Topic 3: Logistic Regression

The *Logistic Regression (LR)* algorithm is a parametric method used for **binary** classification [Coelho and Richert, 2015, Chapter 5] of the data which are linearly separable.

Logistic regression is a huge topic which a lot of statistical inference theory which can be found in Hosmer et al. [2013] and Agresti [2002].

The generalisation of LR is multinomial LR, ElasticNet (unfortunately Python use LR instead of this correct term) as well as neural networks.

Credit scoring and behavioural scoring are techniques for financial institutes to decide on the granting of credit to applicants. One of the widely technique is the logistic regression model [Thomas, 2000]. Other applications are the classification of email spams, modelling marketing responses, etc.

3.1 Logistic Regression

The logistic regression [Cox, 1958] avoids the out-of-range problem in linear regression by modelling $\mathbb{P}(Y = 1|X)$ using the `https://en.wikipedia.org/wiki/Logistic_function` [Berkson, 1944]:

$$S\ :\ (-\infty,\infty) \to (0,1), \quad S(x) = \frac{e^x}{1+e^x} = \frac{1}{1+e^{-x}} \tag{3.1}$$

leading to a "multiple" or "multivariate" logistic regression:

$$\begin{aligned}\mathbb{P}(Y = 1|X_1 = x_1, \cdots, X_p = x_p) &= \frac{1}{1+\exp(-(\beta_0+\beta_1 X_1+\cdots+\beta_p X_p))} \\ &= S(\beta_0+\beta_1 X_1+\cdots+\beta_p X_p).\end{aligned} \tag{3.2}$$

It can be written in vector form:

$$\mathbb{P}(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = S(\beta^T \tilde{\boldsymbol{x}})$$

where $\boldsymbol{\beta} = (\beta_0, \cdots, \beta_p)$ and $\widetilde{\boldsymbol{x}}_j = (1, \boldsymbol{x}_j)$.

Given an input $\boldsymbol{x}$, the LR model provides a prediction as follows based on the conditional probability (assuming the cut-off is 0.5):

$$h(\boldsymbol{x}) = \begin{cases} 0, & \mathbb{P}(Y = 1|X = \boldsymbol{x}) < 0.5 \\ 1, & \mathbb{P}(Y = 1|X = \boldsymbol{x}) \geq 0.5 \end{cases}$$

or based the log-odds (or logit or 'link'?):

$$h(\boldsymbol{x}) = \begin{cases} 0, & \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p < 0 \\ 1, & \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p \geq 0 \end{cases}$$

3.1.1 Estimating the Regression Coefficients

The parameters/coefficients β_i in the model (3.2) are **unknown**, and have to be estimated based on the training data $(\boldsymbol{x}_i, y_i)$, $i = 1, \cdots, n$ using **maximum likelihood estimation** (MLE), i.e. we estimate the parameters β_i so that the **likelihood function** of $\beta_0, \cdots, \beta_p$ is maximised:

$$L(\beta_0, \cdots, \beta_p;\ y_1, \cdots, y_n | \boldsymbol{x}_1, \cdots, \boldsymbol{x}_n) = \prod_{i=1}^{n} \mathbb{P}(Y = y_i | \boldsymbol{X} = \boldsymbol{x}_i) \tag{3.3}$$

where Y is binary and follows a **Bernoulli distribution**, the feature data is p-dimensional $\boldsymbol{x}_i = (x_1^{(i)}, \cdots, x_p^{(i)})$.

According to `https://en.wikipedia.org/wiki/Bernoulli_distribution`, if $X \sim Bernoulli(p)$, then the probability mass function of observing $x \in \{0, 1\}$ is given by $\mathbb{P}(x) = p^x(1-p)^{1-x}$. For $Y \sim Bernoulli(\mathbb{P}(Y = 1|\boldsymbol{X}))$, we have

$$\mathbb{P}(Y = y_i | \boldsymbol{X} = \boldsymbol{x}_i) = \left(\frac{e^{\widetilde{\boldsymbol{x}}_i^T \boldsymbol{\beta}}}{1 + e^{\widetilde{\boldsymbol{x}}_i^T \boldsymbol{\beta}}}\right)^{y_i} \left(1 - \frac{e^{\widetilde{\boldsymbol{x}}_i^T \boldsymbol{\beta}}}{1 + e^{\widetilde{\boldsymbol{x}}_i^T \boldsymbol{\beta}}}\right)^{1-y_i} = e^{y_i \widetilde{\boldsymbol{x}}_i^T \boldsymbol{\beta}} \cdot (1 + e^{\widetilde{\boldsymbol{x}}_i^T \boldsymbol{\beta}})^{-y_i} \cdot (1 + e^{\widetilde{\boldsymbol{x}}_i^T \boldsymbol{\beta}})^{-(1-y_i)}$$

where $\boldsymbol{\beta} = (\beta_0, \cdots, \beta_p)$ and $\widetilde{\boldsymbol{x}}_i = (1, \boldsymbol{x}_i)$.

Substituting it into (3.3), we have

$$L := L(\beta_0, \cdots, \beta_p;\ y_1, \cdots, y_n | \boldsymbol{x}_1, \cdots, \boldsymbol{x}_n) = \prod_{i=1}^{n} (e^{y_i \widetilde{\boldsymbol{x}}_i^T \boldsymbol{\beta}})(1 + e^{\widetilde{\boldsymbol{x}}_i^T \boldsymbol{\beta}})^{-1}.$$

Taking natural log leads to

$$\ln L = \sum_{i=1}^{n} y_i \widetilde{\boldsymbol{x}}_i^T \boldsymbol{\beta} - \sum_{i=1}^{n} \ln(1 + e^{\widetilde{\boldsymbol{x}}_i^T \boldsymbol{\beta}}). \tag{3.4}$$

If there is a maximum $\hat{\boldsymbol{\beta}}$ such that $\ln L$ is maximum, then Calculus theory tells us that:

$$\begin{aligned} &\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\operatorname{argmax}}\, L = \underset{\boldsymbol{\beta}}{\operatorname{argmax}} \ln L \\ \Rightarrow\ &\frac{\partial}{\partial \boldsymbol{\beta}}(\ln L)\bigg|_{\boldsymbol{\beta} = \hat{\boldsymbol{\beta}}} = \frac{\partial}{\partial \boldsymbol{\beta}} \left(\sum_{i=1}^{n} y_i \widetilde{\boldsymbol{x}}_i^T \boldsymbol{\beta} - \sum_{i=1}^{n} \ln(1 + e^{\widetilde{\boldsymbol{x}}_i^T \boldsymbol{\beta}}) \right)\bigg|_{\boldsymbol{\beta} = \hat{\boldsymbol{\beta}}} = \mathbf{0}. \end{aligned}$$

leading to

$$\sum_{i=1}^{n} y_i x_k^{(i)} - \sum_{i=1}^{n} \frac{x_k^{(i)} e^{\widetilde{\boldsymbol{x}}_i^T \boldsymbol{\beta}}}{1 + e^{\widetilde{\boldsymbol{x}}_i^T \boldsymbol{\beta}}} = 0, \quad k = 0, 1, \cdots, p$$

where $x_0^{(i)}$ is defined to be 1.

This is a system of nonlinear equations which can be solved using numerically such as applying `https://en.wikipedia.org/wiki/Newton's_method` to estimate $\hat{\beta}_i$.

A special case ($p = 1$) of the above mathematical derivation was asked in the past final exam.

Example 3.1.1 (Final Exam May 2019, Q5(a))**.** The parameters β in logistic regression can be estimated through maximum likelihood estimation. The estimation can be done by solving the equations from maximized log-likelihood functions, i.e. $\frac{\partial l(\beta)}{\partial \beta_i} = 0$, through numerical methods. For logistic regression with one predictor, show that the differentiated log-likelihood functions for β_0 and β_1 respectively are

$$\begin{aligned} \frac{\partial l(\beta)}{\partial \beta_0} &= \sum_{i=1;y_i=1}^{n} 1 - \sum_{i=1}^{n} \frac{e^{\beta_0+\beta_1 x_i}}{1+e^{\beta_0+\beta_1 x_i}} \\ \frac{\partial l(\beta)}{\partial \beta_1} &= \sum_{i=1;y_i=1}^{n} x_i - \sum_{i=1}^{n} \frac{x_i e^{\beta_0+\beta_1 x_i}}{1+e^{\beta_0+\beta_1 x_i}}. \end{aligned}$$

Your proof shall start from stating probability of Class 1, $\mathbb{P}(y_i = 1)$ and probability of Class 0, $\mathbb{P}(y_i = 0)$. (10 marks)

Solution: The probabilities for $\mathbb{P}(Y = 1)$ and $\mathbb{P}(Y = 0)$ are modelled by

$$\begin{aligned} \mathbb{P}(Y = 1) &= \frac{e^{\beta_0+\beta_1 x_i}}{1+e^{\beta_0+\beta_1 x_i}} \\ \mathbb{P}(Y = 0) &= 1 - \frac{e^{\beta_0+\beta_1 x_i}}{1+e^{\beta_0+\beta_1 x_i}} = \frac{1}{1+e^{\beta_0+\beta_1 x_i}} \end{aligned}$$

Likelihood function, $\mathbb{L}(\beta|\boldsymbol{Y})$

$$\mathbb{L}(\beta|\boldsymbol{Y}) = \prod_{i=1;y_i=1}^{n} \mathbb{P}(y_i = 1) \prod_{i=1;y_i=0}^{n} \mathbb{P}(y_i = 0) = \prod_{i=1;y_i=1}^{n} e^{\beta_0+\beta_1 x_i} \prod_{i=1;y_i=0}^{n} \frac{1}{1+e^{\beta_0+\beta_1 x_i}}$$

Log-likelihood function, $l(\beta)$,

$$l\beta) = \ln \mathbb{L}(\beta|\boldsymbol{Y}) = \sum_{i=1;y_i=1}^{n} (\beta_0 + \beta_1 x_i) - \sum_{i}^{n} \ln(1+e^{\beta_0+\beta_1 x_i})$$

Differentiate $l(\beta)$ with respect to β_0 and β_1 leads to

$$\begin{aligned} \frac{\partial l(\beta)}{\partial \beta_0} &= \sum_{i=1;y_i=1}^{n} 1 - \sum_{i=1}^{n} \frac{e^{\beta_0+\beta_1 x_i}}{1+e^{\beta_0+\beta_1 x_i}} \\ \frac{\partial l(\beta)}{\partial \beta_1} &= \sum_{i=1;y_i=1}^{n} x_i - \sum_{i=1}^{n} \frac{x_i e^{\beta_0+\beta_1 x_i}}{1+e^{\beta_0+\beta_1 x_i}}. \end{aligned}$$

3.1.2 Hypothesis Testing and Inference

For most predictive models, it is impossible to develop the hypothesis testing theory for them. However, statisticians have developed the hypothesis testing theory for LR to regarding the confidence of the model and the parameters β_i.

The *Z-statistic* tests the null hypothesis against the alternative hypothesis:

$$H_0 : \beta_i = 0 \quad \text{vs} \quad H_1 : \beta_i \neq 0.$$

`https://en.wikipedia.org/wiki/Wald_test`: With large "n",

$$\frac{\hat{\beta}_i - 0}{SE(\hat{\beta})} \sim Normal(0, 1),$$

The *standard error* $SE(\hat{\beta})$ is the inverse of the estimated information matrix with a shape $(p+1) \times (p+1)$:

$$SE(\hat{\beta}) = \left[\frac{\partial^2}{\partial \boldsymbol{\beta}^2} \left(\sum_{i=1}^{n} y_i \widetilde{\boldsymbol{x}}_i^T \boldsymbol{\beta} - \sum_{i=1}^{n} \ln(1 + e^{\widetilde{\boldsymbol{x}}_i^T \boldsymbol{\beta}}) \right) \right]^{-1}$$

- **Z-statistic large $\Rightarrow$ *p-value* small.**

  $\Rightarrow$ null hypothesis should be rejected (when p-value is less than some significance level, 5%, for example).

  $\Rightarrow$ X is associated with Y

  $\Rightarrow$ X is a significant factor.

- **Z-statistic small $\Rightarrow$ *p-value* large.**

  $\Rightarrow$ null hypothesis should not be rejected (when (when p-value > 0.05).

  $\Rightarrow$ X and Y is most likely not related.

  $\Rightarrow$ X is an unimportant factor to Y.

- The interception $\hat{\beta}_0$ is typically not of interest and only for fitting data.

A $(1 - \frac{\alpha}{2}) \times 100\%$ confidence interval for β_i, $i = 1, \cdots, p$, can be calculated using the Z-statistic:

$$\hat{\beta}_i \pm Z_{1-\alpha/2} SE(\hat{\beta}_i).$$

A 95% confidence interval is defined as a range of values such that with 95% probability, the range will contain the true unknown value of the parameter. In this case, $\alpha = 0.05$ so $Z_{1-\alpha/2} =$ `qnorm(1-0.05/2)` $= 1.959964 \approx 1.96$, therefore, the 95% confidence interval for β_i takes the form

$$[\hat{\beta}_i - 1.96 \cdot SE(\hat{\beta}_i),\ \hat{\beta}_i + 1.96 \cdot SE(\hat{\beta}_i)]. \tag{3.5}$$

The implementation of the above statistical estimates are encoded in R as the algorithm for generalised linear model (GLM).

Logistic Regression in R's GLM

```
glm(formula, family = gaussian, data, weights, subset,
    na.action, start = NULL, etastart, mustart, offset,
    control = list(...), model = TRUE, method = "glm.fit",
    x = FALSE, y = TRUE, contrasts = NULL, ...)

# iteratively reweighted least squares
glm.fit(x, y, weights = rep(1, nobs),
        start = NULL, etastart = NULL, mustart = NULL,
        offset = rep(0, nobs), family = gaussian(),
        control = list(), intercept = TRUE)
```

To set GLM to LR mode, we need to set `family=binomial`. The `start` can be used if we know the range of the parameters β_i.

Deviance is a measure of the badness of fit for GLM — higher numbers indicate worse fit. R reports two forms of deviance — the *null deviance*

$$= 2(LL(Saturated\_Model) - LL(Null\_Model)) \text{ on df} = df\_Sat - df\_Null$$

and the *residual deviance*

$$= 2(LL(Saturated\_Model) - LL(Proposed\_Model)) \text{ on df} = df\_Sat - df\_Proposed$$

where LL is the log-likelihood in (3.4).

- The Saturated Model is a model that assumes each data point has its own parameters (which means we have n parameters to estimate.)
- The Null Model assumes one parameter for all of the data points, which means we only estimate 1 parameter.
- The Proposed Model assumes we can explain our data points with p parameters + an intercept term, so we have $p+1$ parameters.

The null deviance shows how well the response variable is predicted by a model that includes only the intercept β_0 while the residual deviance shows how well the response variable is predicted by our estimated LR model.

The ***Akaike Information Criterion (AIC)*** provides a method for assessing the quality of our model through comparison of related models. It is based on the deviance and intent to prevent us from including irrelevant predictors. The AIC number itself is not meaningful. If we have more than one similar candidate models (where all of the variables of the simpler model occur in the more complex models), then *we should select the model that has the smallest AIC.*

Example 3.1.2 (LR on Default Data with a Numeric Input)**.** Consider the **Default** data set from R's ISLR package, where the response variable Default falls into one of two categories, Yes or No. Consider just using the predictor `balance` to estimate the probability of default using *logistic regression.* The R script to train the logistic regression model will give the estimates of the parameters and the hypothesis testing of the model.

Solution:

```
library(ISLR)
data(Default)
Prob.Default = as.numeric(Default$default=="Yes")
#pdf("t4-cly-011.pdf")
plot(Default$balance,Prob.Default,xlab="Balance",pch='+',
  xlim=c(0,2750),ylim=c(-0.2,1.2))
model = glm(default ~ balance, data=Default, family=binomial)
print(summary(model)) #print(coef(model))
newdata = data.frame(balance=seq(-1,2750,1))
newdata$Prob.of.Default = predict(model,newdata,type="response")
lines(Prob.of.Default ~ balance, newdata, col="green4", lwd=3)
```

Here's the statistical analysis (involving the Wald test Z-statistic) produced by R:

```
Call:
glm(formula = default ~ balance, family = binomial, data = Default)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-2.2697  -0.1465  -0.0589  -0.0221   3.7589

Coefficients:
              Estimate Std. Error z value Pr(>|z|)
(Intercept) -1.065e+01  3.612e-01  -29.49   <2e-16 ***
balance      5.499e-03  2.204e-04   24.95   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 2920.6  on 9999  degrees of freedom
Residual deviance: 1596.5  on 9998  degrees of freedom
AIC: 1600.5
```

Example 3.1.3 (LR Predictive Model with a Numeric Feature)**.** Consider the **Default** data set with the statistical analysis given in Example 3.1.2, write down the mathematical formulation of the predictive model.

Example 3.1.4. Consider the logistic model for the **Default** data set in Example 3.1.3, predict the default probability for an individual with a balance of (a) \$1000, (b) \$2000.

Example 3.1.5. Consider the **Default** data set with the results given, compute the 95% confidence interval for β_0 and β_1.

Solution: Based on (3.5), there is an approximately 95% chance that the interval

$$[-10.6513 - 1.96 \cdot 0.3612,\ -10.6513 + 1.96 \cdot 0.3612] = [-11.3593, -9.9433]$$

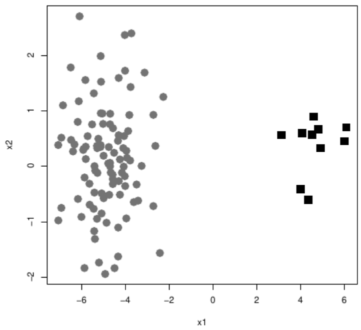
will contain the true value of β_0; and there is an approximately 95% chance that the interval

$$[0.0055 - 1.96 \cdot 0.0002, 0.0055 + 1.96 \cdot 0.0002] = [0.0051, 0.0059]$$

will contain the true value of β_1.

Example 3.1.6 (Completely Separable 2D Data)**.** Consider a simulated data below:

```
set.seed(2023)
cls1_x1 = rnorm(10, mean=5)
cls1_x2 = rnorm(10, mean=0)
cls1_y  = rep(0, length(cls1_x1))

cls2_x1 = rnorm(100, mean=-5)
cls2_x2 = rnorm(100, mean=0)
cls2_y  = rep(1, length(cls2_x1))

d.f = data.frame(x1=c(cls1_x1, cls2_x1),
                 x2=c(cls1_x2, cls2_x2),
                  y=c(cls1_y, cls2_y))
```



Fitting the data with logistic regression model leads to the following summary:

```
Warning messages:
1: glm.fit: algorithm did not converge
2: glm.fit: fitted probabilities numerically 0 or 1 occurred
```

```
Call:
glm(formula = y ~ ., family = binomial, data = d.f)

Deviance Residuals:
       Min          1Q      Median          3Q         Max
-2.231e-05   2.110e-08   2.110e-08   2.110e-08   2.774e-05

Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept)     3.085  23013.497   0.000    1.000
x1             -8.100   8369.842  -0.001    0.999
x2              0.199  19039.246   0.000    1.000

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 6.7020e+01  on 109  degrees of freedom
Residual deviance: 1.7484e-09  on 107  degrees of freedom
AIC: 6
```

- The p-value indicates that the features does not explain the output — This is due to the (3.4) being unbounded when the data is separable by a hyperplane.
- The small residual deviance indicates that the model fits OK. □

Example 3.1.7 (May 2022 Semester Final Exam, Q5(a))**.** The data from a study of low birth weight infants in a neonatal intensive care unit is used to examine the development of bronchopulmonary dysplasia (BPD), a chronic lung disease, in a sample of 223 infants weighing less than 1750 grams. The response variable is binary, denoting whether an infant develops BPD by day 28 of life (where BPD is defined by both oxygen requirement and compatible chest radiograph). Consider the trained logistic regression model is summarised below.

```
Call:
glm(formula = bpd ~ ., family = binomial, data=d.f.train)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-2.0171  -0.6617  -0.3138   0.6840   2.2970

Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept) 12.983392   3.797733   3.419 0.000629 ***
brthwght    -0.003521   0.001091  -3.227 0.001249 **
gestage     -0.314217   0.146186  -2.149 0.031601 *
toxemia     -2.268523   0.909026  -2.496 0.012576 *
---
Signif.:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 172.77  on 132  degrees of freedom
Residual deviance: 112.47  on 129  degrees of freedom
AIC: 120.47

Number of Fisher Scoring iterations: 5
```

In the logistic regression model, the output `bpd` is either 0 (representing no) or 1 (representing yes). The predictors are listed below:

- `brthwght`: birth weight in number of grams;
- `gestage`: gestational age in number of weeks;
- `toxemia`: a condition in pregnancy characterised by abrupt hypertension, albuminuria and edema. This is a binary variable with 0 = no, 1 = yes.

(i) Write down the mathematical expression of the logistic regression model for the given data with the coefficient values. (4 marks)

Solution: Let Y denote the `bpd`, X_1 denote `brthwght`, X_2 denote `gestage` and X_3 denote `toxemia`. The logistic model is

$$P(Y = 1|X_1 = x_3, X_2 = x_2, X_3 = x_3) = \frac{1}{1 + \exp(-\beta^T \boldsymbol{x})} \qquad \text{[2 marks]}$$

where

$$\beta^T \boldsymbol{x} = 12.983392 - 0.003521x_1 - 0.314217x_2 - 2.268523x_3 \qquad \text{[2 marks]}$$

(ii) For an infant with a birth weight of 1020 grams, with a gestational age is 29 weeks and the pregnancy does not have toxemia, by calculating the **conditional probability** of the logistic regression model, determine if the infant has a BPD problem. (7 marks)

(iii) According to the three-predictor model, `brthwght` has the lowest p-value. If only the predictor `brthwght` is used to fit the logistic regression model, the following analysis is obtained.

```
Call:
glm(formula = bpd ~ brthwght, family = binomial,
      data = d.f.train)

Deviance Residuals:
    Min        1Q    Median        3Q       Max
-1.7404   -0.7517   -0.4019    0.8288    2.5192

Coefficients:
              Estimate Std. Error z value Pr(>|z|)
(Intercept)  4.6805219  0.9477546   4.939 7.87e-07 ***
brthwght    -0.0046773  0.0008549  -5.471 4.47e-08 ***
---
Signif.:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)
```

```
    Null deviance: 172.77  on 132  degrees of freedom
Residual deviance: 128.67  on 131  degrees of freedom
AIC: 132.67

Number of Fisher Scoring iterations: 5
```

Investigate the infant with a birth weight of 1020 grams from part (ii) again by calculating the conditional probability to determine if the infant has a BPD problem. (4 marks)

(iv) Comment on the results from part (ii) and part (iii) and use CRISP-DM framework to explain which model we should choose. Provide proper justification. (2 marks)

Solution: The conditional probabilities are different but around 0.5, so the two models provide different prediction. According CRISP-DM framework, the crucial decision on selecting a predictive model is based on validation. A good model should pass the cross-validation test. .... [2 marks]

3.1.3 Qualitative Predictors

When a predictor (or factor) is **qualitative**, we need to introduce **dummy variable(s)**. When the predictor has C levels, $C-1$ dummy variables will be created — this is called **(nearly) one-hot encoding**. Note that some books refer to the encoding of all levels as one-hot encoding. Here, we will remove the reference level because it is not essential in the computation.

For example, "gender" has two levels 0 (male) and 1 (female), a dummy variable `gender1` is created with 0 as reference:

$$\text{gender1} = \begin{cases} 1, & \text{if gender} = 1 \\ 0, & \text{if gender} = 0 \end{cases}$$

For example, "blood type" has four levels A, AB, B, O and 3 dummy variables will be created with A as reference (R usually uses alphabetical ordering):

$$\text{bloodtypeAB} = \begin{cases} 1, & \text{if bloodtype} = \text{AB} \\ 0, & \text{if bloodtype} \neq \text{AB} \end{cases}, \quad \text{bloodtypeB} = \begin{cases} 1, & \text{if bloodtype} = \text{B} \\ 0, & \text{if bloodtype} \neq \text{B} \end{cases},$$

$$\text{bloodtypeO} = \begin{cases} 1, & \text{if bloodtype} = \text{O} \\ 0, & \text{if bloodtype} \neq \text{O} \end{cases}$$

Example 3.1.8 (One-Hot Encoding in R)**.** Consider the data X:

gender	bloodtype
0	A
1	B
1	AB
0	B
0	O

It can be encoded in R and the one-hot encoding can be computed using the `model.matrix` command.

```
d.f = data.frame(gender=c("0", "1", "1", "0", "0"),
                 bloodtype=c("A", "B", "AB", "B", "O"))
model.matrix(~ gender + bloodtype, d.f)
```

The one-hot encoded matrix of the data X is

```
  (Intercept) gender1 bloodtypeAB bloodtypeB bloodtypeO
1           1       0           0          0          0
2           1       1           0          1          0
3           1       1           1          0          0
4           1       0           0          1          0
5           1       0           0          0          1
```

When a qualitative predictor X_j has C levels, logistic regression can be generalised to work with X_j by working with the $(C-1)$ **dummy variables** X_j.level2, $\cdots$, X_j.level$C$

$$\mathbb{P}(Y=1|\boldsymbol{X}=\boldsymbol{x}) = \frac{1}{1+\exp(-(\beta_0+\cdots+\beta_j^{(2)}x_j.\text{level2}+\cdots+\beta_j^{(C)}x_j.\text{level}C+\cdots))}$$

where

$$x_j.\text{level}\ell = \begin{cases} 1, & x_j = \text{level } \ell, \\ 0, & \text{otherwise}, \end{cases} \qquad \ell = 2, \cdots, C.$$

The reason for LR to work with categorical feature is due to the notion of **odds**:

$$\frac{\mathbb{P}(Y=1|\boldsymbol{X}=\boldsymbol{x})}{\mathbb{P}(Y=0|\boldsymbol{X}=\boldsymbol{x})} = \frac{\mathbb{P}(Y=1|\boldsymbol{X}=\boldsymbol{x})}{1-\mathbb{P}(Y=1|\boldsymbol{X}=\boldsymbol{x})} = \exp(\tilde{\boldsymbol{x}}^T\boldsymbol{\beta}). \tag{3.6}$$

It quantifies the relative probability of odds as compared to $\mathbb{P}(Y=0|X=\boldsymbol{x})$ as follows:

Value of odds	Relative Probability of $\mathbb{P}(Y=1|X)$
≥ 1	Higher
< 1	Lower

By taking the logarithm of both sides of (3.6), we obtain the **log-odds** or **logit**, which is linear with respect to the input features:

$$\ln\frac{\mathbb{P}(Y=1|\boldsymbol{X}=\boldsymbol{x})}{1-\mathbb{P}(Y=1|\boldsymbol{X}=\boldsymbol{x})} = \beta_0+\beta_1X_1+\cdots+\beta_pX_p. \tag{3.7}$$

In this case, Y can be inferred linearly from inputs $\boldsymbol{X}$. This means that a unit increase in x_j changes the logit by β_j.

β_i	OR	Relative probability of $\mathbb{P}(Y=1|x_j=x)$	Probability to be classified into $Y=1$
>0	≥ 1	Higher	$X_j=b$ has higher chance than $X_j=a$
<0	<1	Lower	$X_j=a$ has higher chance than $X_j=b$

where the **odds ratio** is the ratio of odds given two inputs:

$$\text{OR} = \frac{\frac{\mathbb{P}(Y=1|X_j=b)}{\mathbb{P}(Y=0|X_j=b)}}{\frac{\mathbb{P}(Y=1|X_j=a)}{\mathbb{P}(Y=0|X_j=a)}} = \frac{\exp(\cdots+\beta_j\cdot b+\cdots)}{\exp(\cdots+\beta_j\cdot a+\cdots)} = \exp(\beta_j(b-a)).$$

Note that $b=1$ and $a=0$ for categorical data.

Example 3.1.9 (LR on Default Data with a Categorical Input)**.** Suppose that the **Default** data set is now depending on another qualitative predictor, `student`. The R script to fit the logistic model is listed below.

```
library(ISLR)
data(Default)
glm.model = glm(default ~ student, data=Default, family=binomial)
print(summary(glm.model))
```

and the output is shown below.

```
Call:
glm(formula = default ~ student, family = binomial, data = Default)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-0.2970  -0.2970  -0.2434  -0.2434   2.6585

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -3.50413    0.07071  -49.55  < 2e-16 ***
studentYes   0.40489    0.11502    3.52 0.000431 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 2920.6  on 9999  degrees of freedom
Residual deviance: 2908.7  on 9998  degrees of freedom
AIC: 2912.7

Number of Fisher Scoring iterations: 6
```

(a) Compare the probability of default for a student with a non-student. Explain.

(b) Predict the probability of default for (i) student (ii) non-student.

Example 3.1.10 (LR on Default Data with a Mix of Numeric and Categorical Inputs)**.** Suppose that the **Default** dataset is now depending on three predictors, `balance`, `income` and `student`. The result from logistic regression is shown below.

```
Call:
glm(formula = default ~ balance + income + student, family = binomial,
    data = Default)
```

```
Deviance Residuals:
    Min       1Q   Median       3Q      Max
-2.4691  -0.1418  -0.0557  -0.0203   3.7383

Coefficients:
              Estimate Std. Error z value Pr(>|z|)
(Intercept) -1.087e+01  4.923e-01 -22.080  < 2e-16 ***
balance      5.737e-03  2.319e-04  24.738  < 2e-16 ***
income       3.033e-06  8.203e-06   0.370  0.71152
studentYes  -6.468e-01  2.363e-01  -2.738  0.00619 **
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 2920.6  on 9999  degrees of freedom
Residual deviance: 1571.5  on 9996  degrees of freedom
AIC: 1579.5

Number of Fisher Scoring iterations: 8
```

Discuss the results involving the significance of each variable based on the coefficients and then the odds.

Solution: Based on the p-value (with 5% significance level), we find that `balance` and `student` are **probably significant** while `income` is **probability insignificant**. A reduced model could be fitted and then compare with the full model to see if a reduced model is better.

The odds of the default

- increases with the balance because $\beta_1 = 5.737 \times 10^{-3} > 0$;
- increases with the income because $\beta_2 = 3.033 \times 10^{-6} > 0$. However, the p-value > 0.05 does not rule out $\beta_2 = 0$ based on the hypothesis testing;
- is lower for students compare to non-students.

Example 3.1.11 (Final Exam Jan 2019, Q4(b)). You are a data analytics consultant to a property investing firm. You task is to help the investment firm make money through property price arbitrage — identify properties that are selling at a lower premium. There is a property listing site that aggregates ready-to-buy properties and quoted prices across the country. You have accumulated data for the properties sold this month along with the features of these properties. Descriptions of the data are shown below:

Dist_train	Distance to nearest train station from the property
Dist_market	Distance to nearest grocery market from the property
Dist_school	Distance to nearest school from the property
Carpet	Carpet area of the property in square feet
Builtup	Built-up area of the property in square feet
Parking	Type of car parking available with the property (Covered; No; Open)
City	Categorization of the city based on population size (A; B; C)
Rainfall	Annual rainfall in the area where property is located
House_price	Is a property sold underpriced? (yes=1; no=0)

A logistic regression model is fitted and results are shown in Table Q4(b).

	Coefficient	Std. error	Z-statistic	p-value
Intercept	0.0054	4.40E+03	12.254	$<$ 2e-16
Dist_train	51.7124	3.1921	1.624	0.1048
Dist_market	16.3212	2.5077	0.651	0.5153
Dist_school	32.7063	3.5612	0.919	0.3586
Carpet	0.5900	4.19E+02	-1.409	0.1592
Builtup	0.5660	3.49E+02	1.621	0.1055
Parking_No	-0.0660	1.65E+03	-4.008	6.87E-05
Parking_Open	0.5165	1.48E+03	-3.816	0.0002
City_B	-0.0408	1.33E+03	-3.068	0.0022
City_C	-0.0176	1.15E+03	-15.271	$<$ 2e-16
Rainfall	0.0279	1.29E+03	-21.681	$<$ 2e-16

Table Q4(b)

With 5% significance,

(i) Comment on the significance of each variable. (2 marks)

(ii) In real-world problem, we will refit the data to a reduced model. However, in this exam environment, you may just pick the coefficients from the full model and then write down the reduced/selected-feature logistic model based on the full model. (2 marks)

Solution: Never-ever write the feature-selected model this way in the real-world calculation and my exam. This answer is used by the previous lecturer because R is not allowed in final exam: The "reduced" logistic regression model based on the p-values are approximately:

$$\mathbb{P}(\text{House\_Price} = 1|\boldsymbol{X}) = \frac{1}{1 + \exp(-(0.0054 + \boldsymbol{w}^T\boldsymbol{X})}$$

where
$$\begin{aligned}\boldsymbol{w}^T\boldsymbol{X} &= -0.0660(\text{Parking\_No}) + 0.5165(\text{Parking\_Open}) \\ &\quad - 0.0408(\text{City\_B}) - 0.0176(\text{City\_C}) + 0.0279(\text{Rainfall}).\end{aligned}$$

(iii) Calculate the odds and compare the probability of underprice for houses with different types of parking based on the reduced model. (5 marks)

Solution: First, note that $Y = 1$ refers to the property sold is underpriced.

There are two **dummy variables** related to the input parking — Parking_No, Parking_Open. They are using Covered as comparison.

Odds ratio	Odds vs Odds	Prob vs Prob
$\frac{odds(Parking=No)}{odds(Parking=Covered)} = e^{-0.0660} = 0.9361 < 1$	Odds of $Y = 1$ is higher for Parking=Covered	Probability of underprice for the house with covered parking will be higher than no parking.
$\frac{odds(Parking=Open)}{odds(Parking=Covered)} = e^{0.5165} = 1.6762 > 1$	Odds of $Y = 1$ is higher for Parking=Open	Probability of underprice for the house with open parking will be higher than covered parking.

Combining the results from the table, the ordering of probability of underprice based on parking is

$$Open > Covered > No$$

(iv) Calculate the odds and compare the probability of underprice for houses with different types of city. (5 marks)

(v) State a possible issue that might be found in the data. Suggest a more suitable solution to solve the stated problem. (2 marks)

Solution: Problem: High correlation between builtup area and carpet area.

Solution: Use PCA instead of original variables.

(vi) State the purposes of principal components. Discuss how principal component achieve the stated purposes. (4 marks)

Solution: Reduce dimension. Consider only the first few principal components which contributes most of the variation.

Avoid correlation. Each principle component is designed to be perpendicular. Hence, there will be no correlation.

Example 3.1.12 (Final Exam May 2019, Q2)**.** (a) The human resource department would like to determine potential employees for promotion. You have collected some data from previous employee promoting records as described below:

exp	Number of years of experience working in the company
sal_mth	Average monthly salary in last 12 months
sal_yr	Yearly salary in last 12 months
pjt	Is there any project involved? [Yes; No]
dpmt	Department [A; B; C; D]
emp_id	Employee ID
promote	Is the employee getting promoted? [Yes=1; No=0]

A logistic regression has been constructed to predict the promotion of an employee. Table Q2(a) shows parts of the results of the logistic regression.

	Coefficient	P-value
Intercept	0.0035	<2e-16
exp_yr	0.7124	<2e-16
sal_mth	-0.0212	0.0057
sal_yr	-0.0363	0.0086
pjt_Yes	0.0330	0.2479
dpmt_B	1.0447	0.0002
dpmt_C	-1.5318	6.87e-05
dpmt_D	2.1539	0.0017
emp_id	-0.0279	0.5245

Table Q2(a)

(i) Write the logistic regression model that compute the probability that an employee get promoted, $\mathbb{P}(Y = 1)$. (3 marks)

(ii) Calculate the odds and compare the probability of promotion for employee with 7 years of working experience and an employee with 2 years of working experience. (3 marks)

(iii) Calculate the odds and compare the probability of promotion for employee in different departments. Arrange the probability of promotion of department from lowest to highest.

(8 marks)

(c) State two possible issues found in the data. Suggest a suitable solution for each of the issue stated. (4 marks)

Solution: Issue 1: emp_id should not be a variable as this shall not affect the result.
Solution 1: Remove emp_id and label as index variable.
Issue 2: sal_mth and sal_yr are highly correlated.
Solution 2: Remove one of the variables / Perform PCA.

3.1.4 Model Evaluation and Classifier Boundary

Example 3.1.13 (Final Exam Jan 2021, Q2(b))**.** The **testing dataset** of a social network advertisement is given in Table 2.2. The variables "Gender", "Age" and "EstimatedSalary" are the predictors and the variable "Purchased" is the response. The "Gender" is a binary categorical data with levels "Male" and "Female", the "Age" and the "EstimatedSalary" are quantitative data. The "Purchased" is a binary response with values 0 (representing "no purchase", assuming **0 is the positive class**) and 1 (representing "purchase").

Table 2.2: The testing data of a social network advertisement.

Gender	Age	EstimatedSalary	Purchased
Male	29	80000	0
Male	45	26000	1
Female	48	29000	1
Male	45	22000	1
Female	47	49000	1
Male	48	41000	1
Male	46	23000	1
Male	47	20000	1
Male	49	28000	1
Female	47	30000	1

Suppose a logistic regression model is trained and the coefficients are stated in Figure 2.1.

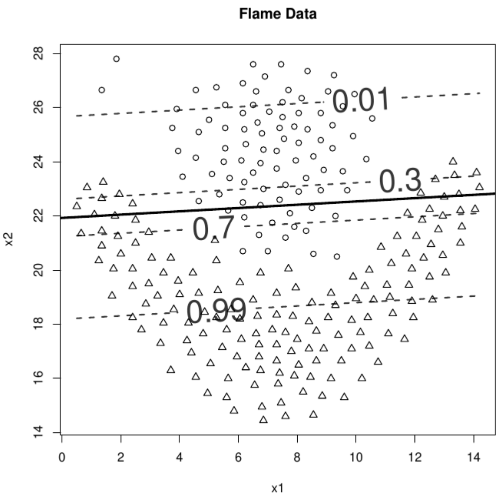
Figure 2.1: The coefficients of the logistic regression based on an insurance claim data.

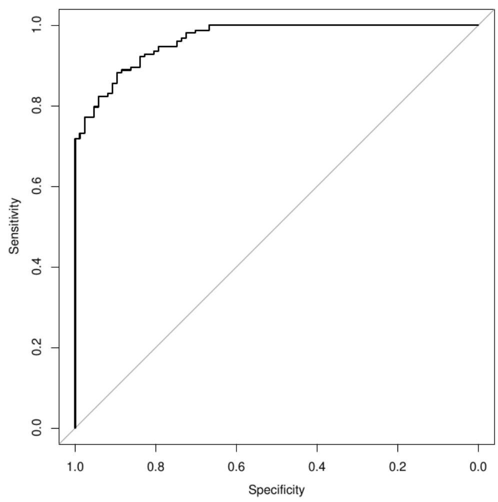
```
glm(formula=Purchased~., family=binomial, data=data.train)

Deviance Residuals:
    Min       1Q   Median      3Q      Max
-2.9882  -0.5640  -0.1372  0.5532  2.1820

Coefficients:
                 Estimate Std. Error z value Pr(>|z|)
(Intercept)     -1.188e+01  2.497e+00  -4.757 1.96e-06 ***
GenderMale       4.221e-01  5.927e-01   0.712 0.476319
Age              2.178e-01  4.751e-02   4.584 4.56e-06 ***
EstimatedSalary  3.868e-05  1.001e-05   3.863 0.000112 ***
```

```
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
(Dispersion parameter for binomial family taken to be 1)
    Null deviance: 135.37  on 99  degrees of freedom
Residual deviance:  74.91  on 96  degrees of freedom
```

Write down the **mathematical formula** of the logistic regression model and then use it to **predict** the variable “Purchase” of the insurance data in Table 2.2 as well as **evaluating** the performance of the model by calculating the confusion matrix, accuracy, sensitivity, specificity, PPV, NPV of the logistic model (assuming 0 is the positive class). [**Note**: The default cut-off is 0.5] (5 marks)

Example 3.1.14 (Decision Boundaries and ROC Curve for (Milely Nonlinear) Flame Data)**.** For the "flame" data, the "boundary" of the classifier is shown in the left figure below as the solid line:





The dashed lines correspond to different "cut-off" 0.01, 0.3, 0.7 and 0.99.

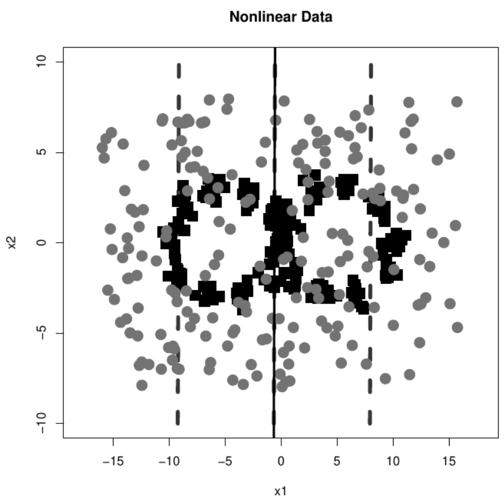
The ROC curve can be understood as the result of varying the "cut-off" and calculating the "sensitivity" (TPR) and "specificity" mentioned in Topic 1. If we calculate out, we have

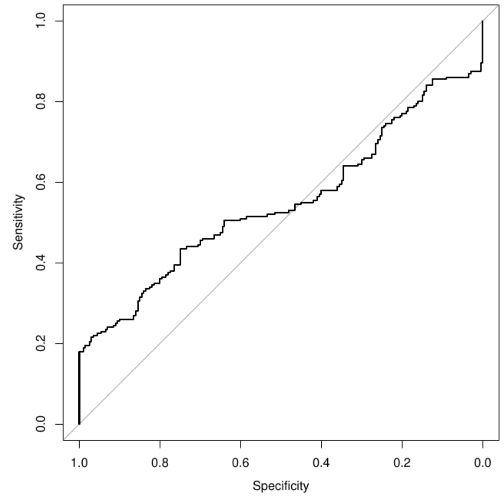
	0.01		0.3		0.7		0.99	
Predicted	1	2	1	2	1	2	1	2
1	19	0	64	6	79	23	87	80
2	68	153	23	147	8	130	0	73
	TPR = 0.2184	FPR = 0	0.7356	0.0392	0.9080	0.1503	1	0.5229

Example 3.1.15 (Decision Boundaries and ROC Curve for LR with Strongly Nonlinear Data)**.** Consider a simulated data generated using the following R script:

```
t = seq(-pi, pi-0.5, length=10)
deterministic = data.frame(x1=c(5*(1+cos(t)),-5*(1+cos(t))),
                           x2=c(   3*sin(t),     3*sin(t)))
x1min = -16; x1max =  16; x2min = -8; x2max =  8
sdev  = 0.5
n = nrow(deterministic)
m = 10
set.seed(2023)
d.f    = data.frame(x1 =
           c(rep(deterministic$x1, each=m) + rnorm(n*m, sd=sdev),
             runif(n*m, min=x1min, max=x1max))
           )
d.f$x2 = c(rep(deterministic$x2, each=m) + rnorm(n*m, sd=sdev),
             runif(n*m, min=x2min, max=x2max))
d.f$y  = c(rep(0,n*m), rep(1,n*m))
```

The decision boudaries is going to be impossible to obtain because the probabilities ranges from around 0.4 to around 0.6 and the ROC curve definitely says that logistic regression model does not fit the model.





Example 3.1.16 (Model Validation using LOOCV)**.** Consider the weather data used in the book Witten et al. [2011] (in Weka arff format from `http://storm.cis.fordham.edu/~gweiss/data-mining/weka-data/weather.arff`). Write an R script to test it using LOOCV.

Solution: A simple script is given below.

```
library(foreign)
d.f = read.arff("weather.arff")
errors = NULL
for(i in 1:nrow(d.f)) {
    d.f.test = d.f[ i,]
    d.f.tran = d.f[-i,]    # Leave-one-out
    logreg.model = glm(play~., family=binomial(link='logit'),
        data=d.f.tran, control=list(maxit=50))
    play.p = predict(logreg.model, newdata=d.f.test, type='response')
    play.p = ifelse(play.p > 0.5,"yes","no")
    errors[i] = (play.p!=d.f.test$play)
}
cat("error rate =", 100*sum(errors)/length(errors), "%\n")
```

Not only that the error rate is 35.71% (high) but the coefficients in the logistic models are all having p-value much larger than 5% which indicates that logistic model is not suitable for modelling the weather data.

```
Coefficients:
              Estimate Std. Error z value Pr(>|z|)
(Intercept)    40.4086  4370.5739   0.009    0.993
outlookrainy  -20.7215  4370.5223  -0.005    0.996
outlooksunny  -21.4922  4370.5222  -0.005    0.996
temperature    -0.0739     0.1957  -0.378    0.706
humidity       -0.1517     0.1229  -1.235    0.217
windyTRUE      -3.6220     2.9590  -1.224    0.221

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 16.0483  on 12  degrees of freedom
Residual deviance:  8.4622  on  7  degrees of freedom
AIC: 20.462
```

3.2 Multinomial Logistic Regression

Multinomial probit or `https://en.wikipedia.org/wiki/Multinomial_logistic_regression` is a classification method that generalises the LR to multiclass problems.

We apply the odds analysis to the output:

$$\begin{cases} \ln \dfrac{\mathbb{P}(Y=2|\boldsymbol{X}=\boldsymbol{x})}{\mathbb{P}(Y=1|\boldsymbol{X}=\boldsymbol{x})} = \boldsymbol{\beta}_2 \cdot \boldsymbol{x} \\ \ln \dfrac{\mathbb{P}(Y=3|\boldsymbol{X}=\boldsymbol{x})}{\mathbb{P}(Y=1|\boldsymbol{X}=\boldsymbol{x})} = \boldsymbol{\beta}_3 \cdot \boldsymbol{x} \\ \qquad\qquad\cdots\cdots \\ \ln \dfrac{\mathbb{P}(Y=K|\boldsymbol{X}=\boldsymbol{x})}{\mathbb{P}(Y=1|\boldsymbol{X}=\boldsymbol{x})} = \boldsymbol{\beta}_K \cdot \boldsymbol{x} \end{cases}$$

Since the sum of the probability of all outputs is one:

$$\begin{aligned} &\mathbb{P}(Y=1|\boldsymbol{X}=\boldsymbol{x}) + \cdots + \mathbb{P}(Y=K-1|\boldsymbol{X}=\boldsymbol{x}) + \mathbb{P}(Y=K|\boldsymbol{X}=\boldsymbol{x}) = 1 \\ \Rightarrow &\mathbb{P}(Y=1|\boldsymbol{X}=\boldsymbol{x}) + \cdots + \mathbb{P}(Y=K|\boldsymbol{X}=\boldsymbol{x})e^{\boldsymbol{\beta}_{K-1}\cdot\boldsymbol{x}} + \mathbb{P}(Y=K|\boldsymbol{X}=\boldsymbol{x})e^{\boldsymbol{\beta}_K\cdot\boldsymbol{x}} = 1, \end{aligned}$$

we obtain the **multinomial LR model**:

$$\begin{aligned} \mathbb{P}(Y=1|\boldsymbol{X}=\boldsymbol{x}) &= \frac{1}{1+\sum_{i=2}^K e^{\boldsymbol{\beta}_i\cdot\boldsymbol{x}}} \\ \mathbb{P}(Y=j|\boldsymbol{X}=\boldsymbol{x}) &= \frac{e^{\boldsymbol{\beta}_j\cdot\boldsymbol{x}}}{1+\sum_{i=2}^K e^{\boldsymbol{\beta}_i\cdot\boldsymbol{x}}}, \quad j=2,\cdots,K. \end{aligned} \tag{3.8}$$

Note that it becomes LR when $K=2$ (we change the labels from 1,2 to 0,1 for LR).

In general, the multinomial LR model requires more data than LR, so when we have little data, this model won't work.

Multinomial LR in R's `nnet`

```
multinom(formula, data, weights, subset, na.action,
         contrasts = NULL, Hess = FALSE, summ = 0,
         censored = FALSE, model = FALSE, ...)
```

Multinomial LR in Python's `statmodels`

```
import statsmodels.api as sm
sm.GLM(endog, exog, family=None, offset=None,
  exposure=None, freq_weights=None,
  var_weights=None, missing='none', **kwargs)

sm.MNLogit(endog, exog, check_rank=True, **kwargs)
```

Note that `endog` stands for endogenous response variable while exogenous variables. See `https://en.wikipedia.org/wiki/Exogenous_and_endogenous_variables`.

In general, for binary classification problem, GLM performs better but when the data is separable like Example 3.1.6.

Example 3.2.1. Analyse the data in Example 3.1.6 using multinomial LR instead of GLM.

Solution: Python statmodels will give similar error to GLM. However, multinom uses convergence algorithm similar to neural network and we obtain the following parameters:

```
Coefficients:
(Intercept)          x1          x2
  45.000000 -266.731095    4.922239
```

```
Residual Deviance: 0
AIC: 6
```

We will also compare the output of `glm` and `multinom` in the practical `p06_logreg2.R`.

A more complex generalisation of LR is the https://en.wikipedia.org/wiki/Elastic_net_regularization.

Elastic Net in R's GLMNET

```
glmnet(x, y, family = c("gaussian", "binomial", "poisson",
  "multinomial", "cox", "mgaussian"), weights = NULL, offset = NULL,
  alpha = 1, nlambda = 100,
  lambda.min.ratio = ifelse(nobs < nvars, 0.01, 1e-04),
  lambda = NULL, standardize = TRUE, intercept = TRUE,
  thresh = 1e-07, dfmax = nvars + 1,
  pmax = min(dfmax * 2 + 20, nvars), exclude = NULL,
  penalty.factor = rep(1, nvars),
  lower.limits = -Inf, upper.limits = Inf, maxit = 1e+05,
  type.gaussian = ifelse(nvars < 500, "covariance", "naive"),
  type.logistic = c("Newton", "modified.Newton"),
  standardize.response = FALSE,
  type.multinomial = c("ungrouped", "grouped"),
  relax = FALSE, trace.it = 0, ...
)
```

Elastic Net in Python's Scikit-Learn

```
class sklearn.linear_model.LogisticRegression(penalty='l2', *,
  dual=False, tol=0.0001, C=1.0, fit_intercept=True,
  intercept_scaling=1, class_weight=None, random_state=None,
  solver='lbfgs', max_iter=100, multi_class='auto', verbose=0,
  warm_start=False, n_jobs=None, l1_ratio=None)

# C -> oo, mode -> LR
```

The implementing the algorithm for finding the parameters βs of the multinomial LR (3.8) is a huge undertaking. A Python implementation of LR is given at http://www.oranlooney.com/post/ml-from-scratch-part-2-logistic-regression/.

According to https://stats.idre.ucla.edu/r/dae/multinomial-logistic-regression/, the following are things to consider when applying the multinomial LR model:

- The Independence of Irrelevant Alternatives (IIA) assumption: Roughly, the IIA assumption means that adding or deleting alternative outcome categories does not affect the odds among the remaining outcomes. There are alternative modelling methods, such as alternative-specific multinomial probit model, or nested logit model to relax the IIA assumption.

- Diagnostics and model fit: Unlike logistic regression where there are many statistics for performing model diagnostics, it is not as straightforward to do diagnostics with multinomial logistic regression models. For the purpose of detecting outliers or influential data points, one can run separate logit models and use the diagnostics tools on each model.

- Sample size: Multinomial regression uses a maximum likelihood estimation method, it requires a large sample size. It also uses multiple equations. This implies that it requires an even larger sample size than ordinal or binary logistic regression.

- Complete or quasi-complete separation: Complete separation means that the outcome variable separate a predictor variable completely, leading perfect prediction by the predictor variable.
- Perfect prediction means that only one value of a predictor variable is associated with only one value of the response variable. But you can tell from the output of the regression coefficients that something is wrong. You can then do a two-way tabulation of the outcome variable with the problematic variable to confirm this and then rerun the model without the problematic variable.
- Empty cells or small cells: You should check for empty or small cells by doing a cross-tabulation between categorical predictors and the outcome variable. If a cell has very few cases (a small cell), the model may become unstable or it might not even run at all.

3.3 (Artificial) Neural Network

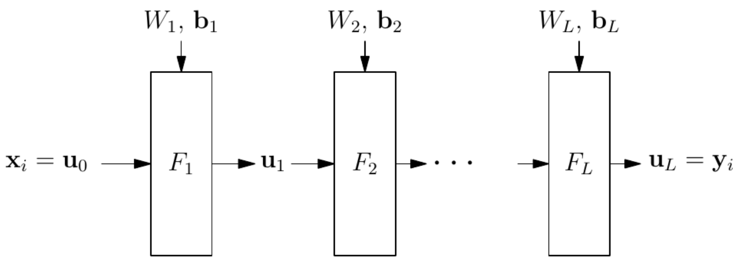
Feed-forward Artificial Neural Networks (ANN) or `https://en.wikipedia.org/wiki/Multilayer_perceptron` (MLP) is a generalisation of the multinomial LR.

A MLP with input $\boldsymbol{x}_i \in \mathbb{R}^p$ and output is $\boldsymbol{y}_i \in \mathbb{R}^m$:

$$\begin{aligned} \boldsymbol{u}_1 &= F_1(W_1\boldsymbol{u}_0 + \boldsymbol{b}_1), \quad \boldsymbol{u}_0 = \boldsymbol{x}_i \\ \boldsymbol{u}_2 &= F_2(W_2\boldsymbol{u}_1 + \boldsymbol{b}_2) \\ &\cdots \\ \hat{\boldsymbol{y}}_i = \boldsymbol{u}_L &= F_L(W_L\boldsymbol{u}_{L-1} + \boldsymbol{b}_L). \end{aligned} \tag{3.9}$$

where L is the number of layers of ANN (with $L-1$ hidden layers).

Horizontal pictorial representation:



When $L = 1$, we obtain a `https://en.wikipedia.org/wiki/Perceptron`:

$$\boldsymbol{u}_1 = F_1(W_1\boldsymbol{x}_i + \boldsymbol{b}_1). \tag{3.10}$$

We can see that when $m = 1$, $\boldsymbol{b}_1 = \beta_0$, $W_1 = (\beta_1, \ldots, \beta_p)$ and $F_1(x) = S(x)$, we obtain the LR. When $m = K - 1$ ($K \geq 2$), we obtain the multinomial LR (3.8) which is how the R's `nnet::multinom` is implemented.

Theorem 3.3.1. *ANNs are univeral approximators (like SVMs, GPs, ...). Theoretically, a ANN with one hidden layer is as expressive as one with many hidden layers in practice if many nodes are used.*

When $L = 2$, we obtain an ANN with a single hidden-layer.

$$\begin{aligned} \boldsymbol{u}_1 &= F_1(W_1\boldsymbol{x}_i + \boldsymbol{b}_1) \\ \boldsymbol{y} = \boldsymbol{u}_2 &= F_1(W_2\boldsymbol{u}_1 + \boldsymbol{b}_2). \end{aligned} \tag{3.11}$$

Single-Hidden-Layer NN in R

```
nnet(x, y, weights, size, Wts, mask,
     linout = FALSE, entropy = FALSE, softmax = FALSE,
     censored = FALSE, skip = FALSE, rang = 0.7, decay = 0,
     maxit = 100, Hess = FALSE, trace = TRUE, MaxNWts = 1000,
     abstol = 1.0e-4, reltol = 1.0e-8, ...)
```

MLP in R

```
neuralnet(formula, data, hidden = 1, threshold = 0.01,
  stepmax = 1e+05, rep = 1, startweights = NULL,
  learningrate.limit = NULL, learningrate.factor = list(minus=0.5,
  plus = 1.2), learningrate = NULL, lifesign = "none",
  lifesign.step = 1000, algorithm = "rprop+", err.fct = "sse",
  act.fct = "logistic", linear.output = TRUE, exclude = NULL,
  constant.weights = NULL, likelihood = FALSE)
```

MLP in Python

```
class sklearn.neural_network.MLPClassifier(
  hidden_layer_sizes=(100,), activation='relu', *, solver='adam',
  alpha=0.0001, batch_size='auto', learning_rate='constant',
  learning_rate_init=0.001, power_t=0.5, max_iter=200,
  shuffle=True, random_state=None, tol=0.0001, verbose=False,
  warm_start=False, momentum=0.9, nesterovs_momentum=True,
  early_stopping=False, validation_fraction=0.1, beta_1=0.9,
  beta_2=0.999, epsilon=1e-08, n_iter_no_change=10, max_fun=15000)
```

The algorithm to estimate the parameters W_ℓ and $\boldsymbol{b}_\ell$ for the layer $\ell = 1, \ldots, L$ is the improvement of **back-propagation algorithm**:

1. $t = 0$;
2. Using the guess parameters $W_\ell^{(t)}$, $\boldsymbol{b}_\ell^{(t)}$, calculate all the intermediate states
$$\boldsymbol{u}_\ell^{(t)} = F_\ell(W_\ell^{(t)} \boldsymbol{u}_{\ell-1}^{(t)} + \boldsymbol{b}_\ell^{(t)})$$
and the output $\hat{\boldsymbol{y}}_i$;
3. The output layer
$$\delta_L = \hat{\boldsymbol{y}}_i - \boldsymbol{y}_i$$
4. Back-Propagation (roughly): For ℓ from L to 1, do
$$\begin{aligned} \delta_{\ell-1} &= \frac{\partial F_\ell}{\partial W_\ell}(\boldsymbol{u}_{\ell-1}^{(t)})\delta_\ell \\ W_\ell^{(t+1)} &= W_\ell^{(t)} + \alpha \times \boldsymbol{u}_{\ell-1}^{(t)} \times \delta_{\ell-1} \end{aligned}$$
5. $t = t + 1$ and go to step 2.

ANNs learn lots of parameters and therefore are prone to overfitting. This is not necessarily a problem as long as regularisation is used. Two popular **reglarisers** are the following:

- Weight Decay: Use ℓ_2 regularisation on all weights (including bias terms).

- Dropout: For each input (or mini-batch) randomly remove each hidden node with probability p (e.g. $p = 0.5$) these nodes stay removed during the backprop pass, however are included again for the next input.

In the training of ANN, local minima need to be avoided by

- Using momentum:

$$\nabla \boldsymbol{w}_t = \Delta \boldsymbol{w}_t + \mu \nabla \boldsymbol{w}_{t-1}, \quad \boldsymbol{w} = \boldsymbol{w} - \alpha \nabla \boldsymbol{w}_t$$

  i.e. still use some portion of previous gradient to keep you pushing out of small local minima.
- Initialising weights cleverly (not all that important). For example, use Autoencoders for unsupervised pre-training.
- Using ReLU instead of sigmoid/tanh (weights don't saturate).

Other tricks and tips in the training of ANN are

- Rescale the data so that all features are within [0,1];
- Lower learning rate;
- Use mini-batch, i.e. stochastic gradient descent with maybe 100 inputs at a time – make sure you shuffle inputs randomly first;
- For image input, use convolution neural network.

Example 3.3.2 (Decision Boundaries and ROC Curve for ANN with Strongly Nonlinear Data)**.** Consider the data from Example 3.1.15. If we use neural network instead of LR, we will face the following problems:

- What neural network to use? 1 hidden layer? 2? 3?
- If we pick 1-hidden layer, how many internal nodes should we have? 5? 10?
- What should the initial guess of the parameters be? I tried the same model with 1 hidden layer, 10 nodes, it sometimes go OK, and some times cannot converge because I forgot to set seed. So far, seed=1 is OK, seed=2023 and seed=202301 are not OK.

The R script is as follows:

```
library(neuralnet)
set.seed(1)   # This works for c(10)
model = neuralnet((y=="1") ~ x1+x2, data=d.f, hidden=c(10),
  linear.output=FALSE)
g.x1 = seq(x1min-2, x1max+2, by=0.1); g.x2 = seq(x2min-2, x2max+2, by=0.1)
d.grid = expand.grid(x1=g.x1, x2=g.x2)
pred = predict(model, newdata=d.grid)
```

The contour plot is complex and the ROC indicates the ANN is a good enough model.