Diabetes Dataset Testing

2023-09-24

Functions

```
count_na_per_column <- function(df) {
    sapply(df, function(x) sum(is.na(x)))
}

# Create a function to calculate metrics
calc_metrics <- function(pred, true) {
  confusion <- table(pred, true)
  TP <- confusion[2, 2]
  FP <- confusion[2, 1]
  TN <- confusion[1, 1]
  FN <- confusion[1, 2]
  Sensitivity <- TP / (TP + FN)
  Specificity <- TN / (TN + FP)
  Accuracy <- (TP + TN) / (TP + FP + TN + FN)
  Precision <- TP / (TP + FP)
  F1 <- 2 * (Precision * Sensitivity) / (Precision + Sensitivity)
  pred_obj <- prediction(as.numeric(pred), as.numeric(true))
  perf <- performance(pred_obj, "auc")
  AUC <- as.numeric(perf@y.values)
  return(c(AUC, Sensitivity, Specificity, F1, Accuracy))
}
```

5. Data Processing

```
# Loading the data
data("PimaIndiansDiabetes2", package = "mlbench")
diabetes <- PimaIndiansDiabetes2
diabetes$diabetes <- as.factor(ifelse(diabetes$diabetes == "pos", 1, 0))
#diabetes$diabetes <- ifelse(diabetes$diabetes == "pos", 1, 0)
kable(t(count_na_per_column(diabetes)))
```

pregnant	glucose	pressure	triceps	insulin	mass	pedigree	age	diabetes
0	5	35	227	374	11	0	0	0

Removing NA's

```
diabetes <- na.omit(diabetes)
kable(t(count_na_per_column(diabetes)))
```

pregnant	glucose	pressure	triceps	insulin	mass	pedigree	age	diabetes
0	0	0	0	0	0	0	0	0

Removing Outliers

```
outliers <- check_outliers(diabetes, method = "mahalanobis")
#plot(outliers)
outliers <- as.vector(outliers)

#diabetes <- diabetes[!outliers, ]
```

Data for models

```
# Split
set.seed(123)
n <- nrow(diabetes)
training.samples <- sample(1:n, size = 0.75 * n)
train.data <- diabetes[training.samples, ]
#train.data <- smote(diabetes ~ ., train.data, perc.over = 1)
test.data <- diabetes[-training.samples, ]
test.data <- na.omit(test.data)



# Handle NA's in training set
#mice <- complete(mice(subset(train.data, select = -c(triceps, insulin)), method='rf', seed = 123))
#mice <- complete(mice(train.data, method='rf', seed = 123))

#train.data$glucose <- mice$glucose
#train.data$pressure <- mice$pressure
#train.data$mass <- mice$mass

#train.data <- na.omit(train.data)

#mice.triceps <- complete(mice(subset(train.data, select = -insulin), method='rf', seed = 123))
#train.data$triceps <- mice.triceps$triceps

#mice.insulin <- complete(mice(train.data, method='rf', seed = 123))
#train.data$insulin <- mice.insulin$insulin

# Train
X.train <- model.matrix(diabetes~., data = train.data)[,-1]
X.train <- scale(X.train)
y.train <- train.data$diabetes

# Test
X.test <- model.matrix(diabetes ~., data = test.data)[,-1]
X.test <- scale(X.test)
y.test <- test.data$diabetes
```

Logistic Regression

```
set.seed(123)
log.model <- glm(diabetes ~., data = train.data, family = "binomial")

# Make predictions
```

```r
probabilities <- predict(log.model, newdata = test.data, type = "response")
predicted.classes.log <- as.factor(ifelse(probabilities > 0.5, 1, 0))

# Accuracy
# mean(predicted.classes == y.test)
confusionMatrix(predicted.classes.log, y.test, positive = "1")
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  0  1
##          0 63 10
##          1  6 19
##
##                Accuracy : 0.8367
##                  95% CI : (0.7484, 0.9037)
##     No Information Rate : 0.7041
##     P-Value [Acc > NIR] : 0.001856
##
##                   Kappa : 0.5919
##
##  Mcnemar's Test P-Value : 0.453255
##
##             Sensitivity : 0.6552
##             Specificity : 0.9130
##          Pos Pred Value : 0.7600
##          Neg Pred Value : 0.8630
##              Prevalence : 0.2959
##          Detection Rate : 0.1939
##    Detection Prevalence : 0.2551
##       Balanced Accuracy : 0.7841
##
##        'Positive' Class : 1
##
```

LASSO

```r
set.seed(123)
cv.lasso.model <- cv.glmnet(X.train, y.train, alpha = 1, family = "binomial",
                            intercept = T)
#plot(cv.lasso.model)
cbind(coef(cv.lasso.model, s = cv.lasso.model$lambda.min), coef(cv.lasso.model, s = cv.lasso.model$lambd
```

```
## 9 x 2 sparse Matrix of class "dgCMatrix"
##                       s1         s1
## (Intercept) -0.8646581 -0.7383796
## pregnant     .          .
## glucose      1.0258065  0.7428165
## pressure     .          .
## triceps      .          .
## insulin      .          .
## mass         0.4231952  0.1340846
## pedigree     0.2695704  .
## age          0.4144144  0.1527177
```

```r
# Make predictions
probabilities <- predict(cv.lasso.model, newx = X.test, s = cv.lasso.model$lambda.min, type = "response
predicted.classes.lasso.min <- as.factor(ifelse(probabilities > 0.5, 1, 0))

probabilities <- predict(cv.lasso.model, newx = X.test, s = cv.lasso.model$lambda.1se, type = "response
predicted.classes.lasso.1se <- as.factor(ifelse(probabilities > 0.5, 1, 0))

# Accuracy
#mean(predicted.classes.lasso.min == y.test)
confusionMatrix(predicted.classes.lasso.min, y.test, positive = "1")
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  0  1
##          0 64  9
##          1  5 20
##
##                Accuracy : 0.8571
##                  95% CI : (0.7719, 0.9196)
##     No Information Rate : 0.7041
##     P-Value [Acc > NIR] : 0.0003264
##
##                   Kappa : 0.6429
##
##  Mcnemar's Test P-Value : 0.4226781
##
##             Sensitivity : 0.6897
##             Specificity : 0.9275
##          Pos Pred Value : 0.8000
##          Neg Pred Value : 0.8767
##              Prevalence : 0.2959
##          Detection Rate : 0.2041
##    Detection Prevalence : 0.2551
##       Balanced Accuracy : 0.8086
##
##        'Positive' Class : 1
##
```

in data: set.seed(123) and train 0.75 all others see(123) i like it a lot. min and 1se very sparse and good pred, just not much difference in amount of sparsity and amount of FN

in data: set.seed(2) and train 0.75 all others see(123) i like it a lot. 1se sparse and more FN but same pred

in data: set.seed(222) and train 0.75 all others see(123) pretty good similar too above

in data: set.seed(6) and train 0.75 all others see(123) gives very sparse 1se lasso and okay pred

in data: set.seed(13) and train 0.75 all others see(123) pretty nice! sparse 1se, but pred is same

in data: set.seed(42) and train 0.75 all others see(123) pretty nice! very very sparse 1se, more FN in 1se

some things we see:

- the more conservative model (1se) usually has more FN —> it makes the safe/conservative choice of going for the class that has 2/3 of observations

Ridge

```
set.seed(123)
cv.ridge.model <- cv.glmnet(X.train, y.train, alpha = 0, family = "binomial", intercept = T)
#plot(cv.ridge)

# Make predictions
probabilities <- predict(cv.ridge.model, newx = X.test, s = cv.ridge.model$lambda.min, type = "response
predicted.classes.ridge <- as.factor(ifelse(probabilities > 0.5, 1, 0))

# Accuracy
#mean(predicted.classes.ridge == y.test)
confusionMatrix(as.factor(predicted.classes.ridge), y.test, positive = "1")
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  0  1
##          0 64 10
##          1  5 19
##
##                Accuracy : 0.8469
##                  95% CI : (0.7601, 0.9117)
##     No Information Rate : 0.7041
##     P-Value [Acc > NIR] : 0.0008073
##
##                   Kappa : 0.6134
##
##  Mcnemar's Test P-Value : 0.3016996
##
##             Sensitivity : 0.6552
##             Specificity : 0.9275
##          Pos Pred Value : 0.7917
##          Neg Pred Value : 0.8649
##              Prevalence : 0.2959
##          Detection Rate : 0.1939
##    Detection Prevalence : 0.2449
##       Balanced Accuracy : 0.7914
##
##        'Positive' Class : 1
##
```

Elastic Net

```
set.seed(123)

# CV and tuning grid

myFolds <- createFolds(y.train, k = 10, list = TRUE)
myControl <- trainControl(index = myFolds)

#cvControl <- trainControl(method = "cv", number = 10)
tuneGrid <- expand.grid(alpha = seq(0, 1, by = 0.05), lambda = 10^seq(1, -3, length=100))
```

```r
# Train model
elasticnet.model <- train(X.train, y.train, method = "glmnet", trControl = myControl,
                          tuneGrid = tuneGrid, intercept = T, family = "binomial")

# Make predictions
probabilities <- predict(elasticnet.model, newdata = X.test, type = "prob") # "raw" already outputs pre
predicted.classes.elasticnet <- ifelse(probabilities$`1` > 0.5, 1, 0)

# Accuracy
# mean(predicted.classes == y.test)
confusionMatrix(as.factor(predicted.classes.elasticnet), y.test, positive = "1")
```

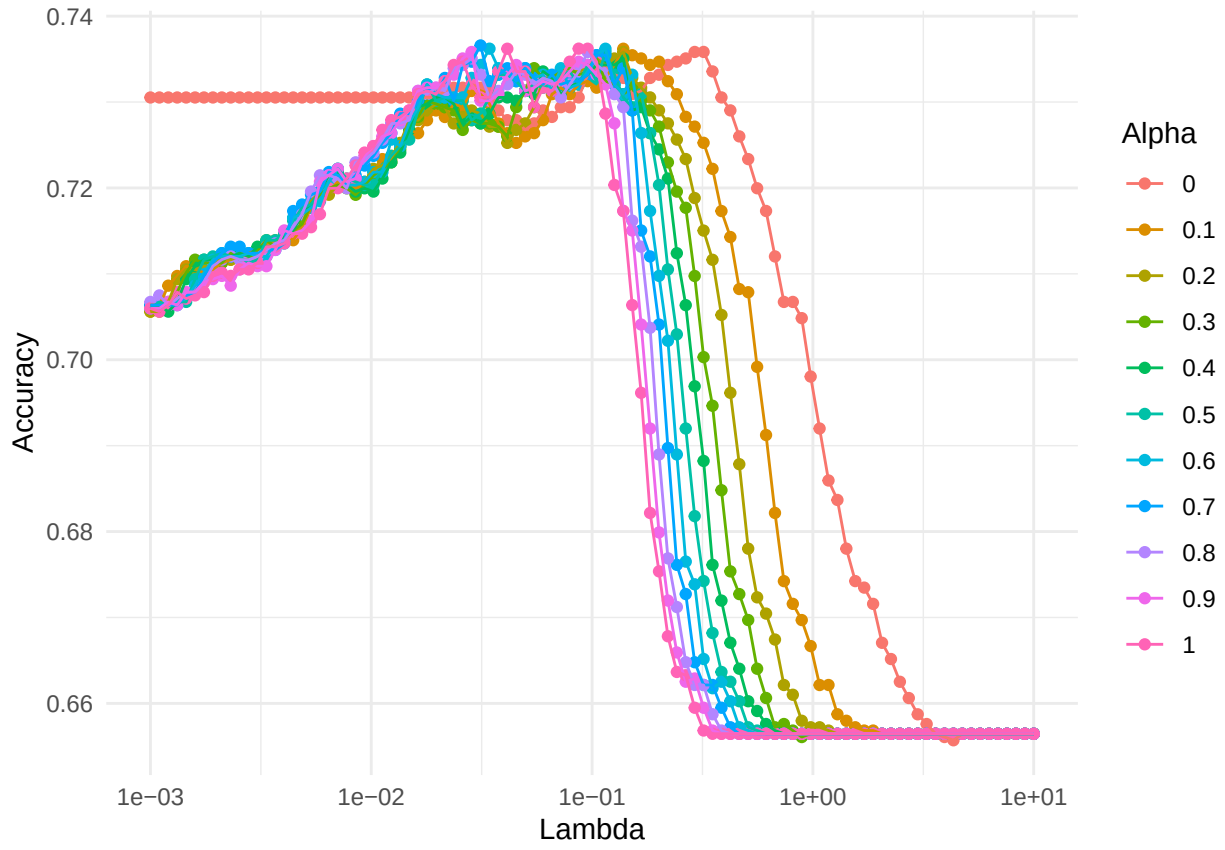
```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  0  1
##          0 65 15
##          1  4 14
##
##                Accuracy : 0.8061
##                  95% CI : (0.7139, 0.879)
##     No Information Rate : 0.7041
##     P-Value [Acc > NIR] : 0.01512
##
##                   Kappa : 0.4773
##
##  Mcnemar's Test P-Value : 0.02178
##
##             Sensitivity : 0.4828
##             Specificity : 0.9420
##          Pos Pred Value : 0.7778
##          Neg Pred Value : 0.8125
##              Prevalence : 0.2959
##          Detection Rate : 0.1429
##    Detection Prevalence : 0.1837
##       Balanced Accuracy : 0.7124
##
##        'Positive' Class : 1
##
```

```r
# Output coefficients
coef(elasticnet.model$finalModel, s = elasticnet.model$bestTune$lambda)
```

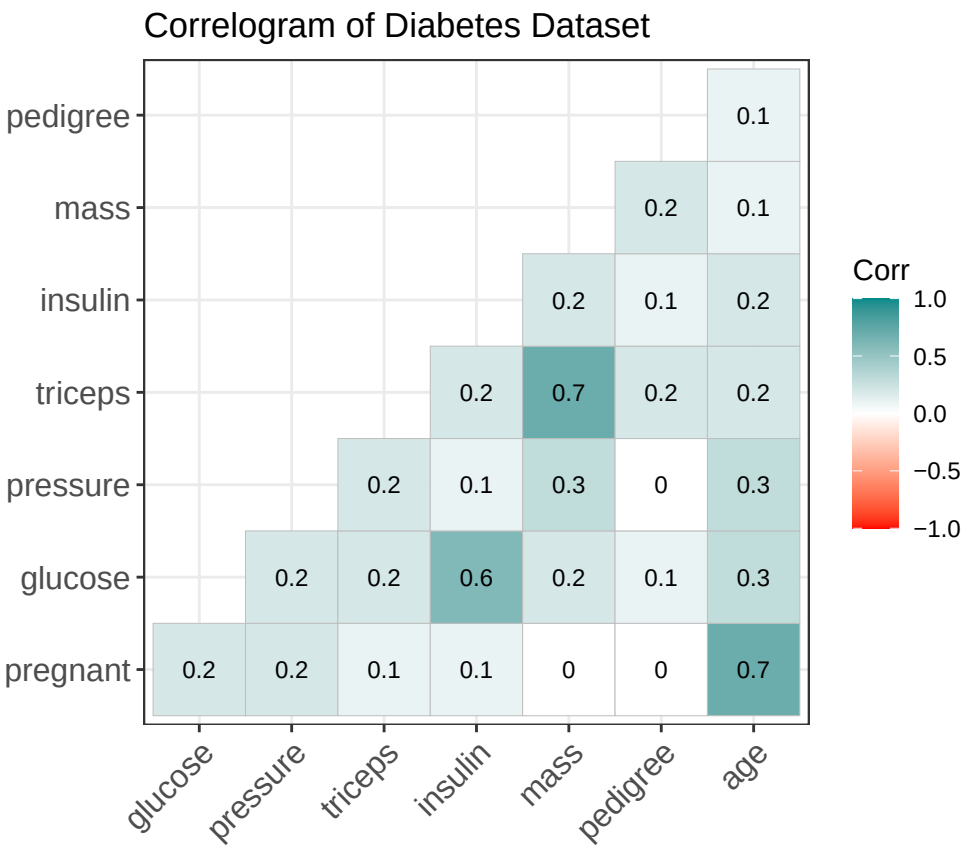
```
## 9 x 1 sparse Matrix of class "dgCMatrix"
##                       s1
## (Intercept) -0.71479062
## pregnant     .
## glucose      0.66381573
## pressure     .
## triceps      .
## insulin      .
## mass         0.06264426
## pedigree     .
## age          0.09478631
```

```r
# Filter data to only include specific alpha values
filtered_data <- subset(elasticnet.model$results, alpha %in% seq(0, 1, by=0.1))

# Create the plot
ggplot(filtered_data, aes(x=lambda, y=Accuracy, color=factor(alpha))) +
  geom_point() +
  geom_line() +
  scale_x_log10() +
  scale_color_discrete(name = "Alpha") +
  labs(x = "Lambda", y = "Accuracy") +
  theme_minimal()
```

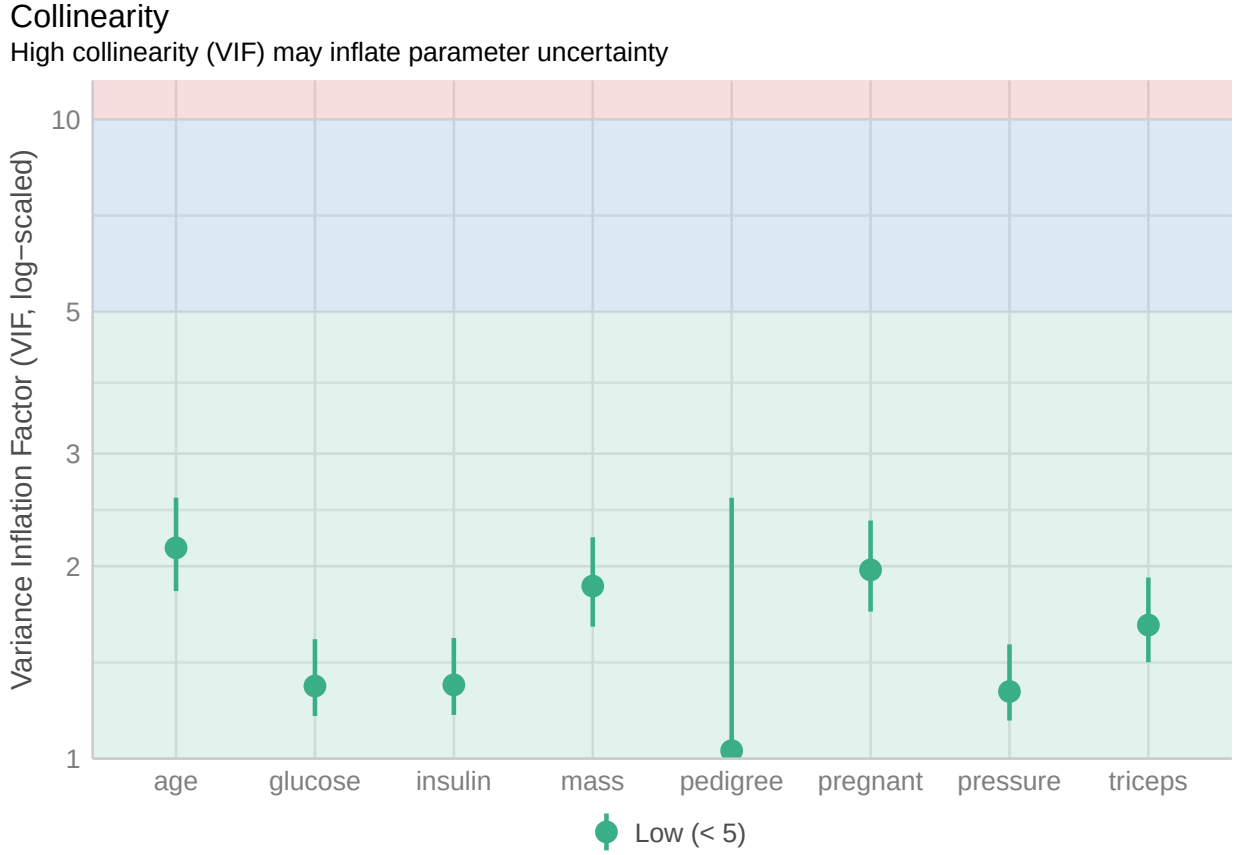



```r
library(ggcorrplot)
# Ensure that all remaining columns after subsetting are numeric
numeric_data <- subset(diabetes, select = -c(diabetes))
corr <- round(cor(numeric_data), 1)
ggcorrplot(corr,
           type = "lower",
           lab = TRUE,
           lab_size = 3,
           colors = c("red", "white", "cyan4"),
           title = "Correlogram of Diabetes Dataset",
           ggtheme = theme_bw())
```



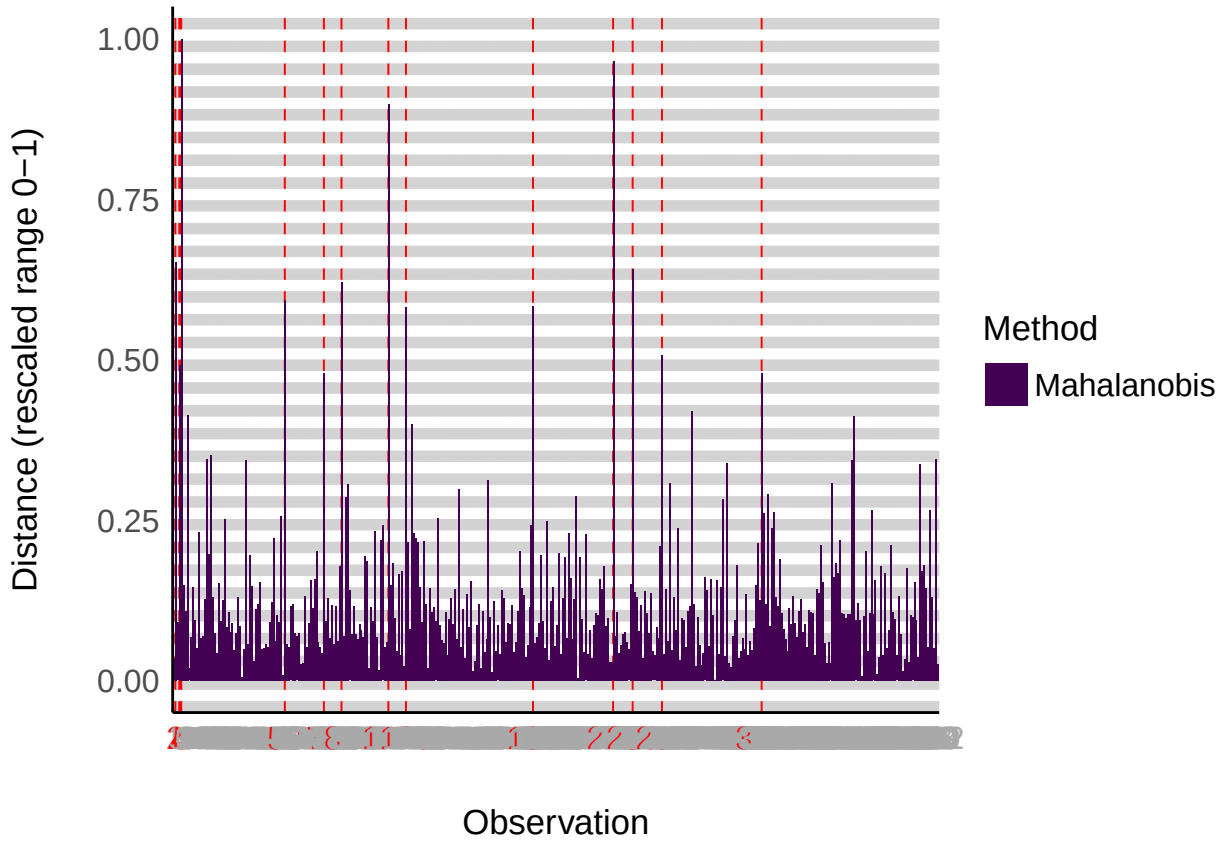

```
result <- check_collinearity(log.model)
plot(result)
```

```
## Variable 'Component' is not in your data frame :/
```



Outliers

```
result <- check_outliers(diabetes, method = "mahalanobis")
plot(result, type = "dots")
```




```
result
```

```
## 13 outliers detected: cases 2, 4, 5, 58, 78, 87, 111, 120, 185, 226,
##   236, 251, 302.
## - Based on the following method and threshold: mahalanobis (30).
## - For variables: pregnant, glucose, pressure, triceps, insulin, mass,
##   pedigree, age.
```

```
as.vector(result)
```

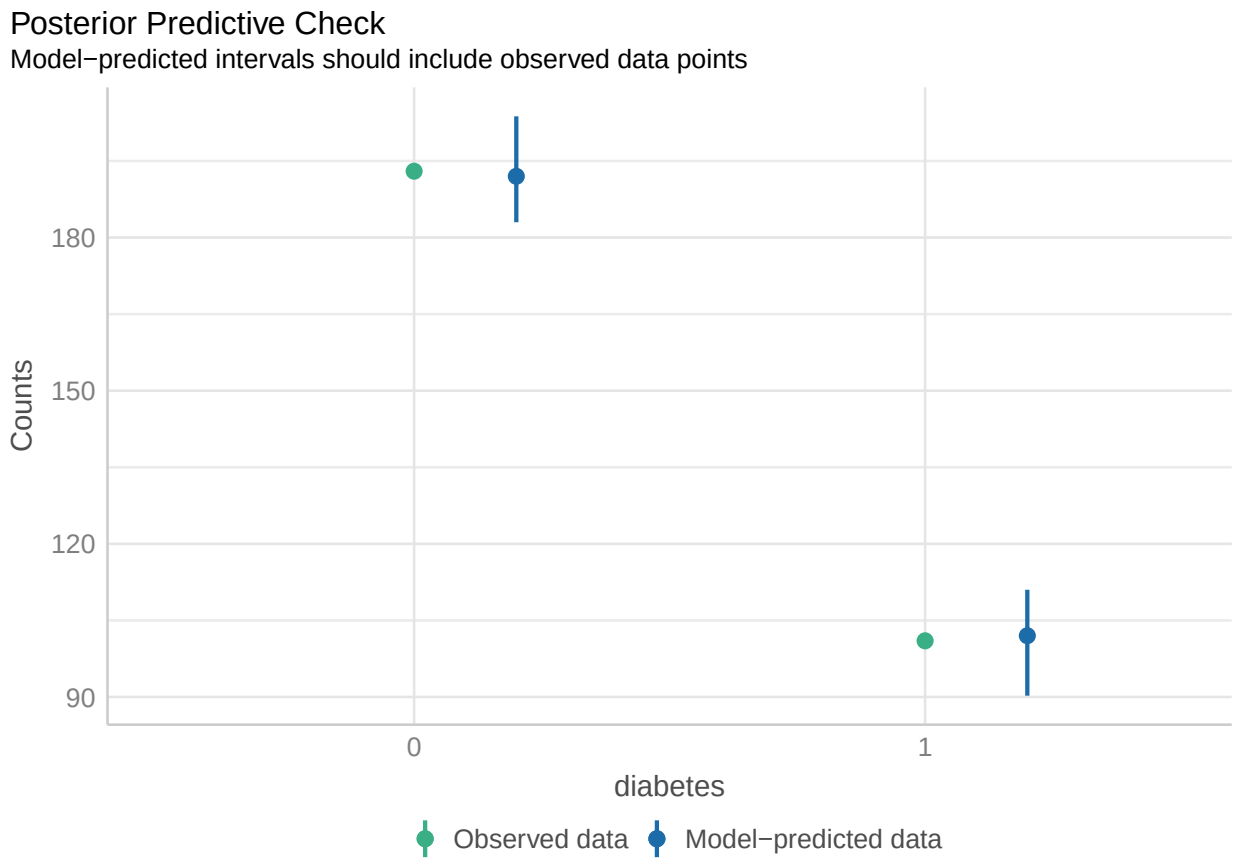
```
##   [1] FALSE  TRUE FALSE  TRUE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
##  [13] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
##  [25] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
##  [37] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
##  [49] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
##  [61] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
##  [73] FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE
##  [85] FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
##  [97] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [109] FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE
## [121] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [133] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [145] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [157] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [169] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [181] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [193] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
```

```
## [205] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [217] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
## [229] FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
## [241] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
## [253] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [265] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [277] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [289] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [301] FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [313] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [325] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [337] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [349] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [361] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [373] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [385] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
```

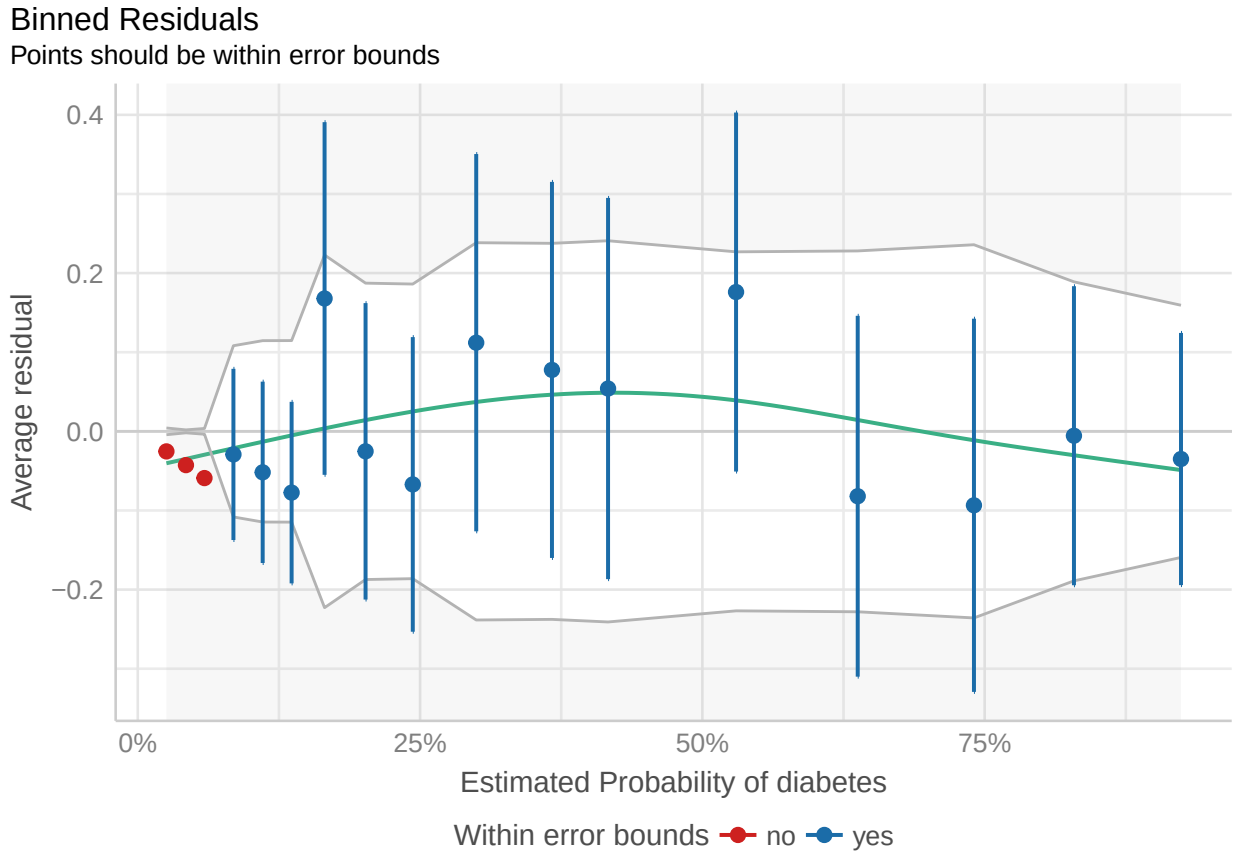
Check model

```
check <- check_model(log.model, panel = F)
plot(check)
```

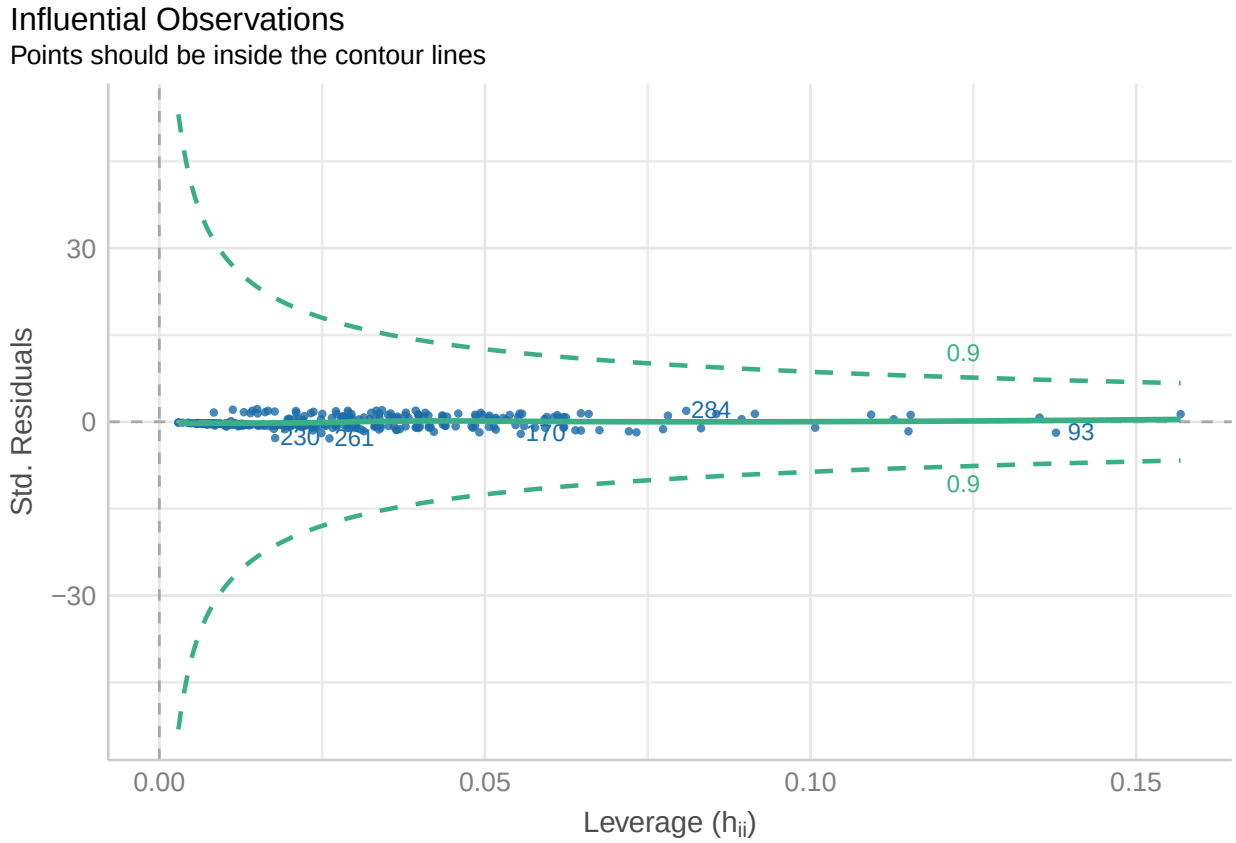
```
## $PP_CHECK
```



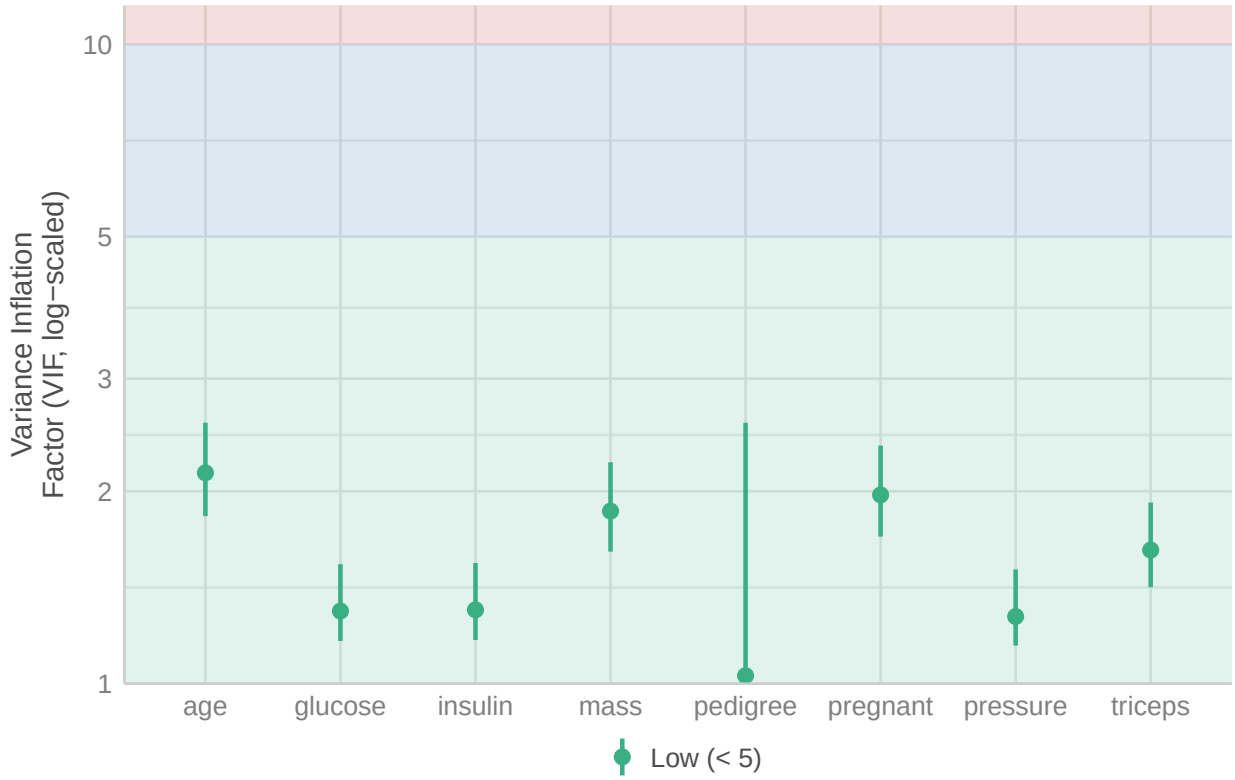

```
##
## $BINNED_RESID
```


Binned Residuals
Points should be within error bounds
0.4
0.2
0.0
−0.2
Average residual
0%
25%
50%
75%
Estimated Probability of diabetes
Within error bounds
no
yes

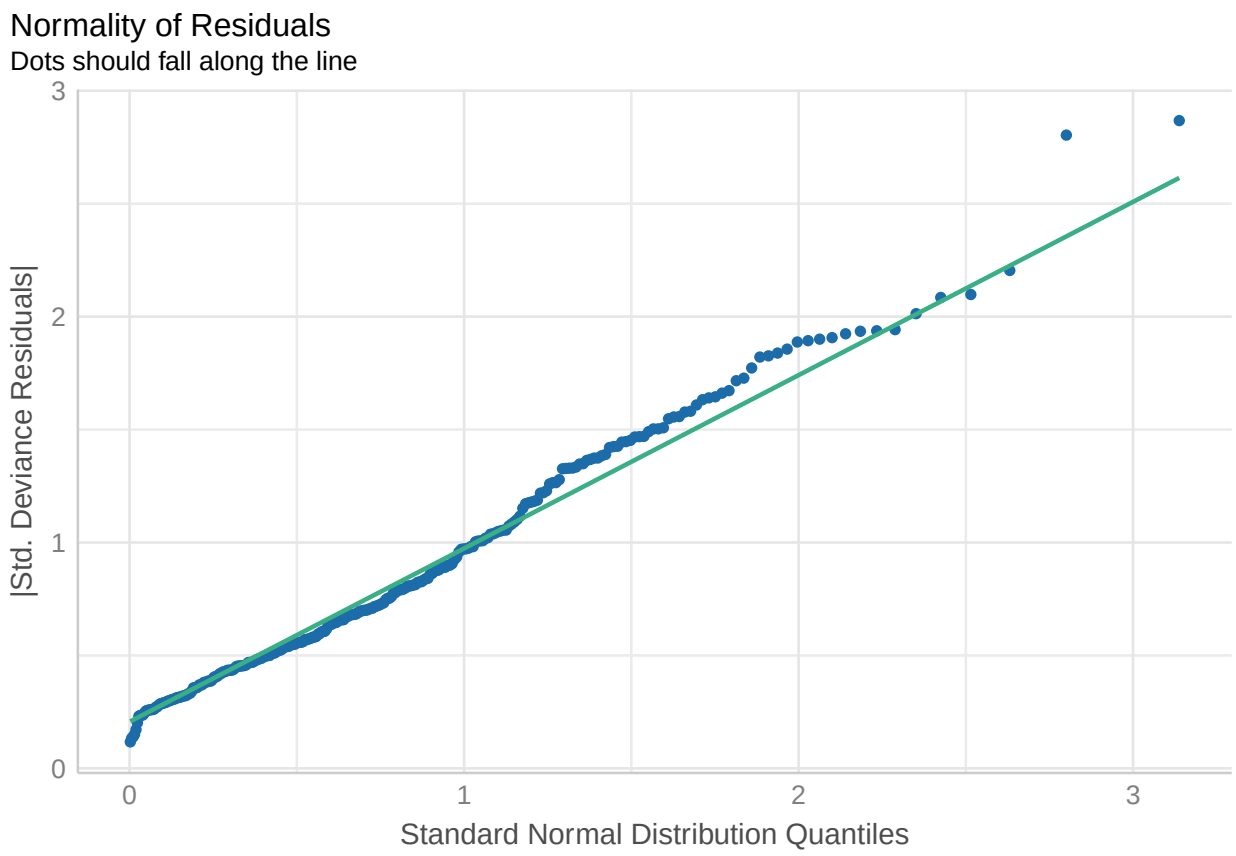
```
##
## $OUTLIERS
```


Influential Observations
Points should be inside the contour lines
Std. Residuals
30
0
−30
0.00
0.05
0.10
0.15
Leverage (h_{ii})
0.9
0.9
284
230
261
170
93

```
##
## $VIF
```


Collinearity
High collinearity (VIF) may inflate parameter uncertainty
Variance Inflation
Factor (VIF, log−scaled)
10
5
3
2
1
age
glucose
insulin
mass
pedigree
pregnant
pressure
triceps
Low (< 5)

```
##
## $QQ
```




```
binned_residuals(log.model)
```

```
## Warning: About 82% of the residuals are inside the error bounds (~95% or higher would be good).
```

Calculate model metrics

```
# Calculate metrics for each model
metrics.log <- calc_metrics(predicted.classes.log, y.test)
metrics.lasso.min <- calc_metrics(predicted.classes.lasso.min, y.test)
metrics.lasso.1se <- calc_metrics(predicted.classes.lasso.1se, y.test)
metrics.ridge <- calc_metrics(predicted.classes.ridge, y.test)
metrics.elasticnet <- calc_metrics(predicted.classes.elasticnet, y.test)

# Store in a dataframe
df_metrics <- as.data.frame(matrix(c(metrics.log, metrics.lasso.min, metrics.lasso.1se, metrics.ridge, m
colnames(df_metrics) <- c("Logistic", "Lasso_min", "Lasso_1se", "Ridge", "ElasticNet")
rownames(df_metrics) <- c("AUC", "Sensitivity", "Specificity", "F1", "Accuracy")
```

Latex Table Metrics

```
metrics_latex <- df_metrics %>%
  kable(format = "latex", booktabs = TRUE, align = c('c'), digits = 3, escape = FALSE,
        col.names = c("Logistic", "Lasso $\\lambda_{\\text{min}}$",
                      "Lasso $\\lambda_{\\text{1se}}$", "Ridge", "ElasticNet")) %>%
  kable_styling(latex_options = c("striped", "scale_down", "hold_position"), position = "center") %>%
  row_spec(0, bold = TRUE) %>%
```

```
  column_spec(1, bold = TRUE) %>%
  add_header_above(c(" " = 1, "Models" = 5), bold = TRUE) %>%
  row_spec(nrow(df_metrics) - 1, extra_latex_after = "\\midrule[.08em]") %>%
  row_spec(nrow(df_metrics), bold = TRUE)

print(metrics_latex)
```

	Models				
	Logistic	**Lasso λ_{min}**	**Lasso λ_{1se}**	**Ridge**	**ElasticNet**
AUC	0.784	0.809	0.757	0.791	0.712
Sensitivity	0.655	0.690	0.586	0.655	0.483
Specificity	0.913	0.928	0.928	0.928	0.942
F1	0.704	0.741	0.667	0.717	0.596
Accuracy	**0.837**	**0.857**	**0.827**	**0.847**	**0.806**

Data Frame of all model coefficients

```
coef.log <- coef(log.model)
coef.lasso.min <- (coef(cv.lasso.model, s = cv.lasso.model$lambda.min))
coef.lasso.1se <- coef(cv.lasso.model, s = cv.lasso.model$lambda.1se)
coef.ridge <- coef(cv.ridge.model)
coef.elasticnet <- coef(elasticnet.model$finalModel, s = elasticnet.model$bestTune$lambda)

# Create a data frame to store coefficients
df_coef <- data.frame(
  Logistic = as.vector(coef.log),
  Lasso_min = as.vector(as.matrix(coef.lasso.min)),
  Lasso_1se = as.vector(as.matrix(coef.lasso.1se)),
  Ridge = as.vector(as.matrix(coef.ridge)),
  ElasticNet = as.vector(as.matrix(coef.elasticnet))
)
options(scipen = 999)
df_coef <- round(df_coef, 4)
df_coef[] <- apply(df_coef, 2, function(x) ifelse(x == 0, '.', x))


# Set the row names to be the names of the coefficients from one of the models
rownames(df_coef) <- names(coef.log)

df_coef
```

```
##             Logistic Lasso_min Lasso_1se   Ridge ElasticNet
## (Intercept) -10.0428   -0.8647   -0.7384 -0.7224    -0.7148
## pregnant      0.0101         .         .  0.093          .
## glucose       0.0376    1.0258    0.7428  0.3495     0.6638
## pressure     -0.0003         .         .  0.0789         .
## triceps       0.0022         .         .  0.1042         .
## insulin      -0.0002         .         .  0.1477         .
```

```
## mass          0.0742    0.4232    0.1341  0.1587     0.0626
## pedigree      1.0681    0.2696         .  0.1316          .
## age           0.0464    0.4144    0.1527   0.187     0.0948
```

Latex Table Coef

```
coef_latex <- df_coef %>%
  kable(format = "latex", booktabs = TRUE, align = c('c'), escape = FALSE,
        col.names = c("Logistic", "Lasso $\\lambda_{\\text{min}}$",
                      "Lasso $\\lambda_{\\text{1se}}$", "Ridge", "ElasticNet")) %>%
  kable_styling(latex_options = c("striped", "scale_down", "hold_position"), position = "center") %>%
  row_spec(0, bold = TRUE) %>%
  column_spec(1, bold = TRUE) %>%
  add_header_above(c(" " = 1, "Models" = 5), bold = TRUE)

print(coef_latex)
```

	Models				
	Logistic	**Lasso λ_{min}**	**Lasso λ_{1se}**	**Ridge**	**ElasticNet**
(Intercept)	-10.0428	-0.8647	-0.7384	-0.7224	-0.7148
pregnant	0.0101	.	.	0.093	.
glucose	0.0376	1.0258	0.7428	0.3495	0.6638
pressure	-0.0003	.	.	0.0789	.
triceps	0.0022	.	.	0.1042	.
insulin	-0.0002	.	.	0.1477	.
mass	0.0742	0.4232	0.1341	0.1587	0.0626
pedigree	1.0681	0.2696	.	0.1316	.
age	0.0464	0.4144	0.1527	0.187	0.0948