Chapter 7. Supervised machine learning for continuous data

[presentation] (./pdf/ppt7.pdf) **[book] (./pdf/book7.pdf)**

CHAPTER OBJECTIVES

Classification analysis is a technique that uses data with known group membership to create a model to determine the group of data with unknown group membership. This chapter introduces the classification analysis for continuous data as follows.

- Bayes classification model, which is the basis of statistical classification analysis.
- Logistic regression model in case of two groups uses multiple linear regression analysis.
- Nearest neighbor classification model, which utilizes distances between observations.
- Neural network model, which is a nonlinear optimization model.
- Support vector machine model, which is a mathematical classification model.
- Ensemble models that synthesize the results of several classification models.

7.1 Bayes Classification Model - Continuous data

In section 6.3.1, we studied the Bayes classification model, which classifies data into groups with high probability by calculating the posterior probability using Bayes theorem. In section 6.3.2, we studied the naive Bayes classification model, which is an application of Bayes classification to categorical data when variables can be assumed to be independent. Suppose there are m random variables $\boldsymbol{X} = (X_1, X_2, \ldots, X_m)$. Let the prior

probabilities of k number of groups, $G_1, G_2, \ldots, G_k$, be $P(G_1), P(G_2), \ldots, P(G_k)$, and let the likelihood probability distribution function for each group be $P(X|G_1), P(X|G_2), \ldots, P(X|G_k)$. Given the observation data $\boldsymbol{x}$ for classification, the posterior probability $P(G_i|\boldsymbol{x})$ that this data comes from the group G_i is as follows.

$$P(G_i|\boldsymbol{x}) = \frac{P(G_i) \times P(\boldsymbol{x}|G_i)}{P(G_1) \times P(\boldsymbol{x}|G_1) + P(G_2) \times P(\boldsymbol{x}|G_2) + \cdots + P(G_k) \times P(\boldsymbol{x}|G_k)}$$

The Bayes classification rule, which uses the posterior probability, is as follow.

Bayes Classification - multiple groups
Suppose that prior probabilities of k number of groups, $G_1, G_2, \ldots, G_k$, are $P(G_1), P(G_2), \ldots, P(G_k)$, and likelihood probability distribution functions for each group are $P(X|G_1), P(X|G_2), \ldots, P(X|G_k)$. Given the observation data $\boldsymbol{x}$ for classification, let the posterior probabilities that $\boldsymbol{x}$ comes from each group be $P(G_1|\boldsymbol{x}), P(G_2|\boldsymbol{x}), \ldots, P(G_k|\boldsymbol{x})$. The Bayes classification rule is as follows.

'Classify $\boldsymbol{x}$ into a group with the highest posterior probability'

If we denote the likelihood probability functions as $f_1(\boldsymbol{x}), f_2(\boldsymbol{x}), \ldots, f_k(\boldsymbol{x})$, since the denominators in the calculation of posterior probabilities are the same, the Bayes classification rule can be written as follows.

'If $P(G_k)f_k(\boldsymbol{x}) \geq P(G_i)f_i(\boldsymbol{x})$ for all $k \neq i$, classify $\boldsymbol{x}$ into group G_k'

If there are only two groups $G_1$and G_2, the Bayesian classification rule is expressed as follows.

'if $\frac{f_1(\boldsymbol{x})}{f_2(\boldsymbol{x})} \geq \frac{P(G_2)}{P(G_1)}$, classify $\boldsymbol{x}$ into group G_1, else into group G_2'

When there are sample data, we can estimate the likelihood probability distribution $f_i(\boldsymbol{x})$ from the sample, the Bayes classification rule can also be estimated using the likelihood distribution. Therefore, the Bayes classification rule can appear in many variations depending on the estimation method of the likelihood probability distribution. Estimating the likelihood probability distribution using samples can be done using either a parametric method, such as maximum likelihood estimation, or a nonparametric method. In the case of categorical data, a multidimensional distribution estimated from the sample is often used, and in the case of continuous data, a multivariate normal distribution is often used. For more information, please refer to the related references.

Example 7.1.1 - Bayes classification with one continuous variable
A survey of customers at a computer store showed the prior probabilities of the purchasing group (G_1) and the non-purchasing group (G_2) are $P(G_1)$ = 0.4 and $P(G_2)$ = 0.6, respectively. Suppose that the likelihood distribution of the age in the purchasing group is a normal distribution with a mean of 35 and a standard deviation of 2, $N(35, 2^2)$, and the non-purchasing group is a normal distribution with a mean of 25 and a standard deviation of 2, $N(25, 2^2)$.
If a customer who visited this store on a certain day is 30 years old, classify the customer using the Bayes classification model whether he will purchase the product or not.

Answer

The functional form of the likelihood probability distribution of the purchasing group G_1 and the non-purchasing group G_2 are as follows.

$$P(x|G_1) = f_1(x) = \frac{1}{\sqrt{2\pi}\,2}\ exp\{-\frac{(x-35)^2}{2\times 2^2}\}$$
$$P(x|G_2) = f_2(x) = \frac{1}{\sqrt{2\pi}\,2}\ exp\{-\frac{(x-25)^2}{2\times 2^2}\}$$

Therefore, the Bayes classification rule is as follows.

$$\text{If } \frac{f_1(x)}{f_2(x)} = exp\{-\frac{(x-35)^2}{2\times 2^2} - \frac{(x-25)^2}{2\times 2^2}\} \geq \frac{P(G_2)}{P(G_1)} = \frac{0.6}{0.4}, \text{ classify } x \text{ into } G_1, \text{ else } G_2.$$

If we organize the above equation by taking the log, the classification rule is as follows.

$$\text{If } x \geq 30.16, \text{ classify } x \text{ into } G_1, \text{ else } G_2.$$

Therefore, the customer whose age is 30 is classified as a non-purchasing group (G_2).

If there are two groups, G_1 and G_2, and the likelihood probability distributions $f_1(\boldsymbol{x})$ and $f_2(\boldsymbol{x})$ for each group follow the multivariate normal distribution $N(\boldsymbol{\mu}_1, \Sigma_1)$ and $N(\boldsymbol{\mu}_2, \Sigma_2)$, the classification rule is as follows.

$$\text{If } d^Q(\boldsymbol{x}) = -\frac{1}{2} ln \frac{|\Sigma_2|}{|\Sigma_1|} - \frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_1)'\Sigma_1^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_1) + \frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_2)'\Sigma_2^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_2) \geq ln \frac{P(G_2)}{P(G_1)}, \text{ classify } x \text{ into } G_1, \text{ else } G_2.$$

$d^Q(\boldsymbol{x})$ is a **quadratic classification function**. If the covariances of groups G_1 and G_2 are the same (i.e., $\Sigma_1 = \Sigma_2 = \Sigma$), the classification function $d^Q(\boldsymbol{x})$ becomes the following **linear classification function** $d^L(\boldsymbol{x})$, which is widely used in the classification of continuous data.

$$\text{If } d^L(\boldsymbol{x}) = (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)' \Sigma^{-1} [\, \boldsymbol{x} - \frac{1}{2}(\boldsymbol{\mu}_1 + \boldsymbol{\mu}_2) \,] \geq ln \frac{P(G_2)}{P(G_1)}, \text{ classify } x \text{ into } G_1, \text{ else } G_2.$$

Since the two means, μ_1 and μ_2, and covariance matrix Σ of the two populations are generally unknown, an estimated classification function is used using the sample means, $\overline{\boldsymbol{x}}_1$ and $\overline{\boldsymbol{x}}_2$, and sample covariance matrix S from each population.

$$\text{If } d^L(\boldsymbol{x}) = (\overline{\boldsymbol{x}}_1 - \overline{\boldsymbol{x}}_2)' S^{-1} [\, \boldsymbol{x} - \frac{1}{2}(\overline{\boldsymbol{x}}_1 + \overline{\boldsymbol{x}}_2) \,] \geq ln \frac{P(G_2)}{P(G_1)}, \text{ classify } x \text{ into } G_1, \text{ else } G_2.$$

Example 7.1.2 Consider a survey of 20 customers at a computer store on age (X_1), monthly income (X_2), and purchasing status, as shown in Table 7.1.1. Assume that these continuous variables are multivariate normal distributions with the same covariance. Find a Bayes classification function and classify a customer who is 33 years old and has a monthly income of 200, whether he will purchase a computer or not.

Table 7.1.1 Survey of customers on age, income, and purchasing status

Number	Age	Income (unit 10,000 won)	Purchase
1	25	150	Yes
2	34	220	No
3	27	210	No
4	28	250	Yes
5	21	100	No
6	31	220	No
7	36	300	Yes
8	20	100	No
9	29	220	No
10	32	250	Yes
11	37	400	Yes
12	24	120	No
13	33	350	No
14	30	180	Yes

15	38	350	Yes
16	32	250	No
17	28	240	No
18	22	220	No
19	39	450	Yes
20	26	150	No

Answer

The sample means of age and income of each group, $\overline{\boldsymbol{x}}_1$ and $\overline{\boldsymbol{x}}_2$, and sample covariance matrix $\boldsymbol{S}$ are calculated as follows.

$$\overline{\boldsymbol{x}}_1 = \begin{bmatrix} 27.250 \\ 200.000 \end{bmatrix}, \quad \overline{x}_2 = \begin{bmatrix} 33.125 \\ 291.250 \end{bmatrix}, \quad \boldsymbol{S} = \begin{bmatrix} 31.621 & 470.105 \\ 470.105 & 9129.211 \end{bmatrix}$$

$\overline{\boldsymbol{x}}_1 - \overline{\boldsymbol{x}}_2$, $\boldsymbol{S}^{-1}$ and $(\overline{\boldsymbol{x}}_1 - \overline{\boldsymbol{x}}_2)'\boldsymbol{S}^{-1}$ is as follows.

$$\overline{\boldsymbol{x}}_1 - \overline{\boldsymbol{x}}_2 = \begin{bmatrix} -5.875 \\ -91.25 \end{bmatrix}, \quad \boldsymbol{S}^{-1} = \begin{bmatrix} 0.134895 & -0.006946 \\ -0.006946 & 0.000467 \end{bmatrix}, \quad (\overline{\boldsymbol{x}}_1 - \overline{\boldsymbol{x}}_2)'\boldsymbol{S}^{-1} = \begin{bmatrix} -0.15865 \\ -0.00182 \end{bmatrix}$$

Assume that the prior probability of non-purchasing group is $P(G_1)$ = 0.6, and the prior probability of purchasing group $P(G_2)$ = 0.4, the sample linear classification function is as follows.

$$\text{If } (-0.15865) \times x_1 + (-0.00182) \times x_2 + 5.64297 \geq 0, \text{ classify } \boldsymbol{x} = (x_1, x_2) \text{ into } G_1, \text{ or } G_2.$$

If the visiting customer's age is 33 and income is 200, the classification function becomes as follows.

$$(-0.15865) * (33) + (0.00182) * (200) + (5.64297) = 0.04251$$

Therefore, the customer is classified into the non-purchasing group G_1.

[Bayes Classification Analysis]

Bayes Classification Analysis

Variable Name		Data Input
Y	Purchase	Yes,No,No,Yes,No,No,Yes,No,No,Yes,Yes,No,No,Yes,Yes,No,No,No,Yes,No
X_1	Age	25,34,27,28,21,31,36,20,29,32,37,24,33,30,38,32,28,22,39,26
X_2	Income	150,220,210,250,100,220,300,100,220,250,400,120,350,180,350,250,240,220,45(
X_3		
X_4		
X_5		

Data partition (Train 100 % : Test 0 %)

Prior probability ◉ sample proportion ○ equal proportion

Execute | Scatter Plot Matrix | Parallel Graph | Erase Data

Graph Save | Classification Table | Table Save

If we can estimate the likelihood probability distribution, Bayes classification can be applied even when the variables are continuous or discrete. If continuous and discrete variables are mixed, the naive Bayes classification can be applied by discretizing the continuous variables.

Variable selection

When there are many variables, selecting only the variables that help classify the groups can reduce the parameter estimation problem and increase accuracy. Stepwise classification analysis is selecting appropriate variables stepwise and classifying them. Variable selection generally uses variables that can best explain group variables, that is, variables with high discriminatory power between groups. For example, when performing an analysis of variance to compare the means between groups, variables with high F values (or t values in the case of two groups) are selected. This type of variable selection can be done by forward selection, which adds variables with high discriminatory power one by one without selecting any variables, and backward elimination, which selects all variables and then removes variables with low discriminatory power one by one. There is also a stepwise method that selects variables using the forward selection method while examining whether the variables already selected can be removed. However, it is not easy to verify whether the 'optimal' variable selection has been made regardless of the method used. For more information, please refer to the references.

Characteristics of Bayes classification

The characteristics of Bayes classification are summarized as follows.

1) Since the Bayes classification model classifies using the posterior probability, which is calculated by the prior probability and the likelihood probability distribution of each group, the risk of model overfitting is low and robust.
2) Bayes classification model can perform stable classification even when incomplete data, outliers, and missing values exist.

7.1.1 R practice - Bayes classification

To analyze Bayes classification using R, we need to install a package called **MASS**. From the main menu of R, select 'Package' => 'Install package(s)', and a window called 'CRAN mirror' will appear. Here, select '0-Cloud [https]' and click 'OK'. Then, when the window called 'Packages' appears, select 'MASS' and click 'OK'. 'MASS' is a package for modeling of Bayes classification model. General usage and key arguments of the function are described in the following table.

Fit a linear discriminant analysis model.	
lda(x, ...) **## S3 method for class 'formula'** **lda(formula, data, ..., subset, na.action)** **## Default S3 method:** **lda(x, grouping, prior = proportions, tol = 1.0e-4,method, CV = FALSE, nu, ...)** **## S3 method for class 'data.frame'** **lda(x, ...)** **## S3 method for class 'matrix'** **lda(x, grouping, ..., subset, na.action)**	
formula	A formula of the form groups ~ x1 + x2 + ... That is, the response is the grouping factor and the right hand side specifies the (non-factor) discriminators.
data	Data frame from which variables specified in formula are preferentially to be taken.
x	(required if no formula is given as the principal argument.) a matrix or data frame or Matrix containing the explanatory variables.
grouping	(required if no formula principal argument is given.) a factor specifying the class for each observation.
prior	the prior probabilities of class membership. If unspecified, the class proportions for the training set are used. If present, the probabilities should be specified in the order of the factor levels.
tol	A tolerance to decide if a matrix is singular; it will reject variables and linear combinations of unit-variance variables whose variance is less than tol^2.
subset	An index vector specifying the cases to be used in the training sample. (NOTE: If given, this argument must be named.)
na.action	A function to specify the action to be taken if NAs are found. The default action is for the procedure to fail. An alternative is na.omit, which leads to rejection of cases with missing values on any required variable.
method	"moment" for standard estimators of the mean and variance, "mle" for MLEs, "mve" to use cov.mve, or "t" for robust estimates based on a t distribution.

An example of R commands for a Bayes classification with purchase as the dependent variable of card data and other variables as independent variables is as follows.

> install.packages('MASS')	copy r command
> library(MASS)	copy r command
> customer <- read.csv('PurchaseByCredit20_Continuous.csv', header=T, as.is=FALSE)	copy r command
> attach(customer)	copy r command

> Purchase
`[1] Yes No  No  Yes No  No  Yes No  No  Yes Yes No  No  Yes Yes No  No  No  Y`
`es`
`[20] No`
`Levels: No Yes`
	copy r command

```
> ldamodel <- lda(Purchase ~ ., customer)
```

copy r command

```
> ldamodel
```

copy r command

```
Call: lda(Purchase ~ ., data = customer)
Prior probabilities of groups:
 No Yes
0.6 0.4
Group means:
       Age Income
No  27.250 200.00
Yes 33.125 291.25
Coefficients of linear discriminants:
               LD1
   Age 0.173328870
Income 0.001994526
```

If we want to classify the group of the customer data using the Bayes model, R commands are as follows.

```
> pred <- predict(ldamodel, customer)"
```

copy r command

```
> pred$class
```

copy r command

```
$class
 [1] No  Yes No  No  No  No  Yes No  No  No  Yes No  Yes No  Yes No  No  No
Yes
[20] No
Levels: No Yes
```

To make a classification cross table, we can use a vector of prediction, pred$class, and Purchase with table command as below. Using this classification table, accuracy of the model is calculated as 0.7 which is (10+4) / (10+2+4+4).

```
> classtable <- table(Purchase,pred$class)
```

copy r command

```
Purchase No Yes
     No  10   2
     Yes  4   4
```

```
> sum(diag(classtable)) / sum(classtable)
```

copy r command

```
[1] 0.7
```

7.2 Logistic regression model

A linear regression model expresses the relationship between m independent variables (explanatory variables) $X_1, X_2, \ldots, X_m$ and the dependent variable (response or target variable) Y as a linear equation as follows.

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots \beta_m X_m + \epsilon$$

Here, the error term ϵ is assumed to be a normal distribution with a mean of 0 and a variance of σ^2. If the target variable Y has values of 0 and 1 representing two groups, the above regression model is not appropriate. For example, Let us consider a simple linear regression model to determine whether a customer will purchase a product (Y = 1) or not (Y = 0) based on monthly income (X).

$$Y = \alpha + \beta X + \epsilon$$

If we estimate the parameters α and β using sample data and apply the above formula to actual test data, since the predicted value of group Y becomes a continuous number, there are cases where it goes beyond the range of [0, 1].

The **logistic regression** is a model that has been modified to fit the classification of two groups by solving this problem of the linear regression model.

When the target variable has the values 1 and 0, the logistic regression model is a linear regression of the log value of the odds ratio, which is the ratio of the probability $P(Y=1\,|x)$ and the probability $P(Y=0\,|x)$ given that $X=x$, as shown below.

$$ln\,\frac{P(Y=1\,|x)}{P(Y=0\,|x)}=\alpha+\beta x$$

Here, ln is the natural logarithm and $P(Y=0\,|x)=1-P(Y=1\,|x)$. If we rearrange the above equation using $P(Y=1\,|x)$, it can be written as follows.

$$P(Y=1\,|x)=\frac{exp(\alpha+\beta x)}{1+exp(\alpha+\beta x)}$$

It means that, if the coefficients α and β of this regression model can be estimated using the least squares method, $P(Y=1\,|x)$ can also be estimated. The estimated probability $P(Y=1\,|x)$ is called the posterior probability of the group 1, and $P(Y=0\,|x)$ is called the posterior probability of the group 0. Data is classified into the group 1 if this posterior probability value is greater than a critical value selected by the analyst, such as 0.5, otherwise it is classified as group 0. The maximum likelihood estimation method is frequently used to estimate the coefficient of the logistic regression model.

The above simple logistic regression model with one variable can be extended to have m variables as follow.

$$ln\,\frac{P(Y=1\mid \boldsymbol{x}=(x_1,x_2,\ldots,x_m))}{1-P(Y=1\mid \boldsymbol{x}=(x_1,x_2,\ldots,x_m))}=\beta_0+\beta_1X_1+\beta_2X_2+\cdots\beta_mX_m$$

If we rearrange the above equation using $P(Y=1\mid \boldsymbol{x}=(x_1,x_2,\ldots,x_m))$, it can be written as follow.

$$P(Y=1\mid \boldsymbol{x}=(x_1,x_2,\ldots,x_m))=\frac{exp(\beta_0+\beta_1X_1+\beta_2X_2+\cdots+\beta_mX_m)}{1+exp(\beta_0+\beta_1X_1+\beta_2X_2+\cdots+\beta_mX_m)}$$

Given the data $\boldsymbol{x}=(x_1,x_2,\ldots,x_m)$ to be classified, the posterior probability $P(Y=1\mid \boldsymbol{x}=(x_1,x_2,\ldots,x_m))$ is estimated using the estimated regression coefficients of $\beta_0,\beta_1,\ldots,\beta_m$. If the estimated posterior probability is greater than the critical value selected by the analyst, it is classified as group 1, otherwise it is classified as group 0.

Let us examine the effect of independent variable X_i on the classification of groups in the logistic regression model. If all other variables are constant and only the variable value x_i is increased by 1 unit (x_i+1), the **incremental odds ratio** is as follows.

$$\begin{aligned}\text{Incremental odds ratio}&=\frac{exp(\beta_0+\beta_1x_1+\cdots+\beta_i(x_i+1)+\cdots+\beta_mx_m)}{exp(\beta_0+\beta_1x_1+\cdots+\beta_ix_i+\cdots+\beta_mx_m)}\\&=exp(\beta_i)\end{aligned}$$

Therefore, when the variable X_i increases by 1 unit, if β_i is positive, the odds ratio increase rate is greater than 1, so $P(Y=1\mid \boldsymbol{x}=(x_1,x_2,\ldots,x_m))$ also increases. On the other hand, if β_i is negative, the odds ratio increase rate is less than 1, so $P(Y=1\mid \boldsymbol{x}=(x_1,x_2,\ldots,x_m))$ decreases. For example, monthly income X is an independent variable and customer purchasing status Y is the target variable, such as purchasing a product $(Y=1)$ or not $(Y=0)$. The estimated logistic regression model is as follow.

$$ln\,\frac{P(Y=1\,|x)}{1-P(Y=1\,|x)}=0.21+1.34x$$

In this case, if the monthly income X increases by 1 unit, the odds ratio increase rate becomes $exp(1.34)$ = 3.82. That is, if monthly income increases by 1 unit, the odd ratio of the probability of purchasing a product to the probability of not purchasing it increases by 3.82 times.

In the case of a logistic regression model with many independent variables, the variable that best explains the target variable must be selected. In order to select variables, a model selection criterion that can compare several models is needed, and the Akaike Information Criteria (AIC) is commonly used. Specific selection methods include forward selection, backward elimination, and stepwise methods, as in the Bayes classification variable selection method. For more information, please refer to a related statistics book.

Example 7.2.1 Using the survey data in Example 7.1.2, find a logistic regression model with product purchase as the target variable and age, monthly income, as independent variables.

Answer

If we perform a logistic regression analysis using R with age (X_1) and monthly income (X_2) as independent variables and purchasing status as a target variable (Y), we will get the results in the following table.

Coefficients:		
(Intercept)	Age	Income
-7.629959	0.223517	0.001918

This means that the logistic regression model is as follows.

$$ln\ \frac{P(Y=1 \mid \boldsymbol{X}=(X_1,X_2))}{1-P(Y=1 \mid \boldsymbol{X}=(X_1,X_2))} = -7.629959 + 0.223517X_1 + 0.001918X_2$$

If we rearrange the above equation using $P(Y=1 \mid \boldsymbol{X}=(X_1,X_2))$, it can be written as follows.

$$P(Y=1 \mid \boldsymbol{X}=(X_1,X_2)) = \frac{exp(-7.629959 + 0.223517X_1 + 0.001918X_2)}{1+exp(-7.629959 + 0.223517X_1 + 0.001918X_2)}$$

If a customer whose age is 20 and income is 200, $\boldsymbol{X}=(20,200)$, the posterior probability $P(Y=1 \mid \boldsymbol{X})$ is as follows.

$$\begin{aligned} P(Y=1 \mid \boldsymbol{X}=(20,200)) &= \frac{exp(-7.629959 + 0.223517 \times 20 + 0.001918 \times 200)}{1+exp(-7.629959 + 0.223517 \times 20 + 0.001918 \times 200)} \\ &= \frac{0.062286}{1+0.062286} \\ &= 0.058634 \end{aligned}$$

If the critical value of the posterior probability is 0.5, then the customer is classified by group 0, which is the non-purchasing group.

7.2.1 R practice - Logistic regression

Let us practice the logistic regression using R commands with the data saved at C:\Rwork\PurchaseByCredit20_Continuous.csv. In order to practice the decision tree using this data, we need to change first the working directory of R as follows.

File > Change Directory > C: > Rwork

If we read the data file in R, it looks like as follows.

# read the data file	
> customer <- read.csv('PurchaseByCredit20_Continuous.csv', header=T, as.is=FALSE)	copy r command

```
> customer
```

```
      Age Income Purchase
1      25    150      Yes
2      34    220       No
3      27    210       No
4      28    250      Yes
5      21    100       No
6      31    220       No
7      36    300      Yes
8      20    100       No
9      29    220       No
10     32    250      Yes
11     37    400      Yes
12     24    120       No
13     33    350       No
14     30    180      Yes
15     38    350      Yes
16     32    250       No
17     28    240       No
18     22    220       No
19     39    450      Yes
20     26    150       No
```

```
> attach(customer)
```

copy r command

```
> Purchase
```

```
 [1] Yes No  No  Yes No  No  Yes No  No  Yes Yes No  No  Yes Yes No  No  No
Yes
[20] No
Levels: No Yes
```

copy r command

```
> logitmodel <- glm(Purchase ~.,family=binomial(link='logit'),data=card)
```

copy r command

```
> logitmodel
```

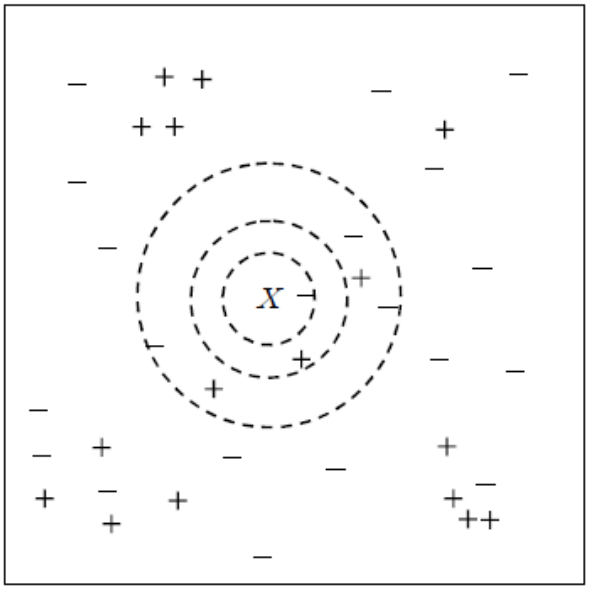
```
Call:  glm(formula = Purchase ~ ., family = binomial(link = "logit"), data =
card)
Coefficients:
(Intercept)          Age       Income
  -7.629959     0.223517     0.001918
Degrees of Freedom: 19 Total (i.e. Null);  17 Residual
Null Deviance:      26.92
Residual Deviance: 20.68        AIC: 26.68
```

copy r command

7.3 Nearest neighbor classification model

Decision tree, Bayes classification, and logistic regression models first establish an appropriate model from the collected data and then apply it to the data to be classified. These models are called eager learners. However, the **nearest neighbor classification model** establishes a model when there is data to be classified and is called a lazy learner. In other words, the nearest neighbor classification model first stores all training data in the computer. When the data is to be classified, it finds a set of k data that are most similar to the variable values of the data and classifies the data into a group with a majority vote in that set. It is called a k-nearest neighbor classification model. The similarity between the data to be classified and the training data uses various mathematical or statistical proximity measures studied in Chapter 3.

<Figure 7.3.1> shows two-dimensional continuous data divided into + and - groups. When the data marked with X in the Figure is to be classified, it shows the 1-nearest neighbor (innermost circle), 2-nearest neighbor (middle circle), and 7-nearest neighbor (outer circle) data points using the two-dimensional Euclidean distance.



<Figure 7.3.1> 1-nearest, 2-nearest, 7-nearest neighbor data for given data marked with X

If only 1-nearest neighbor is used for classification, there is one - group, and the data X is classified as the - group. If 2-nearest neighbors are used, there are one + group and one - group data, so it is difficult to classify the data X and it can be classified into either group. If 7-nearest neighbors are used, since there are three + groups and four - groups, the majority rule is used to classify X into the - group. As seen in these cases, the appropriate selection of k has a great influence on the classification result. If k is too small, the data may be incorrectly classified due to the noise of the data. If k is too large, the data may not be classified into a group close to the data.

An algorithm for the nearest neighbor classification model can be summarized as follows.

[Algorithm for the k nearest neighbor classification]

Suppose there are n number of training data with m variables $\boldsymbol{x}_i$ and group variable y_i as $D = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \ldots, (\boldsymbol{x}_n, y_n)\}$. The algorithm first calculates the similarity distance between the test data $\boldsymbol{x}$ to be classified and all training data. If there is a lot of training data, the calculation of the similarity distance may take a lot of time. After finding the k adjacent neighbors $D_{\boldsymbol{x}}$ using the calculated distance, the test data $\boldsymbol{x}$ is classified into a majority group of these adjacent neighbors, which can be expressed in the following formula.

$$y = argmax_v \sum_{(\boldsymbol{x}_i, y_i) \in D_{\boldsymbol{x}}} I(v = y_i)$$

Step 1	Let $\boldsymbol{x}$ be the test data, and $D = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \ldots, (\boldsymbol{x}_n, y_n)\}$ be the training data.
Step 2	**for** test data $\boldsymbol{x}$ **do**
Step 3	**for** i = 1 to n **do**
Step 4	Calculate the distance $d(\boldsymbol{x}, \boldsymbol{x}_i)$ between $\boldsymbol{x}$ and $\boldsymbol{x}_i$
Step 5	**end for**
Step 6	Find the training data set $D_{\boldsymbol{x}}$ that is the k nearest neighbor of $\boldsymbol{x}$
Step 7	Classify $\boldsymbol{x}$ into the majority group of $D_{\boldsymbol{x}}$, that is $y = argmax_v \sum_{(\boldsymbol{x}_i, y_i) \in D_{\boldsymbol{x}}} I(v = y_i)$
Step 8	**end for**

In this algorithm, when the test data $\boldsymbol{x}$ is classified into the majority group of the k-nearest neighbor data $D_{\boldsymbol{x}}$, the distance between $\boldsymbol{x}$ and neighbors $\boldsymbol{x}_i$ was not considered. A distance-weighted classification method can be used to compensate for this shortcoming, that has a weighting coefficient $\frac{1}{d(\boldsymbol{x},\boldsymbol{x}_i)^2}$ which is inversely proportional to the distance.

Example 7.3.1 Using the survey data in Example 7.1.2, classify a customer whose age is 33 years old and has a monthly income of 190 whether he will buy a product or not, using the 5-nearest neighbor classification model.

Answer

Age and monthly income have different measurement units, so they must be converted to the same unit. Here, the standardization transformation was used using the sample average of age 29.6 and its sample standard deviation of 5.623, and the sample average of monthly income 236.5, and sample standard deviation 95.547 as Table 7.3.1. The standardized value of the customer's data (33, 190) becomes (0.605, -0.487), and Table 7.3.1 shows the squared Euclidean distance between the customer data and all data. 5-nearest neighbors were colored as yellow background which included 3 of 'No's and 2 of 'Yes's. Therefore, the customer is classified into 'No" which means he will not purchase a product.

Table 7.3.1 Standardized data of age and income, and squared Euclid distance of the customer

Number	Age	Income (unit 10,000 won)	Purchase	Standardized Age	Standardized Income	Squared Euclid Distance of customer
1	25	150	Yes	-0.818	-0.905	2.199
2	34	220	No	0.782	-0.173	0.130
3	27	210	No	-0.462	-0.277	1.182
4	28	250	Yes	-0.285	0.141	1.185
5	21	100	No	-1.529	-1.429	5.441
6	31	220	No	0.249	-0.173	0.225
7	36	300	Yes	1.138	0.665	1.610
8	20	100	No	-1.707	-1.429	6.232
9	29	220	No	-0.107	-0.173	0.605
10	32	250	Yes	0.427	0.141	0.426
11	37	400	Yes	1.316	1.711	5.337
12	24	120	No	-0.996	-1.219	3.098
13	33	350	No	0.605	1.188	2.804
14	30	180	Yes	0.071	-0.591	0.296
15	38	350	Yes	1.494	1.188	3.595
16	32	250	No	0.427	0.141	0.426
17	28	240	No	-0.285	0.037	1.064
18	22	220	No	-1.352	-0.173	3.925
19	39	450	Yes	1.672	2.235	8.543
20	26	150	No	-0.640	-0.905	1.725

Selection of k on the neighbor classification

The selection of k in the nearest neighbor classification model is important for an accurate classification. The following module of eStatU makes it possible to search for a k value, which shows better accuracy, sensitivity or specificity on the nearest neighbor classification. k is selected when there is no significant increase in accuracy. Since the number of data is small in this example, it is not easy to decide k. If we select k = 5, eStat shows the classification result of all training data.

[Nearest neighbor classification]

K Nearest Neighbor Classification

Menu

Variable Name		Data Input
Y	Purchase	Yes,No,No,Yes,No,No,Yes,No,No,Yes,Yes,No,No,Yes,Yes,No,No,No,Yes,No
X_1	Age	25,34,27,28,21,31,36,20,29,32,37,24,33,30,38,32,28,22,39,26
X_2	Income	150,220,210,250,100,220,300,100,220,250,400,120,350,180,350,250,240,220,45(
X_3		
X_4		
X_5		

Nearest Neighbor (•) Search K (max=n/20 or 20) ( ) Fixed K = 5

[x] **Data standardization** **Distance measure** (•) $(Euclid)^2$ ( ) Manhattan

Data partition (Train 100 % : Test 0 %)

Execute | Scatter Plot Matrix | Parallel Graph | Erase Data

Graph Save | Classification Table | Table Save

Characteristics of the neighbor classification model

The characteristics of the nearest neighbor classification model are summarized as follows.

1) The nearest neighbor classification method is based on the data to be classified, so it does not require a special model, and only requires a measurement of the similarity between this data and the training data. If the training data increases, it takes a lot of time and effort to calculate the similarity measure, and, if an appropriate similarity measure is not used, the classification may not be accurate.
2) The nearest neighbor classification method classifies only using local information of the nearest neighbors of the data to be classified, so if k is small and there is much noise in the data, the classification may not be accurate.
3) Since the decision boundary determined by the nearest neighbor classification method is not a function, it is more flexible than the straight or rectangular classification boundary of a decision tree or other models. However, a boundary that is too dependent on the training data may not help the stability of the classification. The number of nearest neighbors should be increased or a distance-weighted classification method should be considered to prevent this problem.

7.3.1 R practice – Nearest neighbor classification

To use k-nearest neighbor (KNN) classification using R, we need to install a package called **DMwR2**. From the main menu of R, select 'Package' => 'Install package(s)', and a window called 'CRAN mirror' will appear. Here, select '0-Cloud [https]' and click 'OK'. Then, when the window called 'Packages' appears, select 'DMwR2' and click 'OK'. General usage and key arguments of the function are described in the following table.

k-nearest neighbor classification model. **This function provides a formula interface to the existing knn() function of package class. On top of this type of convinient interface, the function also allows standardization of the given data.**	
kNN(form, train, test, stand = TRUE, stand.stats = NULL, ...)	
form	An object of the class formula describing the functional form of the classification model.
train	The data to be used as training set.

test	The data set for which we want to obtain the k-NN classification, i.e. the test set.
stand	A boolean indicating whether the training data should be previously normalized before obtaining the k-NN predictions (defaults to TRUE).
stand.stats	This argument allows the user to supply the centrality and spread statistics that will drive the standardization. If not supplied they will default to the statistics used in the function scale(). If supplied they should be a list with two components, each beig a vector with as many positions as there are columns in the data set. The first vector should contain the centrality statistics for each column, while the second vector should contain the spread statistc values.

An example of R commands for a k-neares neighbor classification with customer data as both training and testing when k= 5 is as follows.

```
> install.packages('DMwR2')
```
copy r command

```
> library(DMwR2)
```
copy r command

```
> customer <- read.csv('PurchaseAgeIncome_Continuous.csv', header=T, as.is=FALSE)
```
copy r command

```
> attach(customer)
```
copy r command

```
> Purchase
  [1] Yes No  No  Yes No  No  Yes No  No  Yes Yes No  No  Yes Yes No  No  No  Y
es
 [20] No
Levels: No Yes
```
copy r command

```
> nn <- kNN(Purchase ~ ., customer, customer, k=5)
```
copy r command

```
> nn
  [1] No  No  No  No  No  No  Yes No  No  No  Yes No  Yes No  Yes No  No  No
Yes No
Levels: No Yes
```
copy r command

To make a classification cross table, we can use a vector of Purchase and nn which is the predicted class with table command as below. Using this classification table, accuracy of the model is calculated as 0.75 which is (11+4) / (11+1+4+4).

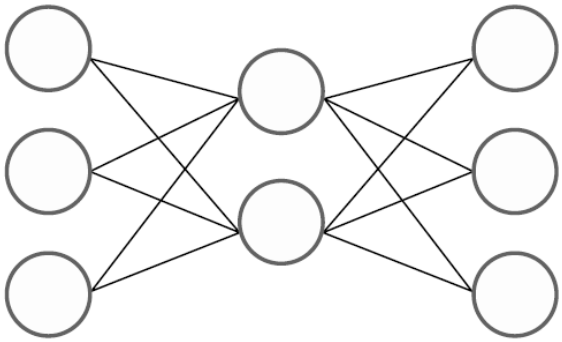
```
> classtable <- table(Purchase, nn)
Purchase No Yes
     No  10   2
     Yes  4   4
```
copy r command

```
> sum(diag(classtable)) / sum(classtable)
[1] 0.75
```
copy r command

7.4 Artificial neural network model

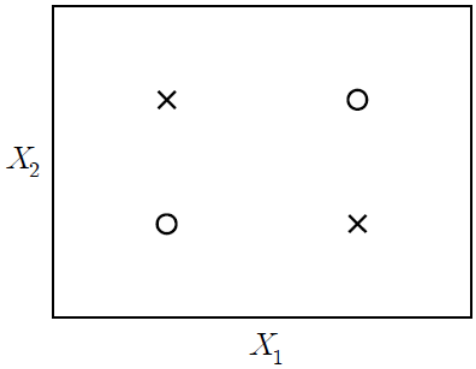
The **artificial neural network** model is a model that imitates the way the human brain makes decisions and classifies them. It is said that the human brain is composed of a neural network in which 10^{11} neurons are connected to each other. When one neuron is stimulated, this stimulation is transmitted to other neurons and the information held by multiple neurons is synthesized to make a decision. The neural network model connects

multiple nodes into a network similar to the human brain and makes decisions to classify data, as in <Figure 7.4.1>.



<Figure 7.4.1> Neural network model connects multiple nodes into a network

The artificial neural network model is a model that uses a generalized nonlinear function as a classification function. The motivation for studying this model is the simple two-group (denoted as o and x) two-dimensional data as in <Figure 7.4.2>. This data cannot be separated into two groups o and x by a single straight line (not linearly separable), and can only be separated by two straight lines or nonlinear functions.



<Figure 7.4.2> Two-dimensional data which cannot be separated into two groups o and x by a single straight line

There are many types of nonlinear functions for classification, so many studies have been conducted on classification models using generalized nonlinear functions. In 1957, Rosenbalatt of Cornell Aeronautical Laboratory in the United States used a **single-layer neural network** model called a **perceptron** for character recognition. However, this perceptron could only solve linear problems, so it did not receive much attention. In 1969, Minsky and Papert of MIT developed a **multilayer neural network** model that introduced a hidden layer to the perceptron neural network and showed that classification was possible with a generalized nonlinear function. In 1982, Hopefield developed a **back-propagation algorithm** that could effectively estimate the weight coefficients of a multilayer neural network. Since then, computer performance has improved, making it easier to estimate weight coefficients using the back-propagation algorithm, and neural network models have been widely used in real-world problems. In Section 7.4.1, a single-layer neural network model is introduced to understand neural network models, and in Section 7.4.2, a multilayer neural network model is explained.

7.4.1 Single-layer neural network

To understand the artificial neural network model, Let us look at the following single-layer neural network example.

Example 7.4.1 (Single-layer neural network)
Suppose y is a group variable where there are two groups, denoted '+1' and '-1', and there are three binary variables x_1, x_2, x_3 which have values either 0 or 1. If two or more of the three binary variables have the value 1, classify them as the group '+1', and if they have one or fewer 1 value, classify them as the group '-1' as in Table 7.4.1. Create a single-layer neural network model that can perform such classification and classify this data.

Table 7.4.1 Possible values of three binary variables x_1, x_2, x_3 and their group y

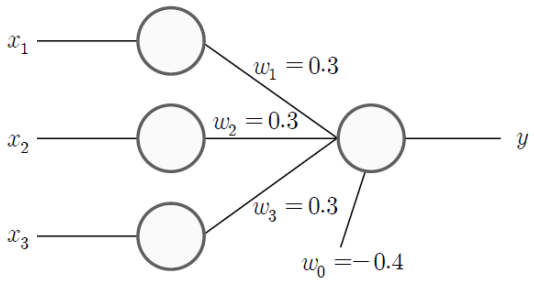
Number	x_1	x_2	x_3	y
1	0	0	0	-1
2	0	0	1	-1
3	0	1	0	-1
4	0	1	1	+1
5	1	0	0	-1
6	1	0	1	+1
7	1	1	0	+1
8	1	1	1	+1

Answer

If the predicted value of the group is $\hat{y}$, the above data can be classified using the following linear function model.

$$\hat{y} = \begin{cases} +1 & if\ \ 0.3x_1 + 0.3x_2 + 0.3x_3 - 0.4 > 0 \\ -1 & if\ \ 0.3x_1 + 0.3x_2 + 0.3x_3 - 0.4 < 0 \end{cases}$$

For example, if $x_1 = 1,\ x_2 = 1,\ x_3 = 0$, then $0.3x_1 + 0.3x_2 + 0.3x_3 - 0.4 = 0.2$, so $\hat{y}$ = +1. If $x_1 = 0,\ x_2 = 1,\ x_3 = 0$, then $0.3x_1 + 0.3x_2 + 0.3x_3 - 0.4 = -0.1$, so $\hat{y}$ = -1. Let us put aside the discussion of how to create such a linear classification model for a moment and if we represent the above model as a neural network in an easy-to-understand way, it is as in <Figure 7.4.3>. This is called a **single-layer neural network** or **perceptron**.



<Figure 7.4.3> Single layer neural network which is a linear classification model

As you can see in the figure, there is an **input node** to display the value of three variables $x_1,\ x_2,\ x_3$ and the **output node** of the model to display the value of the group variable y. The nodes are also called **neurons** in neural networks as the human brain. Each input node is connected to the output node with a weight coefficient, which describes the connections between neurons in the brain. Just as neurons in the brain can learn and make decisions, neural networks use data to train the optimal weight coefficients (in the figure, $w_1 = 0.3, w_2 = 0.3, w_3 = 0.3$) that connect the relationship between input nodes and output nodes. The output node of the neural network calculates the value $\hat{y}$ of the group by adding a constant $w_0 = -0.4$ to the linear combination using the weight coefficients of each input node to calculate the value $w_0 + w_1x_1 + w_2x_2 + w_3x_3$, which is called a **linear combination function**. The constant w_0 is called a **bias factor**. The sign function $sign(x)$ is used to investigate the sign of the calculated linear combination function value which is called an **activation function**.

In general, when there are m variables $x_1, x_2, \ldots, x_m$ and the weighting coefficients for each variable are $w_1, w_2, \ldots, w_m$ and the constant term (bias) is w_0, the classification function of a single-layer neural network model, such as Example 7.4.1, can be expressed as a nonlinear function as follows.

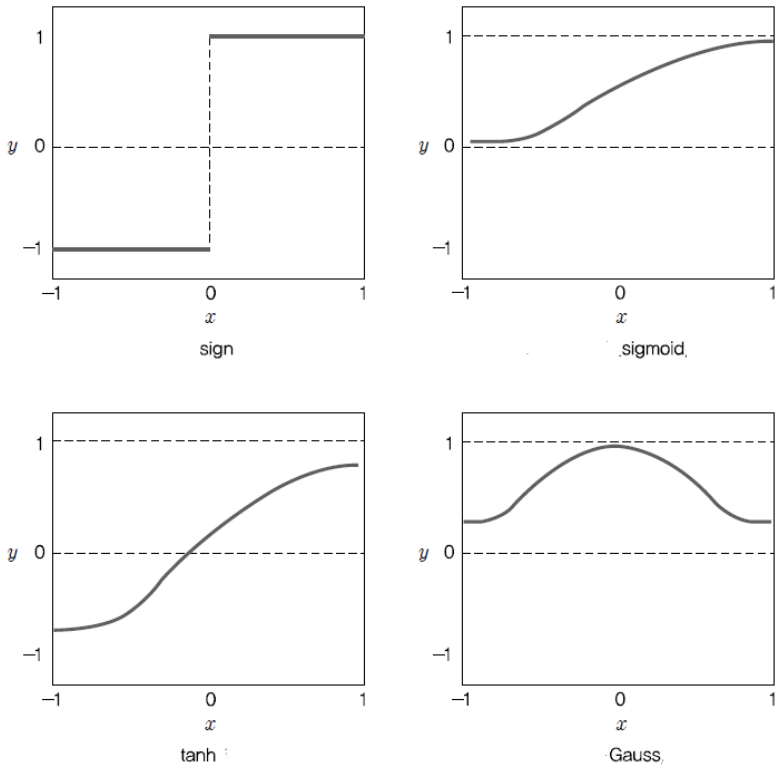
$$\hat{y} = sign(w_0 + w_1x_1 + w_2x_2 + \cdots + w_mx_m)$$

Here, the linear combination (or weighted sum) of each variable $w_0 + w_1x_1 + w_2x_2 + \cdots + w_mx_m$ is called a **combination function**. The sign function, $sign(x)$ that has a value of +1 when x is positive and a value of -1 when x is negative, is called an **activation function**. The activation function is a function that converts the input combination function value back into a certain range of values. The classification function of single-layer neural network is a composite function of a linear combination function with the sign function.

In the example above, a weighted sum of input information was used as the combination function, but there are other combination functions such as simple sums of input information, maximum values, minimum values, or logical ANDs and ORs, but the weighted sum is the most commonly used. In addition to the sign function $sign(x)$, examples of frequently used activation functions are as in Table 7.4.2, and <Figure 7.4.4> shows shapes of these activation functions.

Table 7.4.2 Examples of activation functions

Name	Activation fuction	Range
$sign$ function	$y = sign(x)$	-1, +1
$sigmoid$ fuction	$y = \frac{1}{1+e^{-x}}$	(0, 1)
$tanh$ function	$y = \frac{e^x - e^{-x}}{e^x + e^{-x}}$	(-1, 1)
$Gauss$ function	$y = e^{-\frac{x^2}{2}}$	(0, 1)



<Figure 7.4.4> Shapes of activation functions

The sigmoid function, which is widely used as an activation function, converts the input value to a value between (0,1). This function has little effect on the value of y when the value of x is very large or very small. When the sigmoid function $y = \frac{1}{1+e^{-x}}$ is differentiated, it has the following good property.

$$\begin{aligned} y' &= \frac{e^{-x}}{(1+e^{-x})^2} \\ &= \frac{1}{1+e^{-x}}(1 - \frac{1}{1+e^{-x}}) \\ &= y(1-y) \end{aligned}$$

It means that the differentiation of the sigmoid function y can be easily calculated as $y(1-y)$. Because of this property of the sigmoid function, it is widely used in optimization problems to obtain the rate of change easily.

Learning algorithm for single layer neural network

In the classification function of the single-layer neural network model, estimating the weight coefficients, $w_1, w_2, \ldots, w_m$ and the constant term w_0 is called a **learning** of the neural network. Let n training data be $D = \{(x_{i1}, x_{i2}, \ldots, x_{im}, y_i),\ i = 1, 2, \ldots, n\}$ and $w_1^{(i)}, w_2^{(i)}, \ldots, w_m^{(i)}$ be the ith iteration estimated values of the weight coefficients. The weight coefficients of the single-layer neural network are estimated using an iterative search algorithm as follows.

[Learning algorithm for the single-layer neural network]

Step 1	Let $D = \{(x_{i1}, x_{i2}, \ldots, x_{im}, y_i),\ i = 1, 2, \ldots, n\}$ be the training data
Step 2	$w_1^{(0)}, w_2^{(0)}, \ldots, w_m^{(0)}$ be the initial estimated value of the coefficients and λ is the learning rate
Step 3	**for** i = 1 to n **do**
Step 4	**for** j = 1 to m **do**
Step 5	Estimate $y_i^{(i)}$ using $w_1^{(i-1)}, w_2^{(i-1)}, \ldots, w_m^{(i-1)}$
Step 6	$w_j^{(i)} = w_j^{(i-1)} + \lambda(y_i - y_i^{(i)})x_{ij}$
Step 7	**end for**
Step 8	**end for**

In step 2 of the algorithm, the initial values of the weight coefficients $w_1^{(0)}, w_2^{(0)}, \ldots, w_m^{(0)}$ usually use random numbers between 0 and 1. λ is called a **learning rate** and has a value between 0 and 1. If the learning rate is close to 1, the estimated value changes a lot, and if it is close to 0, the estimated value changes slowly. In step 5, $y_i^{(i)}$ is the estimated value when the group value y_i is estimated i times repeatedly. When this algorithm is repeated as many times as the number of data ($i = 1, 2, \ldots, n$), we say that 'the neural network has been trained'. In step 6, the search algorithm for weight coefficients such as $w_j^{(i)} = w_j^{(i-1)} + \lambda(y_i - y_i^{(i)})x_{ij}$ can be intuitively easily understood. The ith estimate $w^{(i)}$ for the weight coefficient of x_j is obtained by adding a value proportional to the current prediction error $(y_i - y_i^{(i)})$ to the previous estimated weight coefficient $w_j^{(i-1)}$. If the prediction is accurate, $(y_i - y_i^{(i)})$ = 0, so the weight coefficient does not change. If the prediction is not accurate, for example, y_i = +1, $y_i^{(i)}$ = -1, then the prediction error $(y_i - y_i^{(i)})$ = 2, so in order to increase the estimated value, the weight coefficient of the input node with a positive value is increased, and the weight coefficient of the input node with a negative value is decreased. On the other hand, if y_i = -1, $y_i^{(i)}$ = +1, then the prediction error $(y_i - y_i^{(i)})$ = -2, so in order to reduce the estimated value, the weight coefficient of the input node with a negative value is increased, and the weight coefficient of the input node with a positive value is decreased.

The above search method is an algorithm that finds weighting coefficients which minimize the sum of square errors when the estimated value $\hat{y}_i$ for each data group is found using the linear combination function $w_0 + w_1x_1 + w_2x_2 + \cdots + w_mx_m$ and the sigmoid activation function. The sum of squared errors in a single-layer neural network with $m+1$ weighting coefficients $\boldsymbol{w} = (w_0, w_1, w_2, \ldots, w_m)$ is as follows.

$$E(\boldsymbol{w}) = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

In order to find $\boldsymbol{w} = (w_0, w_1, w_2, \ldots, w_m)$ that minimizes the sum of squared errors, we can differentiate $E(\boldsymbol{w})$ partially with respect to each w_j as follows.

$$\frac{\partial E(\boldsymbol{w})}{\partial w_j} = -2 \sum_{i=1}^{n} (y_i - \hat{y}_i) \frac{\partial \hat{y}_i}{\partial w_j}$$

Therefore, one way to search for the weight coefficient w_j that minimizes the sum of squared errors is to move in the direction of the partial derivatives as follows.

$$w_j \leftarrow w_j - \lambda \frac{\partial E(\boldsymbol{w})}{\partial w_j}$$

In the case of the linear combination function and sigmoid activation function, the algorithm for searching weight coefficients can be created as follows.

$$w_j \leftarrow w_j - \lambda (y_i - \hat{y}_i) x_{ij}$$

For more information on the algorithm, please refer to the relevant literature, and let us examine the learning of a single-layer neural network using the following example.

Example 7.4.2 For the single-layer neural network of Example 7.4.1, train the neural network with the initial values for the weight coefficients as $w_1^{(0)}$ = 0.2, $w_2^{(0)}$ = 0.1, $w_3^{(0)}$ = 0.1, the bias w_0 = -0.4, and the learning rate λ = 0.1.

Answer

Table 7.4.3 is the application of the learning algorithm to the single-layer neural network, which calculates the weighted linear combination $\boldsymbol{w}^{(i)} = w_0 + w_1^{(i-1)}x_1 + w_2^{(i-1)}x_2 + w_3^{(i-1)}x_3$ and the estimation of group value $\hat{y}_i = sign(\boldsymbol{w}^{(i)})$ using the given initial values.

Table 7.4.3 Application of learning algorithm to the sigle-layer neural network

iteration	data				linear combination function	activation function	modified coefficients		
i	x_{i1}	x_{i2}	x_{i3}	y_i	$\boldsymbol{w}^{(i)} = w_0 + w_1^{(i-1)}x_1 + w_2^{(i-1)}x_2 + w_3^{(i-1)}x_3$	$\hat{y}_i = sign(\boldsymbol{w}^{(i)})$	$w_1^{(i)}$	$w_2^{(i)}$	$w_3^{(i)}$
1	0	0	0	-1	-0.4	-1	0.2	0.1	0.1
2	0	0	1	-1	-0.3	-1	0.2	0.1	0.1
3	0	1	0	-1	-0.3	-1	0.2	0.1	0.1
4	0	1	1	+1	-0.2	-1	0.2	0.3	0.3
5	1	0	0	-1	-0.2	-1	0.2	0.3	0.3
6	1	0	1	+1	0.1	+1	0.2	0.3	0.3
7	1	1	0	+1	0.1	+1	0.2	0.3	0.3
8	1	1	1	+1	0.4	+1	0.2	0.3	0.3

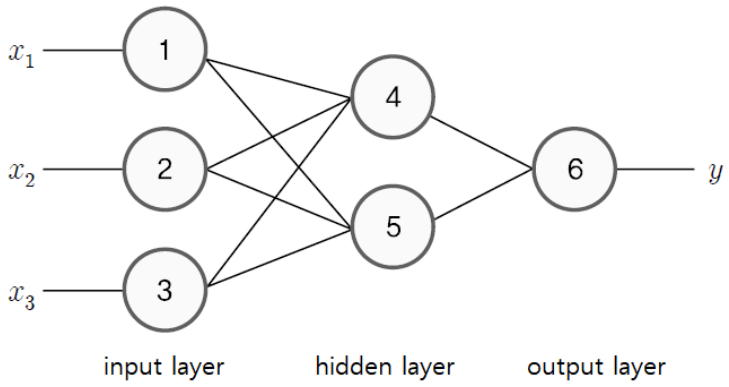
Looking at the table, if the actual group value y_i and the estimated value $\hat{y}_i$ are the same, there is no change in the weight coefficient (iterations 1, 2, and 3). In iteration 4, since the error is $(y_4 - \hat{y}_4)$ = 2, the weight coefficient of the variable with x_2 = 1 and x_3 = 1 is increased by $\lambda \times (y_4 - \hat{y}_4) \times x_{4j}$ = 0.2. Since the

other data have the same group value and predicted value, there is no change in the weight coefficient, so the estimated final weight coefficient is w_1 = 0.2, w_2 = 0.3, w_3 = 0.3. That is, the final neural network model is $\hat{y} = sign(-0.4 + 0.2x_1 + 0.3x_2 + 0.3x_3)$. If this estimation formula is applied to all data, the groups are accurately classified.

It should be noted that the estimation algorithm for the weight coefficients of a single-layer neural network can have different solutions depending on the initial value and learning rate. For example, if the initial values are the same and the learning rate is λ = 0.05, the final weight coefficients are w_1 = 0.2, w_2 = 0.25, w_3 = 0.25, and this solution also correctly classifies all data.

7.4.2 Multilayer neural network

The single-layer neural network model classifies data between two groups as a linear classification function. However, it is not suitable when the data cannot be classified as a linear function, as in <Figure 7.4.2>. In this case, a **multilayer neural network** model which classifies data using a nonlinear function is useful. <Figure 7.4.5> is an example of Example 7.4.1 expressed as a multilayer neural network. As shown in the figure, a multilayer neural network consists of an **input layer** consisting of input nodes, a **hidden layer** that is a set of intermediate nodes that synthesize the nodes of the input layer, and an **output layer** that synthesizes the nodes of the hidden layer. A neural network like <Figure 7.4.5> has only one hidden layer, but can create multiple hidden layers, and each layer can have multiple nodes, so various types of networks can appear.



<Figure 7.4.5> Example of multilayer neural network

The neural network in <Figure 7.4.5> can be expressed as a formula as follows. Let the weight coefficients from the input node ① to the hidden nodes ④ and ⑤ be w_{14} and w_{15}, let the weight coefficients from the input node ② to the hidden nodes ④ and ⑤ be w_{24} and w_{25}, and let the weight coefficients from the input node ③ to the hidden nodes ④ and ⑤ be w_{34} and w_{35}. In the same way, let the weight coefficient from the hidden node ④ to the output node ⑥ be w_{46}, and let the weight coefficient from the hidden node ⑤ to the output node ⑥ be w_{56}. And if the bias constants of nodes ④, ⑤, and ⑥ are w_{04}, w_{05}, w_{06} and the activation function is f_4, f_5, f_6, then the output values O_4 and O_5 calculated from hidden nodes ④ and ⑤ are as follows.

$$O_4 = f_4(w_{04} + w_{14}x_1 + w_{24}x_2 + w_{34}x_3)$$
$$O_5 = f_5(w_{05} + w_{15}x_1 + w_{25}x_2 + w_{35}x_3)$$

The value of the output node ⑥, i.e., the estimated value of y, is the value of the activation function for linear combination of O_4 and O_5 as follows.

$$\hat{y} = f_6(w_{06} + w_{46}O_4 + w_{56}O_6)$$

If we combine the above equations, the estimated value of y becomes the following complex nonlinear function.

$$\hat{y} = f_6(w_{06} + w_{46}f_4(w_{04} + w_{14}x_1 + w_{24}x_2 + w_{34}x_3) + w_{56}f_5(w_{05} + w_{15}x_1 + w_{25}x_2 + w_{35}x_3))$$

In the above example, if there are multiple hidden layers, more hidden nodes, and multiple output nodes, the nonlinear function that represents the final output becomes more complex. Therefore, the design of a multilayer neural network should always consider the following:

- How many hidden layers should there be?
- How many nodes should each hidden layer have?
- Is there a nonlinear function represented by these hidden layers and hidden nodes?

Let us assume that values of all variables, $\boldsymbol{x} = (x_1, x_2, \ldots, x_m)$, can be converted to values between [0,1]. The following theorem shows the existence of a nonlinear function represented by the multilayer neural network.

Theorem 7.4.1 Approximation of a continuous function (Kolmogorov)
When a continuous function $f(\boldsymbol{x})$ is defined on $[0,1]^m$, this function can be expressed as follows.

$$f(\boldsymbol{x}) = \sum_{k=1}^{2m+1} \Theta_k \left[\sum_{j=1}^{m} \phi_{jk}(x_j) \right]$$

Here, Θ_k and ϕ_{jk} are appropriately chosen functions.

This theorem can be interpreted as a neural network as follows. For the input nodes of variables $x_1, x_2, \ldots, x_m$, $(2m+1)$ hidden nodes receive the sum of nonlinear functions $\phi_{jk}(x_j)$. Each hidden node receiving this value outputs a nonlinear function Θ_k, and the final output node calculates the sum of these. In other words, assuming that there is a nonlinear function $y = f(\boldsymbol{x})$, this function can be approximated by a composite function of combination functions and activation functions, such as equation in the Theorem 7.4.1. A neural network model consisting of this complex approximation function is often called a black box. It is not known exactly how many hidden nodes can approximate the function $y = f(\boldsymbol{x})$ well.

Design of multilayer neural network model

The neural network model is experimented with various combinations of the number of hidden layers and the number of nodes through trial and error, and the general design method is as follows.

1) Data preparation
In the case of continuous variables, units of variables may be different, so the variable values are usually converted to be between 0 and 1. A simple conversion method is to subtract the minimum value from the actual data value and then divide it by the possible range of the variable (maximum value - minimum value). For ordinal variables, the smallest ordinal value is set to 0, the larger ordinal value is set to 1, and the ordinal values in between are converted proportionally. In the case of categorical variables, each category value is usually treated as one variable, and a binomial value of 0 or 1 is used depending on the presence or absence of the category value. It is desirable to have a certain number of data for each category value, but if the number of data is small, it is sometimes combined with adjacent category values. Missing values are either removed or replaced by estimating a value appropriate for the data.

2) Number of input nodes
If the variable is binomial or continuous data, assign one input node to each variable. If the variable is categorical, assign one input node to each categorical value.

3) Number of output nodes
If there are two groups, one output node is sufficient. If there are K groups, assign K output nodes.

4) Number of hidden layers and number of hidden nodes

Determining the number of hidden layers and number of hidden nodes is a problem of determining the nonlinear function of the neural network model. If the number of hidden layers and hidden nodes increases, the model may be overfitted, so if possible, it is good to have a model that can classify satisfactorily with a small number of hidden layers and hidden nodes. However, there is no exact method to find the optimal number of hidden layers and hidden nodes. Usually, after setting the number of hidden layers and hidden nodes sufficiently, we reduce them one by one and select a model with high accuracy and a small number of hidden layers and hidden nodes. At this time, model selection criteria such as AIC (Akaike information criteria) can be used.

If possible, it is good to obtain the classification function by setting the number of hidden layers to 1. However, if too many nodes are created in one hidden layer, the number of hidden layers is set to two, and the number of nodes in each layer is reduced. It is usually done so that the number of nodes in each layer does not exceed twice the number of nodes in the input layer. Experiments to determine the number of hidden layers and nodes take the most time in artificial neural network models.

5) Selection of activation function

Among the activation functions in Table 7.4.2, the sigmoid function, which is useful for the estimation algorithm of weight coefficients, is often used. The activation function is known to affect the algorithm speed during the training process of a neural network but does not have a significant effect on the results.

6) Initial value problem

Algorithms that estimate the weight coefficients of a multilayer neural network model require initial values, and most of them randomly generate values between -1 and 1. Since there is a possibility that a given initial value will find a local solution, it is necessary to experiment several times to find the same weight coefficients by trying various initial values.

7) Interpretation of output variables

If there are two groups and one output node, the output value is a continuous value, so it can be classified based on an appropriate boundary value. If there are multiple groups, the number of output nodes is usually the same as the number of groups, and the group is classified based on the value of the output node that is large (or small).

8) Sensitivity analysis

After obtaining the solution of the neural network using training data, it is a good idea to conduct sensitivity analysis to determine the relative importance of the input variables. Change the value of the input variable from the minimum to the maximum and examine the change in the output value.

Learning algorithm of multilayer neural networks

The process of estimating the weight coefficients of a multilayer neural network model is called learning of the neural network. Since a multilayer neural network is a complex nonlinear function model, estimating the weight coefficients is not easy. The learning algorithm for a single-layer neural network is not suitable for a multilayer neural network with a nonlinear function that has many weight coefficients. The estimation of the weight coefficients in a multilayer neural network uses the **gradient descent method**.

Let the input node values of a multilayer neural network with m input variables be $\boldsymbol{x} = (x_1, x_2, \ldots, x_m)$. Let the weight coefficient connecting node j to node k in the neural network be w_{jk}, the constant coefficient at this time be w_{0k}, and let all the weight coefficients appearing in this neural network be $\boldsymbol{w}$. The output of the neural network can be expressed as $\hat{y} = f(\boldsymbol{x} : \boldsymbol{w})$, where the function f is a composite function of several combination functions and activation functions as in Theorem 7.4.1. In order to find the weight coefficient $\boldsymbol{w}$ of the multilayer neural network, it is reasonable to minimize the distance $d(y_i, \hat{y}_i)$ between the observed group value y_i of all data and the estimated value $\hat{y}_i$ of the neural network. If we use the Euclidean square distance, we find the weight coefficient that minimizes the error sum of squares $E(\boldsymbol{w})$ as follows.

$$E(\boldsymbol{w}) = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

To find $\boldsymbol{w}$ that minimizes the error sum of squares, we differentiate $E(\boldsymbol{w})$ with respect to each w_{jk} as follows.

$$\frac{\partial E(\boldsymbol{w})}{\partial w_{jk}} = -2 \sum_{i=1}^{n} (y_i - \hat{y}_i) \frac{\partial \hat{y}_i}{\partial w_{jk}}$$

If $\hat{y}_i$ is estimated using the sigmoid activation function, the rate of change of the estimated value, $\frac{\partial \hat{y}_i}{\partial w_{jk}}$, is proportional to $\hat{y}_i(1 - \hat{y}_i)$ due to the differentiation characteristic of the sigmoid function. Therefore, we can create an algorithm to search for weight coefficients as follows.

$$w_{jk} \leftarrow w_{jk} - \lambda \frac{\partial E(\boldsymbol{w})}{\partial w_{jk}}$$

Here, λ is the learning rate, which has a value between 0 and 1. $\frac{\partial E(\boldsymbol{w})}{\partial w_{jk}}$ means the gradient descent rate, which implies that the estimation of weight coefficients should be adjusted in the direction that decreases the total error sum of squares. If the output value of input node j is O_j and the error at output node k is E_k, the above update of weight coefficients is as follows.

$$w_{jk} \leftarrow w_{jk} - \lambda E_k O_j$$

Here, $\lambda E_k O_j$ is the change amount of the weight coefficient, which is the same concept as the estimation of the weight coefficient of the single-layer neural network. That is, the weight coefficient is updated as a learning rate λ proportional to the input O_j from node j by considering the error E_k of node k. In a similar way, the bias constant w_{0k} is updated as follows.

$$w_{0k} \leftarrow w_{0k} - \lambda E_k$$

In this algorithm, the estimation of E_k and O_j is not easy when applied to the hidden nodes in the multilayer neural network model, so the **back-propagation algorithm** developed by Hopefield is used. The back-propagation algorithm sets a criterion for optimizing the initial weight coefficients and the objective function, and divides it into the forward step and the backward step to repeatedly update the weight coefficients. In the forward step, the estimated weight coefficients are used to calculate the output values of all nodes, and the output values of the nodes in the layer l are used to calculate the output values of the nodes in the layer $l + 1$. In the backward step, the output values and error values for the nodes in the calculated layer $l + 1$ are used to estimate the error values for the nodes in the layer l and the weight coefficients are updated. This method is repeatedly applied until the weight coefficients hardly change or the objective function value is optimized, and the algorithm is stopped.

When the sigmoid activation function is used in the multilayer neural network in <Figure 7.4.5>, let us estimate the weight coefficients by applying the back-propagation algorithm. First, the initial weight coefficients are used to obtain the output values $O_1, O_2, \ldots, O_6$ of each node. Here, O_1, O_2, O_3 are the values of the input variable x_1, x_2, x_3. The key is how to obtain the error E_k of each node. In the back-propagation algorithm, it is estimated by considering the weighted sum of the errors of all nodes connected to node k. In the case of a sigmoid function, the rate of change $\frac{\partial \hat{y}_i}{\partial w_{jk}}$ is proportional to $\hat{y}_i(1 - \hat{y}_i)$, so the error E_6 of the output node ⑥ is estimated as follows.

$$E_6 = O_6(1 - O_6)(y_i - O_6)$$

Here, $O_6(1 - O_6)$ denotes the rate of change $\hat{y}_i(1 - \hat{y}_i)$, and the $(y_i - O_6)$ term denotes the estimation error $(y_i - \hat{y}_i)$. That is, the meaning of the error E_6 is the estimation error $(y_i - O_6)$ multiplied by the error change rate $O_6(1 - O_6)$. The error E_5 of hidden node ⑤ is calculated by multiplying the error change rate $O_5(1 - O_5)$ by the weighted sum of errors of all nodes connected to node ⑤, which is called the back-propagation of the error. That is,

$$E_5 \;=\; O_5(1-O_5)\sum_k w_{5k}E_k$$

After calculating the error E_4 of hidden node ④ in a similar way, the weight coefficients are updated. Let us look at the back-propagation algorithm for estimating the weight coefficient of a multilayer neural network through the following example.

Example 7.4.3 (Learning algorithm of the multilayer neural network)
For the multilayer neural network model in Figure 7.4.5, let the input data be group 1 and the variable values be (x_1, x_2, x_3) = (1, 0, 1). Let us find the weight coefficient and bias of the model equation using the back-propagation algorithm of the gradient descent method. The same sigmoid function, f(x), is used for all activation functions, and the initial values of the weight coefficient and bias are set as follows using a random number between (-1,1). Let the learning rate be λ = 0.1.

Table 7.4.4 Initial values of the weight coefficients for the multilayer neural network in Figure 7.4.5

w_{14}	w_{15}	w_{24}	w_{25}	w_{34}	w_{35}	w_{46}	w_{56}	w_{04}	w_{05}	w_{06}
-0.51	-0.99	0.35	-0.45	0.39	0.19	0.27	0.71	-0.75	-0.09	0.18

Answer

The forward step of the back-propagation algorithm calculates the output values of all nodes using the given initial values. In the neural network of <Figure 7.4.5>, the output values O_1, O_2, O_3 of nodes ①, ②, and ③ are the values of the input variables x_1, x_2, x_3, and the output valuesof nodes ④, ⑤, and ⑥ are as follows, using the given initial weight coefficients.

$$\begin{aligned}
O_4 &= f(w_{14}x_1 + w_{24}x_2 + w_{34}x_3 + w_{04}) \\
&= f(-0.51\times 1 \;+\; 0.35\times 0 \;+\; 0.39\times 1 \;-\; 0.75 \\
&= f(-0.87) = 0.2953 \\
O_5 &= f(w_{15}x_1 + w_{25}x_2 + w_{35}x_3 + w_{05}) \\
&= f(-0.99\times 1 \;-\; 0.45\times 0 \;+\; 0.19\times 1 \;-\; 0.09 \\
&= f(-0.89) = 0.2911 \\
O_6 &= f(w_{46}O_4 + w_{56}O_6 + w_{06}) \\
&= f(0.27\times 0.2953 \;+\; 0.71\times 0.2911 \;+\; 0.18 \\
&= f(0.4664) = 0.6145
\end{aligned}$$

The backward step of the back-propagation algorithm first estimates the error E_6 of node ⑥, and then estimates the errors of nodes ④ and ⑤. The estimation of the error E_6 of node ⑥ is as follows.

$$\begin{aligned}
E_6 \;&=\; O_6(1-O_6)(y_i - O_6) \\
&=\; 0.6145\times(1-0.6145)\times(1-0.6145) = 0.0913
\end{aligned}$$

Here, the $O_6(1-O_6)$ term is the rate of change from the differentiation of the sigmoid function and y is the actual group value. The meaning of the error E_6 is the estimation error, $y_i - O_6$, multiplied by the error change rate $O_6(1-O_6)$. The error E_5 of hidden node ⑤ is calculated by multiplying the error change rate $O_5(1-O_5)$ by the error weighted sum of all nodes connected to node ⑤, which is called back-propagation of the error. That is,

$$E_5 \;=\; O_5(1-O_5)\sum_k w_{5k}E_k$$

In this problem, since there is only node ⑥ connected to node ⑤, E_5 is as follows. The error E_4 of node ④ is also calculated in the same way.

$$\begin{aligned}
E_5 \;&=\; O_5(1-O_5)w_{56}E_6) \\
&=\; 0.2911\times(1-0.2911)\times 0.71\times 0.0913 = 0.0134 \\
E_4 \;&=\; O_4(1-O_4)w_{46}E_6) \\
&=\; 0.2953\times(1-0.2953)\times 0.27\times 0.0913 = 0.0051
\end{aligned}$$

Therefore, the updated weight coefficients and biases are as follows.

$$
\begin{aligned}
w_{46} &\leftarrow w_{46} + \lambda E_6 O_4 = 0.27 + 0.1 \times 0.0913 \times 0.2953 = 0.2727 \\
w_{56} &\leftarrow w_{56} + \lambda E_6 O_5 = 0.71 + 0.1 \times 0.0913 \times 0.2911 = 0.7127 \\
w_{14} &\leftarrow w_{14} + \lambda E_4 x_1 = -0.51 + 0.1 \times 0.0051 \times 1 = -0.5095 \\
w_{15} &\leftarrow w_{15} + \lambda E_5 x_1 = -0.99 + 0.1 \times 0.0134 \times 1 = -0.9887 \\
w_{24} &\leftarrow w_{24} + \lambda E_4 x_2 = +0.35 + 0.1 \times 0.0051 \times 0 = 0.3500 \\
w_{25} &\leftarrow w_{25} + \lambda E_5 x_2 = -0.99 + 0.1 \times 0.0134 \times 0 = -0.4500 \\
w_{34} &\leftarrow w_{34} + \lambda E_4 x_3 = +0.39 + 0.1 \times 0.0051 \times 1 = 0.3905 \\
w_{35} &\leftarrow w_{35} + \lambda E_5 x_3 = +0.19 + 0.1 \times 0.0134 \times 1 = 0.1913 \\
w_{04} &\leftarrow w_{04} + \lambda E_4 = -0.75 + 0.1 \times 0.0051 = -0.7495 \\
w_{05} &\leftarrow w_{06} + \lambda E_5 = -0.09 + 0.1 \times 0.0134 = -0.0887 \\
w_{06} &\leftarrow w_{06} + \lambda E_6 = +0.18 + 0.1 \times 0.0913 = 0.1891
\end{aligned}
$$

In the back-propagation algorithm, it should be noted that the estimation of weight coefficients can vary depending on the initial value and learning rate. If the learning rate λ is increased, the weight coefficients change quickly, and if the learning rate is decreased, the weight coefficients change slowly. It is recommended to conduct experiments with a high learning rate at first, and then gradually conduct experiments with a lower learning rate. Usually, a learning rate value between 0.05 and 0.7 is often used.

When the back-propagation algorithm is repeated as many times as the number of data, it is said that the 'neural network has learned', but if the neural network is complex, the global optimal solution of the objective function may not be obtained, but a local optimal solution may be obtained, so caution is required. In algorithms that handle nonlinear functions, the final solution may be a local optimal value or a global optimal value depending on the initial value, so experiments should be conducted repeatedly through trial and error. Usually, as an initial value, a random number is selected from a uniform distribution in a certain area, and after an experiment, the initial value that shows the best result is selected.

Deep learning

If there are many hidden layers in a multilayer neural network, the back-propagation algorithm often cannot find the weight coefficients successfully because of vanishing gradients where data disappears and learning does not proceed well. However, in 2006, Professor Geoffrey Hinton of the University of Toronto solved the vanishing gradient problem through the pretraining of neural networks and drop-out data, and began calling the neural network model that applied this algorithm as **deep learning**. This algorithm is beyond the scope of this book and please refer related references.

Characteristics of neural network models

The characteristics of neural network models are summarized as follows.

1) In real data for classification, neural network models are evaluated to show somewhat better results than other models. In particular, they are more useful when the number of variables is large and the input and output variables have complex nonlinear function forms.
2) Since it is not easy to explain why the neural network model was classified that way for the classification results, this model is sometimes called a black box. The difficulty in interpreting the model can be considered a disadvantage of neural networks because it can be difficult to modify the model.
3) Multilayer neural networks estimate nonlinear classification functions and require at least one hidden layer. Determining the appropriate number of hidden layers and hidden nodes is very important to avoid overfitting the model. Neural network models show satisfactory results in training data, but in actual applications, classification is sometimes inaccurate. This is mainly due to overfitting of the model.
4) Neural networks do not show a sensitive response even if there is noise in the training data. Therefore, it is not easy to identify errors in input information.
5) The gradient descent method used to estimate the weight coefficients of neural networks can find local solutions. Therefore, it is necessary to investigate whether it is a local solution or not by various methods such as changing the initial value or analyzing the sensitivity of the data.

6) The training process of a neural network is a very time-consuming task when the number of hidden layers and nodes is large. However, after training, test data can be classified quickly.

7.4.3 R practice - Neural network

To use the neural network model using R, we need to install a package called **nnet**. From the main menu of R, select 'Package' => 'Install package(s)', and a window called 'CRAN mirror' will appear. Here, select '0-Cloud [https]' and click 'OK'. Then, when the window called 'Packages' appears, select 'nnet' and click 'OK'. 'nnet' is a package for modeling of the neural network classification model. General usage and key arguments of the function are described in the following table.

nnet {nnet}	**Fit Neural Networks** **Fit single-hidden-layer neural network, possibly with skip-layer connections.**
## S3 method for class 'formula' **nnet(formula, data, weights, ..., subset, na.action, contrasts = NULL)** **## Default S3 method:** **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, ...)**	
formula	A formula of the form class ~ x1 + x2 + ...
x	matrix or data frame of x values for examples.
y	matrix or data frame of target values for examples.
weights	(case) weights for each example – if missing defaults to 1.
size	number of units in the hidden layer. Can be zero if there are skip-layer units.
data	Data frame from which variables specified in formula are preferentially to be taken.
subset	An index vector specifying the cases to be used in the training sample.
na.action	A function to specify the action to be taken if NAs are found. The default action is for the procedure to fail. An alternative is na.omit, which leads to rejection of cases with missing values on any required variable.
contrasts	a list of contrasts to be used for some or all of the factors appearing as variables in the model formula.
Wts	initial parameter vector. If missing chosen at random.
mask	logical vector indicating which parameters should be optimized (default all).
linout	switch for linear output units. Default logistic output units.
entropy	switch for entropy (= maximum conditional likelihood) fitting. Default by least-squares.
softmax	switch for softmax (log-linear model) and maximum conditional likelihood fitting. linout, entropy, softmax and censored are mutually exclusive.
censored	A variant on softmax, in which non-zero targets mean possible classes. Thus for softmax a row of (0, 1, 1) means one example each of classes 2 and 3, but for censored it means one example whose class is only known to be 2 or 3.
skip	switch to add skip-layer connections from input to output.
rang	Initial random weights on [-rang, rang]. Value about 0.5 unless the inputs are large, in which case it should be chosen so that rang * max(|x|) is about 1.
decay	parameter for weight decay. Default 0.
maxit	maximum number of iterations. Default 100.

Hess	If true, the Hessian of the measure of fit at the best set of weights found is returned as component Hessian.
trace	switch for tracing optimization. Default TRUE.
MaxNWts	The maximum allowable number of weights. There is no intrinsic limit in the code, but increasing MaxNWts will probably allow fits that are very slow and time-consuming.
abstol	Stop if the fit criterion falls below abstol, indicating an essentially perfect fit.
reltol	Stop if the optimizer is unable to reduce the fit criterion by a factor of at least 1 - reltol.

An example of R commands for the single-layer neural network model using the data as in Example 7.4.2 is as follows.

> install.packages('nnet') copy r command

> library(nnet) copy r command

> singleNNdata <- read.csv('singleNN.csv', header=T, as.is=FALSE) copy r command

> attach(signleNNdata) copy r command

> singleNNdata copy r command

```
  x1 x2 x3 y
1  0  0  0 -1
2  0  0  1 -1
3  0  1  0 -1
4  0  1  1  1
5  1  0  0 -1
6  1  0  1  1
7  1  1  0  1
8  1  1  1  1
```

```
# create a training data using the 8 data.
> train <- singleNNdata[1:8,]
```
copy r command

```
# create a testing data using the same 8 data
> test <- singleNNdata[1:8,]
```
copy r command

> train.nnet <- nnet(y~x1+x2+x3,data=train, size=2, rang=0.1, decay=5e-4, maxit=100) copy r command

```
# weights:  11
initial  value 10.068006
iter  10 value 7.626637
iter  20 value 4.217955
iter  30 value 4.133499
iter  40 value 4.129743
iter  50 value 4.129625
iter  60 value 4.129609
iter  70 value 4.129607
iter  80 value 4.129601
final  value 4.129595
converged
```

```
> summary(train.nnet)
```

copy r command

```
a 3-2-1 network with 11 weights
options were - decay=5e-04
 b->h1 i1->h1 i2->h1 i3->h1
  4.14  -3.06  -3.06  -3.06
 b->h2 i1->h2 i2->h2 i3->h2
  4.05  -3.01  -3.01  -3.01
 b->o h1->o h2->o
 4.63 -7.37 -7.17
```

In the summary, 3-2-1 network implies that there are 3 input layers (i1, i2, i3) - 2 hidden layers (h1, h2) - 1 output layer (o). There are 11 weights and b->h1 implies the bias constant to the hidden layer h1 which is 4.14. i1->h1 implies the weight coefficient from input layer i1 to the hidden layer h1 which is -3.06 etc. Therefore, the linear combination function to h1 is 4.14 - 3.06 × i1 - 3.06 × i2 - 3.06 × i3, the linear combination function to h2 is 4.05 - 3.01 × i1 - 3.01 × i2 - 3.01 × i3, and the linear combination function to o is 4.63 - 7.37 × h1 - 7.17 × h2.
The R command to classify the groups by testing all 8 data using the above model is as follows. First, if we classify the test data using the predict command with default activation function, the result will be a number.

```
> predict(train.nnet,test)
```

copy r command

```
          [,1]
1 0.0000619568
2 0.0020718984
3 0.0020859221
4 0.9453979298
5 0.0020719570
6 0.9452023418
7 0.9453977511
8 0.9893836166
```

If we observe this and classify the data using 0.1 as the reference value, all data will be classified accurately.

```
> nnetpred <- (predict(train.nnet,test) >= 0.01)
```

copy r command

```
> table(nnetpred,y)
```

copy r command

```
        y
nnetpred -1 1
   FALSE  4 0
   TRUE   0 4
```

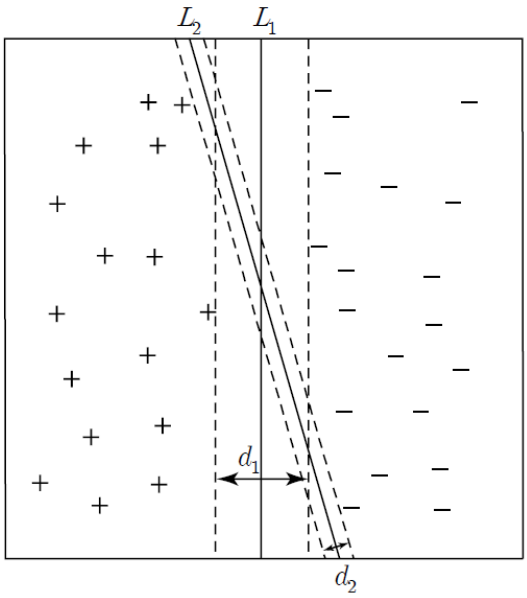
7.5 Support vector machine model

Support vector machine (SVM) model determines a classification function, called a support vector, using training data. The SVM model has recently attracted attention and has been applied in many fields. The SVM model is divided into the **linear SVM** that uses a linear classification function and the **nonlinear SVM** that uses a nonlinear classification function.

7.5.1 Linear support vector machine

Consider the two-dimensional training data for two groups, indicated as '+' and '-' group, as in <Figure 7.5.1>. In this data, the two groups can be classified well without misclassification using a single straight line, but there are too many possible straight lines that can accurately classify two groups. Therefore, we need to consider which straight line can lead to less misclassification of the test data. Let us compare the two straight lines L_1 and L_2 in

the figure. L_1 is a straight line that bisects the point on the far right of the '+' group and the point on the far left of the '-' group on the x-axis, and the distance between the straight lines passing through the two points is d_1. L_2 is a straight line that bisects the point on the far right of the '+' group and the point on the far left of the '-' group, and the distance between the straight lines passing through the two points is d_2. If these two straight lines are used to classify the test data, the distance (margin) d_1 is larger than the distance d_2, so L_1 has less possibility of misclassification in actual classification. Linear SVM is a method to determine a linear classification function so that the distance, such as d_1, is maximized.



<Figure 7.5.1> Comparison of two lines for classification
The distance d_1 of L_1 is larger than d_2 of L_2, so L_1 has less possibility of misclassification.

Linear SVM can be explained by dividing the data of two groups into cases where they can be linearly separable using a linear classification function as shown in <Figure 7.5.1> and cases where they cannot be linearly separable.

A. Linearly separable case

Suppose that there are two groups denoted '+1' and '-1' groups, m independent variables $\boldsymbol{x} = (x_1, x_2, \ldots, x_m)$ and a targent (group) variable y. The n training data observed for these variables are denoted as $D = \{(\boldsymbol{x}_i, y_i),\ i = 1, 2, \ldots, n\}$ using vector notation, where $\boldsymbol{x}_i = (x_{i1}, x_{i2}, \ldots, x_{im})$ and the target variable y_i can have a value of +1 or -1. The linear classification equation for m variables is expressed as follows.

$$w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_m x_m = 0$$

This is a general hyperplane equation in m-dimensional space, and $w_0, w_1, w_2, \ldots, w_m$ are the parameters to be estimated. Using a vector notation $\boldsymbol{w} = (w_1, w_2, \ldots, w_m)$ and an inner product notation, $\cdot$, of vectors, the above equation can be expressed as follows.

$$\boldsymbol{w} \cdot \boldsymbol{x} + w_0 = 0$$

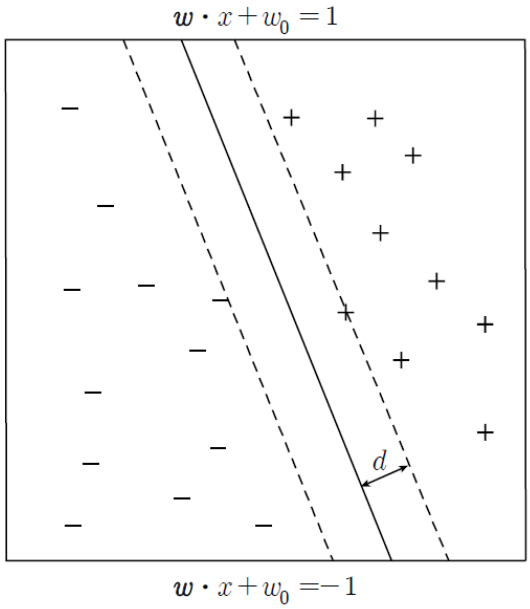
If the data $\boldsymbol{x}_i$ is on this hyperplane, then $\boldsymbol{w} \cdot \boldsymbol{x}_i + w_0 = 0$. If the data $\boldsymbol{x}_i$ is above the hyperplane, then $\boldsymbol{w} \cdot \boldsymbol{x}_i + w_0 > 0$, and if it is below the hyperplane, then $\boldsymbol{w} \cdot \boldsymbol{x}_i + w_0 < 0$. If the value of w_0 is adjusted appropriately, the classification formula that distinguishes the two groups can be written as follows.

$$\begin{aligned} &\text{if } \boldsymbol{w} \cdot \boldsymbol{x} + w_0 \geq 1, \quad \text{classify } \boldsymbol{x} \text{ into } y = 1 \\ &\text{if } \boldsymbol{w} \cdot \boldsymbol{x} + w_0 \leq -1, \quad \text{classify } \boldsymbol{x} \text{ into } y = -1 \end{aligned}$$

Here, $\boldsymbol{w} \cdot \boldsymbol{x}_i + w_0 = 1$ is a hyperplane passing through the points on the boundary of the group $y = +1$, and $\boldsymbol{w} \cdot \boldsymbol{x}_i + w_0 = -1$ is a hyperplane passing through the points on the boundary of the group $y = -1$. These two hyperplanes are called **support vectors**, and the distance d between the two groups is the distance between these two hyperplanes. The classification equation above, which applies to data, can be expressed as follows.

$$y_i \left(\boldsymbol{w} \cdot \boldsymbol{x}_i + w_0 \right) \geq 1, \quad i = 1, 2, \ldots, n$$

As shown in <Figure 7.5.2>, there can be multiple hyperplanes that can classify the two groups in data and the one that has the largest distance of margin between the data on the boundaries of the two groups on the hyperplane can minimize misclassification error.



<Figure 7.5.2> A hyperplane that can classify two groups in data.
The hyperplane that maximizes the distance (margin d) is likely to have less misclassification in actual classification.

If $\boldsymbol{x}_1$ lies in the hyperplane $\boldsymbol{w} \cdot \boldsymbol{x}_i + w_0 = 1$, then $\boldsymbol{w} \cdot \boldsymbol{x}_1 + w_0 = 1$, and if $\boldsymbol{x}_2$ lies in the hyperplane $\boldsymbol{w} \cdot \boldsymbol{x}_i + w_0 = -1$, then $\boldsymbol{w} \cdot \boldsymbol{x}_2 + w_0 = -1$. Therefore, we have the followings.

$$\boldsymbol{w} \cdot (\boldsymbol{x}_1 - \boldsymbol{x}_2) = 2$$

If we denote lengths of vectors $\boldsymbol{w}$ and $(\boldsymbol{x}_1 - \boldsymbol{x}_2)$ are $||\boldsymbol{w}||$ and $||\boldsymbol{x}_1 - \boldsymbol{x}_2||$ respectively, and the angle between two vectors is θ, the inner product of the two vectors is defined as follows.

$$\boldsymbol{w} \cdot (\boldsymbol{x}_1 - \boldsymbol{x}_2) = ||\boldsymbol{w}|| \, ||\boldsymbol{x}_1 - \boldsymbol{x}_2|| \, cos \, \theta$$

Since the vector $\boldsymbol{w}$ is perpendicular to two hyperplanes and the vector $(\boldsymbol{x}_1 - \boldsymbol{x}_2)$ connects two points $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$, the shortest distance $d = ||\boldsymbol{x}_1 - \boldsymbol{x}_2||$ between two hyperplanes occurs when the two vectors are parallel, that is $\theta = 0$ ($cos \, \theta = 1$). In case of the shortest distance, the above equation becomes as follows.

$$||\boldsymbol{w}|| \times d = 2, \quad \text{that is } d = \frac{2}{||\boldsymbol{w}||}$$

We want find a hyperplane which maximizes this distance $d = \frac{2}{||\boldsymbol{w}||}$, which is equivalent to maximizing $d^2 = \frac{2^2}{||\boldsymbol{w}||^2}$ or minimizing $\frac{||\boldsymbol{w}||^2}{2^2}$. Therefore, finding the support vector when the data of the two groups can be completely separated using the hyperplane is equivalent to finding the solution to the following nonlinear optimization problem.

$$\text{Find } \boldsymbol{w}, w_0 \text{ which minimizes } \frac{||\boldsymbol{w}||^2}{2^2}$$
$$\text{subject to}$$
$$y_i\ (\boldsymbol{w}\ \cdot\ \boldsymbol{x}_i\ +\ w_0)\ \geq\ 1,\ \ i = 1, 2, \ldots, n$$

It is a quadratic optimization problem where the objective function is a quadratic function and the constraints are linear functions. This optimization problem can be solved by the standard Lagrangian multiplier method, and the objective function is as follows.

$$f(\boldsymbol{w}, w_0)\ =\ \frac{||\boldsymbol{w}||^2}{2^2}\ -\ \sum_{i=1}^{n} \lambda_i\ [\ y_i\ (\boldsymbol{w}\ \cdot\ \boldsymbol{x}_i\ +\ w_0)\ -\ 1\ ]$$

Here, λ_i is called the Lagrange multiplier. In order to find the value that minimizes the objective function, we must set the partial derivatives for each unknown parameter to 0 and then solve the system of linear equations.

$$\frac{\partial f}{\partial \boldsymbol{w}} = 0 \qquad \Rightarrow \qquad 2\boldsymbol{w}\ =\ \sum_{i=1}^{n} \lambda_i\ y_i \boldsymbol{x}_i$$
$$\frac{\partial f}{\partial w_0} = 0 \qquad \Rightarrow \qquad \sum_{i=1}^{n} \lambda_i\ y_i\ =\ 0$$

The detailed solution of this nonlinear system of equations is beyond the level of this book, so please refer to a book on quadratic programming. When the optimal solutions $\boldsymbol{w}^*$ and w_0^* are obtained, the classification equation using linear support vectors is as follows.

$$\text{If } \boldsymbol{w}^*\ \cdot\ \boldsymbol{x}\ +\ w_0^*\ \geq\ 0,\ \ \text{classify } \boldsymbol{x} \text{ into } '+1' \text{ group, else } '-1' \text{group.}$$

Let us look at the following example of the linear support vector.

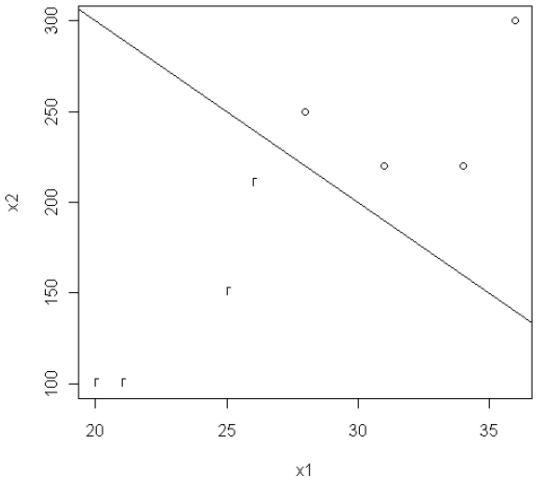
Example 7.5.1
When there are eight data for two variables x_1 (age), x_2 (monthly income) and group variable y (+1: purchase, -1: non-purchase) as in Table 7.5.1, find the classification equation using a linear support vector model.

Table 7.5.1 Eight data with two variables and their group

number	Age x_1	Income x_2	Group y
1	25	150	-1
2	34	220	+1
3	26	210	-1
4	28	250	+1
5	21	100	-1
6	31	220	+1
7	36	300	+1
8	20	100	-1

Answer

If we draw a scatter plot for the data in Table 7.5.1, it is a case where linear separation is possible as in <Figure 7.5.3>. In the figure, o means + group and r means - group, and we can see that there are many straight lines that can classify the two groups.



<Figure 7.5.3> Linearly separable data.

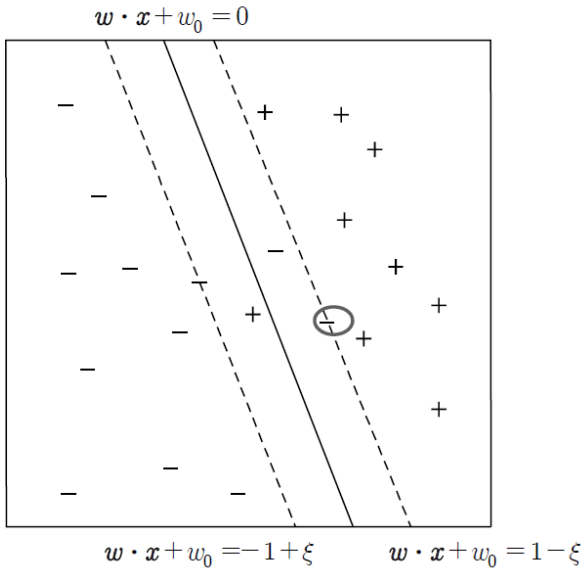
If we find the solution to the quadratic programming of the linear support vector, the classification function is 0.333 x_1 + 0.033 x_2 - 16.667 = 0 which is the line in <Figure 7.5.3> Therefore, the decision rule is as follows.

$$\text{If } \ 0.333x_1 + 0.033x_2 - 16.667 \ \geq \ 0, \ \ \text{classify } '+1' \text{ group, else } '-1' \text{group.}$$

B. Linearly not separable case

<Figure 7.5.4> shows a case where separating the two groups by a straight line is impossible. In this case, we can create a similar optimization problem by introducing a slack variable to the classification equation for the case where linear separation is possible. That is, by subtracting the slack variable ξ which is positive from the right side of the $\geq$ inequality in the classification equation, adding the slack variable ξ from the right side of the $\leq$ inequality, and then finding the hyperplane that minimizes the slack variable. The classification equation minimizes misclassification.

$$\begin{aligned} if \ \boldsymbol{w} \cdot \boldsymbol{x} \ + \ w_0 \ \geq \ 1 - \xi, \quad y = 1 \\ if \ \boldsymbol{w} \cdot \boldsymbol{x} \ + \ w_0 \ \leq \ -1 + \xi, \ \ y = -1 \end{aligned}$$



<Figure 7.5.4> Linearly not separable data and a slack variable.

In <Figure 7.5.4>, the slack variable ξ means that the hyperplane ($\boldsymbol{w} \cdot \boldsymbol{x} + w_0 = -1$) where linear classification is possible has moved parallel to the hyperplane $\boldsymbol{w} \cdot \boldsymbol{x} + w_0 = -1 + \xi$ that can include the data of the - group, which is indicated by a circle. The distance between these two hyperplanes can be shown to be $\frac{\xi}{||\boldsymbol{w}||}$, and the nonlinear optimization problem to minimize misclassification in the case of linearly non-separable is as follows.

$$\text{Find } \boldsymbol{w}, w_0, \xi_i \text{ which minimize} \frac{||\boldsymbol{w}||^2}{2^2} + C(\sum_{i=1}^{n} \xi_i)^k$$

subject to

$$y_i \left(\boldsymbol{w} \cdot \boldsymbol{x}_i + w_0\right) \geq 1 - \xi_i, \quad i = 1, 2, \ldots, n$$

Here, the function $C(x)$ is a penalty function that minimizes the slack variable, which means an error, and $C(x)$ and k can be selected arbitrarily by the user. This nonlinear optimization problem can also be solved by the Lagrangian multiplier method, but the details are beyond the level of this book, so we will omit them.

In this section, we introduce the SVM model for the case of two groups, but it can be extended to the case of multiple groups.

7.5.2 Nonlinear support vector machine

In the previous section, we studied the method of separating two groups using a linear function, and if we extend this concept, we can easily understand the nonlinear SVM model. The basic idea is to nonlinearly transform the coordinate space of data $\boldsymbol{x}$ into a new space $\Phi(\boldsymbol{x})$. At this time, the classification function can take various forms such as a circle, an ellipse, or a curve. The general optimization model of nonlinear SVM is as follows. M

$$\text{Find } \boldsymbol{w} \text{ which minimize} \frac{||\boldsymbol{w}||^2}{2^2}$$

subject to

$$y_i \left(\boldsymbol{w} \cdot \Phi(\boldsymbol{x}_i)\right) \geq 1, \quad i = 1, 2, \ldots, n$$

This nonlinear optimization problem can also be solved using the Lagrangian multiplier method, but the details are beyond the level of this book, so we will omit them.

Characteristics of the support vector machine model

The SVM model is a model that has been widely used recently and has the following characteristics.

1) The optimization problem for solving the linear SVM model is a minimization problem of a convex function, and the algorithm for finding the global minimum is well-developed.
2) In cases where linear separation is impossible, the SVM model may have the disadvantage of requiring the user to determine the penalty function.

7.5.3 R practice - Support vector machine

To use the suport vector machine model using R, we need to install a package called **e1071**. From the main menu of R, select 'Package' => 'Install package(s)', and a window called 'CRAN mirror' will appear. Here, select '0-Cloud [https]' and click 'OK'. Then, when the window called 'Packages' appears, select 'e1071' and click 'OK'. 'e1071' is a package for modeling of the support vector machine classification model. General usage and key arguments of the function are described in the following table.

svm {e1071}	Fit support vector machine

# S3 method for formula, svm(formula, data = NULL, ..., subset, na.action =na.omit, scale = TRUE) # S3 method for default svm(x, y = NULL, scale = TRUE, type = NULL, kernel = "radial", degree = 3, gamma = if (is.vector(x)) 1 else 1 / ncol(x), coef0 = 0, cost = 1, nu = 0.5, class.weights = NULL, cachesize = 40, tolerance = 0.001, epsilon = 0.1, shrinking = TRUE, cross = 0, probability = FALSE, fitted = TRUE, ..., subset, na.action = na.omit)	
formula	A formula of the form class ~ x1 + x2 + ...
data	an optional data frame containing the variables in the model. By default the variables are taken from the environment which ‘svm’ is called from.
x	a data matrix, a vector, or a sparse matrix (object of class Matrix provided by the Matrix package, or of class matrix.csr provided by the SparseM package, or of class simple_triplet_matrix provided by the slam package).
y	a response vector with one label for each row/component of x. Can be either a factor (for classification tasks) or a numeric vector (for regression).
scale	A logical vector indicating the variables to be scaled. If scale is of length 1, the value is recycled as many times as needed. Per default, data are scaled internally (both x and y variables) to zero mean and unit variance. The center and scale values are returned and used for later predictions.
type	svm can be used as a classification machine, as a regression machine, or for novelty detection. Depending of whether y is a factor or not, the default setting for type is C-classification or eps-regression, respectively, but may be overwritten by setting an explicit value. Valid options are: C-classification nu-classification one-classification (for novelty detection) eps-regression nu-regression
kernel	the kernel used in training and predicting. We might consider changing some of the following parameters, depending on the kernel type. linear: polynomial: radial basis: sigmoid:
degree	parameter needed for kernel of type polynomial (default: 3)
gamma	parameter needed for all kernels except linear (default: 1/(data dimension))
coef0	parameter needed for kernels of type polynomial and sigmoid (default: 0)
cost	cost of constraints violation (default: 1)---it is the ‘C’-constant of the regularization term in the Lagrange formulation
nu	parameter needed for nu-classification, nu-regression, and one-classification
class.weights	a named vector of weights for the different classes, used for asymmetric class sizes. Not all factor levels have to be supplied (default weight: 1). All components have to be named. Specifying "inverse" will choose the weights inversely proportional to the class distribution.
cachesize	cache memory in MB (default 40)
tolerance	tolerance of termination criterion (default: 0.001)
epsilon	epsilon in the insensitive-loss function (default: 0.1)
shrinking	option whether to use the shrinking-heuristics (default: TRUE)
cross	if a integer value k>0 is specified, a k-fold cross validation on the training data is performed to assess the quality of the model: the accuracy rate for classification and the Mean Squared Error for regression
fitted	logical indicating whether the fitted values should be computed and included in the model or not (default: TRUE)
probability	logical indicating whether the model should allow for probability predictions.

subset	An index vector specifying the cases to be used in the training sample. (NOTE: If given, this argument must be named.)
na.action	A function to specify the action to be taken if NAs are found. The default action is na.omit, which leads to rejection of cases with missing values on any required variable. An alternative is na.fail, which causes an error if NA cases are found. (NOTE: If given, this argument must be named.)

An example of R commands for the single-layer neural network model using the data as in Example 7.4.2 is as follows.

> install.packages('e1071') copy r command

> library(e1071) copy r command

> svmdata <- read.csv('svmdata.csv', header=T, as.is=FALSE) copy r command

> attach(svmdata) copy r command

> svmdata copy r command

```
  x1  x2  y
1 25 150 -1
2 34 220  1
3 26 210 -1
4 28 250  1
5 21 100 -1
6 31 220  1
7 36 300  1
8 20 100 -1
```

```
# create a training data using the 8 data.
> train <- svmdata[1:8,]
```
copy r command

```
# create a testing data using the same 8 data
> test <- svmdata[1:8,]
```
copy r command

> train.svm = svm(y~x1+x2,type="C-classification", data=train) copy r command

> train.svm copy r command

```
Call:
svm(formula = y ~ x1 + x2, data = train, type = "C-classification")
Parameters:
   SVM-Type:  C-classification
 SVM-Kernel:  radial
       cost:  1
Number of Support Vectors:  6
```

The R command to reclassify the entire 8 data into groups using the above model is as follows. Classifying the test data shows that all data are classified correctly.

```
> svmpred = predict(train.svm,test)
> svmpred
```
copy r command

```
 1  2  3  4  5  6  7  8
-1  1 -1  1 -1  1  1 -1
Levels: -1 1
```

> z = table(svmpred,y) copy r command

```
> z
```

copy r command

```
       y
svmpred -1 1
     -1  4 0
      1  0 4
```

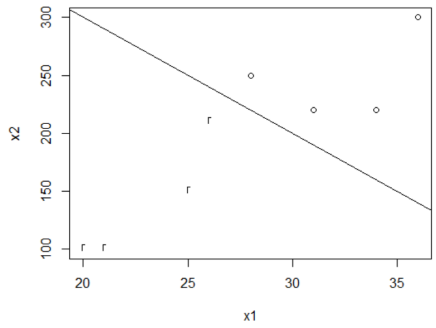
The R command to draw a scatter plot of x1, x2, labeled with the values of y, and a classification line 500 - 10 x1 on the scatter plot is as follows.

```
> plot(x1,x2,pch=y)
```

copy r command

```
> abline(500,-10)
```

copy r command



7.6 Ensemble model

The classification models studied so far have used a single classification function to predict the group of data whose affiliation is unknown. This section introduces an **ensemble model** that combines the results of multiple classification models to increase classification accuracy. Let us call a classification model established using training data a classifier. The ensemble model is a method that creates multiple classifiers from the training data, applies each classifier to classify the group when classifying data whose group affiliation is unknown, and then determines the final group by a majority vote of the resulting groups.

The ensemble model can obtain better classification results than a single classifier. For example, suppose five classifiers classify two groups, and each has a misclassification rate of 5%. If the five classifiers are independent models, the ensemble model will misclassify if more than half of the classifiers are misclassified. In other words, the misclassification rate $e_{ensemble}$ of the ensemble model is as follows.

$$e_{ensemble} = \sum_{i=3}^{5} {}_5C_i \, (0.05)^i (1-0.05)^{5-i} = 0.0001$$

Therefore, the misclassification rate of the ensemble model is smaller than that of each classifier. For the ensemble model to have better classification results than each classifier, each classifier must be independent, and the misclassification rate must be at least less than 50%. In practice, it is often difficult to say that each classifier is completely independent, but even in such cases, the classification results of the ensemble model are known to be good.

Each classifier used in the ensemble model can be any classification model. However, while applying one model, we can create multiple classifiers by adjusting the data, adjusting the number of variables, or adjusting the group name.

A. Adjust the number of data

This method creates multiple training data sets from the data using an appropriate sampling method, and one classifier from each data set is created. A **bagging** method described in Section 7.6.1 and a **boosting** method described in Section 7.6.2 are representative methods for adjusting data and ensembling them.

B. Control the number of variables

This method creates training data by selecting a subset of variables from the entire set of variables. Experts can randomly extract or select the subset of variables. It is known to be effective when there are many unnecessary variables, and an ensemble classification method called a **random forest** is introduced in Section 7.6.3.

C. Control group names

If there are many types of groups, we can classify them by grouping them into a small number of groups, or we can apply an ensemble model by creating a classifier that only classifies whether or not they belong to each group.

D. Adjust classification model assumptions

A classification model can be divided into several different classification models by changing the assumptions about parameters or algorithms, we can synthesize them into an ensemble model. For example, in a neural network model, we can create different classifiers by changing the assumptions about the network shape or the initial weight coefficients. In a decision tree model, we can create different classifiers by changing the criteria for selecting branching variables or tree expansion criteria.

7.6.1 Bagging

Bagging is an abbreviation for bootstrap aggregating that generates a classifier for each sample using simple random sampling with replacement repeatedly from the training data and then ensembling the results. Since the repeated sampling with replacement is used, same data can be extracted multiple times in a sample, and some data may not be extracted in all samples. When there are n data, if n samples are repeatedly extracted by simple random sampling with replacement, the probability that each data will be extracted again is $1-(1-\frac{1}{n})^n$. If n is sufficiently large, this probability converges to $1-\frac{1}{e}$, which is approximately 0.632. The general bagging algorithm is as follows.

[Bagging algorithm]

Step 1	Let R be the number of bootstrap samples, and n be the sample size
Step 2	**for** k = 1 to R **do**
Step 3	Generate bootstrap samples D_k of size n
Step 4	Create classifier C_k using bootstrap samples D_k
Step 5	**end for**
Step 6	Classify an unknown data $\boldsymbol{x}$ into the majority vote of all classifiers, that is, $$C^*(\boldsymbol{x}) = argmax_y \sum_{k=1}^{R} I(C_k(\boldsymbol{x}) = y)$$

Example 7.6.1 (Bagging)
A survey of 10 people who visited a store showed monthly income x and purchasing status y (purchasers have a value of 1 and non-purchasers have a value of -1), as shown in Table 7.6.1. We want to use a simple decision tree classifier such that 'If $x \leq c$, classify x into purchaser group 1, otherwise classify into non-purchaser group -1'. This is called a **decision stump**, and c is determined so that the entropy is minimized (see Section 6.2). Classify this data using the bagging method.

Table 7.6.1 Ten customer data with income x and purchase status y										
x	100	120	160	180	186	190	210	250	270	300
y	1	1	1	-1	-1	-1	-1	1	1	1

Answer

In the above data, the branching that minimizes entropy is c = 170 or 200 (see Section 6.2). In both cases, the classification accuracy is 70%. Table 7.6.2 shows ten bootstrap samples and their classifiers that minimize entropy for applying the bagging method.

Table 7.6.2 Ten bootstrap samples and each classifier												
number	Bootstrap sample											Classifier
Sample 1	x	100	120	120	160	180	180	186	190	270	270	If $x \leq 170$, then y = 1, else y = -1
	y	1	1	1	1	-1	-1	-1	-1	1	1	
Sample 2	x	100	120	160	180	186	250	270	300	300	300	If $x \leq 300$, then y = 1, else y = -1
	y	1	1	1	-1	-1	1	1	1	1	1	
Sample 3	x	100	120	160	180	180	186	210	210	250	270	If $x \leq 170$, then y = 1, else y = -1
	y	1	1	1	-1	-1	-1	-1	-1	1	1	
Sample 4	x	100	100	120	180	180	186	186	210	250	270	If $x \leq 150$, then y = 1, else y = -1
	y	1	1	1	-1	-1	-1	-1	-1	1	1	
Sample 5	x	100	100	120	186	190	190	190	300	300	300	If $x \leq 153$, then y = 1, else y = -1
	y	1	1	1	-1	-1	-1	-1	1	1	1	
Sample 6	x	120	180	186	190	210	210	210	250	270	300	If $x \leq 230$, then y = -1, else y = 1
	y	1	-1	-1	-1	-1	-1	-1	1	1	1	
Sample 7	x	100	180	180	190	210	250	270	270	270	300	If $x \leq 230$, then y = -1, else y = 1
	y	1	-1	-1	-1	-1	1	1	1	1	1	
Sample 8	x	100	120	186	186	186	210	210	250	270	300	If $x \leq 230$, then y = -1, else y = 1
	y	1	1	-1	-1	-1	-1	-1	1	1	1	
Sample 9	x	100	160	180	180	190	210	210	250	300	300	If $x \leq 230$, then y = -1, else y = 1
	y	1	1	-1	-1	-1	-1	-1	1	1	1	
Sample 10	x	100	100	100	100	160	160	250	250	270	270	If $x \leq 50$, then y = -1, else y = 1
	y	1	1	1	1	1	1	1	1	1	1	

Table 7.6.3 shows the final classification results by majority vote after classifying the original 10 data by classifiers obtained from each sample. we can obtain the final classification results using a majority vote by adding the classified group of each classifier and examining the sign. The ensemble classification results by bagging accurately classify all data.

Table 7.6.3 Classification results of each data by bagging 10 classifier										
Classifier of each sample	Income data x									
	100	120	160	180	186	190	210	250	270	300
Classifier 1	1	1	1	-1	-1	-1	-1	-1	-1	-1
Classifier 2	1	1	1	1	1	1	1	1	1	1
Classifier 3	1	1	1	-1	-1	-1	-1	-1	-1	-1

Classifier 4	1	1	1	-1	-1	-1	-1	-1	-1	-1
Classifier 5	1	1	1	-1	-1	-1	-1	-1	-1	-1
Classifier 6	-1	-1	-1	-1	-1	-1	-1	1	1	1
Classifier 7	-1	-1	-1	-1	-1	-1	-1	1	1	1
Classifier 8	-1	-1	-1	-1	-1	-1	-1	1	1	1
Classifier 9	-1	-1	-1	-1	-1	-1	-1	1	1	1
Classifier 10	1	1	1	1	1	1	1	1	1	1
Total	2	2	2	-6	-6	-6	-6	2	2	2
Sign of Total	1	1	1	-1	-1	-1	-1	1	1	1
Actual group y	1	1	1	-1	-1	-1	-1	1	1	1

The bagging ensemble method can reduce misclassification by reducing the variance of each classifier. The performance of bagging depends on the stability of each classifier. If each classifier is not stable, bagging reduces the error related to the random variability in the training data. Since the bagging ensemble method has the same probability of extracting each data, it does not focus on classifying abnormal data such as extreme values. Therefore, problems such as model overfitting do not occur even in noisy data.

7.6.2 R practice - Bagging

To use the bagging ensemble model using R, we need to install a package called **adabag**. From the main menu of R, select 'Package' => 'Install package(s)', and a window called 'CRAN mirror' will appear. Here, select '0-Cloud [https]' and click 'OK'. Then, when the window called 'Packages' appears, select 'adabag' and click 'OK'. 'adabag' is a package for modeling of the bagging and adaboosting ensemble model. General usage and key arguments of the function are described in the following table.

bagging {adabag}	**Applies the Bagging algorithm to a data set** **Fits the Bagging algorithm proposed by Breiman in 1996 using classification trees as single classifiers.**
bagging(formula, data, mfinal = 100, control, par=FALSE,...)	
formula	a formula, as in the lm function.
data	a data frame in which to interpret the variables named in the formula
mfinal	an integer, the number of iterations for which boosting is run or the number of trees to use. Defaults to mfinal=100 iterations.
control	options that control details of the rpart algorithm. See rpart.control for more details.
par	if TRUE, the cross validation process is runned in parallel. If FALSE (by default), the function runs without parallelization.
Details: Unlike boosting, individual classifiers are independent among them in bagging	
Value: An object of class bagging, which is a list with the following components:	
formula	the formula used.
trees	the trees grown along the iterations.
votes	a matrix describing, for each observation, the number of trees that assigned it to each class.
prob	a matrix describing, for each observation, the posterior probability or degree of support of each class. These probabilities are calculated using the proportion of votes in the final ensemble.

class	the class predicted by the ensemble classifier.
samples	the bootstrap samples used along the iterations.
importance	returns the relative importance of each variable in the classification task. This measure takes into account the gain of the Gini index given by a variable in each tree.

An example of R commands for the bagging ensemble model using the iris data stored in R is as follows.

> install.packages('adbag') copy r command

> library(adabag) copy r command

> data(iris) copy r command

mfinal is an integer which is the number of iterations for which boosting is run
> iris.bagging <- bagging(Species~., data=iris, mfinal = 10)) copy r command

list the importance of variable in the classification
> iris.bagging$importance copy r command

```
Petal.Length  Petal.Width Sepal.Length  Sepal.Width
    79.46481     20.53519      0.00000      0.00000
```

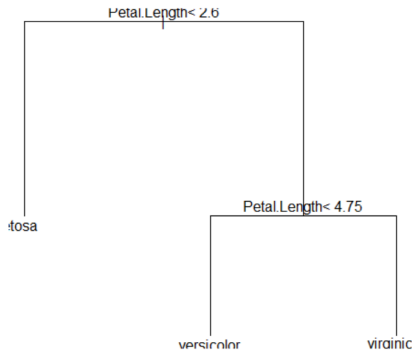
list the trees grown along the iterations.
> iris.bagging$trees copy r command

```
[[1]]
n= 150
node), split, n, loss, yval, (yprob)
      * denotes terminal node
1) root 150 94 virginica (0.32666667 0.30000000 0.37333333)
  2) Petal.Length< 2.45 49  0 setosa (1.00000000 0.00000000 0.00000000) *
  3) Petal.Length>=2.45 101 45 virginica (0.00000000 0.44554455 0.55445545)
    6) Petal.Width< 1.75 49  4 versicolor (0.00000000 0.91836735 0.08163265)
      12) Petal.Length< 4.95 42  0 versicolor (0.00000000 1.00000000 0.000000
00) *
       13) Petal.Length>=4.95 7  3 virginica (0.00000000 0.42857143 0.5714285
7) *
    7) Petal.Width>=1.75 52  0 virginica (0.00000000 0.00000000 1.00000000) *
...
...
...
[[10]]
n= 150
node), split, n, loss, yval, (yprob)
      * denotes terminal node
1) root 150 92 setosa (0.38666667 0.34666667 0.26666667)
  2) Petal.Length< 2.6 58  0 setosa (1.00000000 0.00000000 0.00000000) *
  3) Petal.Length>=2.6 92 40 versicolor (0.00000000 0.56521739 0.43478261)
    6) Petal.Length< 4.75 46  1 versicolor (0.00000000 0.97826087 0.02173913)
*
     7) Petal.Length>=4.75 46  7 virginica (0.00000000 0.15217391 0.84782609)
*
```

plot the decision tree after iteration 10 data
> plot(iris.bagging$trees[[10]]) copy r command

```
> text(iris.bagging$trees[[10]])
```

copy r command



The R command to reclassify the entire iris data using the bagging model is as follows.

```
# classify the iris data using the bagging model
> baggingpred <- predict(iris.bagging, newdata=iris)
```

copy r command

```
> table(baggingpred$class, iris[,5])
```

copy r command

```
             setosa versicolor virginica
  setosa         50          0         0
  versicolor      0         47         1
  virginica       0          3        49
```

```
# calculate the misclassification error
> baggingtb <- table(baggingpred$class, iris[,5])
```

copy r command

```
> baggingerror.rpart <- 1-(sum(diag(baggingtb))/sum(baggingtb))
```

copy r command

```
# misclassification error is 2.67%
> baggingerror.rpart
```

copy r command

```
[1] 0.02666667
```

7.6.3 Boosting

In bagging, data is resampled with the same probability of being selected. **Boosting** is a method of extracting data by weighting data depending on whether it is classified correctly or not in the previous stage, so they are more likely to be selected as samples. In boosting, after samples are extracted and a classifier is made, the classification results are used to modify the probability of each data being selected in the next bootstrap sampling.

When there are n training data, the boosting method first gives each data an equal probability of being selected as $\frac{1}{n}$, just like bagging, and then extracts n bootstrap data with replacement. After creating a classifier using this bootstrap data, the original training data is classified by this classifier, either as a correct classification or a misclassification. If the data is misclassified, the probability of this data being selected is increased, so it is more likely to be selected in the next stage, and if the data is correctly classified, the probability of being selected in the next stage is decreased. Since the data that was not extracted is also likely to be misclassified, the probability of being selected is also increased. If this method is used repeatedly, data that is continuously misclassified will be more focused.

Recently, many types of research on boosting algorithms have been studied, and the algorithms differ depending on (1) 'How do we modify the probability of extracting data in each boosting round?' and (2) 'How do we synthesize the classifiers determined in each boosting round to make the final classification?'. We introduce the widely used adaptive boosting algorithm called **AdaBoosting**.

AdaBoosting algorithm

Let $D = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \ldots, (\boldsymbol{x}_n, y_n)\}$ be the set of training data and the probability of each data being selected is $p_1, p_2, \ldots, p_n$. When selecting the bootstrap sample for the first time, the probability of extracting each data is made the same, that is, $p_i = \frac{1}{n}, i = 1, 2, \ldots, n$. Let the bootstrap samples be selected R times and the classifier obtained from each bootstrap sample be $C_1, C_2, \ldots, C_R$. The Adaboosting algorithm calculates the misclassification rate ϵ_k of each classifier C_k as follows.

$$\epsilon_k \ = \ \frac{1}{n} \left[\sum_{i=1}^{n} p_i \ I\{C_k(\boldsymbol{x}_i) \ \neq \ y_i\} \right], \ \ k = 1, 2, \ldots, R$$

Here, $C_k(\boldsymbol{x}_i)$ is the result of the classifier C_k estimating the group of data $\boldsymbol{x}_i$, and $I\{C_k(\boldsymbol{x}_i) \ \neq \ y_i\}$ has a value of 1 when the classifier C_k fails to classify the data $\boldsymbol{x}_i$ into the original group y_i, and 0 otherwise. In other words, ϵ_k is the error rate that weights the probability of selecting the data for each misclassification of data by the classifier C_k. The importance α_k of the classifier C_k is determined as follows.

$$\alpha_k \ = \ \frac{1}{2} \ ln \ \frac{1 - \epsilon_k}{\epsilon_k}, \ \ k = 1, 2, \ldots, R$$

If the misclassification rate ϵ_k is close to 0, the importance α_k value increases, and conversely, if ϵ_k is close to 1, the α_k value decreases. The importance α_k of the classifier C_k is used to adjust the probability of data being selected. If $p_i^{(k)}, i = 1, 2, \ldots, n$ is the probability when kth bootstrap sample is selected, the adjusted probability for selecting $(k+1)$th bootstrap sample is as follows.

$$\begin{aligned} p_i^{(k+1)} \ &= \ \frac{p_i^{(k)}}{Z_k} \times e^{-\alpha_k} \quad if \ C_k(\boldsymbol{x}_i) \ = \ y_i \\ &= \ \frac{p_i^{(k)}}{Z_k} \times e^{\alpha_k} \quad if \ C_k(\boldsymbol{x}_i) \ \neq \ y_i \end{aligned}$$

This equation means that if the data $\boldsymbol{x}_i$ is misclassified, then this data will be used for the next bootstrap sampling, and it increases the probability of being selected so that it is more likely to be extracted, and if the data is correctly classified, it decreases the probability of being selected in the next bootstrap sampling. Here, Z_k is a constant that makes the sum of $p_1^{(k+1)}, p_2^{(k+1)}, \ldots, p_n^{(k+1)}$ becomes one as follows.

$$\sum_{i=1}^{n} p_i^{(k+1)} \ = \ 1$$

If the misclassification rate exceeds 50% during the boosting round, the probability of each data being selected is returned to $p_i = \frac{1}{n}$ and selection with replacement is performed.

The method of synthesizing the classification results of the R classifiers generated for the data $\boldsymbol{x}$ of which the group is unknown does not use majority voting, but uses the result of weighting each classification result by the importance α_k.

$$C^*(\boldsymbol{x}) = argmax_v \sum_{k=1}^{R} \alpha_k \ I(C_k(\boldsymbol{x}) = v)$$

The Adaboosting algorithm that synthesizes the above explanations is as follows.

[AdaBoosting algorithm]

Step 1	Let $D = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \ldots, (\boldsymbol{x}_n, y_n)\}$ be the set of training data
Step 2	Let the initial probability being selected be $p_i^{(1)} = \frac{1}{n}, i = 1, 2, \ldots, n.$
Step 3	Let R be the number of bootstrap samples.

Step 4	**for** k = 1 to R**do**
Step 5	Generate bootstrap samples D_k of size n using $p_i^{(k)}$
Step 6	Create classifier C_k using bootstrap samples D_k
Step 7	Apply C_k to each data of D whether it classifies correctly or not
Step 8	calculates the misclassification rate $\epsilon_k = \frac{1}{n}\left[\sum_{i=1}^{n} p_i\, I\{C_k(\boldsymbol{x}_i) \neq y_i\}\right]$
Step 9	**If** $\epsilon_k > 0.5$ **then**
Step 10	Set again initial probability $p_i^{(1)} = \frac{1}{n}, i = 1, 2, \ldots, n$
Step 11	Go back to Step 4
Step 12	**end if**
Step 13	$\alpha_k = \frac{1}{2}\, ln\, \frac{1-\epsilon_k}{\epsilon_k}$
Step 14	$p_i^{(k+1)} = \frac{p_i^{(k)}}{Z_k} \times e^{-\alpha_k} \quad if\ C_k(\boldsymbol{x}_i) = y_i$ $= \frac{p_i^{(k)}}{Z_k} \times e^{\alpha_k} \quad if\ C_k(\boldsymbol{x}_i) \neq y_i$ Z is a constant that makes the sum of probability becomes 1.
Step 15	**end for**
Step 16	Classify an unknown data $\boldsymbol{x}$ into the weighted majority vote of each classifier, $C^*(\boldsymbol{x}) = argmax_v \sum_{k=1}^{R} \alpha_k\, I(C_k(\boldsymbol{x}) = v)$

Example 7.6.2 (AdaBoosting)
Classify the data in Table 7.6.1 of Example 7.6.1 below using the Adaboosting ensemble method. The classifier in each round uses a minimum entropy decision stump.

Table 7.6.1 10 customer data with income x and purchase status y

x	100	120	160	180	186	190	210	250	270	300
y	1	1	1	-1	-1	-1	-1	1	1	1

Answer

Since the number of data is n = 10, at first, as in bagging, the probability of each data being selected is given equally as $\frac{1}{10}$ = 0.1, and then 10 new bootstrap sampling data are extracted with replacement. Assume that the data extracted by this method are as follows, the minimum entropy classifier C_1 is as shown in Table 7.6.4.

Table 7.6.4 (Sample 1) 10 bootstrap samples for AdaBoosting and classifier C_1

number	Bootstrap sample											Classifier C_1
Sample 1	x	100	180	186	190	190	210	216	210	250	300	If $x \leq 230$, then y = -1, else y = 1
	y	1	-1	-1	-1	-1	-1	-1	-1	1	1	

The classification results of the original data using the classifier C_1 and the process of updating the new probability of selection are as in Table 7.6.5.

Table 7.6.5 Process of updating the new probability of selection using C_1

Selction probability $p_i^{(1)}$	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
x_i	100	120	160	180	186	190	210	250	270	300
y_i	1	1	1	-1	-1	-1	-1	1	1	1

Classification by $C_1(x_i)$	-1	-1	-1	-1	-1	-1	-1	1	1	1
$I(C_1(x_i) \neq y_i)$	1	1	1	0	0	0	0	0	0	0
$p_i^{(1)}\ I(C_1(x_i) \neq y_i)$	0.1	0.1	0.1	0	0	0	0	0	0	0
	$\epsilon_1 = 0.03, \quad \alpha_1 = \frac{1}{2}\ ln\ \frac{1-\epsilon_1}{\epsilon_1}$ = 1.738									
$e^{-\alpha_1} \quad if\ C_1(\boldsymbol{x}_i) = y_i$ $e^{\alpha_1} \quad if\ C_1(\boldsymbol{x}_i) \neq y_i$	5.686	5.686	5.686	0.176	0.176	0.176	0.176	0.176	0.176	0.176
$p_i^{(1)}$ × above row	0.569	0.569	0.569	0.018	0.018	0.018	0.018	0.018	0.018	0.018
	$Z_1 = 1.829$									
New selction probability $p_i^{(2)}$	0.311	0.311	0.311	0.010	0.010	0.010	0.010	0.010	0.010	0.010

The 10 new bootstrap sampling data extracted with replacement using the new selection probability and the classifier C_2 at this time are as shown in Table 7.6.5.

Table 7.6.5 (Sample 2) 10 bootstrap samples for AdaBoosting and classifier C_2

number	Bootstrap sample											Classifier C_2
Sample 2	x	100	120	120	120	120	120	160	160	160	160	If $x \leq 50$, then y = -1, else y = 1
	y	1	1	1	1	1	1	1	1	1	1	

The classification results of the original data using the classifier C_2 and the process of updating the new probability of selection are as in Table 7.6.6.

Table 7.6.6 Process of updating the new probability of selection using C_2

Selction probability $p_i^{(2)}$	0.311	0.311	0.311	0.010	0.010	0.010	0.010	0.010	0.010	0.010
x_i	100	120	160	180	186	190	210	250	270	300
y_i	1	1	1	-1	-1	-1	-1	1	1	1
Classification by $C_2(x_i)$	1	1	1	1	1	1	1	1	1	1
$I(C_2(x_i) \neq y_i)$	0	0	0	1	1	1	1	0	0	0
$p_i^{(2)}\ I(C_2(x_i) \neq y_i)$	0	0	0	0.010	0.010	0.010	0.010	0	0	0
	$\epsilon_2 = 0.004, \quad \alpha_2 = \frac{1}{2}\ ln\ \frac{1-\epsilon_2}{\epsilon_2}$ = 2.758									
$e^{-\alpha_2} \quad if\ C_2(\boldsymbol{x}_i) = y_i$ $e^{\alpha_2} \quad if\ C_2(\boldsymbol{x}_i) \neq y_i$	0.063	0.063	0.063	15.78	15.78	15.78	15.78	0.063	0.063	0.063
$p_i^{(2)}$ × above row	0.02	0.02	0.02	0.158	0.158	0.158	0.158	0.006	0.006	0.006
	$Z_2 = 0.6922$									
New selction probability $p_i^{(3)}$	0.028	0.028	0.028	0.228	0.228	0.228	0.228	0.001	0.001	0.001

The 10 new bootstrap sampling data extracted with replacement using the new selection probability and the classifier C_3 at this time are as shown in Table 7.6.7.

Table 7.6.7 (Sample 3) 10 bootstrap samples for AdaBoosting and classifier C_3

number	Bootstrap sample											Classifier C_3
Sample 3	x	120	120	180	180	180	180	186	190	190	210	If $x \leq 150$, then y = 1, else y = -1
	y	1	1	-1	-1	-1	-1	-1	-1	-1	-1	

The classification results of the original data using the classifier C_3 and the process of updating the new probability of selection are as in Table 7.6.8.

Table 7.6.8 Process of updating the new probability of selection using C_3										
Selction probability $p_i^{(3)}$	0.028	0.028	0.028	0.228	0.228	0.228	0.228	0.001	0.001	0.001
x_i	100	120	160	180	186	190	210	250	270	300
y_i	1	1	1	-1	-1	-1	-1	1	1	1
Classification by $C_3(x_i)$	1	1	1	-1	-1	-1	-1	-1	-1	-1
$I(C_3(x_i) \neq y_i)$	0	0	0	0	0	0	0	1	1	1
$p_i^{(3)}\ I(C_3(x_i) \neq y_i)$	0	0	0	0	0	0	0	0.001	0.001	0.001
	$\epsilon_3 = 0.0003, \quad \alpha_3 = \frac{1}{2}\ ln\ \frac{1-\epsilon_3}{\epsilon_3}$ = 4.0557									
$e^{-\alpha_3} \quad if\ C_3(\boldsymbol{x}_i) = y_i$ $e^{\alpha_3} \quad if\ C_3(\boldsymbol{x}_i) \neq y_i$	0.017	0.017	0.017	0.017	0.017	0.017	0.017	57.73	57.73	57.73
$p_i^{(3)} \times$ above row	0.0005	0.0005	0.0005	0.004	0.004	0.004	0.004	0.058	0.058	0.058
	$Z_3 = 0.1904$									
New selction probability $p_i^{(4)}$	0.003	0.003	0.003	0.021	0.021	0.021	0.021	0.303	0.303	0.303

For classification results of each classifier, the weighted sum is calculated using the classifier importance α_k , and the sign is examined to perform the final classification as shown in Table 7.6.9. Each classifier has an accuracy of about 70% at best, but it can be seen that all data are classified accurately due to AdaBoosting method.

Table 7.6.9 Final classification results using AdaBootstrap											
x_i	100	120	160	180	186	190	210	250	270	300	Classifier importance
$C_1(x_i)$ classification result	-1	-1	-1	-1	-1	-1	-1	1	1	1	$\alpha_1 = 1.738$
$C_2(x_i)$ classification result	1	1	1	1	1	1	1	1	1	1	$\alpha_2 = 2.758$
$C_3(x_i)$ classification result	1	1	1	-1	-1	-1	-1	-1	-1	-1	$\alpha_3 = 4.055$
Weighted sum of classification result	5.08	5.08	5.08	-3.04	-3.04	-3.04	-3.04	0.44	0.44	0.44	
Final classification result (sign)	1	1	1	-1	-1	-1	-1	1	1	1	

7.6.4 R practice - Adaboosting

R practice

To use the adaboosting ensemble model using R, we need to install a package called **adabag**. From the main menu of R, select 'Package' => 'Install package(s)', and a window called 'CRAN mirror' will appear. Here, select '0-Cloud [https]' and click 'OK'. Then, when the window called 'Packages' appears, select 'adabag' and click 'OK'. 'adabag' is a package for modeling of the bagging and adaboosting ensemble model. General usage and key arguments of the function are described in the following table.

boosting {adabag}	**Applies the AdaBoost.M1 and SAMME algorithms to a data set** **Fits the AdaBoost.M1 (Freund and Schapire, 1996) and SAMME (Zhu et al., 2009) algorithms using classification trees as single classifiers.**
boosting(formula, data, boos = TRUE, mfinal = 100, coeflearn = 'Breiman', control,...)	
formula	a formula, as in the lm function.
data	a data frame in which to interpret the variables named in the formula

boos	if TRUE (by default), a bootstrap sample of the training set is drawn using the weights for each observation on that iteration. If FALSE, every observation is used with its weights.
mfinal	an integer, the number of iterations for which boosting is run or the number of trees to use. Defaults to mfinal=100 iterations.
coeflearn	if 'Breiman'(by default), alpha=1/2ln((1-err)/err) is used. If 'Freund' alpha=ln((1-err)/err) is used. In both cases the AdaBoost.M1 algorithm is used and alpha is the weight updating coefficient. On the other hand, if coeflearn is 'Zhu' the SAMME algorithm is implemented with alpha=ln((1-err)/err)+ ln(nclasses-1).
control	options that control details of the rpart algorithm. See rpart.control for more details.
Details: AdaBoost.M1 and SAMME are simple generalizations of AdaBoost for more than two classes. In AdaBoost-SAMME the individual trees are required to have an error lower than 1-1/nclasses instead of 1/2 of the AdaBoost.M1	
Value: An object of class boosting, which is a list with the following components:	
formula	the formula used.
trees	the trees grown along the iterations.
weights	a vector with the weighting of the trees of all iterations.
votes	a matrix describing, for each observation, the number of trees that assigned it to each class, weighting each tree by its alpha coefficient.
prob	a matrix describing, for each observation, the posterior probability or degree of support of each class. These probabilities are calculated using the proportion of votes in the final ensemble.
class	the class predicted by the ensemble classifier.
importance	returns the relative importance of each variable in the classification task. This measure takes into account the gain of the Gini index given by a variable in a tree and the weight of this tree.

An example of R commands for the adaboosting ensemble model using the iris data stored in R is as follows.

```
> install.packages('adbag')
```
copy r command

```
> library(adabag)
```
copy r command

```
> data(iris)
```
copy r command

```
# mfinal is an integer which is the number of iterations for which boosting is run
> iris.adaboost <- boosting(Species~., data = iris, boos = TRUE, mfinal = 10)
```
copy r command

```
# list the importance of variable in the classification
> iris.adaboost$importance
```
copy r command

```
Petal.Length  Petal.Width Sepal.Length  Sepal.Width
   61.558263    26.329296     5.586443     6.525997
```

list the trees grown along the iterations.
> iris.adaboost$trees

copy r command

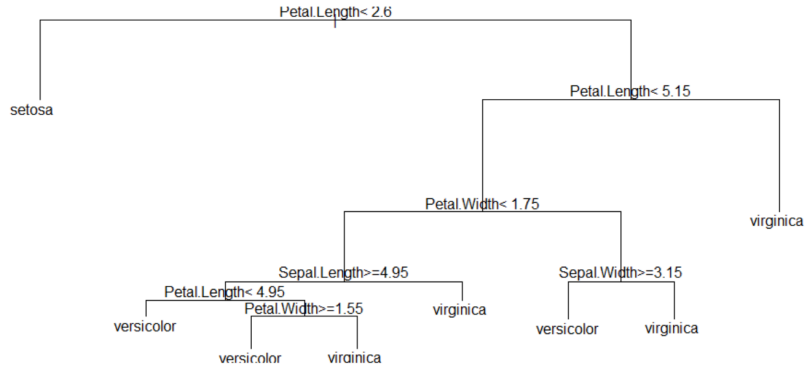
```
[[1]]
n= 150
node), split, n, loss, yval, (yprob)
      * denotes terminal node
 1) root 150 94 virginica (0.32666667 0.30000000 0.37333333)
   2) Petal.Length< 2.45 49  0 setosa (1.00000000 0.00000000 0.00000000) *
   3) Petal.Length>=2.45 101 45 virginica (0.00000000 0.44554455 0.55445545)
     6) Petal.Width< 1.75 49  4 versicolor (0.00000000 0.91836735 0.08163265)
      12) Petal.Length< 4.95 42  0 versicolor (0.00000000 1.00000000 0.000000
00) *
      13) Petal.Length>=4.95 7  3 virginica (0.00000000 0.42857143 0.5714285
7) *
     7) Petal.Width>=1.75 52  0 virginica (0.00000000 0.00000000 1.00000000)
*
...
...
...
[[10]]
n= 150
node), split, n, loss, yval, (yprob)
      * denotes terminal node
[[10]]
n= 150
node), split, n, loss, yval, (yprob)
      * denotes terminal node
 1) root 150 77 virginica (0.1133333 0.4000000 0.4866667)
   2) Petal.Length< 2.6 17  0 setosa (1.0000000 0.0000000 0.0000000) *
   3) Petal.Length>=2.6 133 60 virginica (0.0000000 0.4511278 0.5488722)
     6) Petal.Length< 5.15 96 36 versicolor (0.0000000 0.6250000 0.3750000)
      12) Petal.Width< 1.75 65 13 versicolor (0.0000000 0.8000000 0.2000000)
        24) Sepal.Length>=4.95 57  7 versicolor (0.0000000 0.8771930 0.122807
0)
          48) Petal.Length< 4.95 34  0 versicolor (0.0000000 1.0000000 0.0000
000) *
          49) Petal.Length>=4.95 23  7 versicolor (0.0000000 0.6956522 0.3043
478)
            98) Petal.Width>=1.55 16  0 versicolor (0.0000000 1.0000000 0.000
0000) *
            99) Petal.Width< 1.55 7  0 virginica (0.0000000 0.0000000 1.00000
00) *
        25) Sepal.Length< 4.95 8  2 virginica (0.0000000 0.2500000 0.7500000)
*
      13) Petal.Width>=1.75 31  8 virginica (0.0000000 0.2580645 0.7419355)
        26) Sepal.Width>=3.15 8  0 versicolor (0.0000000 1.0000000 0.0000000)
*
        27) Sepal.Width< 3.15 23  0 virginica (0.0000000 0.0000000 1.0000000)
*
     7) Petal.Length>=5.15 37  0 virginica (0.0000000 0.0000000 1.0000000) *
```

plot the decision tree after iteration 10 data
> plot(iris.adaboost$trees[[10]])

copy r command

```
> text(iris.adaboost$trees[[10]])
```

copy r command



The R command to reclassify the entire iris data using the bagging model is as follows.

```
# classify the iris data using the adaboosting model
> adaboostpred <- predict(iris.adaboost, newdata=iris)
```

copy r command

```
> table(adaboostpred$class, iris[,5])
```

copy r command

```
            setosa versicolor virginica
  setosa        50          0         0
  versicolor     0         50         0
  virginica      0          0        50
```

```
# calculate the misclassification error
> adaboosttb <- table(adaboostpred$class, iris[,5])
```

copy r command

```
> adaboosterror <- 1-(sum(diag(adaboosttb))/sum(adaboosttb))
```

copy r command

```
# misclassification error is 2.67%
> adaboosterror
```

copy r command

```
[1] 0
```

7.6.5 Random forest

Random forest is an ensemble method designed to combine the classification results of several decision tree models. However, it is also used when there are many variables. Each decision tree is created using a subset of variables independently selected from all variables and then synthesized. The generation of the subset of variables can use random or probability distributions. The bagging method using decision trees can be considered a special case of random forest. The general random forest algorithm is as follows.

[Random forest algorithm]

Step 1	Let $D = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \ldots, (\boldsymbol{x}_n, y_n)\}$ be the set of training data, and m be the number of variables.
Step 2	Let R be the number of random forest samples.
Step 3	**for** k = 1 to R**do**
Step 4	Generate random forest samples D_k with the subset of all variables.
Step 5	Create classifier C_k using random forest samples D_k
Step 6	**end for**
Step 7	Classify an unknown data $\boldsymbol{x}$ by the majority vote of each classifier.

The ensemble method using random forests may not be efficient if each decision tree classifier is related to each other. In other words, selecting a good set of variables is the key to creating an efficient random forest ensemble. There have been many studies on selecting a set of variables and expanding the decision tree using it. Please refer to the relevant references.

There have been many comparative studies on various ensemble methods. It is known that the efficiency of the Adaboosting method and the random forest method is relatively good as a result of experiments using actual data.

7.6.6 R practice - Random forest

This is a method that adds a random process to bagging. The process of extracting bootstrap samples from the original data and forming a tree for each bootstrap sample is similar to bagging, but instead of selecting the optimal split among all predictors for each node, it randomly extracts predictors and creates the optimal split among the extracted variables. In other words, if all variables are used, it becomes bagging, and if variables are randomly extracted and split, it becomes a random forest. Predictions for new data are made by majority vote in the case of classification and by taking the average in the case of regression, which is the same as other ensemble models.

To use the random forest ensemble model using R, we need to install a package called **randomForest**. From the main menu of R, select 'Package' => 'Install package(s)', and a window called 'CRAN mirror' will appear. Here, select '0-Cloud [https]' and click 'OK'. Then, when the window called 'Packages' appears, select 'randomForest' and click 'OK'. 'randomForest' is a package for modeling of the random forest ensemble model. General usage and key arguments of the function are described in the following table.

randomForest {randomForest}	**Classification and Regression with Random Forest randomForest implements Breiman's random forest algorithm (based on Breiman and Cutler's original Fortran code) for classification and regression. It can also be used in unsupervised mode for assessing proximities among data points.**
## S3 method for class 'formula' randomForest(formula, data=NULL, ..., subset, na.action=na.fail) ## Default S3 method: randomForest(x, y=NULL, xtest=NULL, ytest=NULL, ntree=500, mtry=if (!is.null(y) && !is.factor(y)) max(floor(ncol(x)/3), 1) else floor(sqrt(ncol(x))), weights=NULL, replace=TRUE, classwt=NULL, cutoff, strata, sampsize = if (replace) nrow(x) else ceiling(.632*nrow(x)), nodesize = if (!is.null(y) && !is.factor(y)) 5 else 1, maxnodes = NULL, importance=FALSE, localImp=FALSE, nPerm=1, proximity, oob.prox=proximity, norm.votes=TRUE, do.trace=FALSE, keep.forest=!is.null(y) && is.null(xtest), corr.bias=FALSE, keep.inbag=FALSE, ...)	
data	an optional data frame containing the variables in the model. By default the variables are taken from the environment which randomForest is called from.
subset	an index vector indicating which rows should be used. (NOTE: If given, this argument must be named.)
na.action	A function to specify the action to be taken if NAs are found. (NOTE: If given, this argument must be named.)
x, formula	a data frame or a matrix of predictors, or a formula describing the model to be fitted (for the print method, an randomForest object).
y	A response vector. If a factor, classification is assumed, otherwise regression is assumed. If omitted, randomForest will run in unsupervised mode.
xtest	a data frame or matrix (like x) containing predictors for the test set.
ytest	response for the test set.
ntree	Number of trees to grow. This should not be set to too small a number, to ensure that every input row gets predicted at least a few times.

mtry	Number of variables randomly sampled as candidates at each split. Note that the default values are different for classification (sqrt(p) where p is number of variables in x) and regression (p/3)
weights	A vector of length same as y that are positive weights used only in sampling data to grow each tree (not used in any other calculation)
replace	Should sampling of cases be done with or without replacement?
classwt	Priors of the classes. Need not add up to one. Ignored for regression.
cutoff	(Classification only) A vector of length equal to number of classes. The 'winning' class for an observation is the one with the maximum ratio of proportion of votes to cutoff. Default is 1/k where k is the number of classes (i.e., majority vote wins).
strata	A (factor) variable that is used for stratified sampling.
samplesize	Size(s) of sample to draw. For classification, if sampsize is a vector of the length the number of strata, then sampling is stratified by strata, and the elements of sampsize indicate the numbers to be drawn from the strata.
nodesize	Minimum size of terminal nodes. Setting this number larger causes smaller trees to be grown (and thus take less time). Note that the default values are different for classification (1) and regression (5).
maxnodes	Maximum number of terminal nodes trees in the forest can have. If not given, trees are grown to the maximum possible (subject to limits by nodesize). If set larger than maximum possible, a warning is issued.
importance	Should casewise importance measure be computed? (Setting this to TRUE will override importance.)
localImp	Should casewise importance measure be computed? (Setting this to TRUE will override importance.)
nPerm	Number of times the OOB data are permuted per tree for assessing variable importance. Number larger than 1 gives slightly more stable estimate, but not very effective. Currently only implemented for regression.
proximity	Should proximity measure among the rows be calculated?
oob.prox	Should proximity be calculated only on "out-of-bag" data?
norm.votes	If TRUE (default), the final result of votes are expressed as fractions. If FALSE, raw vote counts are returned (useful for combining results from different runs). Ignored for regression.
do.trace	If set to TRUE, give a more verbose output as randomForest is run. If set to some integer, then running output is printed for every do.trace trees.
keep.forest	If set to FALSE, the forest will not be retained in the output object. If xtest is given, defaults to FALSE.
corr.bias	perform bias correction for regression? Note: Experimental. Use at your own risk.
keep.inbag	Should an n by ntree matrix be returned that keeps track of which samples are "in-bag" in which trees (but not how many times, if sampling with replacement)
Value: An object of class randomForest, which is a list with the following components:	
call	the original call to randomForest
type	one of regression, classification, or unsupervised.
predicted	the predicted values of the input data based on out-of-bag samples.

importance	a matrix with nclass + 2 (for classification) or two (for regression) columns. For classification, the first nclass columns are the class-specific measures computed as mean descrease in accuracy. The nclass + 1st column is the mean descrease in accuracy over all classes. The last column is the mean decrease in Gini index. For Regression, the first column is the mean decrease in accuracy and the second the mean decrease in MSE. If importance=FALSE, the last measure is still returned as a vector.
importanceSD	The “standard errors” of the permutation-based importance measure. For classification, a p by nclass + 1 matrix corresponding to the first nclass + 1 columns of the importance matrix. For regression, a length p vector.
localImp	a p by n matrix containing the casewise importance measures, the [i,j] element of which is the importance of i-th variable on the j-th case. NULL if localImp=FALSE.
ntree	number of trees grown.
mtry	number of predictors sampled for spliting at each node.
forest	(a list that contains the entire forest; NULL if randomForest is run in unsupervised mode or if keep.forest=FALSE.
err.rate	(classification only) vector error rates of the prediction on the input data, the i-th element being the (OOB) error rate for all trees up to the i-th.
confusion	(classification only) the confusion matrix of the prediction (based on OOB data).
votes	(classification only) a matrix with one row for each input data point and one column for each class, giving the fraction or number of (OOB) ‘votes’ from the random forest.
oob.times	number of times cases are ‘out-of-bag’ (and thus used in computing OOB error estimate)
proximity	if proximity=TRUE when randomForest is called, a matrix of proximity measures among the input (based on the frequency that pairs of data points are in the same terminal nodes).
mse	(regression only) vector of mean square errors: sum of squared residuals divided by n.
rsq	(regression only) “pseudo R-squared”: 1 - mse / Var(y).
test	if test set is given (through the xtest or additionally ytest arguments), this component is a list which contains the corresponding predicted, err.rate, confusion, votes (for classification) or predicted, mse and rsq (for regression) for the test set. If proximity=TRUE, there is also a component, proximity, which contains the proximity among the test set as well as proximity between test and training data.

An example of R commands for the random forest ensemble model using the iris data stored in R is as follows.

```
> install.packages('randomForest')
```
copy r command

```
> library(randomForest)
```
copy r command

```
> data(iris)
```
copy r command

```
> iris.forest <- randomForest(Species~., data=iris, ntree = 100, proximity=TRUE)
```
copy r command

The R command to reclassify the entire iris data using the random forest model is as follows.

```
# classify the iris data using the bagging model
> table(predict(iris.forest), iris[,5])
```
copy r command

```
             setosa versicolor virginica
  setosa         50          0         0
  versicolor      0         47         6
  virginica       0          3        44
```

# calculate the misclassification error > foresttb <- table(predict(iris.forest), iris[,5])	copy r command
> foresterror <- 1-(sum(diag(foresttb))/sum(foresttb))	copy r command
# misclassification error is 2.67% > foresterror `[1] 0.06`	copy r command

7.7 Classification of multiple groups

Support vector machines and Adaboosting classification models were designed as a two-group classification method. However, in reality, classification problems of multiple groups often occur, so a method of applying a two-group classification model to classification problems of multiple groups has been studied.

When there are K classification groups, Let us denote them as $G_1, G_2, \ldots, G_K$. One way to apply a two-group classification method to the classification of multiple groups is to view the remaining groups as one group for each group G_i, and view it as a two-group problem of $\{G_i$, other groups$\}$. This is called the $(1 : K-1)$ method. The second method is to classify the K groups into two pairwise groups $\{G_i, G_j\}$, which requires the creation of ${}_KC_2 = \frac{K(K-1)}{2}$ classifiers, and it is called the (1:1) method. When creating a classifier, data that do not belong to two groups $\{G_i, G_j\}$ are ignored. When classifying data whose group membership is unknown, a method of applying multiple classifiers and classifying them into one group by majority vote is often used. There is a possibility of obtaining equal votes when using a majority vote. To prevent this, if the results of the two-group classification are expressed as the probability of belonging to each group, then these are combined to classify them into the group with the higher probability.

Example 7.7.1 (Classification of multiple groups)
Suppose there are 4 classification groups $\{G_1, G_2, G_3, G_4\}$ and Let us apply the (1:3) method. For example, if $(G_1 : \{G_2, G_3, G_4\})$, was applied to one data whose group affiliation was unknown, it was classified into G_1 group, Let us denote it as + group. if $(G_2 : \{G_1, G_3, G_4\})$ was applied to the data, it was classified into $\{G_1, G_3, G_4\}$ group, Let us denote it as - group. Similarly, if $(G_3 : \{G_1, G_2, G_4\})$ was applied to the data, it was classified into $\{G_1, G_2, G_4\}$ group, which is - group, if $(G_4 : \{G_1, G_2, G_3\})$ was applied to the data, it was classified into $\{G_1, G_2, G_3\}$ group, which is - group. The classification results are summarized as in Table 7.7.1. What is the final classification result of the data using (1:3) method?

Table 7.7.1 Classification results of (1:3) method

Method (1:3) groups	+ : G_1 - : $\{G_2, G_3, G_4\}$	+ : G_2 - : $\{G_1, G_3, G_4\}$	+ : G_3 - : $\{G_1, G_2, G_4\}$	+ : G_4 - : $\{G_1, G_2, G_3\}$
Classification result	+	-	-	-

When we applied the (1:1) method to the same data, there are 6 classification and their classification results are summarized as in Table 7.7.2. What is the final classification result of the data using (1:1) method?

Table 7.7.2 Classification results of (1:3) method

Method (1:1) groups	+ : G_1 - : G_2	+ : G_1 - : G_3	+ : G_1 - : G_4	+ : G_2 - : G_3	+ : G_2 - : G_4	+ : G_3 - : G_4
Classification result	+	+	-	+	-	+

Answer

The classification results of (1:3) method ,as shown in Table 7.7.1 means that G_1 group receives 4 votes and the other groups receive 2 votes. Therefore, the data is classified into the G_1 group by the majority vote.

When applying the (1:1) method, the G_1 and G_4 groups receive 2 votes, and the G_2 and G_3 groups receive 1 vote, and are classified into the G_1 or G_4 group.

7.8 Exercise

7.1 The SAT scores (out of 100) and essay scores of 10 accepted applicants, denoted P, for a college, 10 failed applicants, denoted F, are as follows.

Group	SAT	Essay
P	96	95
P	86	83
P	76	88
P	73	89
P	85	80
P	83	81
P	92	80
P	93	95
P	87	90
P	92	90
N	76	70
N	82	70
N	80	80
N	70	85
N	65	75
N	71	72
N	72	80
N	70	65
N	64	70
N	73	80

1) Assuming that the distributions of the two groups are multivariate normal distributions with the same covariance, find a Bayesian classification function. Assume that the prior probability of each group is 0.5. Classify whether a student with an 80 SAT and an essay score of 80 will enter the university.
2) Find a Logistic regression function. Classify whether a student with an 80 SAT and an essay score of 80 will enter the university.
3) Classify whether a student with an 80 SAT and an essay score of 80 will enter the university using the 3-nearest neighbor classification model.
4) Apply a neural network model. Classify whether a student with an 80 SAT and an essay score of 80 will enter the university.
5) Apply a support vector model. Classify whether a student with an 80 SAT and an essay score of 80 will enter the university.

7.2 The following is a survey of 10 people visiting a department store to determine whether they purchased a product and their age. Those who purchased were denoted as Y, those who did not purchase were denoted as N. The data were sorted in ascending order of age. We want to divide age into two groups to apply a decision tree model. What is the best boundary value for the division?

Group	Age
N	25
N	27
N	31
Y	33
N	35
Y	41
N	43
Y	49
Y	51
Y	55