	1
190	51	0	0	130	305	0	1	142	1	1.2	1	0	3	0
90	48	1	2	124	255	1	1	175	0	0.0	2	2	2	1
166	67	1	0	120	229	0	0	129	1	2.6	1	2	3	0

https://www.kaggle.com/ronitf/heart-disease-uci

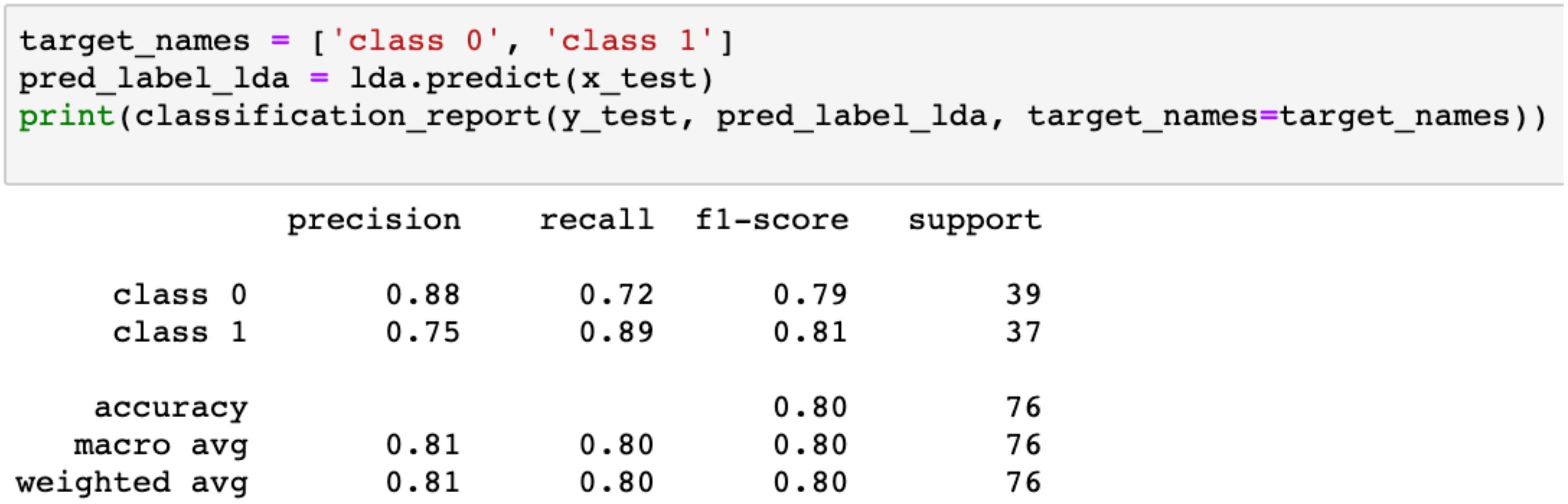
Lab LDA



```python
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis
lda = LinearDiscriminantAnalysis()
lda.fit(x_train, y_train)
print('Priors:')
print(lda.priors_)
print('Means:')
print(lda.means_)
print('Coefficients:')
print(lda.coef_)
print('Test Accuracy:')
print(lda.score(x_test, y_test))
```

```
Priors:
[0.41409692 0.58590308]
Means:
[[5.70744681e+01 8.19148936e-01 4.78723404e-01 1.34882979e+02
  2.49031915e+02 1.27659574e-01 4.36170213e-01 1.40021277e+02
  5.21276596e-01 1.62446809e+00 1.18085106e+00 1.24468085e+00
  2.57446809e+00]
 [5.24060150e+01 5.48872180e-01 1.36090226e+00 1.29548872e+02
  2.45052632e+02 1.27819549e-01 5.93984962e-01 1.59195489e+02
  1.35338346e-01 5.84962406e-01 1.64661654e+00 3.30827068e-01
  2.12030075e+00]]
Coefficients:
[[-5.12655671e-03 -1.65128336e+00  9.42708811e-01 -1.63429905e-02
  -8.26945654e-05  3.61220910e-01  6.53320414e-01  2.61543171e-02
  -1.10225766e+00 -5.26885663e-01  9.83938578e-01 -1.00983532e+00
  -1.16829536e+00]]
Test Accuracy:
0.8026315789473685
```

LDA Metrics



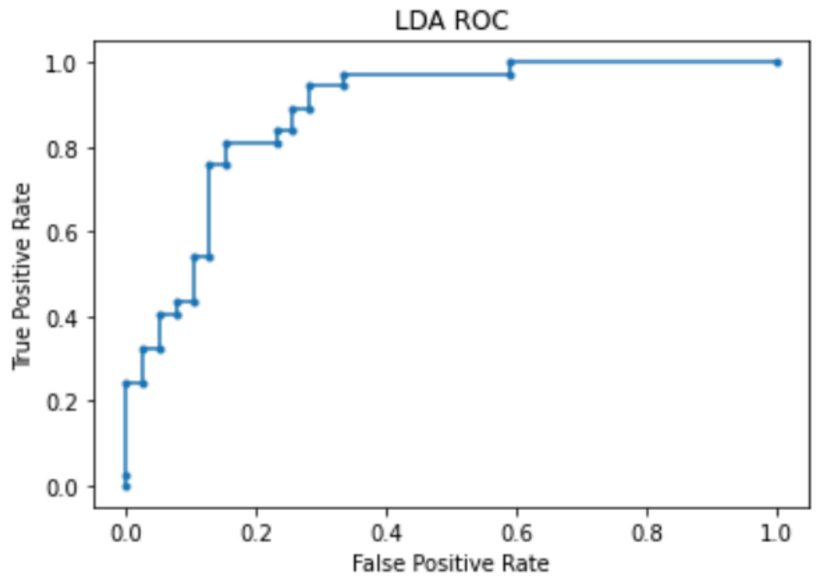
```python
target_names = ['class 0', 'class 1']
pred_label_lda = lda.predict(x_test)
print(classification_report(y_test, pred_label_lda, target_names=target_names))
```

```
              precision    recall  f1-score   support

     class 0       0.88      0.72      0.79        39
     class 1       0.75      0.89      0.81        37

    accuracy                           0.80        76
   macro avg       0.81      0.80      0.80        76
weighted avg       0.81      0.80      0.80        76
```

LDA ROC Curve

```python
pred_lda = lda.predict_proba(x_test)[:,1]
r_auc_lda = roc_auc_score(y_test, pred_lda)
print("AUC=",r_auc_lda)

lda_fpr, lda_tpr, _ = roc_curve(y_test, pred_lda)
pyplot.plot(lda_fpr, lda_tpr, marker='.', label='Logistic')
pyplot.xlabel('False Positive Rate')
pyplot.ylabel('True Positive Rate')
pyplot.title('LDA ROC')
```

```
AUC= 0.8842688842688843
```



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- Density Estimation
- Naïve Bayes classifier

Essential probability concepts

- Marginalization: $P(B) = \sum_{v \in \text{values}(A)} P(B \wedge A = v)$
- Conditional Probability: $P(A \mid B) = \frac{P(A \wedge B)}{P(B)}$
- Bayes' Rule: $P(A \mid B) = \frac{P(B \mid A) \times P(A)}{P(B)}$
- Independence:

$$\begin{aligned} A \perp\!\!\!\perp B &\leftrightarrow P(A \wedge B) = P(A) \times P(B) \\ &\leftrightarrow P(A \mid B) = P(A) \\ A \perp\!\!\!\perp B \mid C &\leftrightarrow P(A \wedge B \mid C) = P(A \mid C) \times P(B \mid C) \end{aligned}$$

Prior and Joint Probabilities

- **Prior probability**: degree of belief without any other evidence
- **Joint probability**: matrix of combined probabilities of a set of variables

Russell & Norvig's Alarm Domain: (boolean RVs)

- A world has a specific instantiation of variables:

  (alarm ∧ theft ∧ ¬earthquake)

- The joint probability is given by:

P(Alarm, Theft) =

	alarm	¬alarm
theft	0.09	0.01
┐theft	0.1	0.8

Prior and Joint Probabilities

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P(Alarm, Theft) =

	alarm	¬alarm
theft	0.09	0.01
¬theft	0.1	0.8

Prior probability of theft

P(theft) = 0.1

by marginalization over Alarm

Computing Prior Probabilities

	alarm		¬alarm	
	earthquake	¬earthquake	earthquake	¬earthquake
theft	0.01	0.08	0.001	0.009
¬theft	0.01	0.09	0.01	0.79

$$P(alarm) = \sum_{b,e} P(alarm \wedge \text{theft} = b \wedge \text{Earthquake} = e)$$

$$= 0.01 + 0.08 + 0.01 + 0.09 = 0.19$$

$$P(\text{theft}) = \sum_{a,e} P(\text{Alarm} = a \wedge \text{theft} \wedge \text{Earthquake} = e)$$

$$= 0.01 + 0.08 + 0.001 + 0.009 = 0.1$$

The Joint Distribution

Recipe for making a joint distribution of d variables:

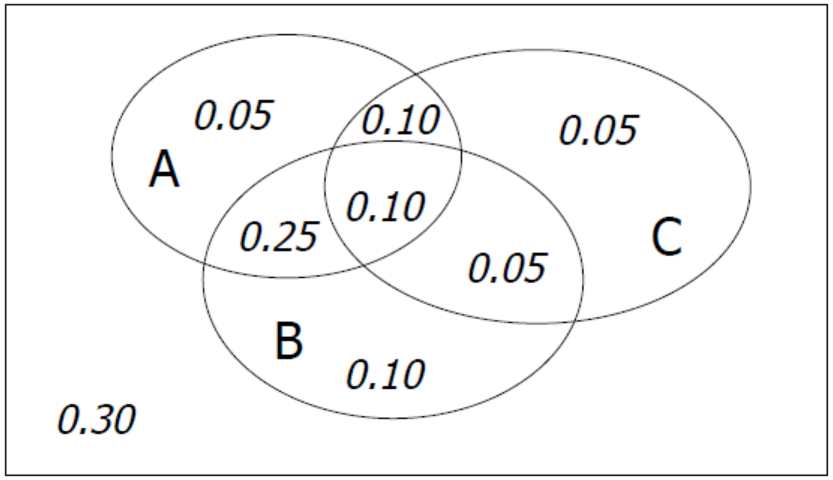
1. Make a truth table listing all combinations of values of your variables (if there are d Boolean variables then the table will have 2^d rows).

2. For each combination of values, say how probable it is.

3. If you subscribe to the axioms of probability, those numbers must sum to 1.

e.g., Boolean variables A, B, C

A	B	C	Prob
0	0	0	0.30
0	0	1	0.05
0	1	0	0.10
0	1	1	0.05
1	0	0	0.05
1	0	1	0.10
1	1	0	0.25
1	1	1	0.10



Slide © Andrew Moore

Learning Joint Distributions

Step 1:
Build a JD table for your attributes in which the probabilities are unspecified

A	B	C	Prob
0	0	0	?
0	0	1	?
0	1	0	?
0	1	1	?
1	0	0	?
1	0	1	?
1	1	0	?
1	1	1	?

Step 2:
Then, fill in each row with:

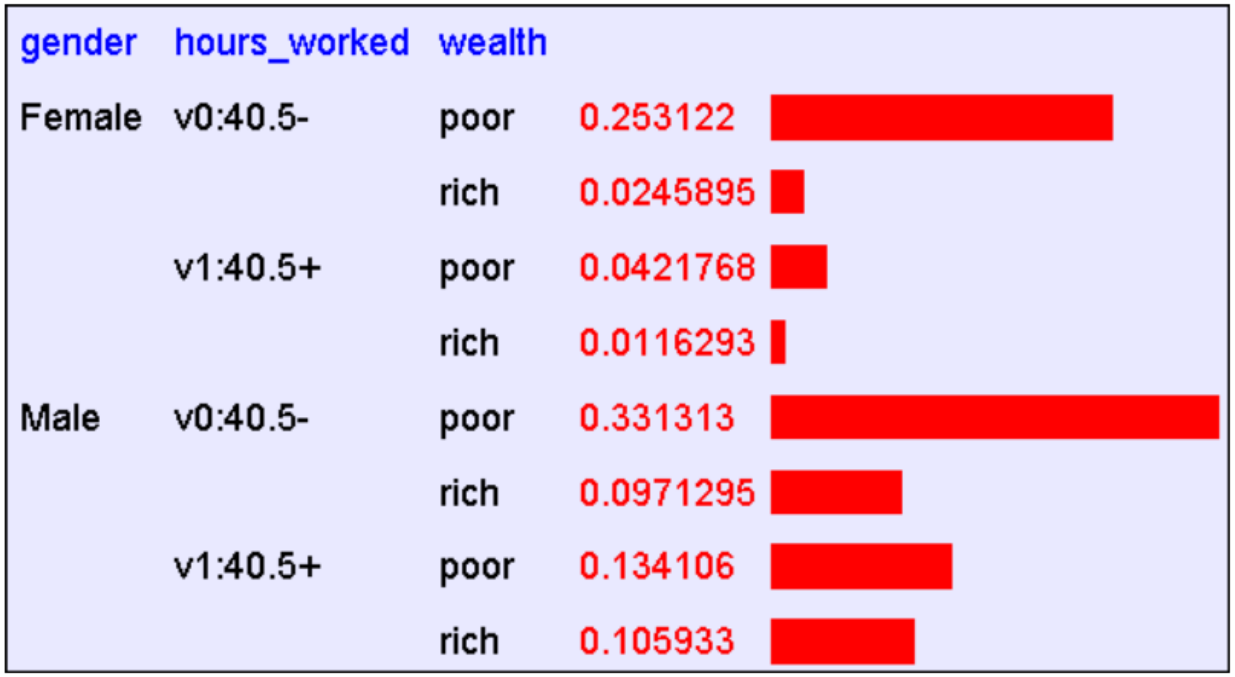
$$\hat{P}(\text{row}) = \frac{\text{records matching row}}{\text{total number of records}}$$

A	B	C	Prob
0	0	0	0.30
0	0	1	0.05
0	1	0	0.10
0	1	1	0.05
1	0	0	0.05
1	0	1	0.10
1	1	0	**0.25**
1	1	1	0.10

Fraction of all records in which A and B are true but C is false

Example – Learning Joint Probability Distribution

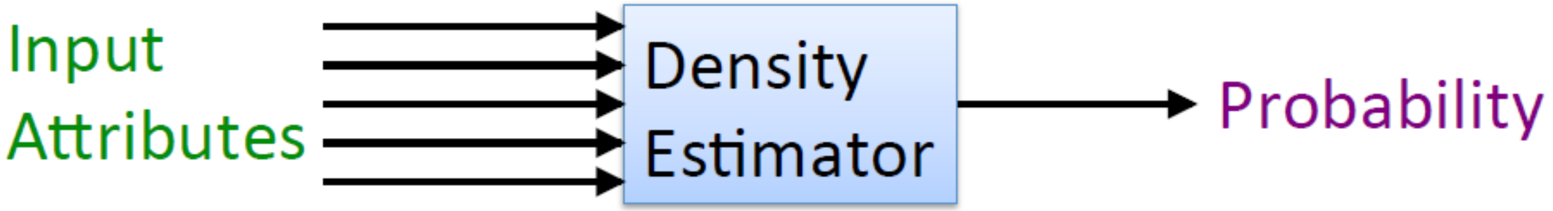
This Joint PD was obtained by learning from three attributes in the UCI "Adult" Census Database [Kohavi 1995]



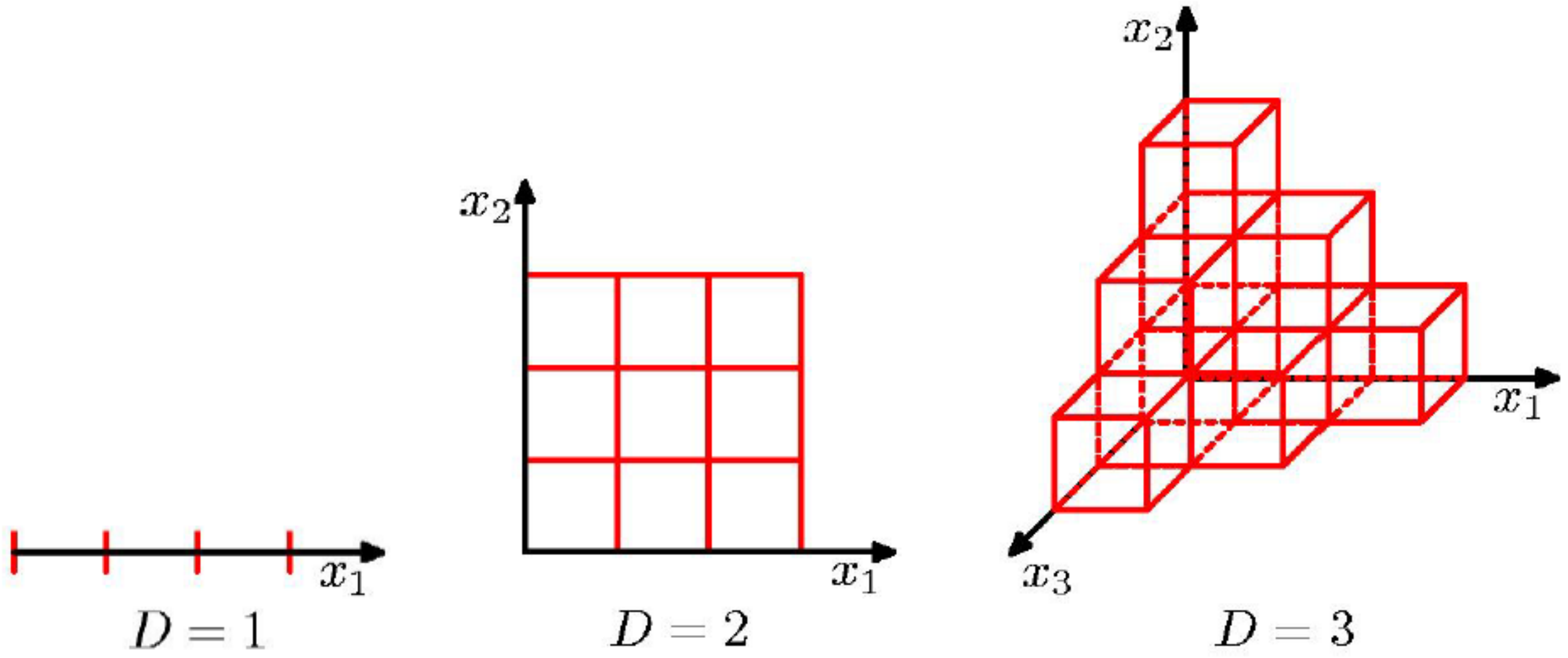
gender	hours_worked	wealth	
Female	v0:40.5-	poor	0.253122
		rich	0.0245895
	v1:40.5+	poor	0.0421768
		rich	0.0116293
Male	v0:40.5-	poor	0.331313
		rich	0.0971295
	v1:40.5+	poor	0.134106
		rich	0.105933

Density Estimation

- Our joint distribution learner is an example of something called **Density Estimation**
- A Density Estimator learns a mapping from a set of attributes to a probability



Curse of Dimensionality



Naïve Bayes Classifier

Idea: Use the training data to estimate

$P(X \mid Y)$ and $P(Y)$.

Then, use Bayes rule to infer $P(Y|X_{\text{new}})$ for new data

---

$$\mathrm{P}[Y=k|X=x] = \frac{\overbrace{\boxed{\mathrm{P}[Y=k]}}^{\text{Easy to estimate from data}}\overbrace{\boxed{\mathrm{P}[X_1=x_1 \wedge \cdots \wedge X_d=x_d|Y=k]}}^{\text{Impractical, but necessary}}}{\underbrace{\boxed{\mathrm{P}[X_1=x_1 \wedge \cdots \wedge X_d=x_d]}}_{\text{Unnecessary, as it turns out}}}$$

- Recall that estimating the joint probability distribution $P(X_1, X_2, \ldots, X_d \mid Y)$ is not practical

Naïve Bayes Classifier

Problem: estimating the joint density isn't practical

- Severely overfits, as we saw before

However, if we make the assumption that the attributes are independent given the class label, estimation is easy!

$$P(X_1, X_2, \ldots, X_d \mid Y) = \prod_{j=1}^{d} P(X_j \mid Y)$$

- In other words, we assume all attributes are *conditionally independent* given Y
- Often this assumption is violated in practice, but more on that later…

Acknowledgements

- Slides made using resources from:
  - Andrew Ng
  - Eric Eaton
  - David Sontag
- Thanks!