BIOST 546 HW 3

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```
# set global options for code chunks
knitr::opts_chunk$set(message = FALSE, warning = FALSE, collapse = TRUE)
knitr::opts_knit$set(root.dir = rprojroot::find_rstudio_root_file())

library(knitr)
library(dplyr)
library(ggplot2)
library(ggcorrplot)
library(caret)
library(pROC)
library(cowplot)
library(MASS)
library(class)
```

As in HW2, we will perform binary classification on the Breast Cancer Wisconsin (Diagnostic) Data Set in the csv file `wdbc.data`. The dataset describes characteristics of the cell nuclei present in n (sample size) images. Each image has multiple attributes, which are described in detail in `wdbc.names`. This time, however, you will predict the attribute in column 2, which we denote by Y, given the columns $\{3, 4, \ldots, 32\}$, which we denote by $X_1, ..., X_{30}$. The variable Y represents the diagnosis (M = malignant, B = benign).

1. Data exploration and Simple Logistic Regression

- 1a. Describe the data: sample size n, number of predictors p, and the number of observations in each class.

```
# load data
wdbc <- read.csv("./dataset/wdbc.data", header = FALSE, stringsAsFactors = TRUE)
wdbc_set <- wdbc[, -1] %>%
    rename(diagnosis = 1)

# rename columns to predictor labels X1, ..., X30
names <- c("diagnosis")
for (i in 1:ncol(wdbc_set[ , -1])) {
  names[i + 1] <- paste("X", i, sep = "")
}
colnames(wdbc_set) <- names

# check for missing values; if returns 0, no missing data in data set
which(complete.cases(wdbc_set) == FALSE)
## integer(0)
```

```r
# count number of observations in each diagnosis class
wdbc_summary <- wdbc_set %>%
  count(diagnosis)
kable(wdbc_summary, caption = "Total observations by diagnosis class")
```

Table 1: Total observations by diagnosis class

diagnosis	n
B	357
M	212

The `wdbc` data set has a sample size of $n = 569$ and $p = 30$ predictors. There are 357 observations in the benign class and 212 observations in the malignant class (as shown in **Table 1**).

- 1b. Divide the data into a training set of 400 observations and a test set.

```r
set.seed(2)
random_sample <- sample(1:nrow(wdbc_set), size = 400, replace = FALSE)

# split data into training and test sets
wdbc_train <- wdbc_set[random_sample, ]
wdbc_test <- wdbc_set[-random_sample, ]
```

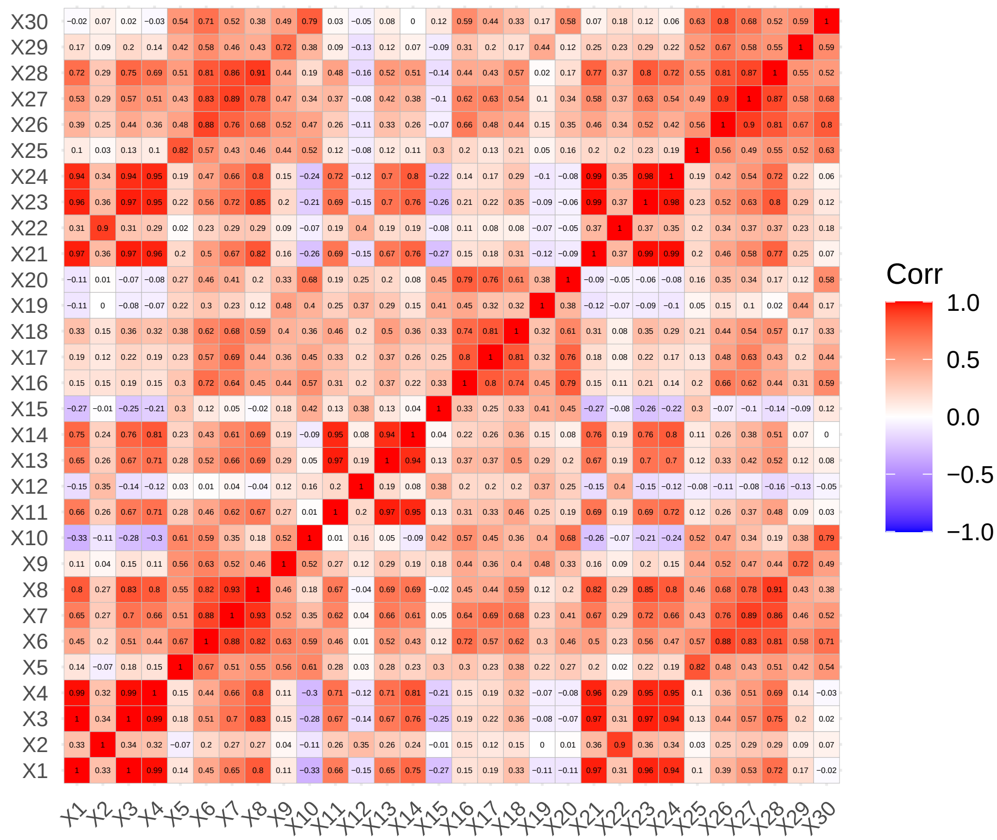
- 1c. Normalize your predictors, i.e. for each variable X_j remove the mean and make each variable's standard deviation 1. Explain why you should perform this step separately in the training set and test set.

```r
# normalize predictors such that each variable has mean = 0 and sd = 1
wdbc_train_scaled <- scale(wdbc_train[ , -1])
wdbc_test_scaled <- scale(wdbc_test[ , -1])
```

We must normalize the predictors of the training and test sets separately to avoid having observations in one set affect the other set. If we were to normalize the predictors of the training and test sets together (i.e. normalize before splitting into train-test sets), the values of the test set will have been affected by the normalization of the training set observations. This renders the test set not completely brand new data for us to validate models fitted with the training set, leading to possible bias in our data.

- 1d. Compute the correlation matrix of your training predictors (command `cor`) and plot it (e.g. command `ggcorrplot` in the library `ggcorrplot`). Inspect the correlation matrix and explain what type of challenges this data set may present?

```r
ggcorrplot(cor(wdbc_train_scaled),
           lab = "TRUE", lab_size = 1,
           tl.cex = 8)
```



Looking at the correlation matrix for the training predictors in the training data set, it looks like we have a number of variables/predictors that are highly correlated with each other.

For example, X_1 and X_3 are perfectly correlated with each other. There are also high correlations between X_1 and X_{21}, X_{23}, X_{24}.

This introduces multicollinearity to the data, which reduces the precision of the estimated individual predictor coefficients in our regression models.

- 1e. Fit a simple logistic regression model to predict Y given $X_1, ..., X_{30}$.
  Inspect and report the correlation between the variables X_1 and X_3; and the magnitude of their coefficient estimates $\hat{\beta}_1$, $\hat{\beta}_3$ with regard to the other coefficients of the model. Comment on their values and relate this to what we have seen in class.

```r
glm_train <- glm(formula = wdbc_train$diagnosis ~ .,
                 family = "binomial",
                 data = as.data.frame(wdbc_train_scaled))

kable(summary(glm_train)$coefficients,
      digits = 3,
      caption = "Training Set: Estimates of Predictor Coefficient")
```

Table 2: Training Set: Estimates of Predictor Coefficient

	Estimate	Std. Error	z value	Pr(>|z|)
(Intercept)	92.461	28281.573	0.003	0.997
X1	-862.997	462270.497	-0.002	0.999
X2	-3.798	13416.446	0.000	1.000
X3	989.130	544553.105	0.002	0.999
X4	-189.766	100538.360	-0.002	0.998
X5	117.778	15574.736	0.008	0.994
X6	-302.085	41791.183	-0.007	0.994
X7	-8.086	39076.942	0.000	1.000
X8	265.443	49259.173	0.005	0.996
X9	-122.564	22339.352	-0.005	0.996
X10	96.252	28237.700	0.003	0.997
X11	559.966	61288.543	0.009	0.993
X12	3.348	9628.505	0.000	1.000
X13	-110.485	70063.531	-0.002	0.999
X14	-540.239	107218.217	-0.005	0.996
X15	31.709	12943.540	0.002	0.998
X16	73.749	13649.606	0.005	0.996
X17	52.341	57193.234	0.001	0.999
X18	90.037	20354.300	0.004	0.996
X19	-93.137	24992.864	-0.004	0.997
X20	-262.422	65894.489	-0.004	0.997
X21	-1030.876	195279.900	-0.005	0.996
X22	105.940	15834.642	0.007	0.995
X23	-502.589	175318.352	-0.003	0.998
X24	2156.153	279421.092	0.008	0.994
X25	-97.368	20531.897	-0.005	0.996
X26	5.471	30882.296	0.000	1.000
X27	106.239	52714.248	0.002	0.998
X28	162.495	25575.212	0.006	0.995
X29	241.662	25846.588	0.009	0.993
X30	-39.356	62867.795	-0.001	1.000

```r
kable(head(summary(glm_train, correlation = TRUE)$correlation)[ , 1:6],
      digits = 3,
      caption = "Training Set: Correlation Values (Partial Table)")
```

Table 3: Training Set: Correlation Values (Partial Table)

	(Intercept)	X1	X2	X3	X4	X5
(Intercept)	1.000	0.119	0.199	-0.126	0.228	-0.469
X1	0.119	1.000	0.034	-0.977	-0.057	-0.134
X2	0.199	0.034	1.000	0.015	0.383	-0.676
X3	-0.126	-0.977	0.015	1.000	-0.084	0.116
X4	0.228	-0.057	0.383	-0.084	1.000	-0.453
X5	-0.469	-0.134	-0.676	0.116	-0.453	1.000

The correlation between variables X_1 and X_3 is -0.9773678. **Table 2** shows that the estimated coefficient values for X_1 and X_3 are $\hat{\beta}_1$ = -862.9974499 and $\hat{\beta}_3$ = 989.1304951, respectively. The coefficient estimates are opposite in sign and nearly equal in magnitude to each other, which makes sense given the correlation between X_1 and X_3 is -0.9773678.

Compared to the other estimated coefficients of the model, the values of $\hat{\beta}_1$ and $\hat{\beta}_3$ are larger compared to the *non-collinear* coefficient estimates (e.g., not compared to X_{21}, X_{23}, X_{24} which are collinear with X_1).

- 1f. Use the glm previously fitted and the Bayes rule to compute the predicted outcome $\hat{Y}$ from the associated probability estimates (computed with `predict`) both on the training and the test set. Then compute the confusion table and prediction accuracy (rate of correctly classified observations) both on the training and test set. Comment on the results.

2. Ridge Logistic Regression

- 2a.From the normalized training set and validation set, contruct a data matrix X (numeric) and an outcome vector y (factor).
- 2b. On the training set, run a ridge logistic regression model with `glmnet` (with the argument `family = "binomial"`) to predict Y given $X_1, ..., X_{30}$. Use the following grid of values for lambda: `10^seq(5, -18, length = 100)`.
- 2c. Plot the values of the coefficients β_1, β_3 (y-axis) in function of `log(lambda)` (x-axis). Comment on the result.
- 2d. Apply 10-fold cross-validation with the previously defined grid of values for lambda. Report the value of lambda that minimizes the CV misclassification error. We will refer to it as the optimal lambda. Plot the misclassification error (y-axis) in function of `log(lambda)` (x-axis). Use `cv.glmnet` with the arguments `family = "binomial"` and `type.measure = "class"`.
- 2e. Report the number of coefficients β_j that are different from 0 for the ridge model with the optimal lambda. Comment on the results.
- 2f. Use the regularized glm previously gitted (with the optimal lambda) and the Bayes rule to compute the predicted outcome $\hat{Y}$ from the associated probability estimates on both the training and test sets. Then compute the confusion table and prediction accuracy both on the training and test set. Comment on the results. Use the command `predict` with argument 'type = "response".
- 2g. Plot the ROC curve, computed on the test set.
- 2h. Compute an estimate of the area under the ROC curve (AUC).

3. Lasso Logistic Regression

Repeat the sub-problems 2b to 2h using a lasso regression model instead of a ridge logistic regression model.

4. Discussion

Discuss the performance of the simple glm, ridge glm, and lasso glm on the Breast Cancer Wisconsin Data Set in terms of prediction accuracy (on the training and test set) and model interpretability.