MATH 567: Mathematical Techniques in Data Science
Logistic regression and Discriminant Analysis

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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).

Logistic regression: Different perspective. Instead of modelling the $\{0, 1\}$ output, we model the probability that $Y = 0, 1$.

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 $x^T\beta$.

We assume

$$\begin{aligned} \operatorname{logit}(P(Y = 1|X = x)) &= \log \frac{P(Y = 1|X = x)}{1 - P(Y = 1|X = x)} \\ &= \log \frac{P(Y = 1|X = x)}{P(Y = 0|X = x)} = x^T\beta. \end{aligned}$$

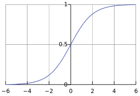
Logistic regression (cont.)

Equivalently,

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

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

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



$\log \frac{P(Y=1|X=x)}{P(Y=0|X=x)}$ is the *log-odds* ratio.

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

Logistic regression (cont.)

In summary, we are assuming:

- $Y|X = x \sim \text{Bernoulli}(p)$.
- $\operatorname{logit}(p) = \operatorname{logit}(E(Y|X = x)) = x^T\beta$.

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 $g(E(Y|X = x)) = \eta$.

Logistic regression: estimating the parameters

In logistic regression, we are assuming a model for Y. We typically estimate the parameter β using maximum likelihood.

Recall: If $Y \sim \mathrm{Bernoulli}(p)$, then

$$P(Y = y) = p^y (1-p)^{1-y}, \qquad y \in \{0, 1\}.$$

Thus, $L(p) = \prod_{i=1}^n p^{y_i}(1-p)^{1-y_i}$.

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

$$L(\beta) = \prod_{i=1}^n p(x_i, \beta)^{y_i}(1 - p(x_i, \beta))^{1-y_i}.$$

Taking the logarithm, we obtain

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

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,

$$\begin{aligned} &\min_\beta -l(\beta) + \alpha\|\beta\|_1 \\ &\min_\beta -l(\beta) + \alpha\|\beta\|_2. \end{aligned}$$

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.
- $P(Y = i|X = x) = p_i$, $0 \le p_i \le 1$, $\sum_{i=1}^K p_i = 1$.
- Each category has its own set of coefficients:

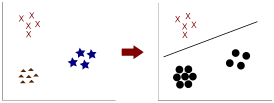
$$P(Y = i|X = x) = \frac{e^{x^T\beta^{(i)}}}{\sum_{i=1}^K e^{x^T\beta^{(i)}}}.$$

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

Multiple classes of data

Other popular approaches to classify data from multiple categories.

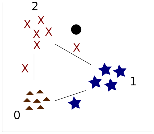
- **One versus all:**(or one versus the rest) Fit the model to separate each class against the remaining classes. Label a new point x according to the model for which $x^T\beta + \beta_0$ is the largest.



Need to fit the model K times.

Multiple classes of data (cont.)

- **One versus one:**
  1. Train a classifier for each possible **pair** of classes.
     Note: There are $\binom{K}{2} = K(K-1)/2$ such pairs.
  2. Classify a new points according to a **majority vote**: count the number of times the new point is assign to a given class, and pick the class with the largest number.



Need to fit the model $\binom{K}{2}$ times (computationally intensive).

Linear discriminant analysis (LDA)

- Categorical data Y. Predictors $X_1, \dots, X_p$.
- We saw how *logistic regression* can be used to predict Y by modelling the log-odds

$$\log \frac{P(Y=1|X=x)}{P(Y=0|X=x)} = x^T\beta.$$

- More now examine other models for $P(Y=i|X=x)$.

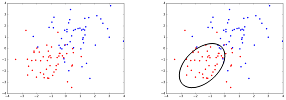
Recall: Bayes' theorem (Rev. Thomas Bayes, 1701–1761). Given two events A, B:

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

Source: Wikipedia (Public Domain).

Using Bayes' theorem

- $P(Y=i|X=x)$ harder to model.
- $P(X=x|Y=i)$ easier to model.



$P(X=x|Y=\mathrm{red})$.

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

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

Then

$$\begin{aligned} P(Y=i|X=x) &= \frac{P(X=x|Y=i)P(Y=i)}{P(X=x)} \\ &= \frac{P(X=x|Y=i)P(Y=i)}{\sum_{j=1}^k P(X=x|Y=j)P(Y=j)} \\ &= \frac{f_i(x)\pi_i}{\sum_{j=1}^k f_j(x)\pi_j}. \end{aligned}$$

- 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:

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

Linear discriminant analysis (LDA): We assume $\Sigma_j = \Sigma$ for all $j = 1, \dots, k$.

Quadratic discriminant analysis (QDA): general case, i.e., Σ_j can be distinct.

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 $(j = 1, \dots, k)$. 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.)

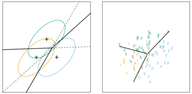


FIGURE 4.5. The left panel shows three Gaussian distributions, with the same covariance and different means. Included are the contours of constant density enclosing 95% of the probability in each case. The Bayes decision boundaries between each pair of classes are shown (broken straight lines), and the 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*:

$$\log \frac{P(Y=l|X=x)}{P(Y=m|X=x)} = \log \frac{f_l(x)}{f_m(x)} + \log \frac{\pi_l}{\pi_m}$$
$$= \log \frac{\pi_l}{\pi_m} - \frac{1}{2}(\mu_l + \mu_m)^T \Sigma^{-1}(\mu_l - \mu_m) + x^T \Sigma^{-1}(\mu_l - \mu_m)$$
$$= \beta_0 + x^T \beta.$$

Note that the previous expression is **linear** in x.
Recall that for logistic regression, we model

$$\log \frac{P(Y=l|X=x)}{P(Y=m|X=x)} = \beta_0 + x^T\beta.$$

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

$$\log \frac{P(Y=l|X=x)}{P(Y=m|X=x)}$$
$$= \log \frac{\pi_l}{\pi_m} + \frac{1}{2}\log \frac{\det \Sigma_m}{\det \Sigma_l}$$
$$- \frac{1}{2}(x-\mu_l)^T \Sigma_l^{-1}(x-\mu_l) - \frac{1}{2}(x-\mu_m)^T \Sigma_l^{-1}(x-\mu_m).$$

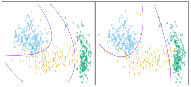


FIGURE 4.6. Two methods for fitting quadratic boundaries. The left plot shows the quadratic decision boundaries for the data in Figure 4.1 (obtained using LDA in the five-dimensional space $X_1, X_2, X_1X_2, X_1^2, X_2^2$). The right plot shows the quadratic decision boundaries found by QDA. The differences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

ESL, Figure 4.6.

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).