Task 4

Task 4: Use 5-fold cross-validation to select the best λ. Compare the prediction performance between the "optimal" model and "full" model.

5-fold CV

We write an **R** function `cv.logit.lasso` to conduct 5-fold cross-validation to select the best λ.

```
cv.logit.lasso <- function(x, y, nfolds = 5, lambda) {
  auc <- data.frame(matrix(ncol = 3, nrow = 0))
  folds <- createFolds(y, k = nfolds)
  for (i in 1:nfolds) {
    valid_index <- folds[[i]]
    x_training <- x[-valid_index, ]
    y_training <- y[-valid_index]
    training_dat <- data.frame(cbind(y_training, x_training))
    x_valid <- cbind(rep(1, length(valid_index)), x[valid_index, ])
    y_valid <- y[valid_index]
    res <- LogisticLASSO(dat = training_dat, start = rep(0, ncol(training_dat)), lambda = lambda)
    for (k in 1:nrow(res)) {
      betavec <- res[k, 2:ncol(res)]
      u_valid <- x_valid %*% betavec
      phat_valid <- sigmoid(u_valid)[, 1]
      roc <- roc(response = y_valid, predictor = phat_valid)
      auc <- rbind(auc, c(lambda[k], i, roc$auc[1]))
    }
  }
  colnames(auc) <- c("lambda", "fold", "auc")
  cv_res <- auc %>%
    group_by(lambda) %>%
    summarize(auc_mean = mean(auc),
              auc_se = sd(auc) / sqrt(5),
              auc_low = auc_mean - auc_se,
              auc_high = auc_mean + auc_se) %>%
    mutate(auc_ranking = min_rank(desc(auc_mean)))
  bestlambda <- max(cv_res$lambda[cv_res$auc_ranking == 1])
  return(cv_res)
}
```

Compare the results of cross-validation using `glmnet` and using our algorithm.

1. Our function `cv.logit.lasso`:

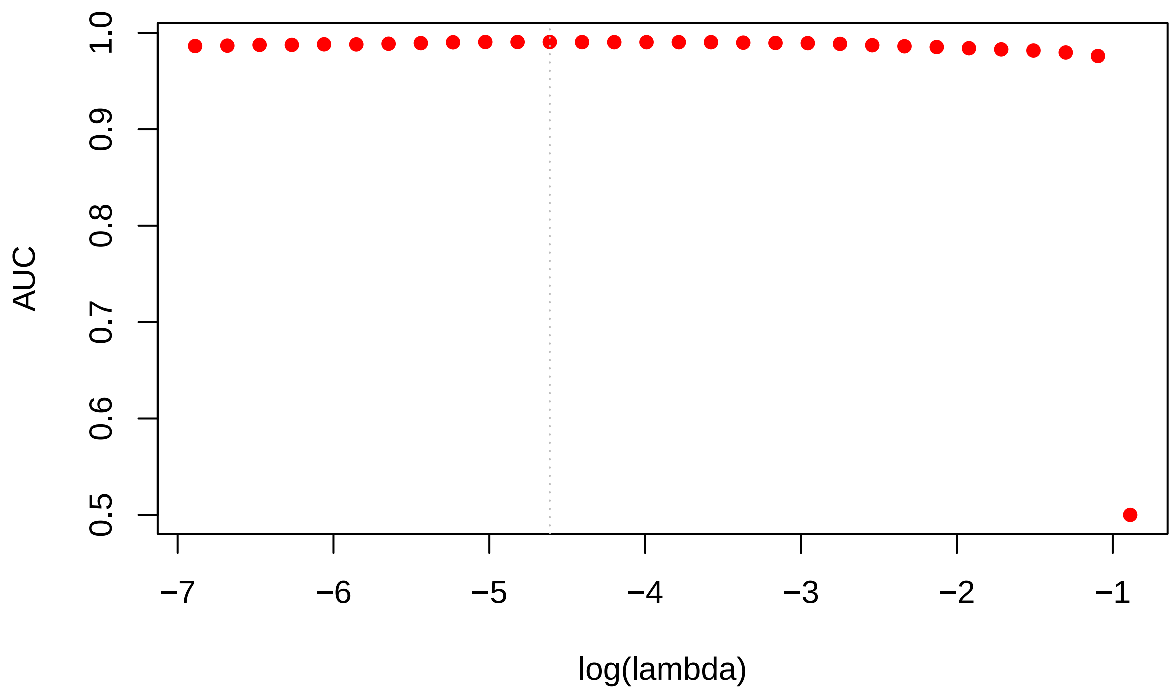
```r
set.seed(1)
folds <- createFolds(y, k = 5)
lambda_max_i <- rep(NA, 5) # lambda_max for each training set in CV (4/5 of the whole training data)
for (i in 1:5) {
    valid_index <- folds[[i]]
    x_training <- x[-valid_index, ]
    y_training <- y[-valid_index]
    lambda_max_i[i] <- max(abs(t(x_training) %*% (y_training - mean(y_training)))) / length(y_training)
    }
lambda_max <- max(lambda_max_i) + 1e-10 # max of lambda_max's so that all beta_i's = 0 except intercept
lambdas <- exp(seq(log(lambda_max), log(lambda_max) - 6, length = 30))

set.seed(1)
res_cv = cv.logit.lasso(x, y, nfolds = 5, lambda = lambdas)
as.matrix(res_cv %>% arrange(-lambda))
```

```
##            lambda  auc_mean      auc_se   auc_low  auc_high auc_ranking
##  [1,] 0.411544526 0.5000000 0.000000000 0.5000000 0.5000000          30
##  [2,] 0.334628402 0.9760054 0.010592380 0.9654130 0.9865978          29
##  [3,] 0.272087611 0.9796678 0.010375900 0.9692919 0.9900437          28
##  [4,] 0.221235460 0.9816903 0.009512584 0.9721777 0.9912029          27
##  [5,] 0.179887384 0.9828852 0.008738249 0.9741469 0.9916234          26
##  [6,] 0.146267108 0.9841071 0.007957927 0.9761492 0.9920651          25
##  [7,] 0.118930336 0.9853029 0.007306301 0.9779966 0.9926092          24
##  [8,] 0.096702703 0.9861031 0.007243727 0.9788594 0.9933468          23
##  [9,] 0.078629332 0.9872060 0.007099766 0.9801063 0.9943058          20
## [10,] 0.063933805 0.9885875 0.006862409 0.9817250 0.9954499          15
## [11,] 0.051984817 0.9893408 0.006624454 0.9827164 0.9959653          12
## [12,] 0.042269050 0.9895397 0.006405661 0.9831340 0.9959454          11
## [13,] 0.034369124 0.9898394 0.006335376 0.9835040 0.9961747          10
## [14,] 0.027945664 0.9903360 0.005905664 0.9844304 0.9962417           5
## [15,] 0.022722724 0.9903354 0.005871355 0.9844640 0.9962067           6
## [16,] 0.018475933 0.9903346 0.005795855 0.9845387 0.9961304           8
## [17,] 0.015022850 0.9903347 0.005776185 0.9845585 0.9961109           7
## [18,] 0.012215136 0.9904332 0.005623032 0.9848102 0.9960562           4
## [19,] 0.009932173 0.9905325 0.005536136 0.9849964 0.9960687           1
## [20,] 0.008075887 0.9905317 0.005476448 0.9850553 0.9960082           3
## [21,] 0.006566534 0.9905324 0.005476956 0.9850554 0.9960093           2
## [22,] 0.005339274 0.9902345 0.005741539 0.9844929 0.9959760           9
## [23,] 0.004341384 0.9893390 0.006354172 0.9829848 0.9956931          13
## [24,] 0.003529995 0.9887423 0.006823535 0.9819188 0.9955659          14
## [25,] 0.002870252 0.9880447 0.007261041 0.9807837 0.9953058          17
## [26,] 0.002333813 0.9881480 0.007498966 0.9806490 0.9956469          16
## [27,] 0.001897632 0.9875518 0.008002341 0.9795495 0.9955542          18
## [28,] 0.001542972 0.9875498 0.007823489 0.9797263 0.9953733          19
## [29,] 0.001254596 0.9867502 0.007946196 0.9788040 0.9946964          21
## [30,] 0.001020117 0.9863500 0.007967195 0.9783828 0.9943171          22
```

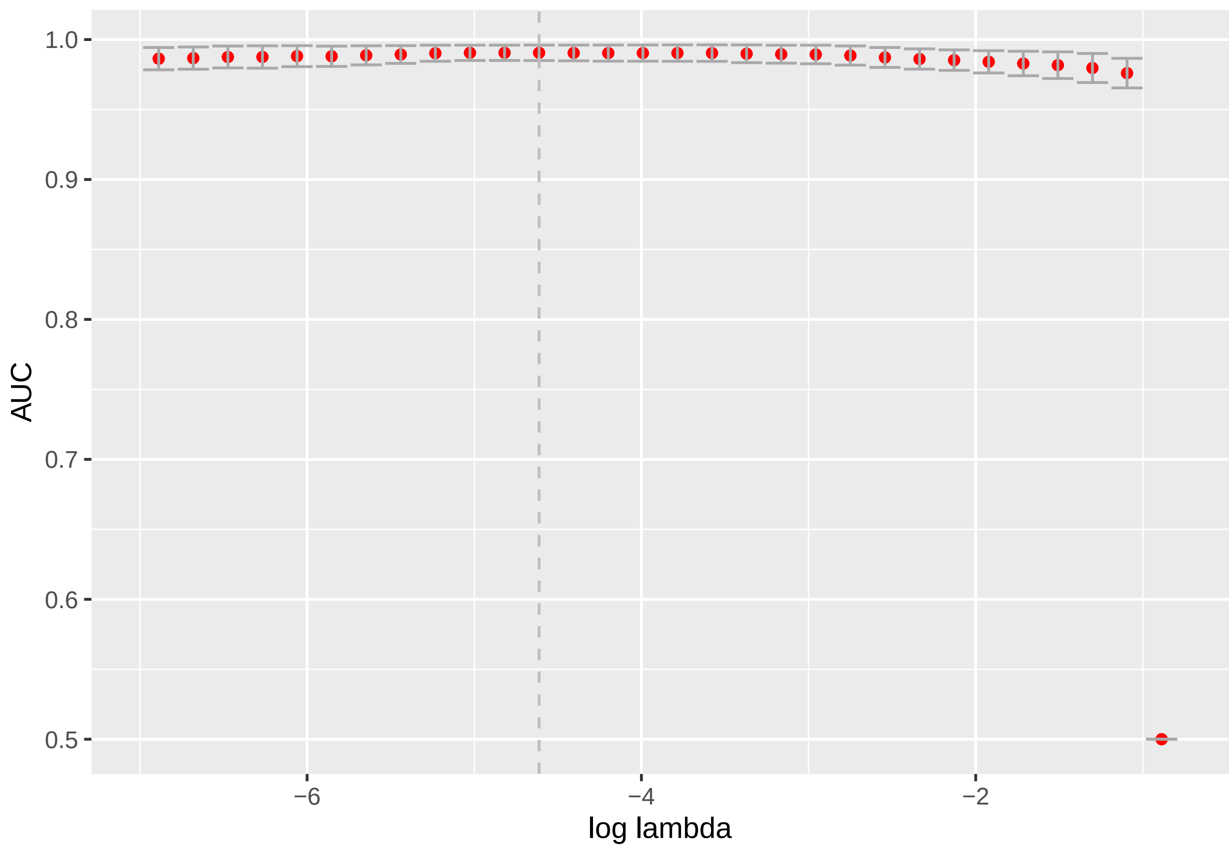
```r
# best lambda
best_lambda <- max(res_cv$lambda[res_cv$auc_ranking == 1])
best_lambda
```

```
## [1] 0.009932173
```

```r
# plot of best lambda
plot(log(res_cv$lambda),
     res_cv$auc_mean,
     pch = 16,
     xlab = "log(lambda)",
     ylab = "AUC",
     col = "red")
abline(v = log(res_cv$lambda[which((res_cv$auc_ranking == 1))]), col = "gray", lty = 3)
```




```r
# plot of best lambda with std.error interval
ggplot(res_cv, aes(log(lambda), auc_mean)) +
  geom_point(col = "red") +
  geom_errorbar(aes(ymin = auc_low, ymax = auc_high), col = "darkgray") +
  geom_vline(aes(xintercept = log(lambda[which((auc_ranking == 1))])), color = "grey", linetype = "dashe
  xlab("log lambda") +
  ylab("AUC")
```

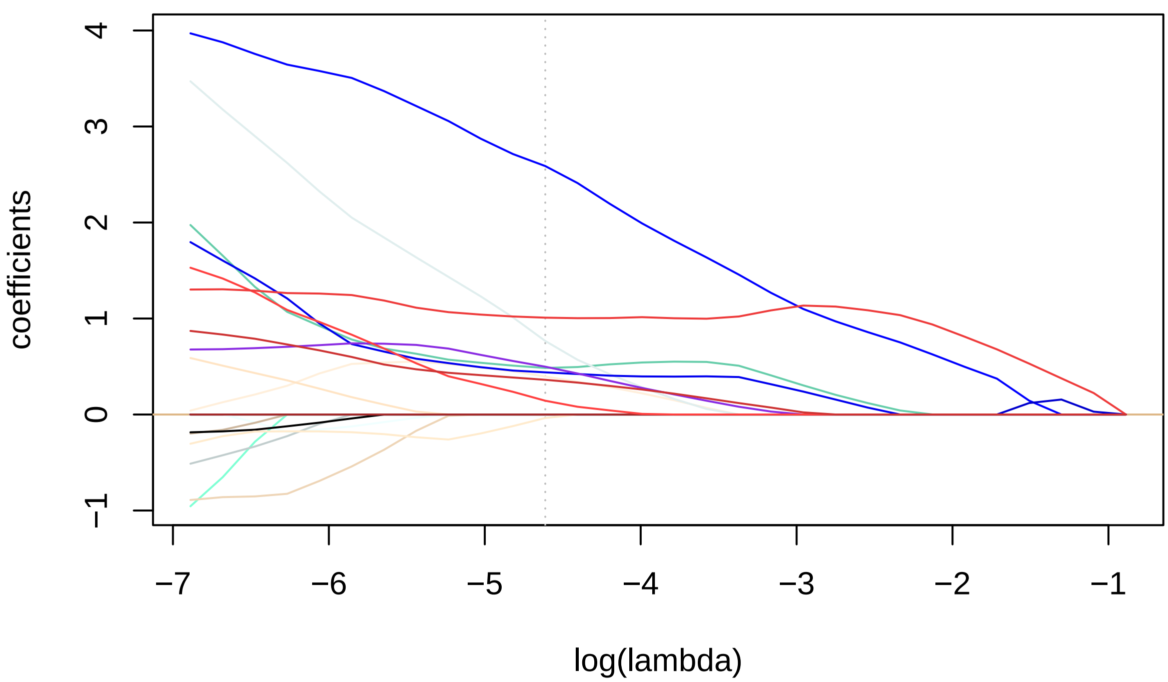



```
# coefficients of the best model
res_coef <- LogisticLASSO(dat = Training, start = rep(0, ncol(Training)),
                          lambda = lambdas) %>% as.data.frame
res_coef[res_coef$lambda == best_lambda, -1]
```

```
##    (Intercept) radius_mean texture_mean perimeter_mean area_mean
## 19   -0.613828           0    0.3958698              0         0
##    smoothness_mean compactness_mean concavity_mean concave.points_mean
## 19               0                0              0           0.4850029
##    symmetry_mean fractal_dimension_mean radius_se texture_se perimeter_se
## 19             0                      0 0.7660262          0            0
##    area_se smoothness_se compactness_se concavity_se concave.points_se
## 19       0             0              0            0                 0
##    symmetry_se fractal_dimension_se radius_worst texture_worst perimeter_worst
## 19           0          -0.03644811     2.587817     0.4394404               0
##    area_worst smoothness_worst compactness_worst concavity_worst
## 19          0        0.4980005                 0        0.143706
##    concave.points_worst symmetry_worst fractal_dimension_worst
## 19             1.008792      0.3617036                       0
```

```
# plot of coefficients
i = 3
plot(log(res_coef$lambda),
     res_coef[, 1],
     type = "l",
```

```r
     xlab = "log(lambda)",
     ylab = "coefficients",
     ylim = c(min(res_coef), max(res_coef)),
     col = colors(1)[1])
abline(h = 0, col = colors(1)[length(res_coef) + 1])
abline(v = log(res_cv$lambda[which((res_cv$auc_ranking == 1))]), col = "gray", lty = 3)
while (i < length(res_coef)) {
  lines(log(res_coef$lambda), res_coef[, i], col = colors(1)[i], lty = 1)
  i = i + 1
}
```

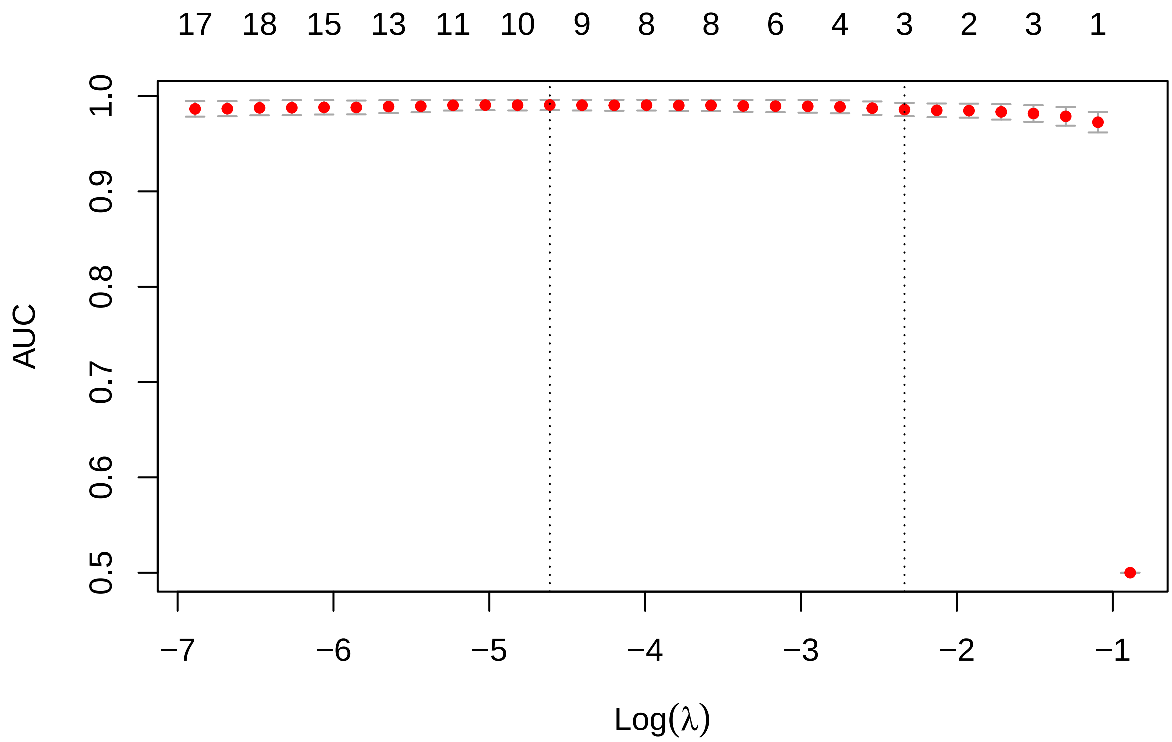


2. `glmnet` from **R** package `caret`

```r
set.seed(1)
fit.logit.lasso <- cv.glmnet(x, y,
                             nfolds = 5, alpha = 1,
                             lambda = lambdas,
                             family = "binomial", type.measure = "auc")
# best lambda
fit.logit.lasso$lambda.min
```

```
## [1] 0.009932173
```

```r
plot(fit.logit.lasso)
```




```r
# coefficients of the best model
coef(fit.logit.lasso, fit.logit.lasso$lambda.min)
```

```
## 31 x 1 sparse Matrix of class "dgCMatrix"
##                                 s1
## (Intercept)            -0.60486590
## radius_mean             .
## texture_mean            0.38113717
## perimeter_mean          .
## area_mean               .
## smoothness_mean         .
## compactness_mean        .
## concavity_mean          .
## concave.points_mean     0.44764990
## symmetry_mean           .
## fractal_dimension_mean  .
## radius_se               0.83791365
## texture_se              .
## perimeter_se            .
## area_se                 .
## smoothness_se           .
## compactness_se          .
## concavity_se            .
```

```
## concave.points_se        .
## symmetry_se              .
## fractal_dimension_se    -0.03686225
## radius_worst             2.57346076
## texture_worst            0.45902449
## perimeter_worst          .
## area_worst               .
## smoothness_worst         0.49454577
## compactness_worst        .
## concavity_worst          0.12532306
## concave.points_worst     1.06926848
## symmetry_worst           0.36416342
## fractal_dimension_worst  .
```

The results are slightly different (mean AUC values).

lambda	ours_AUC	cv.glmnet_AUC
0.4115445	0.5000000	0.5000000
0.3346284	0.9760054	0.9725915
0.2720876	0.9796678	0.9787526
0.2212355	0.9816903	0.9817053
0.1798874	0.9828852	0.9834002
0.1462671	0.9841071	0.9847216
0.1189303	0.9853029	0.9850192
0.0967027	0.9861031	0.9858166
0.0786293	0.9872060	0.9873215
0.0639338	0.9885875	0.9887026
0.0519848	0.9893408	0.9892575
0.0422691	0.9895397	0.9894566
0.0343691	0.9898394	0.9896556
0.0279457	0.9903360	0.9902522
0.0227227	0.9903354	0.9901527
0.0184759	0.9903346	0.9904508
0.0150229	0.9903347	0.9903518
0.0122151	0.9904332	0.9904501
0.0099322	0.9905325	0.9906491
0.0080759	0.9905317	0.9904501
0.0065665	0.9905324	0.9905479
0.0053393	0.9902345	0.9903485
0.0043414	0.9893390	0.9893569
0.0035300	0.9887423	0.9889618
0.0028703	0.9880447	0.9880654
0.0023338	0.9881480	0.9881674
0.0018976	0.9875518	0.9877693
0.0015430	0.9875498	0.9876669
0.0012546	0.9867502	0.9867649
0.0010201	0.9863500	0.9865655

The best λ's are the same, and the coefficients are very similar.

```
## [1] 0.009932173
```

```
## [1] 0.009932173
```

predictor	ours_coef	cv.glmnet_coef
(Intercept)	-0.6138280	-0.6048659
radius_mean	0.0000000	0.0000000
texture_mean	0.3958698	0.3811372
perimeter_mean	0.0000000	0.0000000
area_mean	0.0000000	0.0000000
smoothness_mean	0.0000000	0.0000000
compactness_mean	0.0000000	0.0000000
concavity_mean	0.0000000	0.0000000
concave.points_mean	0.4850029	0.4476499
symmetry_mean	0.0000000	0.0000000
fractal_dimension_mean	0.0000000	0.0000000
radius_se	0.7660262	0.8379136
texture_se	0.0000000	0.0000000
perimeter_se	0.0000000	0.0000000
area_se	0.0000000	0.0000000
smoothness_se	0.0000000	0.0000000
compactness_se	0.0000000	0.0000000
concavity_se	0.0000000	0.0000000
concave.points_se	0.0000000	0.0000000
symmetry_se	0.0000000	0.0000000
fractal_dimension_se	-0.0364481	-0.0368622
radius_worst	2.5878169	2.5734608
texture_worst	0.4394404	0.4590245
perimeter_worst	0.0000000	0.0000000
area_worst	0.0000000	0.0000000
smoothness_worst	0.4980005	0.4945458
compactness_worst	0.0000000	0.0000000
concavity_worst	0.1437060	0.1253231
concave.points_worst	1.0087922	1.0692685
symmetry_worst	0.3617036	0.3641634
fractal_dimension_worst	0.0000000	0.0000000

Prediction performance comparison

Below is the prediction performance on the test data.

```r
# test data
X_test <- cbind(rep(1, nrow(Test)), model.matrix(diagnosis ~ ., Test)[, -1])
y_test <- Test$diagnosis

# logistic model
res_logit <- NewtonRaphson(dat = Training, func = logisticstuff, start = rep(0, ncol(Training)))
```

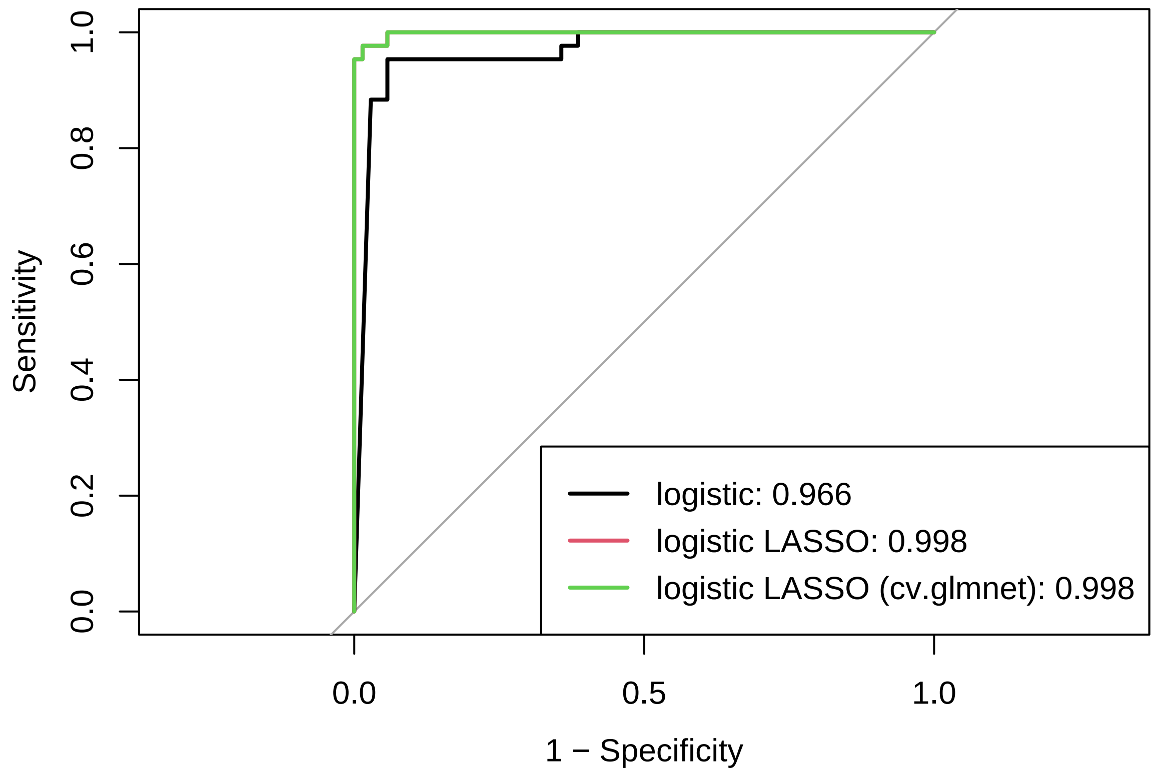
```
## Warning in NewtonRaphson(dat = Training, func = logisticstuff, start = rep(0, :
## Complete separation occurs. Algorithm does not converge.
```

```r
betavec_logit <- res_logit[nrow(res_logit), 3:ncol(res_logit)]
u <- X_test %*% betavec_logit
phat <- sigmoid(u)[, 1]
roc.logit <- roc(response = y_test, predictor = phat)
```

```r
logit_spec <- specificity(as.factor(y_test), as.factor(round(phat)))
logit_sens <- sensitivity(as.factor(y_test), as.factor(round(phat)))

# logistic LASSO model
betavec_logit.lasso <- res_coef[res_coef$lambda == best_lambda, -c(1, 2)]
col_nonzero <- names(betavec_logit.lasso)[betavec_logit.lasso != 0]
df_nonzero <- Training[c("diagnosis", col_nonzero)]
refit_logit <- NewtonRaphson(dat = df_nonzero, func = logisticstuff, start = rep(0, ncol(df_nonzero)))
betavec_lasso.refit <- refit_logit[nrow(refit_logit), 3:ncol(refit_logit)]
betavec_lasso.refit <- bind_rows(betavec_logit.lasso, betavec_lasso.refit)[2,] %>% select("(Intercept)"
betavec_lasso.refit[is.na(betavec_lasso.refit)] <- 0
betavec_lasso.refit <- as.numeric(betavec_lasso.refit)
u <- X_test %*% betavec_lasso.refit
phat <- sigmoid(u)[, 1]
roc.logitlasso <- roc(response = y_test, predictor = phat)
ll_spec <- specificity(as.factor(y_test), as.factor(round(phat)))
ll_sens <- sensitivity(as.factor(y_test), as.factor(round(phat)))

# logistic LASSO model (cv.glmnet)
betavec_logit.lasso.glm_temp <- coef(fit.logit.lasso, fit.logit.lasso$lambda.min)
betavec_logit.lasso.glm <- betavec_logit.lasso.glm_temp %>% as.vector
names(betavec_logit.lasso.glm) <- betavec_logit.lasso.glm_temp@Dimnames[[1]]
col_nonzero <- names(betavec_logit.lasso.glm)[betavec_logit.lasso.glm != 0][-1]
df_nonzero <- Training[c("diagnosis", col_nonzero)]
refit_logit.glm <- NewtonRaphson(dat = df_nonzero, func = logisticstuff, start = rep(0, ncol(df_nonzero)
betavec_lasso.refit.glm <- refit_logit.glm[nrow(refit_logit.glm), 3:ncol(refit_logit.glm)]
betavec_lasso.refit.glm <- bind_rows(betavec_logit.lasso, betavec_lasso.refit.glm)[2,] %>% select("(Inte
betavec_lasso.refit.glm[is.na(betavec_lasso.refit.glm)] <- 0
betavec_lasso.refit.glm <- as.numeric(betavec_lasso.refit.glm)
u <- X_test %*% betavec_lasso.refit.glm
phat <- sigmoid(u)[, 1]
roc.logitlasso.glm <- roc(response = y_test, predictor = phat)

# draw rocs
auc <- c(roc.logit$auc[1], roc.logitlasso$auc[1], roc.logitlasso.glm$auc[1])
auc
```

```
## [1] 0.9661130 0.9983389 0.9983389
```

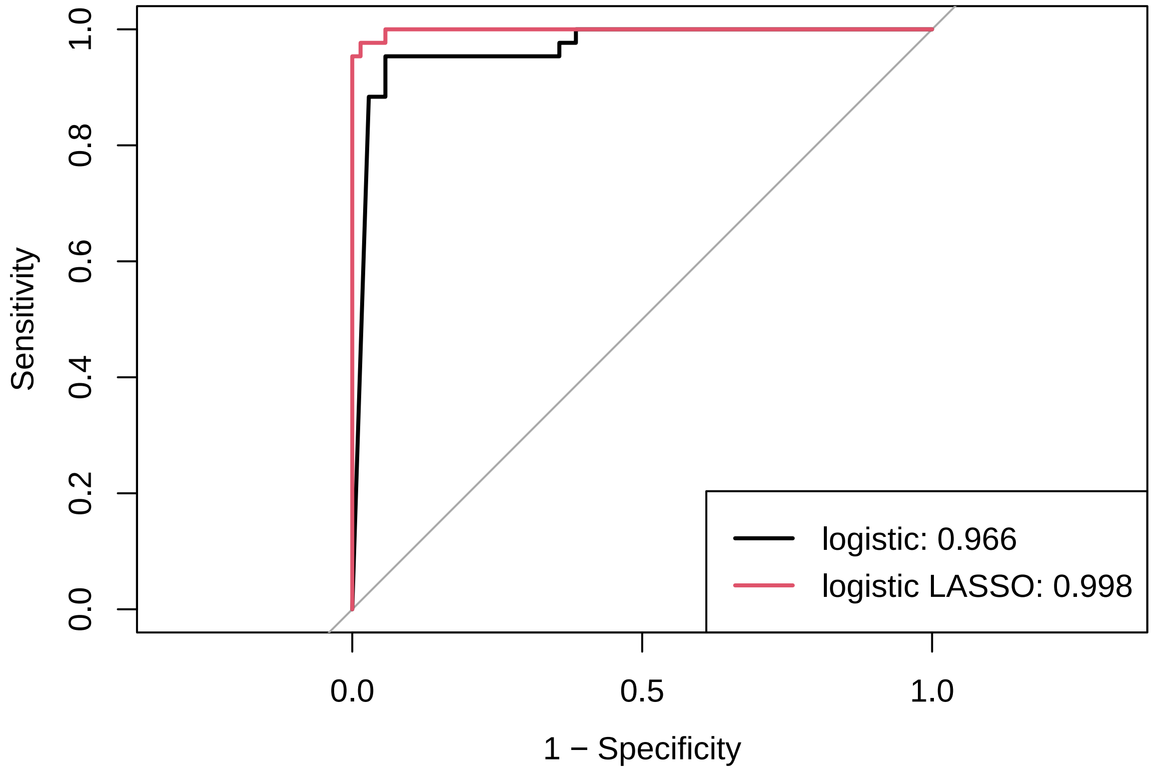
```r
plot(roc.logit, legacy.axes = TRUE)
plot(roc.logitlasso, col = 2, add = TRUE)
plot(roc.logitlasso.glm, col = 3, add = TRUE)
modelNames <- c("logistic", "logistic LASSO", "logistic LASSO (cv.glmnet)")
legend("bottomright", legend = paste0(modelNames, ": ", round(auc, 3)),
col = 1:3, lwd = 2)
```




```
# draw rocs(only 2)
auc <- c(roc.logit$auc[1], roc.logitlasso$auc[1])
auc
```

```
## [1] 0.9661130 0.9983389
```

```
plot(roc.logit, legacy.axes = TRUE)
plot(roc.logitlasso, col = 2, add = TRUE)
modelNames <- c("logistic", "logistic LASSO")
legend("bottomright", legend = paste0(modelNames, ": ", round(auc, 3)),
col = 1:2, lwd = 2)
```

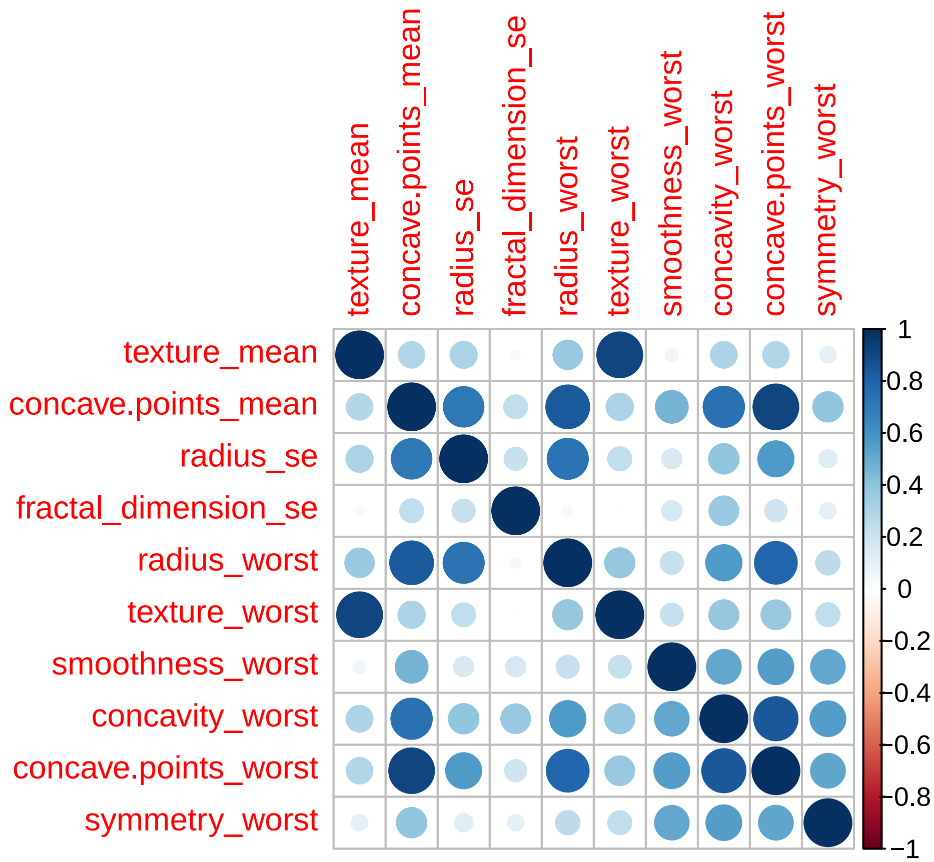



```
tibble(Model = c("full", "optimal"),
       specificity = c(logit_spec, ll_spec),
       sensitivity = c(logit_sens, ll_sens),
       AUC = c(roc.logit$auc[1], roc.logitlasso$auc[1])) %>%
  knitr::kable(
  )
```

Model	specificity	sensitivity	AUC
full	0.9268293	0.9305556	0.9661130
optimal	0.9545455	0.9855072	0.9983389

Correlation Plot

```
corrplot::corrplot(cor(Training[names(betavec_logit.lasso)[betavec_logit.lasso != 0]]))
```



LASSO model coefficients

Re-fit the logistic regression with the predictors selected by LASSO.

```
refit_logit[nrow(refit_logit), 3:ncol(refit_logit)]
```

```
##          (Intercept)         texture_mean  concave.points_mean
##          -0.09092737           0.94392378           0.84754704
##            radius_se fractal_dimension_se         radius_worst
##           3.77040802          -1.12476354           6.01510669
##        texture_worst     smoothness_worst      concavity_worst
##           1.23805580           1.67539455           1.19425400
## concave.points_worst       symmetry_worst
##           1.87249528           0.69899461
```