

資料科學期末報告

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- 專案簡介
- 資料輸入輸出與前處理
- 模型設定及處理
- 實驗結果
- 參考出處



專案簡介

- 若鐵達尼存活預測是
 - 初入資料科學、Kaggle競賽的熱門入門題
 - 初入特徵工程，了解其過程及特徵選取
 - 瞭解資料科學的運作過程
- 那此次的心臟病分類預測競賽就是
 - 正式實作資料科學的流程
 - 較深入進行特徵工程，用各種假設檢定、熵來了解特徵之間對答案及模型的重要性
 - 遇到實務上的問題並嘗試著解決

資料輸入輸出

- 共有欄位如下：

Id	Max rate
Age	Exercise angina
Sex	St depression
Chest pain	Slope
Resting bp	Vessels
Cholestorol	Thalium scan
High sugar	Heart disease
Ecg	

資料前處理

- 轉換之前
- 為什麼要轉換
- 如何轉換與處理資料
- 各欄位原始格式
- 預期各欄位轉換後格式
- 資料觀察
- 轉換後的資料
 - 訓練
 - 測試

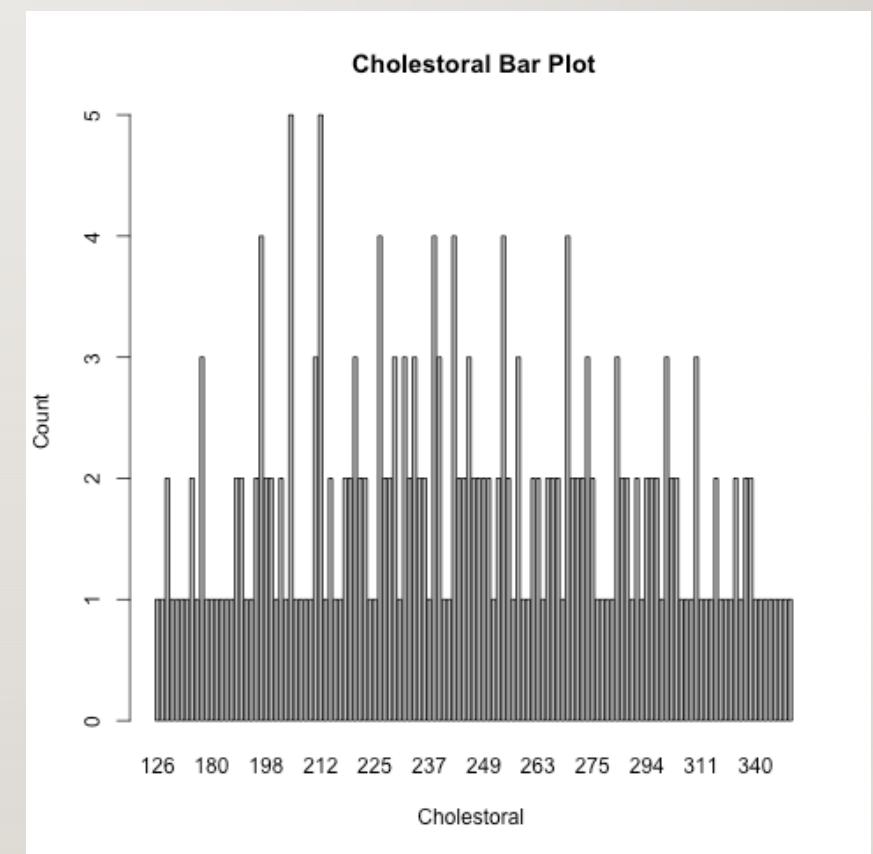
資料前處理 – 轉換之前

- 理解、觀察各欄位資料
- 進行適當的轉換於特定欄位
- 觀察轉換後的分佈，例如
 - 受試者的年齡區間分佈
 - 受試者的性別分佈
 - 受試者的總膽固醇區間分佈
 - 各個欄位與心臟病的關係程度為何
 - ...等



資料前處理 – 為什麼要轉換

- 多數欄位原始型態是數值型
- 資料範圍相當大時，觀察其分佈會有些困難
- 因此需要做適當的資料轉換



資料前處理 – 如何轉換與處理資料

- 前處理：
 - Outlier : ($>$ 第三四分位 + $0.5 \times IQR$; $<$ 第一四分位 - $0.5 \times IQR$)
 - 將個欄位 outlier 的 index 記錄起來，找將共同的 id 的資料並移除
 - 其他 outlier 則用最大值或最小值補齊，避免訓練時讓模型訓練錯誤
 - NA Numbers :
 - 找到 NA 的欄位資料，並用 median 來填補（因為沒有連續型數值變數有 NA，所以對類別變數則用 median）
 - Normalize :
 - 這部分未處理，已包含在建模裡面

資料前處理 – 如何轉換與處理資料

- 數值變數：
 - 區間化：利用 kmeans 方法，找到最大組間距離、最小組內距離的 K 點。並利用 cut 針對 K 個中心找到相對應的區間，Label 化
- 類別變數：
 - 連結變數與答案之間的關係，算出 contingency table
 - 變數間的重要性與相關性
 - Chi Square 假設檢定：
 - 當 p value 小於 alpha (0.05)，則拒絕 H0，也就是兩變數之間相關；反之則接受 H0，即兩變數獨立
 - Mutual Information：
 - 利用相互資訊熵，來觀察變數對於答案 Label 的重要程度

$$I(X;Y) = \sum_{y \in Y} \sum_{x \in X} p(x,y) \log \left(\frac{p(x,y)}{p(x)p(y)} \right),$$

資料前處理 – 各欄位原始格式

Input	Format
id	integer
age	numeric
sex	binary
chest_pain	multinomial
resting_bp	numeric
cholesterol	numeric
high_sugar	binary
ecg	multinomial

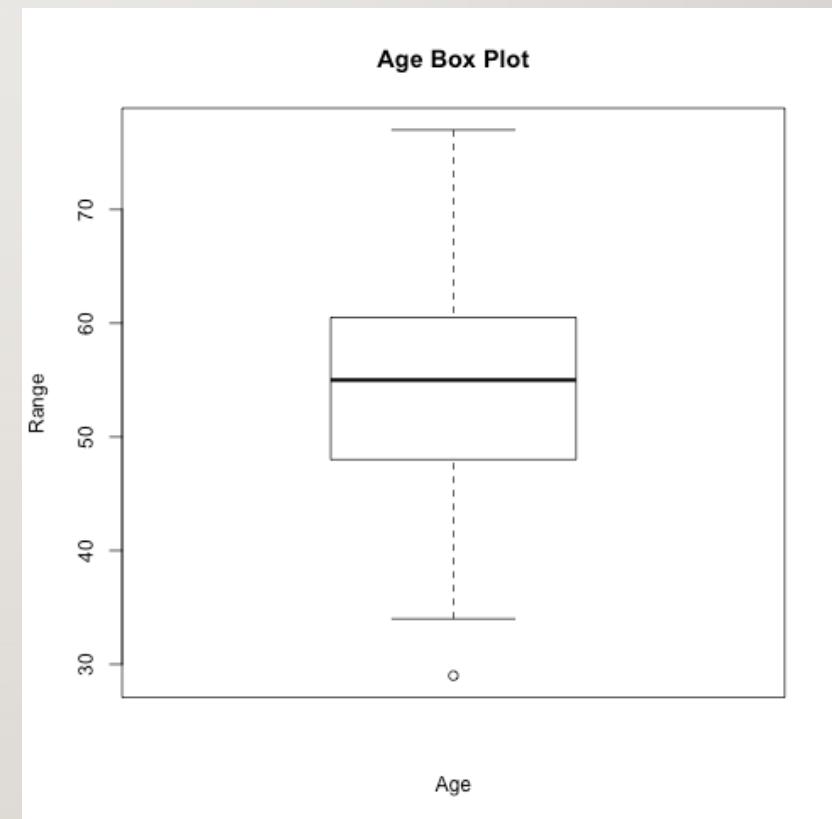
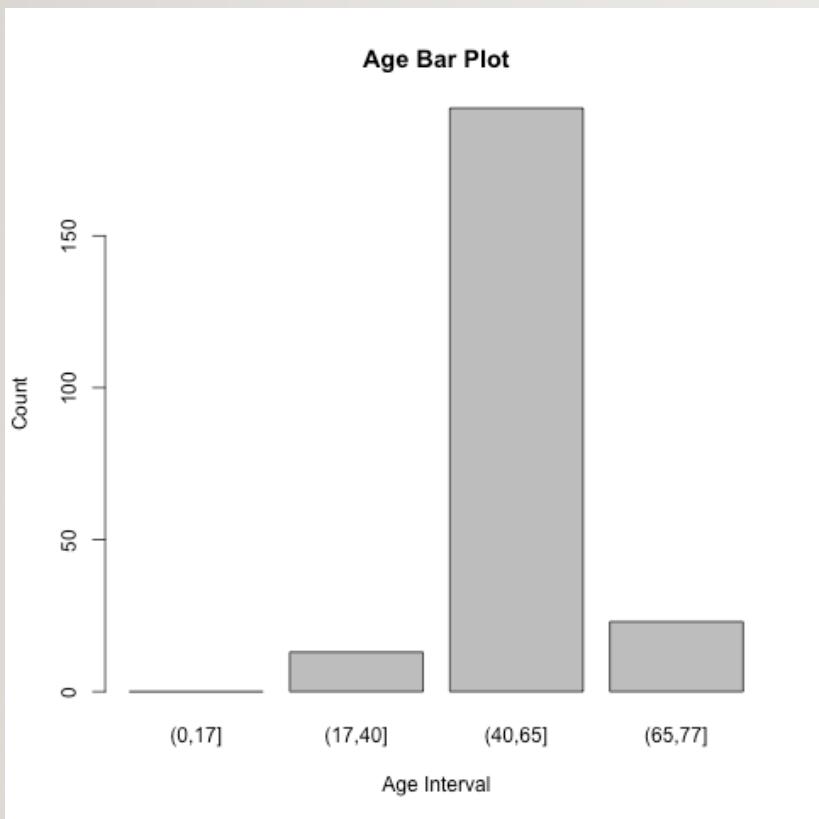
資料前處理 – 各欄位原始格式

Input	Format
max_rate	numeric
exercise_angina	binary
st_depression	binary
slope	multinomial
vessels	multinomial
thalium_scan	multinomial
Heart_disease	binary

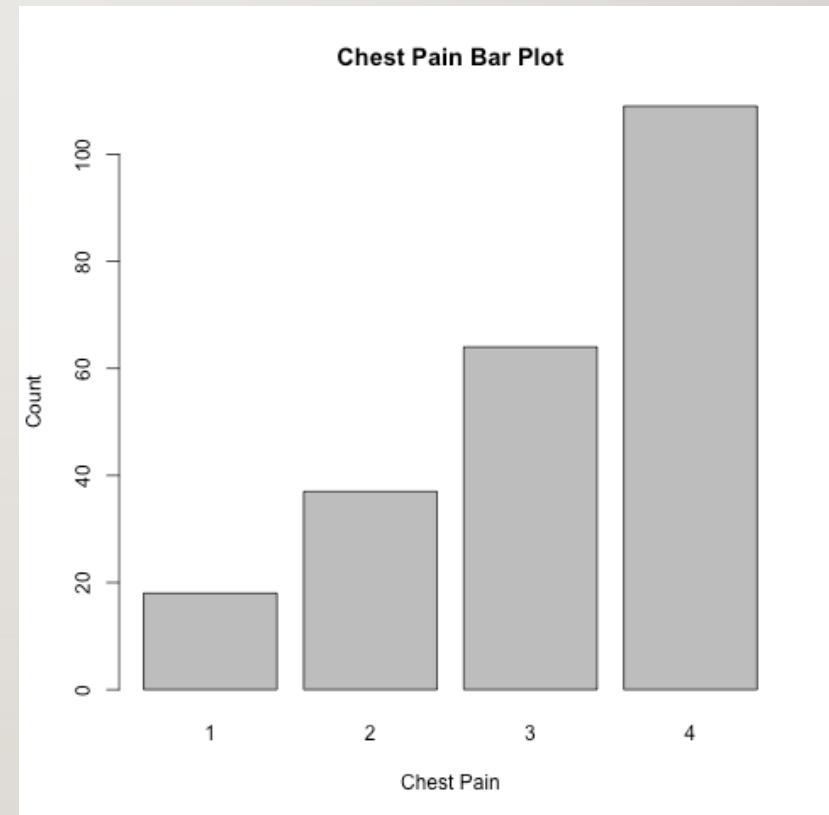
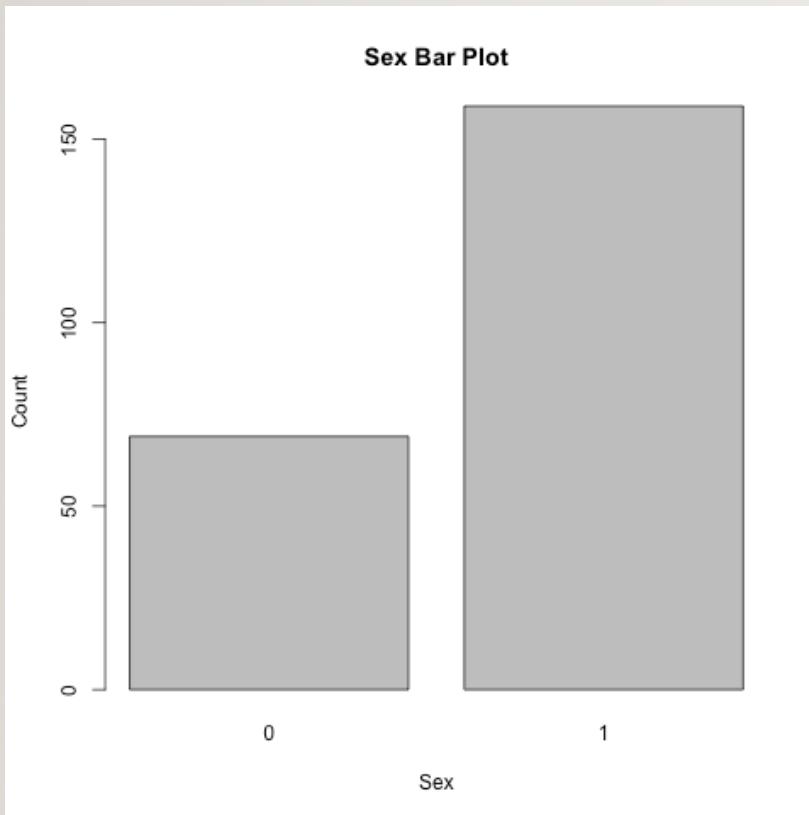
資料前處理 – 預期各欄位轉換後格式

Input	Format	Remark
age_interval	multinomial	利用設定區間進行標籤化 P.S: 0, 17, 40, 65, max_value
resting_bp_interval	multinomial	利用設定區間進行標籤化 P.S: 0, 120, 139, max_value
cholestorol_interval	multinomial	利用設定區間進行標籤化 P.S: 0, 129, 200, 239, max_value
max_rate	multinomial	利用 Kmeans 進行標籤化 P.S: 113, 121, 152, 177, 202
st_depression	multinomial	利用 Kmeans 進行標籤化 P.S: 0, 0.03, 0.51, 0.81, 1.11, 1.48, 1.97, max_value
vessels	multinomial	Filling up NA
thalium_scan	multinomial	Filling up NA, (3, 6, 7) ->(1,2,3)

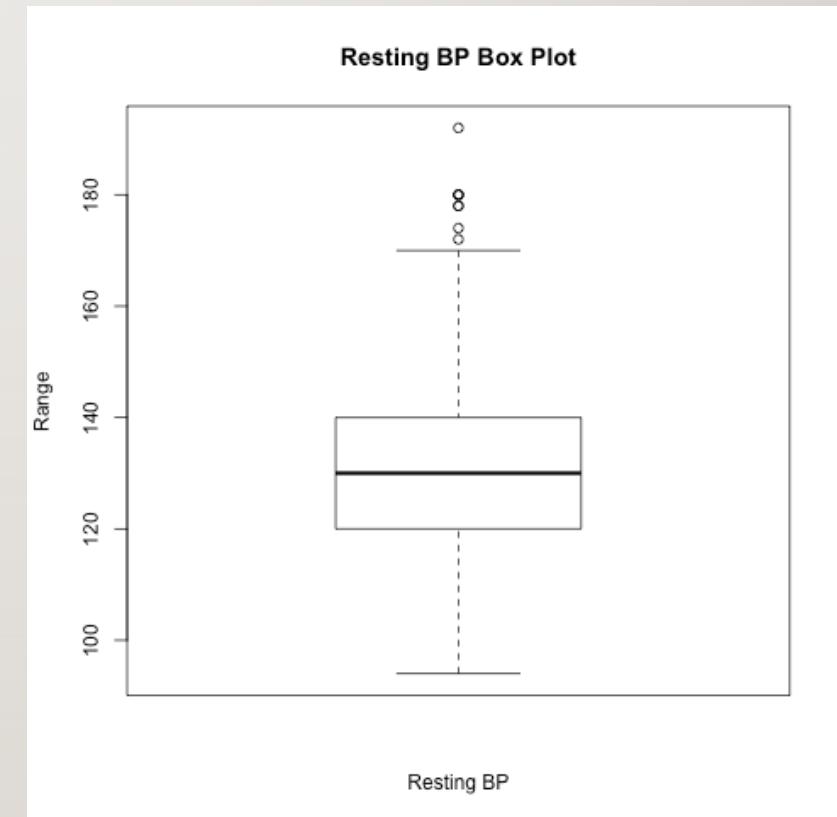
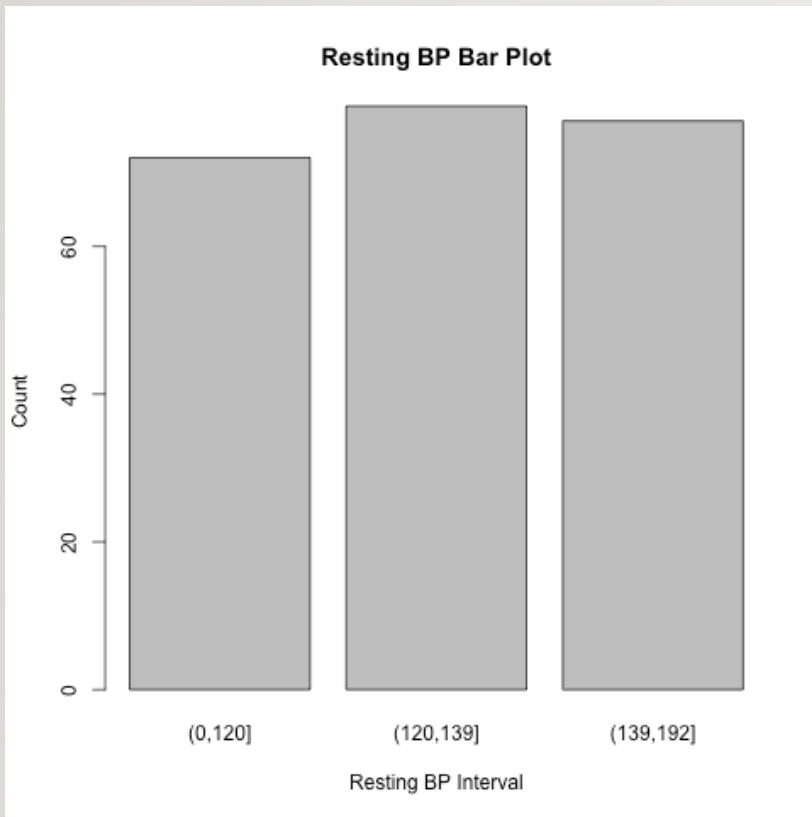
資料前處理 - 資料觀察



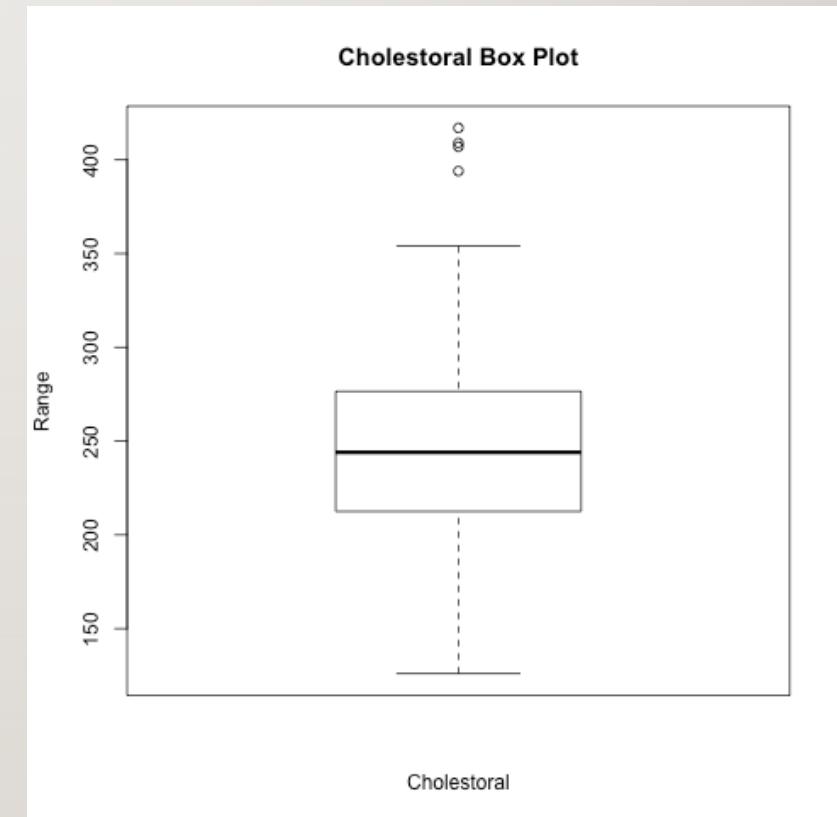
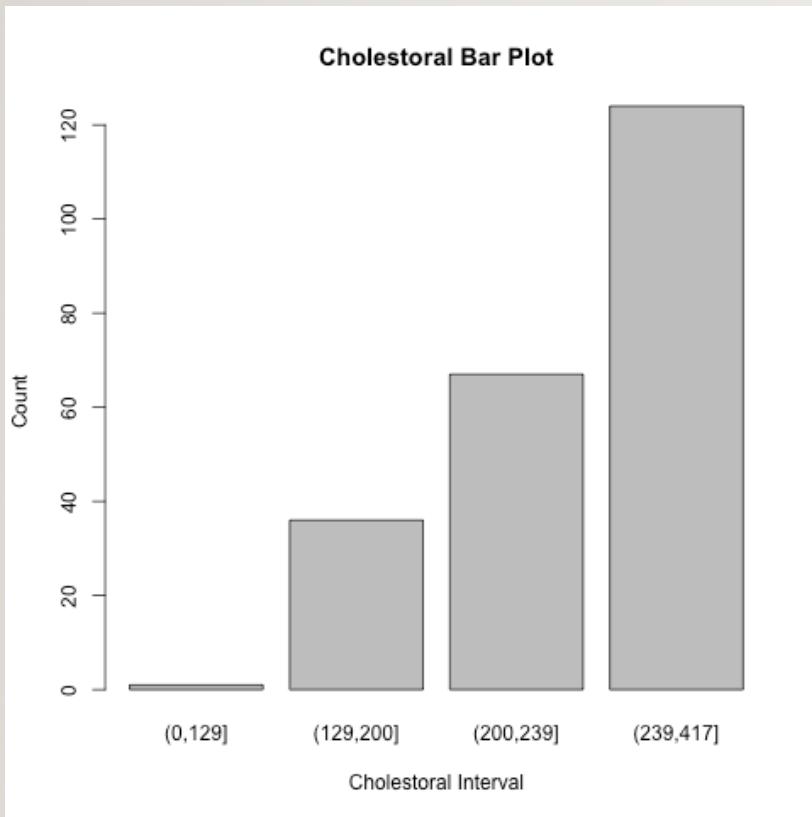
資料前處理 - 資料觀察



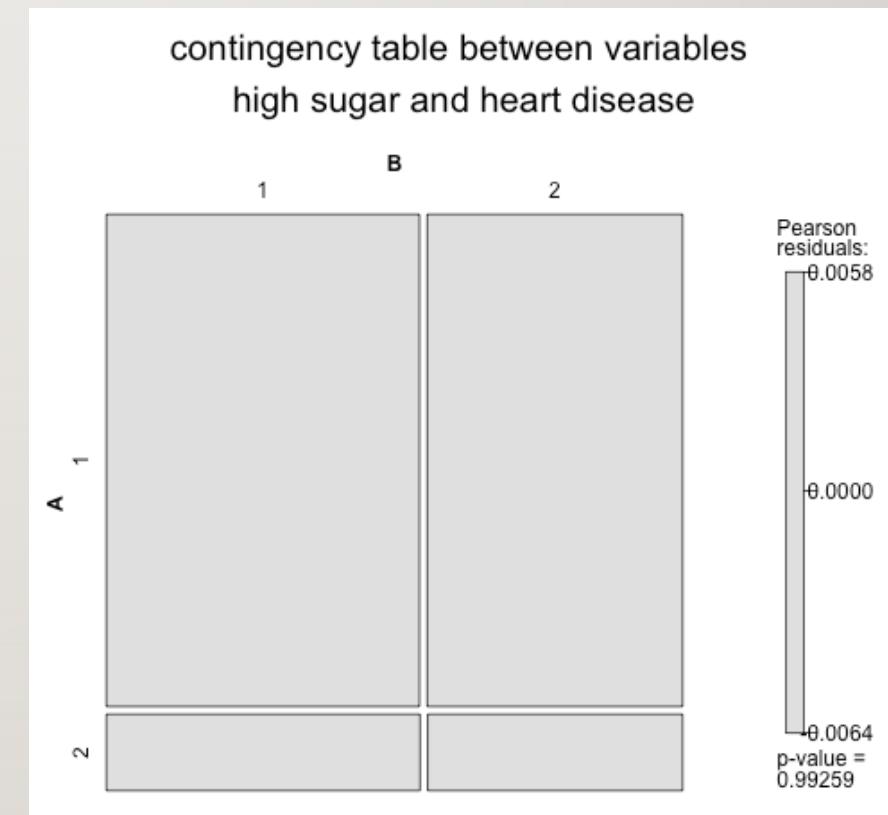
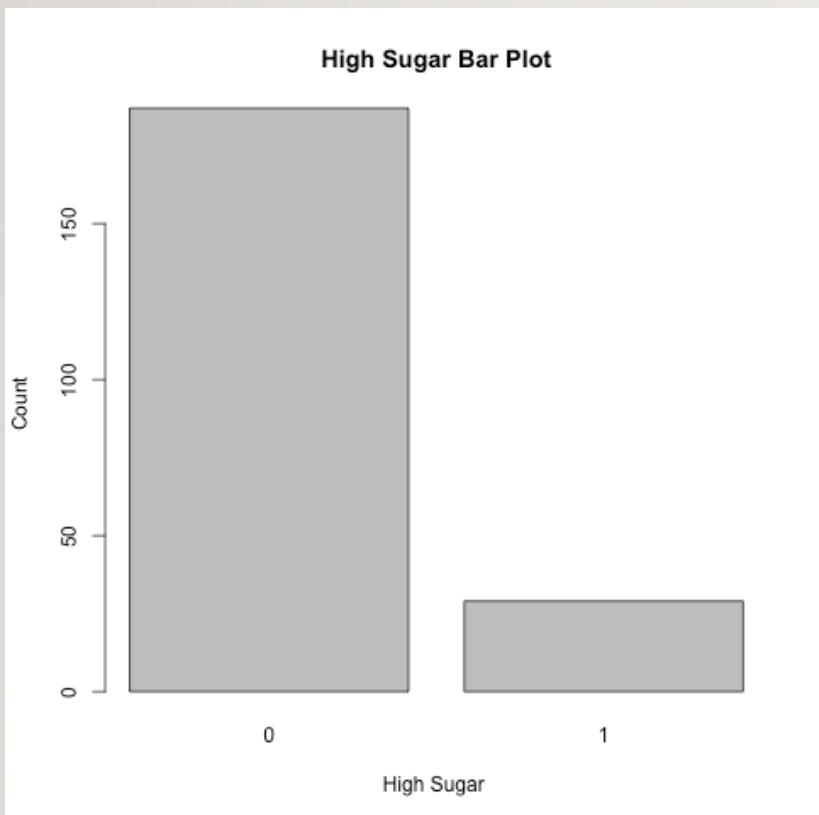
資料前處理 – 資料觀察



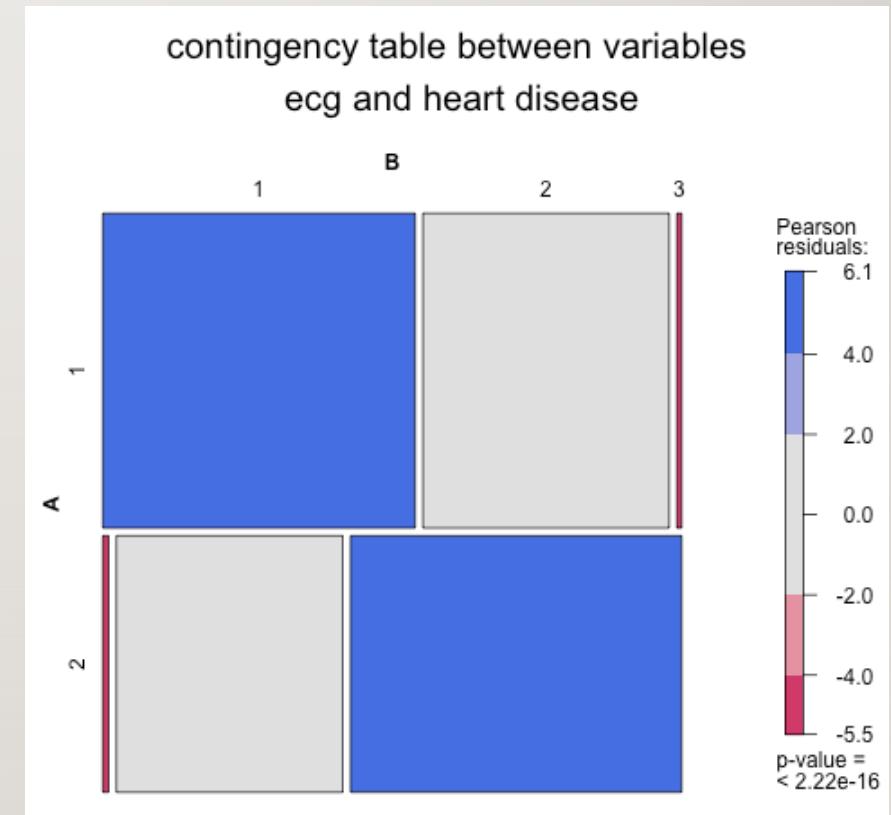
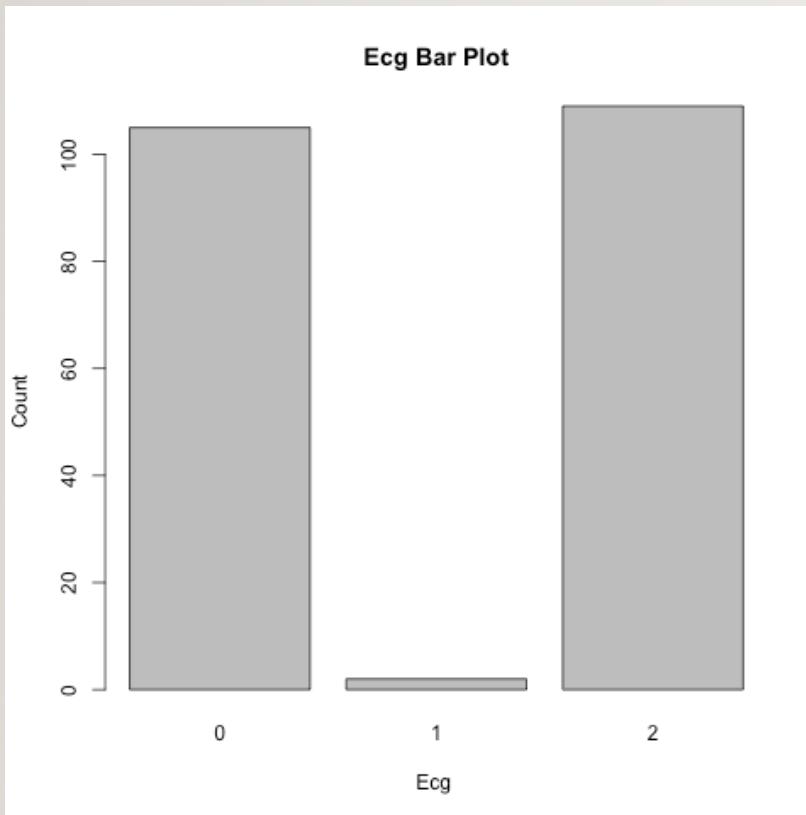
資料前處理 – 資料觀察



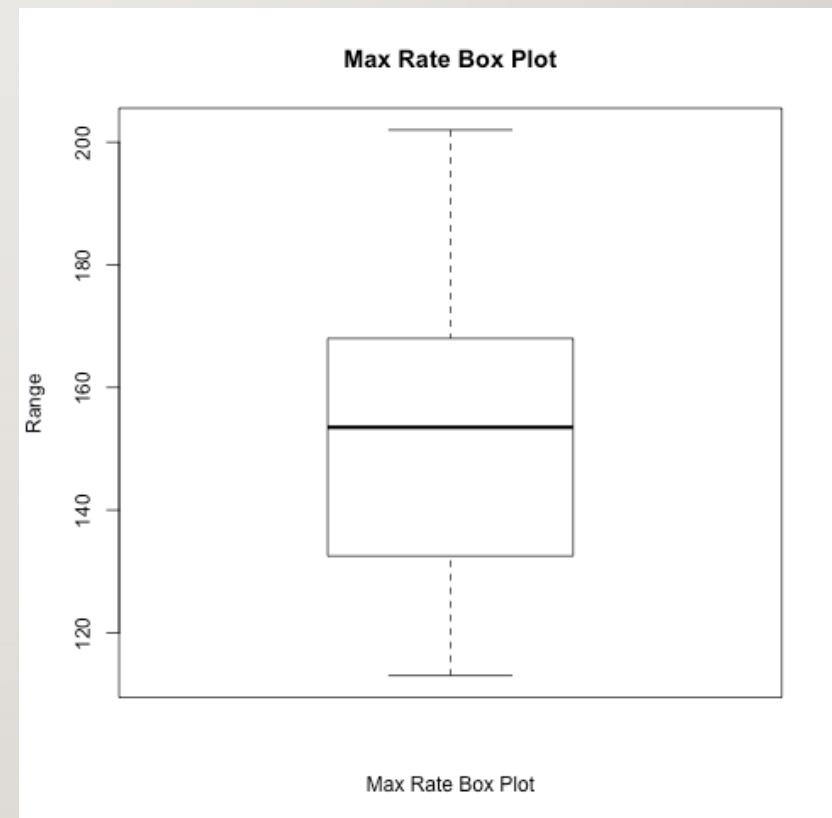
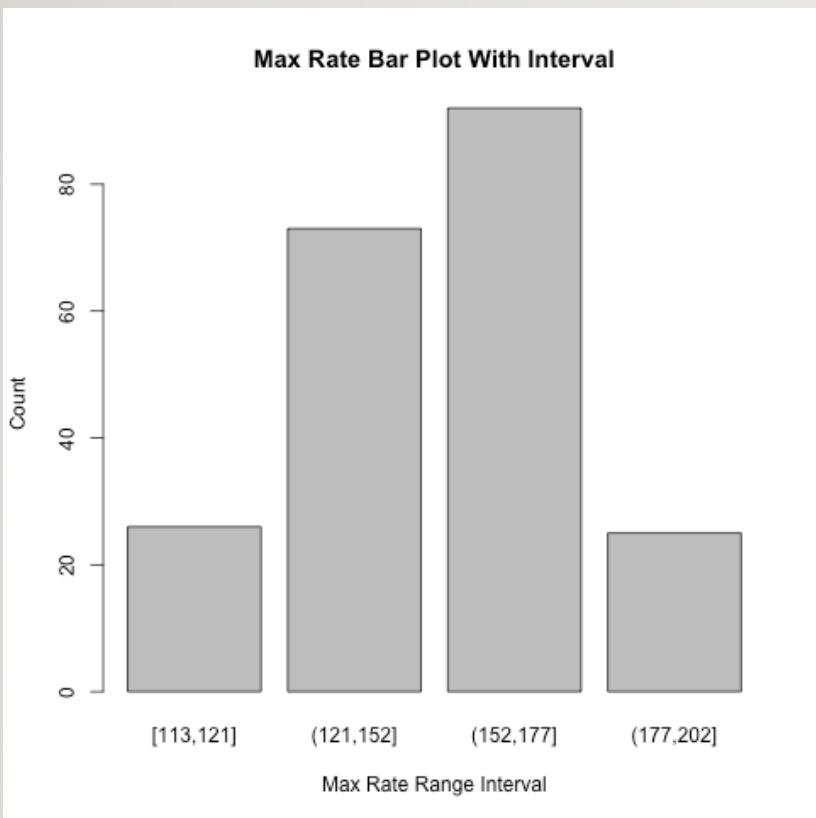
資料前處理 – 資料觀察



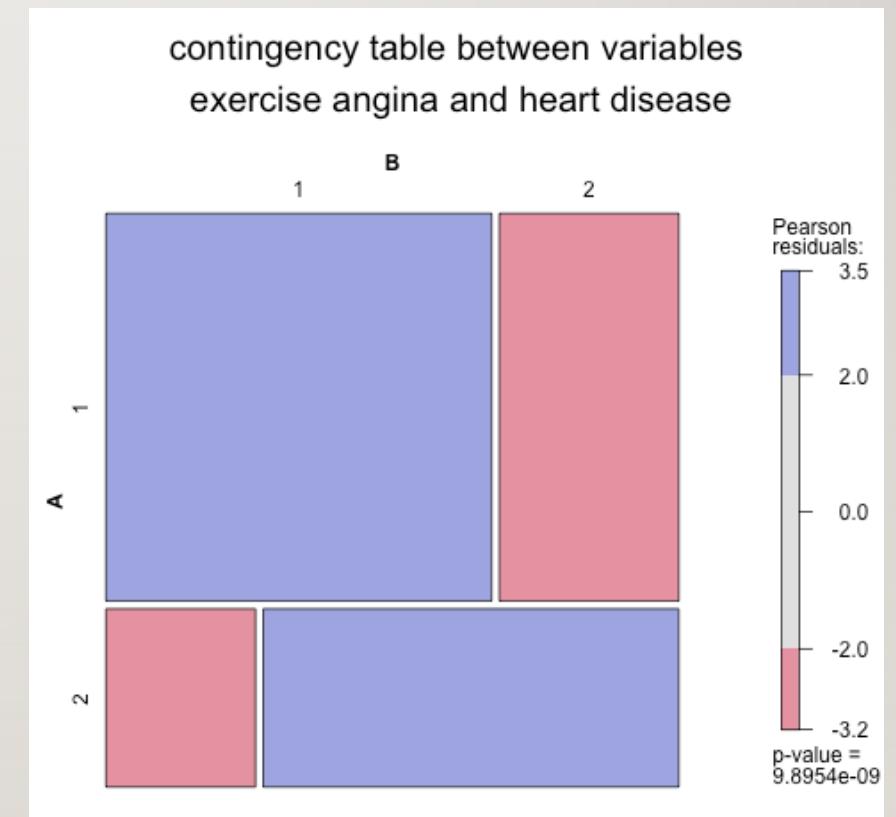
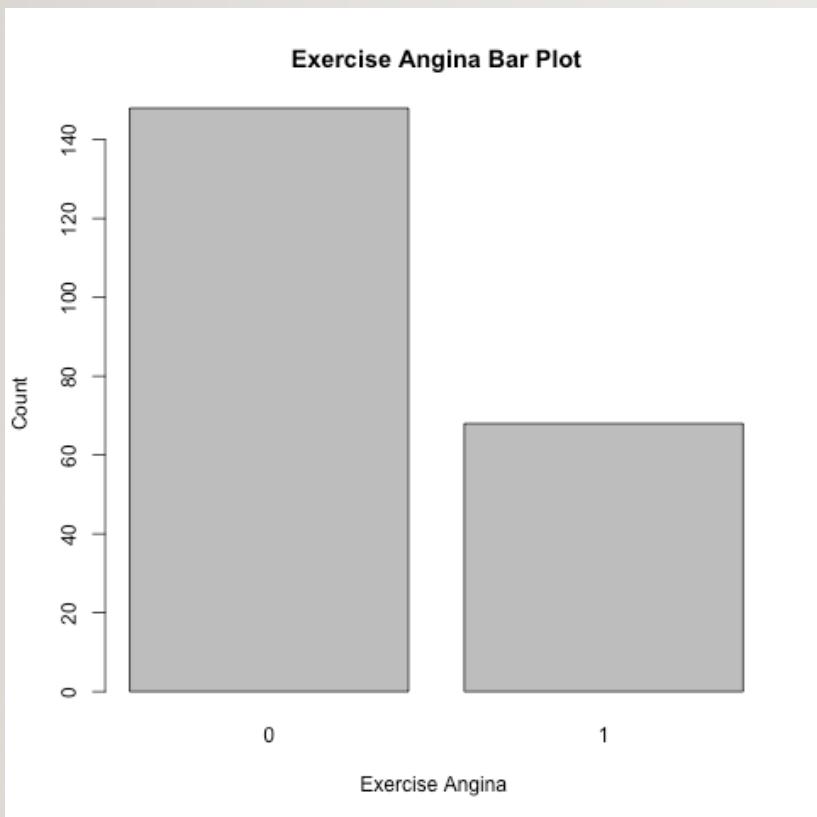
資料前處理 – 資料觀察



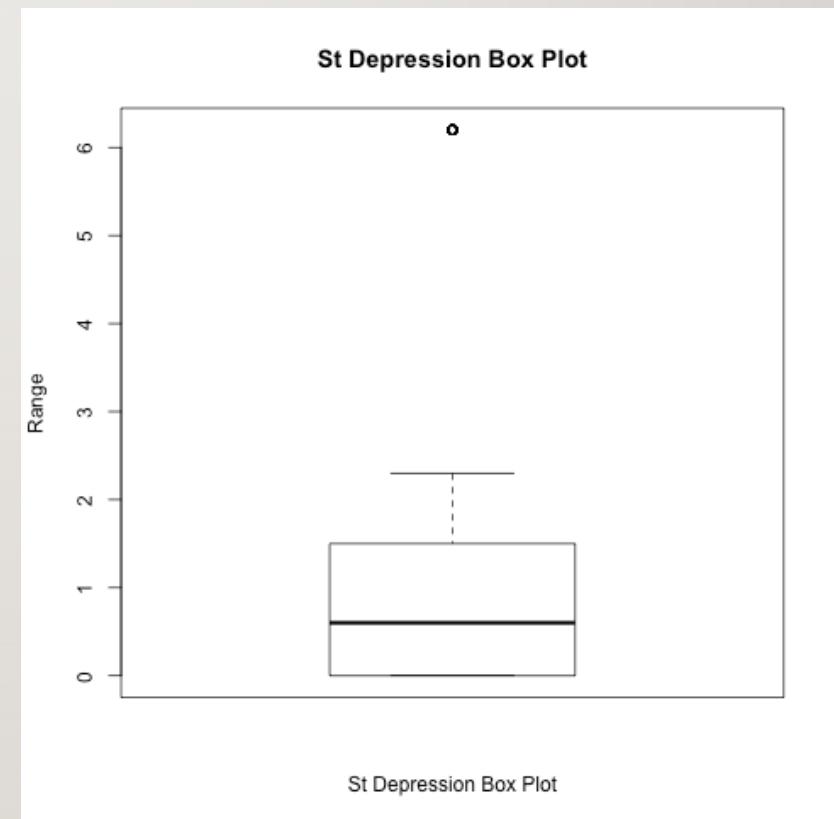
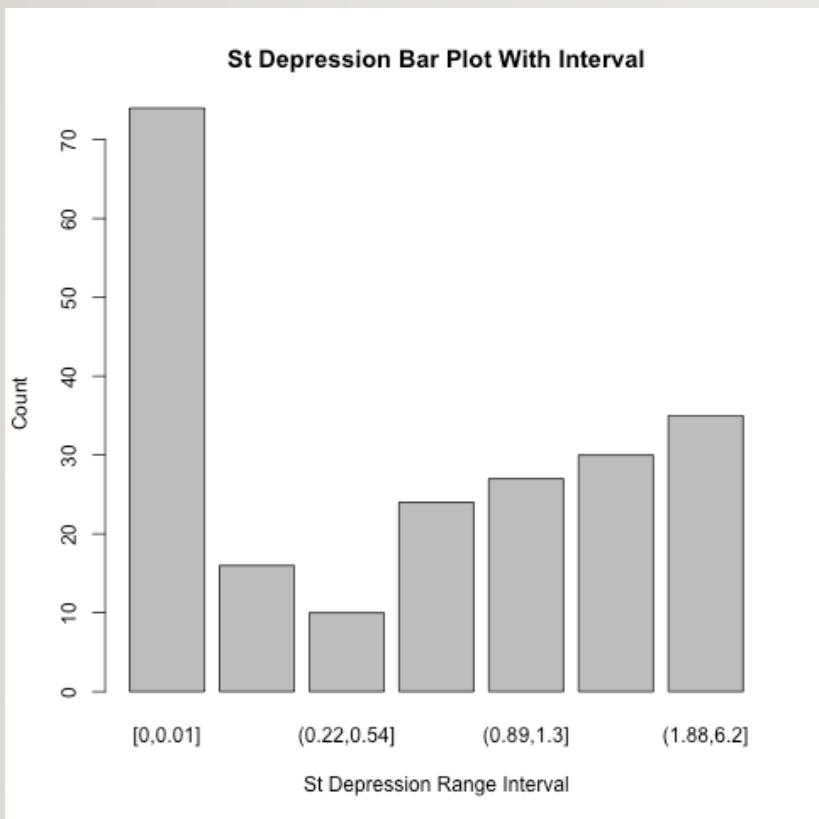
資料前處理 - 資料觀察



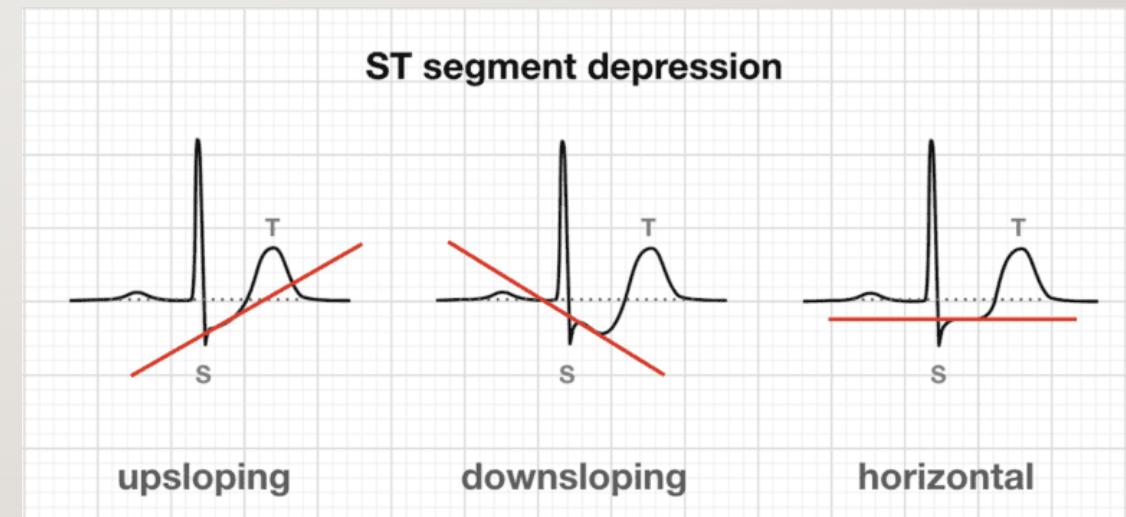
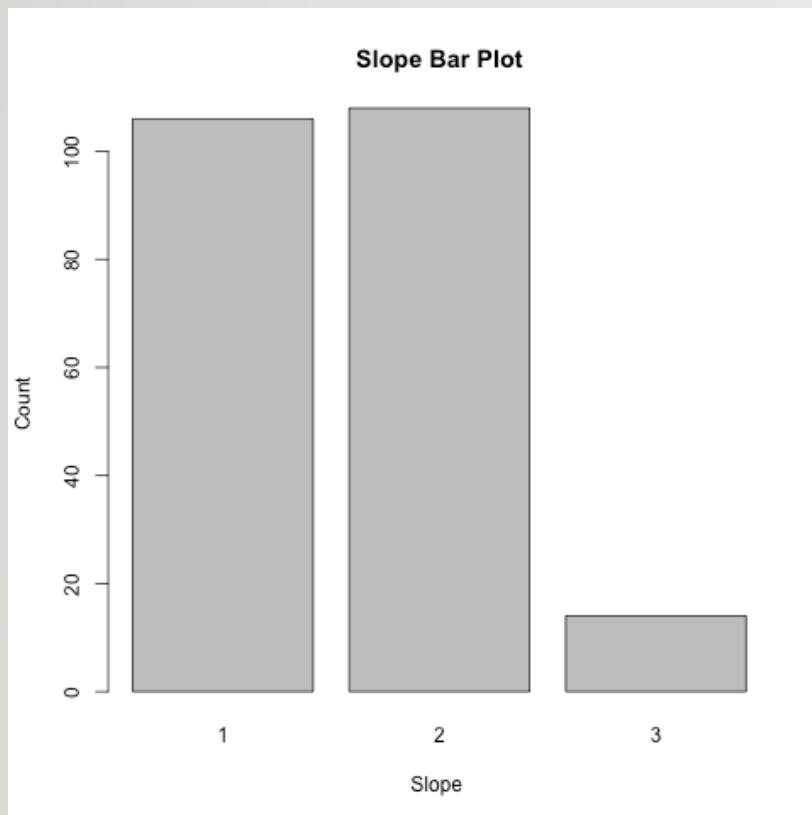
資料前處理 – 資料觀察



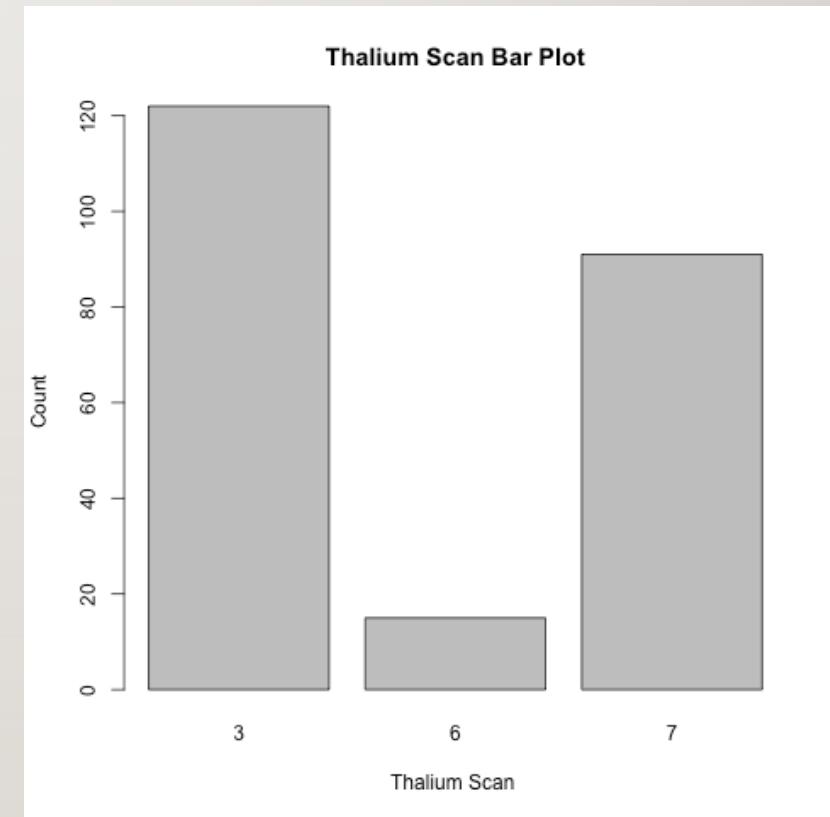
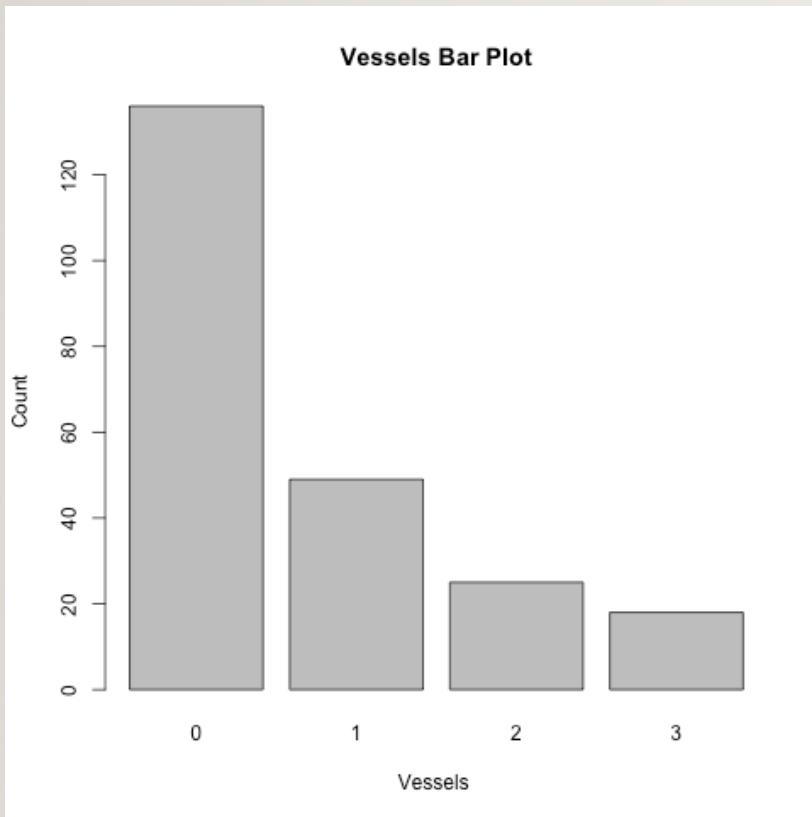
資料前處理 - 資料觀察

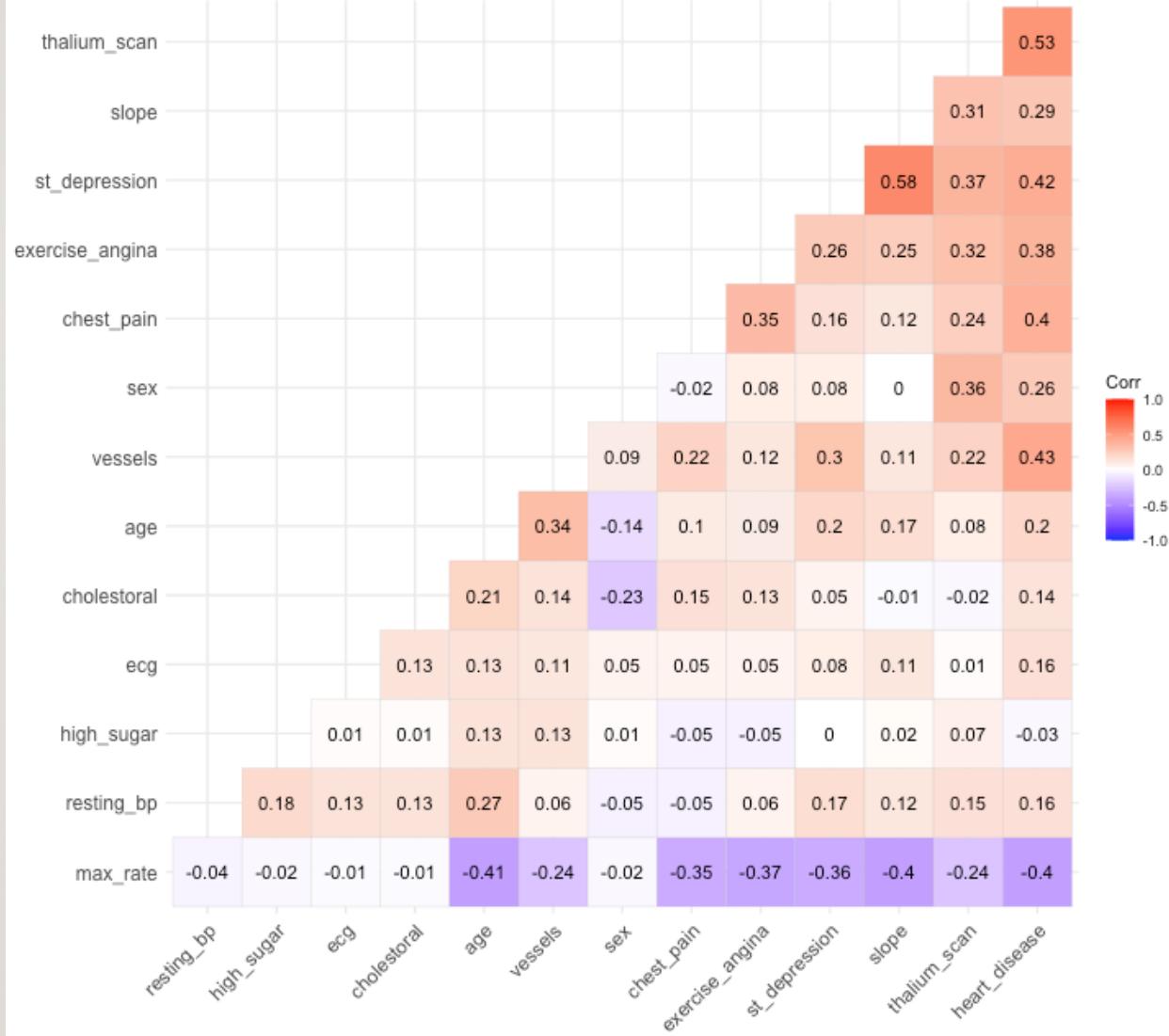


資料前處理 – 資料觀察



資料前處理 - 資料觀察





資料前處理 – 轉換後的訓練資料

id	cholesterol	cholesterol_with_label	cholesterol_without_label	high_sugar	ecg	max_rate	max_rate_with_label	max_rate_without_label	exercise_angina	st_depression	st_depression_with_label	st_depression_without_label	heart_disease
1	233	2	(198,239]	1	2	150	2	(121,152]	0	2.3	7	(1.88,6.2]	0
2	286	4	(282,417]	0	2	113	1	[113,121]	1	1.5	6	(1.3,1.88]	1
3	229	2	(198,239]	0	2	129	2	(121,152]	1	6.2	7	(1.88,6.2]	1
5	204	2	(198,239]	0	2	172	3	(152,177]	0	1.4	6	(1.3,1.88]	0
6	236	2	(198,239]	0	0	178	4	(177,202]	0	0.8	4	(0.54,0.89]	0
8	417	4	(282,417]	0	0	163	3	(152,177]	1	0.6	4	(0.54,0.89]	0
9	254	3	(239,282]	0	2	147	2	(121,152]	0	1.4	6	(1.3,1.88]	1
10	203	2	(198,239]	1	2	155	3	(152,177]	1	6.2	7	(1.88,6.2]	1
11	192	1	[182,198]	0	0	148	2	(121,152]	0	0.4	3	(0.22,0.54]	0
12	294	4	(282,417]	0	2	153	3	(152,177]	0	1.3	5	(0.89,1.3]	0
15	199	2	(198,239]	1	0	162	3	(152,177]	0	0.5	3	(0.22,0.54]	0
17	229	2	(198,239]	0	0	168	3	(152,177]	0	1	5	(0.89,1.3]	1
18	239	3	(239,282]	0	0	160	3	(152,177]	0	1.2	5	(0.89,1.3]	0
19	275	3	(239,282]	0	0	139	2	(121,152]	0	0.2	2	(0.01,0.22]	0
20	266	3	(239,282]	0	0	171	3	(152,177]	0	0.6	4	(0.54,0.89]	0
21	211	2	(198,239]	0	2	144	2	(121,152]	1	1.8	6	(1.3,1.88]	0
24	224	2	(198,239]	0	2	173	3	(152,177]	0	6.2	7	(1.88,6.2]	1
27	417	4	(282,417]	0	0	172	3	(152,177]	0	0	1	[0,0.01]	0
28	226	2	(198,239]	0	0	114	1	[113,121]	0	6.2	7	(1.88,6.2]	0
29	247	3	(239,282]	0	0	171	3	(152,177]	0	1.5	6	(1.3,1.88]	0
31	239	3	(239,282]	0	0	151	2	(121,152]	0	1.8	6	(1.3,1.88]	0
33	417	4	(282,417]	0	0	158	3	(152,177]	0	0	1	[0,0.01]	1

資料前處理 – 轉換後的測試資料

id	cholestorol	cholestorol_with_label	cholestorol_without_label	high_sugar	ecg	max_rate	max_rate_with_label	max_rate_without_label	exercise_angina	st_depression	st_depression_with_label	st_depression_without_label
179	564	6	(287,564]	0	0	162	6	(161,166]	0	1.9	3	(1.26,2.15]
14	263	5	(260,287]	0	0	173	8	(172,187]	0	0	1	[0,0.14]
195	211	3	(209,234]	0	2	131	1	[131,132]	0	1.5	3	(1.26,2.15]
118	183	1	[177,186]	0	0	187	8	(172,187]	0	1.4	3	(1.26,2.15]
299	264	5	(260,287]	0	0	132	2	(132,142]	0	1.2	2	(0.14,1.26]
229	206	2	(186,209]	0	2	131	1	[131,132]	1	0	1	[0,0.14]
244	234	3	(209,234]	0	0	145	3	(142,151]	0	2.6	4	(2.15,4]
302	236	4	(234,260]	0	2	174	8	(172,187]	0	0	1	[0,0.14]
153	564	6	(287,564]	0	2	160	5	(156,161]	0	1.6	3	(1.26,2.15]
90	256	4	(234,260]	0	2	149	3	(142,151]	0	0.5	2	(0.14,1.26]
91	564	6	(287,564]	0	2	151	4	(151,156]	0	0.4	2	(0.14,1.26]
256	209	2	(186,209]	0	0	173	8	(172,187]	0	0	1	[0,0.14]
197	234	3	(209,234]	1	2	131	1	[131,132]	0	0.1	1	[0,0.14]
26	219	3	(209,234]	0	0	158	5	(156,161]	0	1.6	3	(1.26,2.15]
7	268	5	(260,287]	0	2	160	5	(156,161]	0	4	4	(2.15,4]
289	221	3	(209,234]	0	2	163	6	(161,166]	0	0	1	[0,0.14]
254	295	6	(287,564]	0	2	157	5	(156,161]	0	0.6	2	(0.14,1.26]
211	215	3	(209,234]	0	0	170	7	(166,172]	0	0	1	[0,0.14]
78	564	6	(287,564]	0	2	142	3	(142,151]	0	1.5	3	(1.26,2.15]
81	208	2	(186,209]	0	2	148	3	(142,151]	1	4	4	(2.15,4]
43	564	6	(287,564]	0	0	162	6	(161,166]	0	0.4	2	(0.14,1.26]

模型設定及處理

- 需求設定：
 - Which method do you use?
 - What is a null model for comparison?
 - How do you perform evaluation? ie. Cross-validation, or extra separated data

模型設定及處理

- XGBoost
- Logistic Regression

模型設定及處理 – XGBOOST

- 特徵選取與特徵轉換：
 - 將 slope 轉換成「binary」型式
 - 將 thalium_scan 轉換成「one-hot encoding」
 - 利用 xgb.importance 的套件，找出較重要的特徵，並訓練模型
- 實驗設定：
 - Cross Validation : 20

Feature	Gain	Frequency
thalium_scan	0.275342017	0.01639344
chest_pain	0.133716699	0.06557377
cholestorol	0.114106357	0.19672131
exercise_angina	0.010420478	0.01639344
High_sugar	0.007573798	0.01639344

模型設定及處理 – LOGISTIC REGRESSION

- 特徵選取與特徵轉換：
 - 原始資料：
 - 根據全部資料，利用 student t test 來找到對應的 t 值 (P value)，選取重要特徵：

- chest_pain
- vessels
- thalium_scan

```
Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -8.198600  4.765700 -1.720 0.085372 .
age          -0.003836  0.043680 -0.088 0.930025
sex           1.204706  0.847649  1.421 0.155249
chest_pain    0.631230  0.319222  1.977 0.047997 *
resting_bp    0.035300  0.019485  1.812 0.070037 .
cholesterol   0.004815  0.007044  0.684 0.494254
high_sugar    -0.244334  0.853651 -0.286 0.774708
ecg            0.377170  0.315155  1.197 0.231394
max_rate      -0.029827  0.017083 -1.746 0.080815 .
exercise_angina -0.055663  0.689874 -0.081 0.935691
st_depression   0.302998  0.404717  0.749 0.454058
slope           -0.235356  0.639480 -0.368 0.712842
vessels         1.402988  0.404926  3.465 0.000531 ***
thalium_scan    0.537693  0.179171  3.001 0.002691 **
---
Signif. codes:  0 '****' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Dispersion parameter for binomial family taken to be 1)

Null deviance: 181.047 on 132 degrees of freedom
Residual deviance: 81.029 on 119 degrees of freedom
AIC: 109.03
```

模型設定及處理 – LOGISTIC REGRESSION

- 特徵選取與特徵轉換：
 - 轉換後資料（非最終模型）：
 - One hot encoding
 - 各別考慮 chest_pain, ecg, , thalium_scan 三變數：0/1
 - Age：
 - cut into bins => nonsignificant
 - linear combinations
 - examine p-value

模型設定及處理 – LOGISTIC REGRESSION

- 特徵選取與特徵轉換：
 - 轉換後資料（最終模型）：
 - 以decision tree, 拿沒有 NA 的 column 項來預測遺失值
 - Vessels ; thalium_scan
 - resting_bp_without_label：
 - 用kmeans 跑區間，最後分出5個區間：(93, 113, 133, 160, 192)

```
# fill na's (vessels,thalium_scan)
vessels.model <- rpart(vessels ~ age+sex+chest_pain+resting_bp+cholestorol+high_sugar
+ecg+max_rate+exercise_angina+st_depression+slope+heart_disease
,data=train[!is.na(train$vessels), ],method='class')

train$vessels[is.na(train$vessels)] <-predict(vessels.model, newdata=train[is.na(train$vessels)],
, type = "class")

thalium_scan.model <- rpart(thalium_scan ~ age+sex+chest_pain+resting_bp+cholestorol+high_sugar+ecg
+max_rate+exercise_angina+st_depression+slope+vessels+heart_disease
, data=train[!is.na(train$thalium_scan), ], method='class')

train$thalium_scan[is.na(train$thalium_scan)] <- predict(thalium_scan.model
, newdata=train[is.na(train$thalium_scan),
, type="class"])
```

模型設定及處理 – LOGISTIC REGRESSION

- 轉換後資料（最終模型，承上）：
 - slope_label：
 - origin category: 0,1,2
 - Since distribution like the table
 - category = 0 => 0 ; category = 1,2 => 1
 - thalium_scan
 - Origin: 3,6,7 => transform to 1,2,3
 - One – hot encoding
 - 雖然有三類，但實際上只需要用兩類來概括資料：thalium_scan_1 + thalium_scan_3 as feature
- 實驗設定：
 - Cross Validation : 5~10
 - 根據 proposed-final 模型，我們設不同的 seed

slope	Heart_disease
0	1
1	2
2	3

模型設定及處理

- 需求回應：
 - Which method do you use?
 - => XGBoost, Logistic Regression
 - What is a null model for comparison?
 - 反之，我們有針對飽和模型進行 Baseline 模型之前的訓練
 - 利用 T Test 找到較重要的特徵後，進行該特徵的強化與處理
 - How do you perform evaluation?
 - => K-Fold Cross-validation
 - => 如上所說，進行不同特徵之下的訓練

實驗結果

- 需求設定：
 - Which metric do you use
 - precision, recall, R-square
 - Is your improvement significant?
 - What is the challenge part of your project?

實驗結果 – LOGISTIC REGRESSION

model	Item set	Private Score	Public Score
XGBoost	thalium_scan、chest_pain、cholestorol、exercise_angina、High_sugar	0.86792	0.90909
Baseline (特徵未經處理)	chest_pain、vessels、thalium_scan、resting_bp、max_rate	0.86363	0.83018
Proposed-A (Slope_label 改為二類)	resting_bp_without_label、slope_label、vessels、chest_pain、thalium_scan	0.81132	0.90909
Proposed-C (chest_pain 改為 one-hot encoding)	resting_bp_without_label、slope_label、vessels、chest_pain_2、chest_pain_3、chest_pain_4、thalium_scan	0.77358	0.86363
Proposed-Final (thalium_scan 改為 one-hot encoding)	resting_bp_without_label、slope_label、vessels、chest_pain、thalium_scan_1、thalium_scan_3	0.86792	0.90909

Accuracy is not always the best choice to choose the test mode !!!!

實驗結果 – LOGISTIC REGRESSION

- 不同的 seed :

seed	public score	private score
4	0.86792	0.90909
10	0.83018	0.81818

[predict_final.csv](#)

34 minutes ago by [流](#)

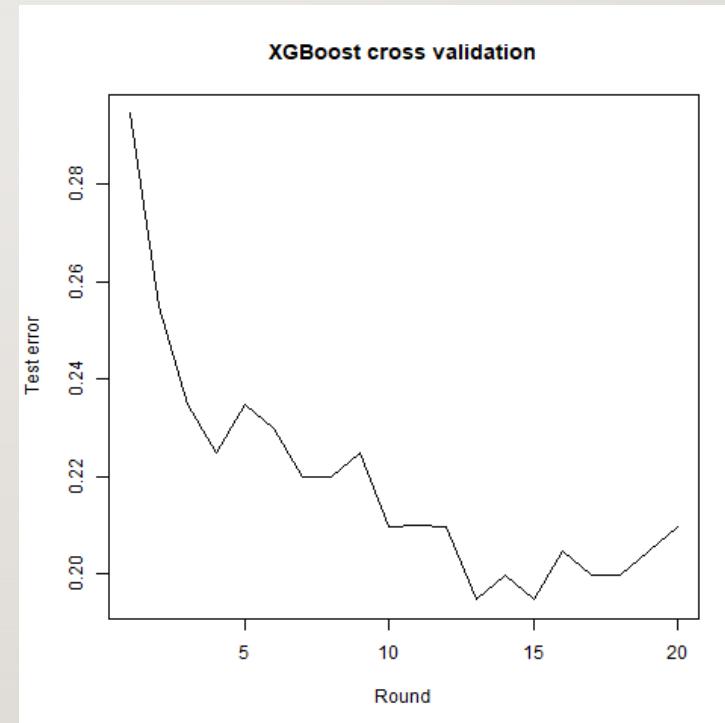
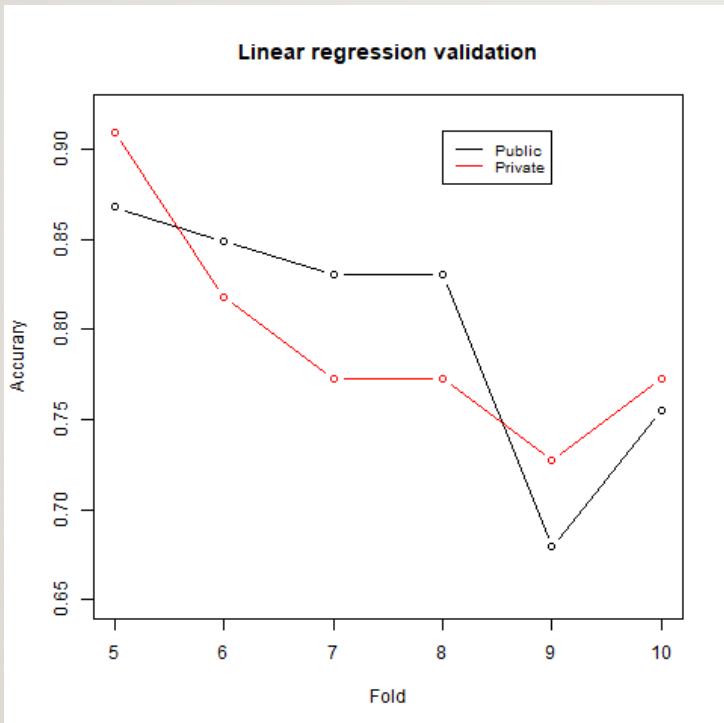
check - seed: 4 (prev: 10)

0.86792

0.90909

The way we cut into fold is important, it can be improved if we make some tricks before cut

實驗結果



實驗結果

- 需求回應：
 - Which metric do you use
 - => Accuracy, Test Error
 - Is your improvement significant?
 - => 針對不同的資料處理及標籤設定，會有不同結果
 - => 不同的模型、seed 也會影響結果。
 - => 綜合以上，我們最後且最佳模型有很大進步
 - What is the challenge part of your project?
 - => 資料的特徵工程及選擇，因為不知道何者是最重要且必要的特徵
 - 訓練時的抽樣方法也需多加研究

參考出處

- Age interval (年齡區間劃分)
 - 出自《老年性生理學和老年的性生活》一書
- Blood pressure interval (血壓區間劃分)
- Cholestral interval (總膽固醇區間劃分)
 - 啟新診所
 - 馬偕醫院
- 資料處理：
 - <https://www.datacamp.com/community/tutorials/contingency-tables-r>
 - <https://www.pluralsight.com/guides/cleaning-up-data-from-outliers>
 - <https://www.gastonsanchez.com/r4strings/formatting.html>
 - <https://www.guru99.com/r-data-frames.html>

參考出處

- 套件引用：
 - <https://cran.r-project.org/web/packages/hash/hash.pdf>
 - <https://stackoverflow.com/questions/23765996/get-all-keys-from-ruby-hash>
 - https://www.rdocumentation.org/packages/tibble/versions/1.4.2/topics/add_column
 - <https://stackoverflow.com/questions/45741498/add-column-in-tibble-with-variable-column-name>
 - <https://statmath.wu.ac.at/projects/vcd/>
 - <https://rdrr.io/cran/infotheo/man/mutinformation.html>
 - <https://cran.r-project.org/web/packages/infotheo/infotheo.pdf>
 - <https://www.rdocumentation.org/packages/stringr>
 - https://stringr.tidyverse.org/reference/str_detect.html
 - <https://www.rdocumentation.org/packages/vcd/>

END