DSA1101 Midterm Notes

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1 R

1.1 Data Types

1.1.1 Vectors

```
c(1,2,3,4,5)

## [1] 1 2 3 4 5

1:5

## [1] 1 2 3 4 5

seq(1,9,2)

## [1] 1 3 5 7 9
```

1.1.2 Matrices

```
matrix(1:6, nrow = 2, ncol = 3, byrow = TRUE)

## [,1] [,2] [,3]
## [1,] 1 2 3
## [2,] 4 5 6
```

1.1.3 Data Frames

```
data.frame(
  id = 1:3,
  name = c('Tom', 'Mary', 'Peter'),
  age = c(26,30,25),
  marital_status = c('married','divorced','single'),
  stringsAsFactors = TRUE
)

## id name age marital_status
## 1 1 Tom 26 married
## 2 2 Mary 30 divorced
## 3 3 Peter 25 single
```

1.2 Logical Vectors

```
random_permutation_one_to_ten <- sample(1:10, 10, replace=FALSE)
random_permutation_one_to_ten

## [1] 10 1 9 5 6 8 7 3 2 4

random_permutation_one_to_ten > 5

## [1] TRUE FALSE TRUE FALSE TRUE TRUE TRUE FALSE FALSE FALSE
```

1.3 Logical Operators

A	В	B A AND B			
TRUE	TRUE	TRUE TRUE			
TRUE	FALSE	FALSE	TRUE		
FALSE	TRUE	FALSE	TRUE		
FALSE	FALSE	FALSE	FALSE		

A	NOT A
TRUE	FALSE
FALSE	TRUE

1.3.1 Logical Operators in R

Operator	Description		
&	Element-wise AND		
	Element-wise OR		
&&	First element AND		
	First element OR		
!	NOT		

1.4 Conditionals

1.4.1 Conditional Statements

```
if (x > 20) {
  print('x is bigger than 20')
} else if (x > 10) {
  print('x is bigger than 10')
} else {
  print('x is smaller than or equal to 10')
}
## [1] "x is smaller than or equal to 10"
```

1.5 Reading CSV Files

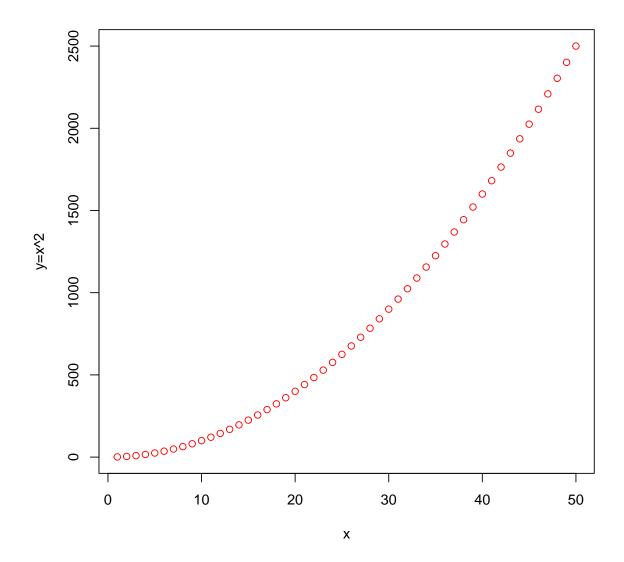
1.6 Data Visualisation

1.6.1 Scatter Plots

```
x <- 1:50

y <- x^2

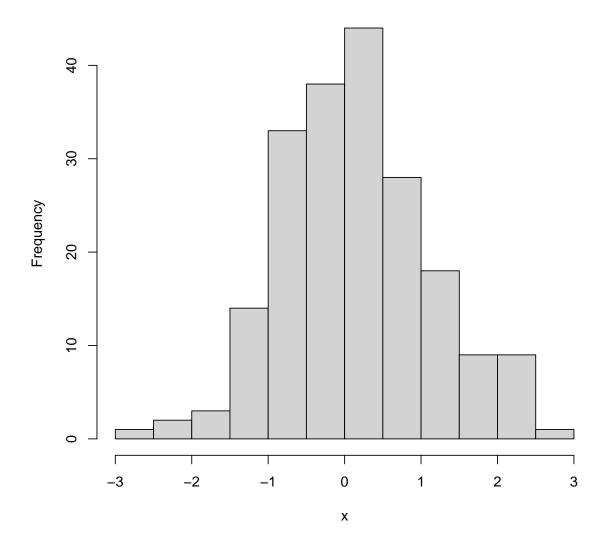
plot(x = x, y = y, xlab = 'x', ylab = 'y=x^2', col = 'red')
```



1.6.2 Histogram

```
n <- 200
x <- rnorm(n)
hist(x = x, breaks = ceiling(sqrt(n)), col = 'lightgray')</pre>
```

Histogram of x



1.7 Iteration

1.7.1 For Loop

```
for (i in 1:5) {
   print(i)
}
```

```
## [1] 1
## [1] 2
## [1] 3
## [1] 4
## [1] 5
```

1.7.2 While Loop

```
i = 1
while (i <= 5) {
  print(i)
  i <- i + 1
}
## [1] 1
## [1] 2
## [1] 3
## [1] 4
## [1] 5</pre>
```

1.7.3 Repeat Loop

```
i = 1
repeat {
  print(i)
  i <- i + 1
  if (i == 6) break
}

## [1] 1
## [1] 2
## [1] 3
## [1] 4
## [1] 5</pre>
```

2 Statistical Measures

2.1 Mean

$$\operatorname{mean}(\mathbf{x}) = \overline{x} = \frac{1}{N} \sum_{i=1}^{N} x_i$$

2.2 Median

$$\operatorname{median}(\mathbf{x}) = \begin{cases} x_{(N+1)/2} & \text{if } N \text{ is odd} \\ \frac{x_{N/2} + x_{N/2+1}}{2} & \text{if } N \text{ is even} \end{cases}$$

2.3 Sample Variance

$$\operatorname{var}(\mathbf{x}) = \frac{1}{N-1} \sum_{i=1}^{N} (x_i - \overline{x})^2$$

2.4 Sample Standard Deviation

$$sd(\mathbf{x}) = \sqrt{var(\mathbf{x})}$$

2.5 Sample Covariance

$$cov(\mathbf{x}, \mathbf{y}) = \frac{1}{N-1} \sum_{i=1}^{N} (x_i - \overline{x})(y_i - \overline{y})$$

2.6 Sample Correlation Coefficient

$$cor(\mathbf{x}, \mathbf{y}) = r_{xy} = \frac{cov(\mathbf{x}, \mathbf{y})}{sd(\mathbf{x}) sd(\mathbf{y})}$$

2.7 Location and Scale Changes to Statistical Measures

Statistical	Location Changes $\mathbf{x} + b$, $\mathbf{y} + c$	Scale Changes ax, dy
Measure		
mean	variant mean(\mathbf{x}) + b	variant $a \cdot \text{mean}(\mathbf{x})$
median	variant	variant
var	invariant $var(\mathbf{x})$	variant $a^2 \cdot \text{var}(\mathbf{x})$
sd	invariant $sd(\mathbf{x})$	variant $ a \cdot \operatorname{sd}(\mathbf{x})$
cov	invariant $cov(\mathbf{x}, \mathbf{y})$	variant
cor	invariant $cor(\mathbf{x}, \mathbf{y})$	invariant $cor(\mathbf{x}, \mathbf{y})$ if $ad >$
		0 else if $ad < 0$ then $-\operatorname{cor}(\mathbf{x}, \mathbf{y})$

3 Diagnostics of Classifiers

3.1 Confusion Matrix

		Predicted Class				
		Positive Negative				
Actual	Positive	True Positive (TP)	False Negative (FN)			
Class Negative		False Positive (FP)	True Negative (TN)			

3.2 Accuracy

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$

3.3 True Positive Rate

$$TPR = \frac{TP}{TP + FN}$$

3.4 False Positive Rate / Type I Error Rate

$$FPR = \frac{FP}{FP + TN}$$

3.5 False Negative Rate / Type II Error Rate

$$FNR = \frac{FN}{TP + FN}$$

3.6 True Negative Rate

$$TNR = \frac{TN}{TN + FP}$$

3.7 Precision

$$\text{Precision} = \frac{TP}{TP + FP}$$

3.7.1 Remarks

- 1. Precision is useful when costly actions will be followed up on the data predicted to be positive,
- 2. because precision gives the proportion of actual positives among those predicted to be positive
- 3. For example, if an insurance company wants to predict potential customers interested in purchasing insurance, and the cost to try to sell an insurance to a potential customer is non-trivial (e.g. insurance agent has to house visit the customer).

3.8 N-Fold Cross Validation

3.8.1 Algorithm

- 1. The entire dataset is randomly split into N datasets of approximately equal size.
- 2. N-1 of these datasets are treated as the training dataset, while the remaining one is the test dataset. A measure of the model error is obtained.
- 3. This process is repeated across the various combinations of N datasets taken N-1 at a time.
- 4. The observed N models errors are averaged across the N folds

3.9 ROC Curve (TPR vs FPR Trade-off)

- 1. Graph of True Positive Rate (TPR) against False Positive Rate (FPR)
- 2. As TPR increases, FPR tend to increase as well
 - (a) Increasing TPR may be a double-edged sword
- 3. TPR = FPR = 0 means binary classifier classifies everything as negative
- 4. TPR = FPR = 1 means binary classifier classifies everything as positive

3.10 Bias-Variance tradeoff

- 1. $error = bias^2 + variance + irreducible error$
- 2. As variance increases, bias decreases, and vice versa

3.11 Calculation Intensive Exam Question & Solution

Midterm Q6. Consider the following confusion matrix for a classifier

		Predicted Class			
		Positive Negati			
Actual	Positive	20	75		
Class	Negative	140	55		

The false negative rate (FNR) of the classifier is _____ (round to 3 decimal places).

Solution

1. Copy paste the following code:

```
gcmfv <- function(tp, fn, fp, tn) {</pre>
  # generates confusion matrix from values
 return (matrix(c(tp, fn, fp, tn), nrow = 2, ncol = 2, byrow = TRUE))
}
tp <- function(m) {</pre>
  # true positive from confusion matrix m
 return (m[1, 1])
fn <- function(m) {</pre>
  # false negative from confusion matrix m
  return (m[1, 2])
}
fp <- function(m) {</pre>
  # false positive from confusion matrix m
  return (m[2, 1])
tn <- function(m) {</pre>
  # true negative from confusion matrix m
  return (m[2, 2])
accuracy <- function(m) {</pre>
  return ((tp(m)+tn(m))/(tp(m)+tn(m)+fp(m)+fn(m)))
tpr <- function(m) {</pre>
 return (tp(m)/(tp(m)+fn(m)))
}
fpr <- function(m) {</pre>
return (fp(m)/(fp(m)+tn(m)))
}
fnr <- function(m) {</pre>
```

```
return (fn(m)/(fn(m)+tp(m)))
}

tnr <- function(m) {
  return (tn(m)/(tn(m)+fp(m)))
}

precision <- function(m) {
  return (tp(m)/(tp(m)+fp(m)))
}</pre>
```

2. Create Confusion Matrix

```
confusion.matrix <- gcmfv(tp=20, fn=75, fp=140, tn=55)
```

3. Get the metric you need

```
fnr(confusion.matrix)
## [1] 0.7894737
```

4 Supervised Learning

4.1 K-nearest Neigbours

4.1.1 Description

- 1. Given training set of size M, N feature values, and 1 binary outcome (0 or 1), we have a table of feature values x_{ij} and a vector of outcome y_i for $1 \le i \le M$, $1 \le j \le N$
- 2. Given any test point x^* , with N feature values x_j^* , for $1 \le j \le N$, calculate euclidean distance of x^* to each training point x_i , i.e. for $1 \le i \le M$, distance_i = $\sqrt{\sum_{j=1}^{N} (x_{ij} x_j^*)^2}$
- 3. Given chosen value k, the k-nearest neighbours/training points x_i to x^* , denoted $N_k(x^*)$, is the set of the first k x_i in the sequence of x_i sorted by increasing distance_i

4.
$$\hat{Y}(x^*) = \frac{1}{k} \sum_{x_i \in N_k(x^*)} y_i$$

5. The predicted outcome for $x^* = y^* = \begin{cases} 1 & \hat{Y} > \sigma \\ 0 & \hat{Y} < \sigma \end{cases}$ where σ is the threshold. $\sigma = 0.5$ in the majority rule.

4.1.2 Choice of σ

- 1. As σ increases,
 - (a) TP, TPR, FP, and FPR decreases or stays the same
 - (b) TN, TNR, FN, and FNR increases or stays the same
- 2. As σ decreases,
 - (a) TP, TPR, FP, and FPR increases or stays the same
 - (b) TN, TNR, FN, and FNR decreases or stays the same
- 3. See Diagnostics of Classifiers ROC Curve for more info

4.1.3 Choice of k

- 1. when k increases, the variance decreases, but bias increases
- 2. when k decreases, the variance increases, but bias decreases
- 3. See Diagnostics of Classifiers Bias-Variance Tradeoff for more info

4.1.4 Prediction Surface

- 1. Boundaries can be curvy
- 2. Can be not axis-aligned

4.1.5 Standardising Variables

- 1. Any variable with a larger scale than others will have a larger effect on the Euclidean distance
- 2. To prevent this problem, we can standardise our data so that all our variables will have mean of zero and standard deviation of one with the scale function in R

```
data <- cbind(</pre>
    1:5,
    seq(100, 500, 100),
    sample(0:1, 5, replace = TRUE)
)
data
   [,1] [,2] [,3]
##
## [1,] 1 100
## [2,] 2 200
## [3,] 3 300 1
## [4,] 4 400 0
## [5,] 5 500
                  1
data[, 1:2] = scale(data[, 1:2])
data
##
              [,1]
                  [,2] [,3]
## [1,] -1.2649111 -1.2649111
## [2,] -0.6324555 -0.6324555
                                0
## [3,] 0.0000000 0.0000000
## [4,] 0.6324555 0.6324555
                                0
## [5,] 1.2649111 1.2649111
```

4.1.6 R Implementation

```
library(class)
data <- matrix(
    c(1, 1, 0,
        1, 2, 0,
        2, 1, 0,
        2, 2, 0,
        2, 3, 0,
        8, 8, 1,
        9, 8, 1,
        8, 7, 1,
        9, 9, 1,
        9, 7, 1), nrow = 10, byrow = TRUE</pre>
```

```
train <- sample(1:10, 5, replace = FALSE)</pre>
train.x <- data[train, 1:2]</pre>
train.y <- data[train, 3]</pre>
cbind(train.x, train.y)
##
             train.y
## [1,] 2 3
                    0
## [2,] 8 8
## [3,] 1 1
                    0
## [4,] 1 2
                    0
## [5,] 9 8
                    1
test.x <- data[-train, 1:2]
test.y <- data[-train, 3]
cbind(test.x, test.y)
##
             test.y
## [1,] 2 1
                  0
## [2,] 2 2
                  0
## [3,] 8 7
                  1
## [4,] 9 9
                  1
## [5,] 9 7
                  1
knn.pred <- knn(train.x, test.x, train.y, k=3)
confusion.matrix <- table(test.y, knn.pred)</pre>
confusion.matrix
##
          knn.pred
## test.y 0 1
        0 2 0
##
        1 0 3
```

4.1.7 Calculation Intensive Exam Questions & Solutions

4.1.7.1 Euclidean Distances, \hat{Y} , and Prediction for 1 Test Data Point

Adapted from Midterm Q17-18. Suppose we have a training set of 5 data points with binary value outcome = c(1,1,0,1,0), $x_1 = c(1,2,1,3,3)$, and $x_2 = c(3,2,1,3,1)$. Using the 3-nearest neighbors classifier and the majority, what is the **fitted outcome value** \hat{Y} and the **predicted outcome value** of $(x_1^*, x_2^*) = (2,4)$?

Solution

1. Copy paste the following code:

```
distance <- function(m, t) {</pre>
  # returns numbered table of euclidean distance of t to each
  # training point in m
  # each column in m is feature variable except last column is
  # outcome y
  if (length(t) != ncol(m)-1) {
    print("test data does not match number of feature variables")
    return
  }
  cd <- function(p1, p2) {</pre>
   return (sqrt(sum((p1-p2)^2)))
  }
  table <- data.frame(id = 1:nrow(m))</pre>
  colnames(m) <- c(paste("x_", 1:(ncol(m)-1), sep = ""), "y")</pre>
  table <- cbind(table, m)
  dist <- rep(1, times<-nrow(m))</pre>
  for (r in 1:nrow(m)) {
    dist[r] \leftarrow cd(m[r, 1:(ncol(m)-1)], t)
  }
  table <- cbind(table, dist)</pre>
 return (table)
}
sorts <- function(d) {</pre>
  # sorts the table output of distance function in increasing
 # euclidean distance
 return (d[order(d[, ncol(d)]), ])
}
y_hat <- function(s, k) {</pre>
# calculate y-hat from table output of sorts function given value of k
return (sum(s[1:k, ncol(s)-1])/k)
}
```

```
predict <- function(y, s) {
    # return predicted class given y-hat y and threshold value s (sigma)
    # assumes y !<- s, i.e. no tie
    return (if (y > s) 1 else 0)
}
```

2. Calculate Euclidean Distances to (2, 4)

3. Sort By Increasing Euclidean Distances

4. Calculate fitted outcome value \hat{Y} based on value of k=3

```
y_hat_value <- y_hat(sorted_dist_matrix, k=3)
y_hat_value
## [1] 1</pre>
```

5. Calculate **predicted outcome value** based on majority rule $\sigma = 0.5$

```
predicted_value <- predict(y_hat_value, s=0.5)
predicted_value
## [1] 1</pre>
```

4.1.7.2 \hat{Y} to Confusion Matrix for n Test Data Points

Adapted from Midterm Q14. Suppose we have k-nearest neighbours classifier for binary outcome Y. The table below shows the actual and fitted outcome for n = 10 test data points.

Actual Y	1	1	0	1	1	0	0	0	1	0
\hat{Y}	0.9	0.8	0.8	0.6	0.5	0.5	0.5	0.3	0.2	0.1

What is the True Positive Rate (TPR) when we predict Y = 1 if $\sigma > 0.7$ Solution

1. Copy paste the following code

```
predict <- function(y, s) {
    # return predicted class given y-hat y and threshold value s (sigma)
    # assumes y !<- s, i.e. no tie
    return (ifelse(y > s, 1, 0))
}
```

2. Obtain predictions for $\sigma = 0.7$

```
predictions <- predict(
   c(0.9, 0.8, 0.8, 0.6, 0.5, 0.5, 0.5, 0.3, 0.2, 0.1), s=0.7
)
predictions
## [1] 1 1 1 0 0 0 0 0 0 0</pre>
```

3. Generate Confusion Matrix

```
table(c(1, 1, 0, 1, 1, 0, 0, 0, 1, 0), predictions)

## predictions
## 0 1
## 0 4 1
## 1 3 2
```

4. Refer to Section 3.11 for metric calculations

4.2 Decision Tree

4.2.1 Graph

- 1. A graph consists of nodes (circles) and edges (lines) connecting the nodes.
- 2. A walk is a sequence of edges which joins a sequence of nodes
- 3. A trail is a walk where all edges are distinct
- 4. A cycle is a trail in which the only repeated nodes are the first and last nodes
- 5. An acyclic graph has no cycles

4.2.2 Tree

- 1. A tree is an acyclic graph.
- 2. A rooted tree has a root node.
- 3. Depth of node in a rooted tree = distance of node from root node
 - (a) depth of root node = 0

4.2.3 Decision Tree

1. Is a rooted tree

4.2.4 Entropy

Given a outcome variable Y, with possible outcomes y_1, y_2, \ldots, y_n which occur with purity $P(y_1), P(y_2), \ldots, P(y_n)$, the entropy of Y is defined as:

$$D(Y) = -\sum_{i=1}^{n} P(y_i) \log_2 P(y_i)$$

4.2.5 Conditional Entropy

Given a feature variable X, with split outcome x_1, x_2 which occur with probability $P(x_1), P(x_2)$, the conditional entropy of Y given X is defined as:

$$D(Y|X) = \sum_{i=1}^{2} P(x_i)D(Y|X = x_i)$$

4.2.6 Decision Tree Algorithm: Entropy

- 1. Start at root node
- 2. Check for termination conditions, if any, e.g.:
 - (a) Minimum purity threshold reached
 - (b) Tree cannot be further split with the preset minimum purity threshold.
 - (c) Any other stopping criterion is satisfied (such as the maximum depth of the tree).
- 3. Calculate entropy for current node (base entropy)
- 4. For each feature variable, for each split outcome, calculate conditional entropy.
- 5. Choose the feature variable and split outcome with the highest entropy reduction = base entropy conditional entropy. Branch the current node by this choice.
- 6. Repeat Step 2-5 for each of the two branched nodes.

4.2.7 Gini Index

Given a outcome variable Y, with possible outcomes y_1, y_2, \ldots, y_n which occur with probability $P(y_1), P(y_2), \ldots, P(y_n)$, the Gini index of Y is defined as:

$$G(Y) = \sum_{i=1}^{n} P(y_i)(1 - P(y_i))$$

4.2.8 Conditional Gini Index

Given a feature variable X, with split outcome x_1, x_2 which occur with probability $P(x_1), P(x_2)$, the conditional Gini index of Y given X is defined as:

$$G(Y|X) = \sum_{i=1}^{2} P(x_i)G(Y|X = x_i)$$

4.2.9 Decision Tree Algorithm: Gini Index

1. Same as Decision Tree Algorithm for Entropy but replace Entropy with Gini Index.

4.2.10 Complexity Parameter C_p

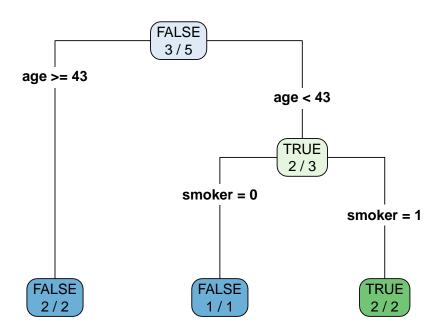
- 1. Smaller values of C_p correspond to decision trees of larger sizes
- 2. Larger values of C_p correspond to decision trees of smaller sizes

4.2.11 Prediction Surface

- 1. Rectangular surfaces
- 2. Can only be axis-aligned

4.2.12 R Implementation

```
library(rpart)
library(rpart.plot)
data <- data.frame(</pre>
  id = 1:5,
  gender = c('M', 'M', 'F', 'M', 'F'),
  age = c(21, 33, 40, 60, 45),
  smoker = c(TRUE, FALSE, TRUE, TRUE, FALSE),
  bmi = c(22, 25, 28, 24, 26),
  diabetes = c(TRUE, FALSE, TRUE, FALSE, FALSE),
  stringsAsFactors = TRUE
)
data
##
     id gender age smoker bmi diabetes
## 1 1
             M 21
                     TRUE 22
                                  TRUE
## 2 2
           M 33 FALSE
                           25
                                 FALSE
## 3 3
            F 40
                   TRUE
                           28
                                  TRUE
## 4 4
                     TRUE
             M 60
                           24
                                 FALSE
             F 45 FALSE 26
## 5 5
                                 FALSE
fit <- rpart(</pre>
  diabetes ~ gender + age + smoker + bmi,
 method = 'class',
  data = data,
  control = rpart.control(minsplit=1),
  parms = list(split = 'information')
```



4.2.13 Calculation Intensive Exam Questions & Solutions

4.2.13.1 Entropy involving n outcomes

Adapted from Midterm Q2. Let X be the outcome variable with n=2 possible outcomes, which occur with purity c(0.5, 0.5). Calculate the entropy of X. Solution.

1. Copy paste the following code

```
entropy <- function(prob) {
   sum <- 0
   for (p in prob) {
      sum <- sum + p * log2(p)
   }
   return (-sum)
}</pre>
```

2. Calculate entropy

```
entropy(c(0.5, 0.5))
## [1] 1
```

4.2.13.2 Gini Index involving n outcomes

Adapted from Midterm Q28. Let X be the outcome variable with n=2 possible outcomes, which occur with purity c(1490/2201, 1-1490/2201). Calculate the Gini index of X.

Solution.

1. Copy paste the following code

```
gini_index <- function(prob) {
   sum <- 0
   for (p in prob) {
      sum <- sum + p * (1-p)
   }
   return (sum)
}</pre>
```

2. Calculate Gini index

```
gini_index(c(1490/2201, 1-1490/2201))
## [1] 0.4373668
```

4.3 Naive Bayes

4.3.1 Probability Laws

4.3.1.1 Bayes' Theorem

$$P(Y|X) = \frac{P(Y \cap X)}{P(X)} = \frac{P(X|Y) \times P(Y)}{P(X)}$$

4.3.1.2 Law of total probability

$$P(A) = P(A \cap B) + P(A \cap \neg B)$$

4.3.2 Naive Bayes

Suppose the categorical outcome variable Y takes on values in the set $\{y_1, y_2, \dots, y_k\}$ and there are m feature variables X_1, X_2, \dots, X_m . By Bayes Theorem, for $j = 1, 2, \dots, k$,

$$P(Y = y_j | X_1 = x_1, X_2 = x_2, \dots, X_m = x_m)$$

$$= \frac{P(X_1 = x_1, X_2 = x_2, \dots, X_m = x_m | Y = y_j) \times P(Y = y_j)}{P(X_1 = x_1, X_2 = x_2, \dots, X_m = x_m)}$$

4.3.2.1 Assume Conditional Independence

$$P(X_1 = x_1, X_2 = x_2, \dots, X_m = x_m | Y = y_j)$$

$$= P(X_1 = x_1 | Y = y_j) P(X_2 = x_2 | Y = y_j) \dots P(X_m = x_m | Y = y_j)$$

$$= \prod_{i=1}^m P(X_i = x_i | Y = y_j)$$

4.3.2.2 Ignore Denominator

$$P(X_1 = x_1, X_2 = x_2, \dots, X_m = x_m)$$

4.3.2.3 Finally

For
$$j = 1, 2, ..., k$$
,

$$P(Y = y_j | X_1 = x_1, X_2 = x_2, \dots, X_m = x_m)$$

 $\propto P(Y = y_j) \times \prod_{i=1}^m P(X_i = x_i | Y = y_j)$

4.3.3 Numerical Underflow

To prevent probability scores from becoming too small to be accurately stored in a computer, we can take logarithm on both sides,

$$\log P(Y = y_i | X_1 = x_1, X_2 = x_2, \dots, X_m = x_m)$$

$$\propto \log P(Y = y_j) + \sum_{i=1}^{m} \log P(X_i = x_i | Y = y_j)$$

4.3.4 R Implementation

4.3.5 Calculation Intensive Exam Questions & Solutions

```
table_to_naiveBayes <- function(features, feature_categories, )

## Error: <text>:1:63: unexpected ')'
## 1: table_to_naiveBayes <- function(features, feature_categories, )
##</pre>
```

4.4 Linear & Logistic Regression

4.4.1 Solving Simultaneous Equations

1. Use solve function in R

- 5 Unsupervised Learning
- 6 Big Data Techniques
- 6.1 MapReduce