Compulsory exercise 1: Group 39

TMA4268 Statistical Learning V2021

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Problem 1

a)

By extending the given univariate regression problem to a multivariate regression problem that allows for several observations, we have that $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$. Hence, we have $\mathsf{E}(\mathbf{Y}) = \mathsf{E}(\mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}) = \mathbf{X}\boldsymbol{\beta}$ and $\mathsf{Cov}(\mathbf{Y}) = \sigma^2 I$, assuming that $\boldsymbol{\varepsilon} \sim N(0, \sigma^2 I)$. Then

$$\mathsf{E}(\widetilde{\boldsymbol{\beta}}) = \mathsf{E}((\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I})^{-1}\mathbf{X}^T\mathbf{Y}) = (\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I})^{-1}\mathbf{X}^T\mathsf{E}(\mathbf{Y}) = (\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I})^{-1}\mathbf{X}^T\mathbf{X}\boldsymbol{\beta}$$

and

$$\begin{split} \mathsf{Cov}(\widetilde{\boldsymbol{\beta}}) &= \mathsf{Cov}((\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I})^{-1}\mathbf{X}^T\mathbf{Y}) = ((\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I})^{-1}\mathbf{X}^T)\mathsf{Cov}(\mathbf{Y})((\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I})^{-1}\mathbf{X}^T)^T \\ &= ((\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I})^{-1}\mathbf{X}^T)\sigma^2I\mathbf{X}(\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I})^{-T} = \sigma^2((\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I})^{-1}\mathbf{X}^T\mathbf{X}(\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I})^{-T}) \\ &= \sigma^2((\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I})^{-1}\mathbf{X}^T\mathbf{X}(\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I})^{-1}), \end{split}$$

where we have used that $(\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I})^{-1} = (\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I})^{-T}$ in the last equality, because $\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I}$ is symmetric. In both these equations it is apparent that the moments are equal to those of the OLS estimator when $\lambda = 0$.

b)

The requested moments of $\widetilde{f}(\mathbf{x}_0) = \mathbf{x}_0^T \widetilde{\boldsymbol{\beta}}$ are

$$\mathsf{E}(\widetilde{f}(\mathbf{x}_0)) = \mathsf{E}(\mathbf{x}_0^T \widetilde{\boldsymbol{\beta}}) = \mathbf{x}_0^T \mathsf{E}(\widetilde{\boldsymbol{\beta}}) = \mathbf{x}_0^T (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^T \mathbf{X} \boldsymbol{\beta}$$

and

$$\begin{aligned} \mathsf{Cov}(\widetilde{f}(\mathbf{x}_0)) &= \mathsf{Cov}(\mathbf{x}_0^T \widetilde{\boldsymbol{\beta}}) = \mathbf{x}_0^T \mathsf{Cov}(\widetilde{\boldsymbol{\beta}}) \mathbf{x}_0 \\ &= \sigma^2 \mathbf{x}_0^T ((\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^T \mathbf{X} (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1}) \mathbf{x}_0. \end{aligned}$$

c)

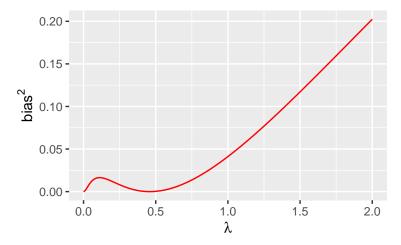
The expected MSE at \mathbf{x}_0 is

```
\begin{split} \mathsf{E}[(y_0 - \widetilde{f}(\mathbf{x}_0))^2] &= [\mathsf{E}(\widetilde{f}(\mathbf{x}_0) - f(\mathbf{x}_0))]^2 + \mathsf{Var}(\widetilde{f}(\mathbf{x}_0)) + \mathsf{Var}(\varepsilon) \\ &= [\mathsf{E}(\widetilde{f}(\mathbf{x}_0)) - \mathsf{E}(f(\mathbf{x}_0))]^2 + \mathsf{Cov}(\widetilde{f}(\mathbf{x}_0)) + \sigma^2 \\ &= [\mathbf{x}_0^T(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{X}\boldsymbol{\beta} - \mathbf{x}_0^T\boldsymbol{\beta}]^2 + \sigma^2\mathbf{x}_0^T((\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{X}(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1})\mathbf{x}_0 + \sigma^2. \end{split}
```

Since there is no obvious way to simplify this, it will be left like this. This is also practical since it is easy to distinguish between the irreducible error, the variance of prediction and the squared bias.

d)

```
id <- "1X_80KcoYbng1XvYFDirxjEWr7LtpNr1m" # Google file ID.
values <- dget(sprintf("https://docs.google.com/uc?id=%s&export=download", id))</pre>
X = values$X
dim(X)
#> [1] 100 81
x0 = values$x0
dim(x0)
#> [1] 81 1
beta=values$beta
dim(beta)
#> [1] 81
sigma=values$sigma
sigma
#> [1] 0.5
bias = function(lambda, X, x0, beta)
 p = ncol(X)
  value <- (t(x0) \% \% solve(t(X) \% \% X + lambda * diag(p)) \% \% t(X) \% X \% beta - t(x0) \% \% beta)^2
  return(value)
lambdas = seq(0, 2, length.out = 500)
BIAS = rep(NA,length(lambdas))
for (i in 1:length(lambdas)) BIAS[i] = bias(lambdas[i], X, x0, beta)
dfBias = data.frame(lambdas = lambdas, bias = BIAS)
ggplot(dfBias, aes(x = lambdas, y = bias)) +
  geom_line(color = "red")+
 xlab(expression(lambda))+
 ylab(expression(bias^2))
```

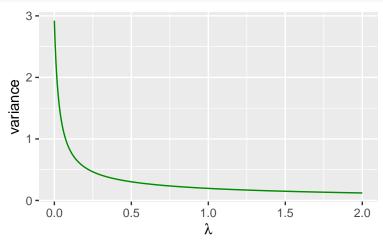


The graph shows that the bias of the ridge regression estimator increases as λ grows. OLS is unbiased, so, as expected, the bias is zero when $\lambda=0$. Note that $\lambda\approx0.5$ appears to be a sweet spot for this estimator when comparing all $\lambda>0$, since the bias is low there. Perhaps this can be useful later.

e)

```
variance = function(lambda, X, x0, sigma)
{
   p = ncol(X)
   inv = solve(t(X)%*%X+lambda*diag(p))
   value = sigma^2*t(x0) %*% (inv %*% t(X) %*% X %*% inv) %*% x0
   return(value)
}
lambdas = seq(0, 2, length.out = 500)
VAR=rep(NA,length(lambdas))
for (i in 1:length(lambdas)) VAR[i]=variance(lambdas[i], X, x0, sigma)
dfVar = data.frame(lambdas = lambdas, var = VAR)
ggplot(dfVar, aes(x = lambdas, y = var))+
   geom_line(color = "green4")+

   xlab(expression(lambda))+
   ylab("variance")
```



The variance begins at ≈ 2.923 and decreases with λ . Hence, it is apparent that the ridge regression estimator is advantageous, when looking at solely variance, compared to the OLS estimator, since the variance is

decreasing with λ . Despite this, when adding the bias and the variance, the OLS estimator may still have a lower expected MSE than the ridge regression estimator. Finally, note that the changes in the variance are larger for $\lambda \in [0, 2]$ than the changes in the bias (compared to the plot in task d)), which indicates that the variance dominates the change in expected MSE for the ridge regression estimation.

f)

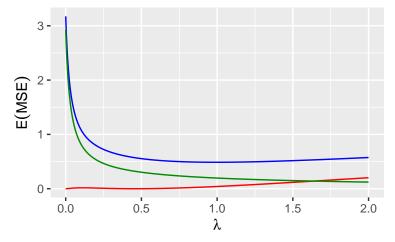
```
exp_mse = BIAS + VAR + sigma^2
lambdas[which.min(exp_mse)]

#> [1] 0.993988

dfAll = data.frame(lambda = lambdas, bias = BIAS, var = VAR, exp_mse = exp_mse)
ggplot(dfAll)+
```

```
dfAll = data.frame(lambda = lambdas, bias = BIAS, var = VAR, exp_mse = exp_mse)
ggplot(dfAll)+
  geom_line(aes(x = lambda, y = exp_mse), color = "blue")+

geom_line(aes(x = lambda, y = bias), color = "red")+
  geom_line(aes(x = lambda, y = var), color = "green4")+
    xlab(expression(lambda))+
    ylab(expression(E(MSE)))
```



Now we are able to conclude that the ridge regression estimator has a lower expected MSE compared to the OLS estimator, as gathered from the blue line in the plot. The optimal value of λ , which minimizes MSE, is ≈ 0.994 . Hence, despite the fact that the bias is higher for the ridge regression estimator, the total expected MSE is lower, since the decrease in variance counters the increase in bias.

Problem 2

```
# Read file.
id <- "1yYlEl5gYY3BEtJ4d7KWaFGI0EweJIn__" # Google file ID.
d.corona <- read.csv(sprintf("https://docs.google.com/uc?id=%s&export=download", id),header=T)
a)
The tables are reported below.</pre>
```

deceased	non_deceased
105	1905

```
table2 <- table(d.corona$country, d.corona$sex)
knitr::kable(table2)</pre>
```

	female	male
France	60	54
indonesia	30	39
japan	120	174
Korea	879	654

```
table3 <- table(d.corona$deceased, d.corona$sex)
rownames(table3) = c("non-deceased", "deceased")
knitr::kable(table3)</pre>
```

	female	male
non-deceased	1046	859
deceased	43	62

```
d.france <- filter(d.corona, country == "France")
table4 <- table(d.france$deceased, d.france$sex)
rownames(table4) = c("non-deceased", "deceased")
knitr::kable(table4)</pre>
```

	female	$_{\mathrm{male}}$
non-deceased	55	43
deceased	5	11

b)

Since we want to understand the probability of decease of covid-19, we fit a logistic regression model as opposed to a linear regression model.

```
glm.fit <- glm(deceased ~ ., family = "binomial", data = d.corona)
summary(glm.fit)</pre>
```

```
#>
#> Call:
#> glm(formula = deceased ~ ., family = "binomial", data = d.corona)
#> Deviance Residuals:
     Min
             1Q Median
                             3Q
#> -0.9050 -0.3508 -0.2761 -0.2144
                                 3.1165
#>
#> Coefficients:
                 Estimate Std. Error z value Pr(>|z|)
#>
#> (Intercept)
                -3.993485 0.462190 -8.640 < 2e-16 ***
                #> sexmale
```

```
0.027134
                                 0.004736
                                            5.729 1.01e-08 ***
#> age
#> countryindonesia -0.411855
                                           -0.749
                                                    0.45400
                                 0.550051
#> countryjapan
                    -1.343383
                                 0.417196
                                           -3.220
                                                    0.00128 **
#> countryKorea
                    -0.773895
                                 0.307980
                                           -2.513
                                                   0.01198 *
#>
                   0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#> Signif. codes:
#>
#>
   (Dispersion parameter for binomial family taken to be 1)
#>
#>
       Null deviance: 824.32
                               on 2009
                                        degrees of freedom
#> Residual deviance: 766.16
                               on 2004
                                        degrees of freedom
  AIC: 778.16
#>
#>
#> Number of Fisher Scoring iterations: 6
anova(glm.fit, test = "Chisq")
#> Analysis of Deviance Table
#>
#> Model: binomial, link: logit
#>
#> Response: deceased
#>
#> Terms added sequentially (first to last)
#>
#>
           Df Deviance Resid. Df Resid. Dev
#>
                                              Pr(>Chi)
#> NULL
                             2009
                                      824.32
                 7.785
#> sex
            1
                             2008
                                      816.54 0.005268 **
            1
                39.311
                             2007
                                      777.23 3.613e-10 ***
#> age
                11.063
                             2004
                                      766.16 0.011390 *
#> country
            3
                   0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#> Signif. codes:
```

(i) The probability to die of covid for a male age 75 living in Korea can be predicted from the model. The prediction is found by

```
x0 <- data.frame(sex = "male", age = 75, country = "Korea")
pred <- predict(glm.fit, newdata = x0, type = "response")
pred
#> 1
```

#> 0.1084912

Hence, the probability to die of covid for a male age 75 living in Korea is ≈ 0.108 .

- (ii) The p-value associated with sexmale is relatively small, and since the coefficient is positive, this constitutes some evidence that males have a higher probability of dying.
- (iii) Yes. From the output of anova we see that country has a low p-value, which could be used as evidence that the country of residence has an influence on the probability of decease. Additionally, we see that both the countryjapan and countryKorea coefficients from the summary have relatively low p-values and are negative, which could be used as evidence that the probability of decease is lower in Japan and Korea compared to the reference category, France. countryIndonesia is not significant (large p-value), so there is no evidence that the probability of decease is any higher in Indonesia than in France.
- (iv) Since we have used logistic regression, the predicted odds of decease, given an observation x, is

$$\frac{p(\boldsymbol{x})}{1 - p(\boldsymbol{x})} = e^{\boldsymbol{x}^T \hat{\boldsymbol{\beta}}}.$$

Thus, the odds of decease increases by a factor of $e^{10\beta_{\rm age}} \approx 1.312$ when age increases by 10 and all other covariates are held constant.

c)

```
log.fit1 <- glm(deceased ~. + sex:age, data = d.corona, family="binomial")</pre>
summary(log.fit1)
#>
#> Call:
#> glm(formula = deceased ~ . + sex:age, family = "binomial", data = d.corona)
#> Deviance Residuals:
                     Median
      Min
                10
                                  30
                                          Max
#> -0.9111 -0.3500 -0.2768 -0.2150
                                        3.1078
#>
#> Coefficients:
                    Estimate Std. Error z value Pr(>|z|)
#>
#> (Intercept)
                   -3.953580 0.571712 -6.915 4.67e-12 ***
#> sexmale
                    0.556745 0.624834
                                         0.891 0.372913
#> age
                    0.026485 0.007261
                                          3.648 0.000265 ***
#> countryindonesia -0.410197   0.550304   -0.745   0.456030
                   -1.344440
#> countryjapan
                               0.417364
                                         -3.221 0.001276 **
#> countryKorea
                   -0.772596
                               0.308244 -2.506 0.012195 *
#> sexmale:age
                    0.001111
                               0.009443
                                          0.118 0.906350
#> ---
#> Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
#>
#> (Dispersion parameter for binomial family taken to be 1)
#>
      Null deviance: 824.32 on 2009 degrees of freedom
#> Residual deviance: 766.15 on 2003
                                      degrees of freedom
#> AIC: 780.15
#>
#> Number of Fisher Scoring iterations: 6
```

(i) As seen above, we have fitted the full logistic regression with an interaction term between age and sex. As the summary shows, the interaction effect between sexmale and age is not significant, since the p-value is large. Hence, although the coefficient is slightly positive, we cannot conclude that age is a greater risk factor for men.

```
log.fit2 <- glm(deceased ~ . + age:country, data = d.corona, family="binomial")
summary(log.fit2)</pre>
```

```
#>
#> Coefficients:
#>
                       Estimate Std. Error z value Pr(>|z|)
                                   1.72789 -4.076 4.58e-05 ***
#> (Intercept)
                       -7.04272
#> sexmale
                        0.62777
                                   0.21056
                                            2.981 0.00287 **
#> age
                        0.06693
                                   0.02124
                                            3.151 0.00163 **
#> countryindonesia
                        4.34249
                                   2.16594
                                            2.005 0.04497 *
#> countryjapan
                        2.13091
                                   2.03299
                                            1.048 0.29456
#> countryKorea
                        2.37162
                                   1.75357
                                            1.352 0.17623
#> age:countryindonesia -0.07189
                                   0.03310 -2.172 0.02986 *
#> age:countryjapan
                       -0.04630
                                   0.02668 -1.736 0.08260
#> age:countryKorea
                       -0.04142
                                   0.02189 -1.892 0.05854 .
#> ---
#> Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
#>
#> (Dispersion parameter for binomial family taken to be 1)
#>
#>
      Null deviance: 824.32 on 2009
                                      degrees of freedom
#> Residual deviance: 759.71 on 2001 degrees of freedom
#> AIC: 777.71
#>
#> Number of Fisher Scoring iterations: 6
```

(ii) As seen above, we have fitted the full logistic regression with an interaction term between age and country. Since France is the reference level, and the interaction-term coefficient age:countryindonesia has the value \approx -0.072 with a somewhat low p-value, we can infer that age is a greater risk factor for the French population than for the Indonesian population.

d)

TRUE, TRUE, TRUE, FALSE.

Problem 3

```
# Read file.
id <- "111cQPeoLLC_FyAHOnnqCnnrSBpn05_h0" # Google file ID.
diab <- dget(sprintf("https://docs.google.com/uc?id=%s&export=download", id))
t = MASS::Pima.tr2
train = diab$ctrain
test = diab$ctest</pre>
```

a)

```
logReg = glm(diabetes~., data = train, family = "binomial")
```

(i) We have that

$$p_{i} = \frac{e^{\beta_{0} + \beta_{1}x_{i1} + \beta_{2}x_{i2} + \dots + \beta_{7}x_{i7}}}{1 + e^{\beta_{0} + \beta_{1}x_{i1} + \beta_{2}x_{i2} + \dots + \beta_{7}x_{i7}}} := \frac{e^{\eta_{i}(x)}}{1 + e^{\eta_{i}(x)}} \implies \frac{p_{i}}{1 - p_{i}} = \frac{\frac{e^{\eta_{i}(x)}}{1 + e^{\eta_{i}(x)}}}{1 - \frac{e^{\eta_{i}(x)}}{1 + e^{\eta_{i}(x)}}} = e^{\eta_{i}(x)}$$

$$\implies \log \operatorname{id}(p_{i}) = \log \left(\frac{p_{i}}{1 - p_{i}}\right) = \eta_{i}(x) = \beta_{0} + \beta_{1}x_{i1} + \beta_{2}x_{i2} + \dots + \beta_{7}x_{i7}$$

(ii) The classification is done below.

```
glm.probs <- predict(logReg, newdata = test, type = "response")
glm.preds <- ifelse(glm.probs > 0.5, 1, 0)
conf.table.glm <- table(predicted = glm.preds, true = test$diabetes)
conf.table.glm</pre>
```

```
#> true
#> predicted 0 1
#> 0 137 29
#> 1 18 48
```

The sensitivity is $48/(48 + 29) \approx 0.623$ and the specificity is $137/(137 + 18) \approx 0.884$.

b)

- (i) π_k is the prior probability for an observation, given by $\pi_k = P(y = k)$. $f_k(\mathbf{x})$ is the gaussian pdf for class k, with mean $\boldsymbol{\mu}_k$ and covariance matrix $\boldsymbol{\Sigma}_k$. In LDA $\boldsymbol{\Sigma}_k = \boldsymbol{\Sigma} \quad \forall k$, whereas in QDA each $\boldsymbol{\Sigma}_k$ are assumed to be class-specific. In this case, the class 1, i.e. presence of diabetes, has the mean vector $\boldsymbol{\mu}_1$ and the class 0, i.e. non-presence of diabetes, has the mean vector $\boldsymbol{\mu}_0$. $\boldsymbol{\Sigma}$ is the covariance matrix of both classes, since we are performing LDA. Hence, $f_1(\mathbf{x})$ is the gaussian pdf for class 1, with mean $\boldsymbol{\mu}_1$ and covariance matrix $\boldsymbol{\Sigma}$, while $f_0(\mathbf{x})$ is the gaussian pdf for class 0, with mean $\boldsymbol{\mu}_0$ and covariance matrix $\boldsymbol{\Sigma}$.
- (ii) The fits are seen below

```
lda.diabetes <- lda(diabetes~., data = train)
qda.diabetes <- qda(diabetes~., data = train)

# Only need the prob if diabetes is present.
lda.diabetes.probs <- predict(lda.diabetes, newdata = test)$posterior[, 2]
lda.preds <- ifelse(lda.diabetes.probs > 0.5, 1, 0)
conf.table.lda.diabetes <- table(predicted = lda.preds, true = test$diabetes)
conf.table.lda.diabetes</pre>
```

```
#>
            true
#> predicted
               0
                   1
#>
           0 138
                  30
#>
           1
             17
                  47
# Only need the prob if diabetes is present.
qda.diabetes.probs <- predict(qda.diabetes, newdata = test) $posterior[, 2]
qda.preds <- ifelse(qda.diabetes.probs > 0.5, 1, 0)
conf.table.qda.diabetes <- table(predicted = qda.preds, true = test$diabetes)</pre>
conf.table.qda.diabetes
```

```
#> true
#> predicted 0 1
#> 0 131 32
#> 1 24 45
```

The sensitivity and specificity for LDA are thus $47/(47 + 30) \approx 0.61$ and $138/(138 + 17) \approx 0.89$, respectively. The sensitivity and specificity of QDA are $45/(45 + 32) \approx 0.584$ and $131/(131 + 24) \approx 0.845$, respectively.

The difference between the methods is that the covariance matrix is assumed to be equal across all classes (in this case: both classes) in LDA, which gives linear discriminant functions and a linear decision boundary, while in QDA the covariance matrix is assumed to be class-specific, which gives a quadratic discriminant function for each class and a quadratic decision boundary.

c)

- (i) In the KNN approach, a new observation is classified by using the k nearest points (in Euclidean distance) to the observation in question. The new observation is classified to the most occurring class among the k nearest points, i.e. to the class with the highest estimated probability.
- (ii) We would choose the tuning parameter k based on a κ -fold cross validation, with $\kappa = 5$ or $\kappa = 10$.
- (iii) The KNN classification fit can be seen below

```
set.seed(123) # For reproducibility, e.g. in case of ties.
knn.diabetes <- knn(train = train, test = test, cl = train$diabetes, k=25, prob=T)
conf.table.knn <- table(predicted = knn.diabetes, true = test$diabetes)
conf.table.knn</pre>
```

```
#> true
#> predicted 0 1
#> 0 144 36
#> 1 11 41
```

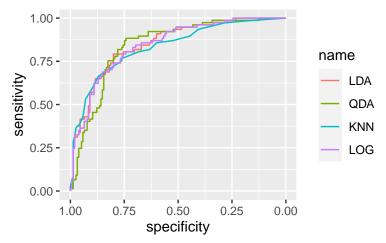
The sensitivity is $41/(41+36) \approx 0.532$ and the specificity is $144/(144+11) \approx 0.929$.

d) ROC curves

```
knn.probs <- ifelse(knn.diabetes == 0, 1 - attributes(knn.diabetes)$prob, attributes(knn.diabetes)$prob
glm.log.probs <- predict(logReg, newdata = test, type="response")

ldaroc = roc(response = test$diabetes, predictor = lda.diabetes.probs, direction = "<")
qdaroc = roc(response = test$diabetes, predictor = qda.diabetes.probs, direction = "<")
knnroc = roc(response = test$diabetes, predictor = knn.probs, direction = "<")
glm.logroc = roc(response = test$diabetes, predictor = glm.log.probs, direction = "<")

ggroc(list(LDA = ldaroc, QDA = qdaroc, KNN = knnroc, LOG = glm.logroc))</pre>
```



The area under the ROC curve is 0.849 for LDA, 0.841 for QDA, 0.833 for KNN and 0.845 for logistic regression (LOG). We see that LDA performs the best with respect to the AUC, which indicates that a linear decision boundary is appropriate. Despite this, if the task is to create an interpretable model, we would choose the logistic regression model, since it has almost as high AUC as LDA and is more interpretable with its readily available coefficients and associated formulas for probability and odds.

Problem 4

a)

$$\begin{split} \hat{y}_{(-i)} &= \mathbf{x}_{i}^{T} \hat{\boldsymbol{\beta}}_{(-i)} \\ &= \mathbf{x}_{i}^{T} (X_{(-i)}^{T} X_{(-i)})^{-1} X_{(-i)}^{T} \mathbf{y}_{(-i)} \\ &= \mathbf{x}_{i}^{T} (X^{T} X - \mathbf{x}_{i} \mathbf{x}_{i}^{T})^{-1} (X^{T} \mathbf{y} - \mathbf{x}_{i} y_{i}) \\ &= \mathbf{x}_{i}^{T} \left[(X^{T} X)^{-1} + \frac{(X^{T} X)^{-1} \mathbf{x}_{i} \mathbf{x}_{i}^{T} (X^{T} X)^{-1}}{1 - \mathbf{x}_{i}^{T} (X^{T} X)^{-1} \mathbf{x}_{i}} \right] (X^{T} \mathbf{y} - \mathbf{x}_{i} y_{i}), \quad \text{Sherman-Morrison} \\ &= \mathbf{x}_{i}^{T} \left[(X^{T} X)^{-1} + \frac{(X^{T} X)^{-1} \mathbf{x}_{i} \mathbf{x}_{i}^{T} (X^{T} X)^{-1}}{1 - h_{i}} \right] (X^{T} \mathbf{y} - \mathbf{x}_{i} y_{i}) \\ &= \mathbf{x}_{i}^{T} (X^{T} X)^{-1} X^{T} \mathbf{y} - \mathbf{x}_{i}^{T} (X^{T} X)^{-1} \mathbf{x}_{i} y_{i} + \mathbf{x}_{i}^{T} \frac{(X^{T} X)^{-1} \mathbf{x}_{i} \mathbf{x}_{i}^{T} (X^{T} X)^{-1}}{1 - h_{i}} X^{T} \mathbf{y} - \mathbf{x}_{i}^{T} \frac{(X^{T} X)^{-1} \mathbf{x}_{i} \mathbf{x}_{i}^{T} (X^{T} X)^{-1}}{1 - h_{i}} \mathbf{x}_{i} y_{i} \\ &= \mathbf{x}_{i}^{T} (X^{T} X)^{-1} X^{T} \mathbf{y} - \mathbf{x}_{i}^{T} \left[\frac{(X^{T} X)^{-1} \mathbf{x}_{i}}{1 - h_{i}} \right] (y_{i} (1 - h_{i}) - \mathbf{x}_{i}^{T} (X^{T} X)^{-1} X^{T} \mathbf{y} + h_{i} y_{i}) \\ &= \mathbf{x}_{i}^{T} \hat{\boldsymbol{\beta}} - \mathbf{x}_{i}^{T} \left[\frac{(X^{T} X)^{-1} \mathbf{x}_{i}}{1 - h_{i}} \right] (y_{i} - \mathbf{x}_{i}^{T} \hat{\boldsymbol{\beta}}). \end{split}$$

This gives

$$y_i - \hat{y}_{(-i)} = y_i - \mathbf{x}_i^T \hat{\boldsymbol{\beta}} + \mathbf{x}_i^T \left[\frac{(X^T X)^{-1} \mathbf{x}_i}{1 - h_i} \right] (y_i - \mathbf{x}_i^T \hat{\boldsymbol{\beta}})$$
$$= (y_i - \mathbf{x}_i^T \hat{\boldsymbol{\beta}}) \left(1 + \frac{h_i}{1 - h_i} \right)$$
$$= \frac{y_i - \hat{y}_i}{1 - h_i},$$

which gives

$$CV = \frac{1}{N} \sum_{i=1}^{N} (y_i - \hat{y}_{(-i)})^2 = \frac{1}{N} \sum_{i=1}^{N} \left(\frac{y_i - \hat{y}_i}{1 - h_i} \right)^2,$$

which completes the proof.

b)

FALSE, TRUE, FALSE, FALSE.

Problem 5

```
id <- "19auu8Y1UJJJUsZY8JZfsCTWzDm6doE7C" # Google file ID.
d.bodyfat <- read.csv(sprintf("https://docs.google.com/uc?id=%s&export=download", id),header=T)</pre>
```

a)

```
lm.fit5 <- lm(bodyfat ~ age + weight + bmi, data = d.bodyfat)</pre>
```

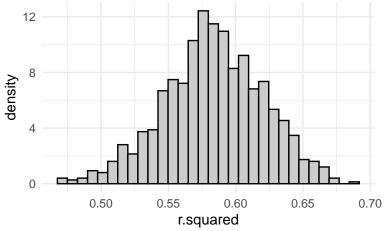
The R^2 is ≈ 0.5803 .

b)

#>

#> 0.5090717 0.6534133

```
set.seed(4268)
boot.fn <- function(data, index) {</pre>
  return(summary(lm(bodyfat ~ age + weight + bmi, data = data, subset = index))$r.squared)
}
B <- 1000
r.squared <- rep(NA, B)
for (b in 1:B){
  r.squared[b] <- boot.fn(d.bodyfat, sample(nrow(d.bodyfat), nrow(d.bodyfat), replace = T))</pre>
}
df = data.frame(r.squared = r.squared, norm_den = dnorm(r.squared, mean(r.squared),
                                                          sd(r.squared)))
ggplot(df) + geom_histogram(aes(x = r.squared, y = ..density..), fill = "grey80",color = "black") +
   theme_minimal()
```



```
sd(r.squared)
#> [1] 0.03705002
quantile(r.squared, c(0.025, 0.975))
        2.5%
                 97.5%
```

The standard error estimated from the bootstrap is 6.385 % of \mathbb{R}^2 . This gives us a measure of the uncertainty in R^2 , which illustrates that the proportion of variance explained by the linear regression is not a fixed number, but depends on the training data.