MATH 637: Mathematical Techniques in Data Science
Logistic regression & Linear Discriminant Analysis

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Announcements

- All classes will be on Zoom until the end of the semester.
- Our assessment plan remains the same.
- Please submit HW2 as soon as possible if you haven't done so already.
- We may have a (Zoom) guest lecture next week (to be confirmed).
- Please start thinking about what you would like to do for your project. More details soon.

Logistic regression

Suppose we work with binary outputs, i.e., $y_i \in \{0, 1\}$.

Linear regression may not be the best model.

- $x^T \beta \in \mathbb{R}$ not in $\{0, 1\}$.
- Linearity may not be appropriate. Does doubling the predictor doubles the probability of $Y = 1$? (e.g. probability of going to the beach vs outdoors temperature).

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Idea: We model $P(Y = 1|X = x)$.

- Now: $P(Y = 1|X = x) \in [0, 1]$ instead of $\{0, 1\}$.
- We want to relate that probability to $x^T\beta$.

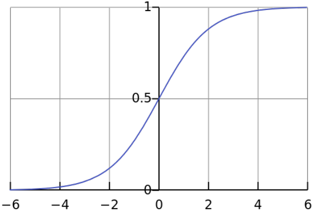
Logistic regression (cont.)

We assume,

$$P(Y = 1|X = x) = \frac{e^{x^T\beta}}{1 + e^{x^T\beta}}$$

$$P(Y = 0|X = x) = 1 - P(Y = 1|X = x) = \frac{1}{1 + e^{x^T\beta}}$$

The function $f(x) = e^x/(1 + e^x) = 1/(1 + e^{-x})$ is called the *logistic function* (or sigmoid function).



- Larger positive values of $x^T\beta \Rightarrow p \approx 1$.
- Larger negative values of $x^T\beta \Rightarrow p \approx 0$.

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- Hence, we are looking for a model for the "odds ratio":

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is called the *odds ratio*.
- Notice we are assuming $Y|X=x \sim \operatorname{Bernoulli}(p)$. Hence,

$$E(Y|X=x) = p.$$

Logistic regression (cont.)

In summary, we are assuming:

- $Y|X = x \sim \text{Bernoulli}(p)$.
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Logistic regression (cont.)

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More generally, one can use a *generalized linear model* (GLM). A GLM consists of:

- A probability distribution for $Y|X = x$ from the exponential family.
- A linear predictor $\eta = x^T\beta$.
- A *link function* g such that $g(E(Y|X = x)) = \eta$.

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If $Y_1, \ldots, Y_n \sim \text{Bernoulli}(p)$ are iid observations, then

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Here $p = p(x_i, \beta) = \frac{e^{x_i^T\beta}}{1+e^{x_i^T\beta}}$. Therefore,

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Taking the logarithm, we obtain

$$\begin{aligned} l(\beta) &= \sum_{i=1}^{n} y_i \log p(x_i, \beta) + (1-y_i) \log(1 - p(x_i, \beta)) \\ &= \sum_{i=1}^{n} y_i (x_i^T \beta - \log(1 + x_i^T \beta)) - (1 - y_i) \log(1 + e^{x_i^T \beta}) \end{aligned}$$

Logistic regression: estimating the parameters

Taking the derivative:

$$\frac{\partial}{\partial \beta_j} l(\beta) = \sum_{i=1}^{n} \left[y_i x_{ij} - x_{ij} \frac{e^{x_i^T \beta}}{1 + e^{x_i^T \beta}} \right].$$

Needs to be solved using numerical methods
(e.g. Newton-Raphson).

Logistic regression often performs well in applications.

As before, penalties can be added to regularize the problem or induce sparsity. For example,

$$\min_{\beta} -l(\beta) + \alpha \|\beta\|_1$$

$$\min_{\beta} -l(\beta) + \alpha \|\beta\|_2.$$

Logistic regression with more than 2 classes

- Suppose now the response can take any of $\{1, \ldots, K\}$ values.
- Can still use logistic regression.
- We use the categorical distribution instead of the Bernoulli distribution.
- $P(Y = i|X = x) = p_i$, $0 \leq p_i \leq 1$, $\sum_{i=1}^{K} p_i = 1$.
- Each category has its own set of coefficients:

$$P(Y = i|X = x) = \frac{e^{x^T \beta^{(i)}}}{\sum_{i=1}^{K} e^{x^T \beta^{(i)}}}.$$

- Estimation can be done using maximum likelihood as for the binary case.

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Recall: Bayes' theorem (Rev. Thomas Bayes, 1701–1761). Given two events A, B:

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

Source: Wikipedia (Public Domain).

Using Bayes' theorem

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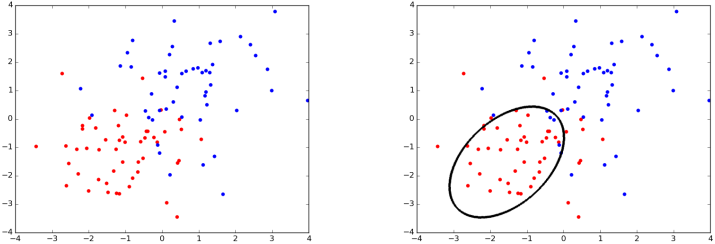

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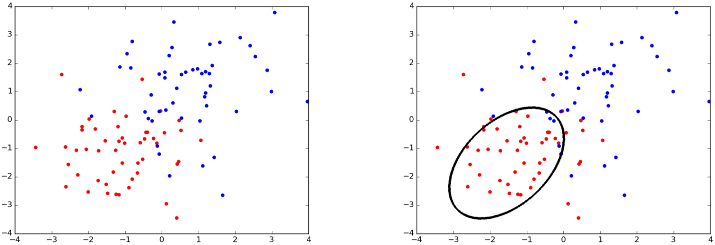

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Going back to our prediction using Bayes' theorem:

$$P(Y = i|X = x) = \frac{P(X = x|Y = i)P(Y = i)}{P(X = x)}$$

Using Bayes' theorem

More precisely, suppose

- $Y \in \{1, \ldots, k\}$.
- $P(Y = i) = \pi_i \qquad (i = 1, \ldots, k)$.
- $P(X = x | Y = i) \sim f_i(x) \qquad (i = 1, \ldots, k)$.

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- We can easily estimate π_i using the proportion of observations in category i.
- We need a model for $f_i(x)$.

Using a Gaussian model: LDA and QDA

A natural model for the f_js is the multivariate Gaussian distribution:

$$f_j(x) = \frac{1}{\sqrt{(2\pi)^p \det \Sigma_j}} e^{-\frac{1}{2}(x-\mu_j)^T \Sigma_j^{-1}(x-\mu_j)}.$$

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Note: When p is large, using QDA instead of LDA can dramatically increase the number of parameters to estimate.

In order to use LDA or QDA, we need:

- An estimate of the class probabilities π_j.
- An estimate of the mean vectors μ_j.
- An estimate of the covariance matrices Σ_j (or Σ for LDA).

Estimating the parameters

LDA: Suppose we have N observations, and N_j of these observations belong to the j category $(j = 1, \ldots, k)$. We use

- $\hat{\pi}_j = N_j/N$.
- $\hat{\mu}_j = \frac{1}{N_j} \sum_{y_i=j} x_i$ (average of x over each category).
- $\hat{\Sigma} = \frac{1}{N-k} \sum_{j=1}^{k} \sum_{y_i=j} (x_i - \hat{\mu}_j)(x_i - \hat{\mu}_j)^T$. (Pooled variance.)

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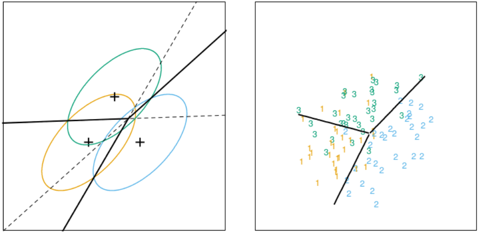

FIGURE 4.5. *The left panel shows three Gaussian distributions, with the same covariance and different means. Included are the contours of constant density enclosing 95% of the probability in each case. The Bayes decision boundaries between each pair of classes are shown (broken straight lines), and the Bayes decision boundaries separating all three classes are the thicker solid lines (a subset of the former). On the right we see a sample of 30 drawn from each Gaussian distribution, and the fitted LDA decision boundaries.*

ESL, Figure 4.5.

LDA: linearity of the decision boundary

In the previous figure, we saw that the decision boundary is linear. Indeed, examining the *log-odds*:

$$\begin{aligned}
&\log \frac{P(Y=l|X=x)}{P(Y=m|X=x)} = \log \frac{f_l(x)}{f_m(x)} + \log \frac{\pi_l}{\pi_m} \\
&= \log \frac{\pi_l}{\pi_m} - \frac{1}{2}(\mu_l + \mu_m)^T \Sigma^{-1}(\mu_l - \mu_m) + x^T \Sigma^{-1}(\mu_l - \mu_m) \\
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How is this different from LDA?

- In LDA, the parameters are more constrained and are not estimated the same way.
- Can lead to smaller variance if the Gaussian model is correct.
- In practice, logistic regression is considered *safer* and *more robust*.
- LDA and logistic regression often return similar results.

QDA: quadratic decision boundary

Let us now examing the log-odds for QDA: in that case no simplification occurs as before

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&= \log \frac{\pi_l}{\pi_m} + \frac{1}{2} \log \frac{\det \Sigma_m}{\det \Sigma_l} \\
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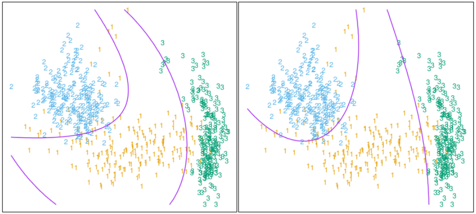

FIGURE 4.6. *Two methods for fitting quadratic boundaries. The left plot shows the quadratic decision boundaries for the data in Figure 4.1 (obtained using LDA in the five-dimensional space $X_1, X_2, X_1X_2, X_1^2, X_2^2$). The right plot shows the quadratic decision boundaries found by QDA. The differences are small, as is usually the case.*

ESL, Figure 4.6.

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Problems when $n < p$:

- Estimating covariance matrices when n is small compared to p is challenging.
- The *sample covariance* (MLE for Gaussian) $S = \frac{1}{n-1} \sum_{j=1}^{n} (x_i - \hat{\mu})(x_i - \hat{\mu})^T$ has rank at most $\min(n, p)$ so is singular when $n < p$.
- This is a problem since Σ needs to be inverted in LDA and QDA.

LDA and QDA

- Despite their simplicity, LDA and QDA often perform very well.
- Both techniques are widely used.

Problems when $n < p$:

- Estimating covariance matrices when n is small compared to p is challenging.
- The *sample covariance* (MLE for Gaussian) $S = \frac{1}{n-1} \sum_{j=1}^{n} (x_i - \hat{\mu})(x_i - \hat{\mu})^T$ has rank at most $\min(n, p)$ so is singular when $n < p$.
- This is a problem since Σ needs to be inverted in LDA and QDA.

Many strategies exist to obtain better estimates of Σ (or Σ_j). Among them:

- Regularization methods. E.g. $\hat{\Sigma}(\lambda) = \hat{\Sigma} + \lambda I$.
- Graphical modelling (discussed later during the course).

Python

LDA:

```
from sklearn.discriminant_analysis import
        LinearDiscriminantAnalysis
```

QDA:

```
from sklearn.discriminant_analysis import
      QuadraticDiscriminantAnalysis
```

–Lab–

Example

South African Heart Disease (ESL):

- Subset of the Coronary Risk-Factor Study (CORIS) baseline survey.
- Carried out in three rural areas of the Western Cape, South Africa (Rousseauw et al., 1983).
- Aim of the study was to establish the intensity of ischemic heart disease risk factors in that high-incidence region
- Data represent white males between 15 and 64, and the response variable is the presence or absence of myocardial infarction (MI) at the time of the survey.
- 160 cases in dataset, and a sample of 302 controls.

Dataset variables

sbp	systolic blood pressure
tobacco	cumulative tobacco (kg)
ldl	low density lipoprotein cholesterol
adiposity	
famhist	family history of heart disease (Present, Absent)
typea	type-A behavior
obesity	
alcohol	current alcohol consumption
age	age at onset
chd	response, coronary heart disease

Example (cont.)

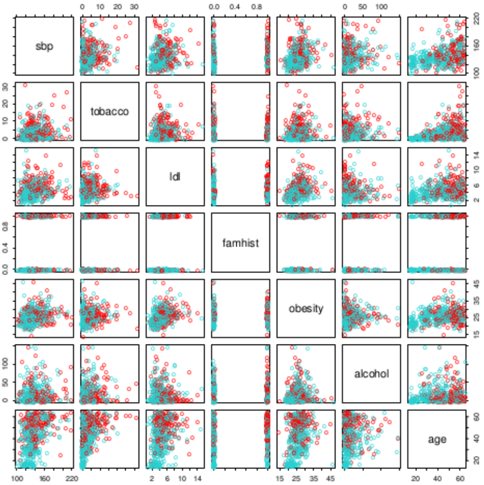

FIGURE 4.12. *A scatterplot matrix of the South African heart disease data. Each plot shows a pair of risk factors, and the cases and controls are color coded (red is a case). The variable* family history of heart disease (`famhist`) *is binary (yes or no).*

ESL

Example (cont.)

```
import pandas as pd
import numpy as np
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import train_test_split

data = pd.read_csv(’./SAheart.csv’)

y = np.array(data[’chd’])
X = np.array(data.drop(’chd’,axis=1))

# Separate data into train/test
N = 100  # Number of repetitions

log_model = LogisticRegression(fit_intercept=True)
score = np.zeros((N,1))
for i in range(N):
    X_train, X_test, y_train, y_test =
     train_test_split(X, y, test_size=0.25)
    log_model.fit(X_train,y_train)
    score[i] = log_model.score(X_test, y_test)

print(score.mean())
print(score.std())
```

We obtain about 72% accuracy with a standard deviation of $\approx 4\%$.

Example: handwritten digits

- Normalized handwritten digits, automatically scanned from envelopes by the U.S. Postal Service.
- Images here have been deslanted and size normalized, resulting in 16 x 16 grayscale images (Le Cun et al., 1990).
- Each line consists of the digit id (0-9) followed by the 256 grayscale values.
- There are 7291 training observations and 2007 test observations.
- The test set is notoriously "difficult", and a 2.5% error rate is excellent.
- These data were kindly made available by the neural network group at AT&T research labs (thanks to Yann Le Cunn).

Exercises

South African Heart Disease.

1. Test the code given on the previous slide to predict heart disease using logistic regression.
2. Repeat the same exercise using LDA and QDA instead of logistic regression.

Handwritten digits.

1. Use logistic regression to predict the handwritten digits. Compute the prediction error of your model on the given test set.
2. Repeat the same exercise using LDA and QDA.

For each dataset, briefly discuss which method works better.

Please submit your work on Canvas by Monday April 6, 11:59 PM. Only one file per team (please indicate the name of all team members).