In-class worksheet 13

March 5, 2019

In this worksheet, we will use the libraries tidyverse, plotROC, and ggthemes:

```
library(tidyverse)
theme_set(theme_bw(base_size=12)) # set default ggplot2 theme
library(plotROC)
library(ggthemes)
```

1. Working with training and test data sets

We continue working with the biopsy data set:

```
biopsy <- read_csv("http://wilkelab.org/classes/SDS348/data_sets/biopsy.csv")
```

```
## Parsed with column specification:
## cols(
##   clump_thickness = col_integer(),
##   uniform_cell_size = col_integer(),
##   uniform_cell_shape = col_integer(),
##   marg_adhesion = col_integer(),
##   epithelial_cell_size = col_integer(),
##   bare_nuclei = col_integer(),
##   bland_chromatin = col_integer(),
##   normal_nucleoli = col_integer(),
##   mitoses = col_integer(),
##   outcome = col_character()
## )
```

```
biopsy$outcome <- factor(biopsy$outcome) # make outcome a factor
```

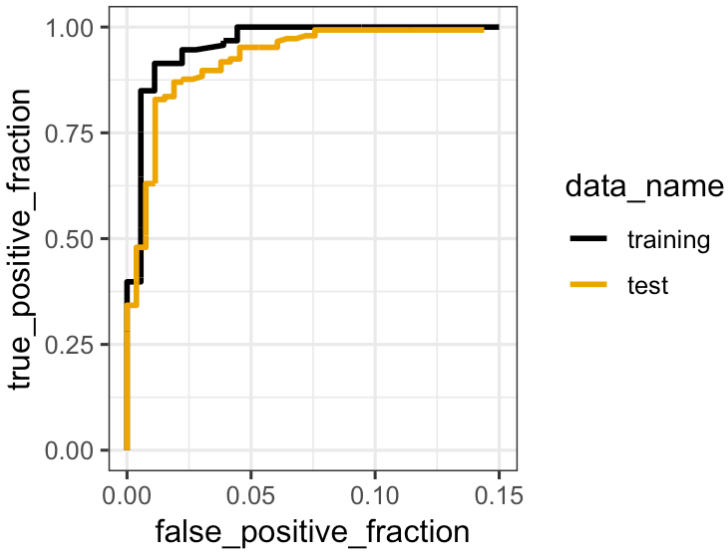
The following code splits the biopsy data set into a random training and test set:

```
train_fraction <- 0.4 # fraction of data for training purposes
set.seed(126)  # set the seed to make the partition reproductible
train_size <- floor(train_fraction * nrow(biopsy)) # number of observations in
training set
train_indices <- sample(1:nrow(biopsy), size = train_size)

train_data <- biopsy[train_indices, ] # get training data
test_data <- biopsy[-train_indices, ] # get test data
```

Fit a logistic regression model on the training data set, then predict the outcome on the test data set, and plot the resulting ROC curves. Limit the x-axis range from 0 to 0.15 to zoom into the ROC curve. (Hint: Do **not** use `coord_fixed()` .)

```
# model to use:
# outcome ~ clump_thickness + uniform_cell_size + uniform_cell_shape

glm_out <- glm(
  outcome ~ clump_thickness + uniform_cell_size + uniform_cell_shape,
  data = train_data,
  family = binomial
)

# results data frame for training data
df_train <- data.frame(
  predictor = predict(glm_out, train_data),
  known_truth = train_data$outcome,
  data_name = "training"
)

# results data frame for test data
df_test <- data.frame(
  predictor = predict(glm_out, test_data),
  known_truth = test_data$outcome,
  data_name = "test"
)

df_combined <- rbind(df_train, df_test)

ggplot(df_combined, aes(d = known_truth, m = predictor, color = data_name)) +
  geom_roc(n.cuts = 0) +
  xlim(0, 0.15) +
  scale_color_colorblind()
```

```
## Warning in verify_d(data$d): D not labeled 0/1, assuming benign = 0 and
## malignant = 1!
```



2. Area under the ROC curves

You can calculate the areas under the ROC curves by running `calc_auc()` on a plot generated with `geom_roc()` (see previous worksheet). Use this function to calculate the area under the training and test curve for the model `outcome ~ clump_thickness`. For this exercise, generate a new set of training and test datasets with a different fraction of training data from before.

```
train_fraction <- 0.2 # fraction of data for training purposes
set.seed(123)  # set the seed to make the partition reproductible
train_size <- floor(train_fraction * nrow(biopsy)) # number of observations in
training set
train_indices <- sample(1:nrow(biopsy), size = train_size)

train_data <- biopsy[train_indices, ] # get training data
test_data <- biopsy[-train_indices, ] # get test data

# fit the model on the training data
glm_out <- glm(
  outcome ~ clump_thickness,
  data = train_data,
  family = binomial
)

# predict outcomes for the training data
df_train <- data.frame(
  predictor = predict(glm_out, train_data),
  known_truth = train_data$outcome,
  data_name = "training"
)

# predict outcomes for the test data
df_test <- data.frame(
  predictor = predict(glm_out, test_data),
  known_truth = test_data$outcome,
  data_name = "test"
)

df_combined <- rbind(df_train, df_test)

p <- ggplot(df_combined, aes(d = known_truth, m = predictor, color = data_name)
) +
  geom_roc(n.cuts = 0)

calc_auc(p)
```

```
## Warning in verify_d(data$d): D not labeled 0/1, assuming benign = 0 and
## malignant = 1!
```

```
##   PANEL group       AUC
## 1     1     1 0.9214427
## 2     1     2 0.9050554
```

3. If this was easy

Write code that combines the AUC values calculated by `calc_auc()` with the correct group names and orders the output in descending order of AUC. (Hint: We have seen similar code in the previous worksheet.)

```
data_name <- unique(df_combined$data_name)
data_info <- data.frame(
  data_name,
  group = order(data_name)
)
left_join(data_info, calc_auc(p)) %>%
  select(-group, -PANEL) %>%
  arrange(desc(AUC))
```

```
## Warning in verify_d(data$d): D not labeled 0/1, assuming benign = 0 and
## malignant = 1!
```

```
## Joining, by = "group"
```

```
##   data_name       AUC
## 1  training 0.9214427
## 2      test 0.9050554
```

Write code that generates an arbitrary number of random subdivisions of the data into training and test sets, fits a given model, calculates the area under the curve for each test data set, and then calculates the average and standard deviation of these values.

```
# function that does the heavy lifting
generate_AUC_values <- function(data, formula, train_fraction)
{
  n_obs <- nrow(data) # number of observations in data set
  train_size <- floor(train_fraction * nrow(data)) # number of observations in
training set
  train_indices <- sample(1:n_obs, size = train_size)

  train_data <- data[train_indices, ] # get training data
  test_data <- data[-train_indices, ] # get test data
  glm_out <- glm(formula, data = train_data, family = binomial)

  df_train <- data.frame(
    predictor = predict(glm_out, train_data),
    known_truth = train_data$outcome,
    data_name = "AUC_train"
  )

  df_test <- data.frame(
    predictor = predict(glm_out, test_data),
    known_truth = test_data$outcome,
    data_name = "AUC_test"
  )

  df_combined <- rbind(df_train, df_test)

  p <- ggplot(df_combined, aes(d = known_truth, m = predictor, color = data_nam
e)) +
    geom_roc(n.cuts = 0)

  data_name <- unique(df_combined$data_name)
  data_info <- data.frame(
    data_name,
    group = order(data_name)
  )
  left_join(data_info, calc_auc(p)) %>%
    select(-group, -PANEL) %>%
    spread(data_name, AUC)
}

# example use
generate_AUC_values(biopsy,  outcome ~ clump_thickness, 0.2)
```

```
## Joining, by = "group"
```

```
##   AUC_train  AUC_test
## 1 0.8968605 0.9121516
```

```
# function that does repeated random subsampling validation
subsample_validate <- function(data, formula, train_fraction, replicates)
{
  reps <- data.frame(rep=1:replicates) # dummy data frame to iterate over
  reps %>% group_by(rep) %>% # iterate over all replicates
    do(generate_AUC_values(data, formula, train_fraction)) %>% # run calc_AUC f
or each replicate
    ungroup() %>%     # ungroup so we can summarize
    summarize(
      mean_AUC_train = mean(AUC_train),        # summarize
      sd_AUC_train = sd(AUC_train),
      mean_AUC_test = mean(AUC_test),
      sd_AUC_test = sd(AUC_test)
    ) %>%
    mutate( # add columns containing meta data
      train_fraction = train_fraction,
      replicates = replicates
    )
}
```

Now that we have these two functions, we can use them to complete the exercise. (We set `message = FALSE` and `warning = FALSE` for this R chunk so that we don't get repeated messages and warnings in the knitted html.)

```
train_fraction <- 0.2 # fraction of data for training purposes
replicates <- 10 # how many times do we want to randomly sample
set.seed(116) # random seed
formula <- outcome ~ clump_thickness + normal_nucleoli # the model we want to f
it
subsample_validate(biopsy, formula, train_fraction, replicates)
```

```
## # A tibble: 1 x 6
##   mean_AUC_train sd_AUC_train mean_AUC_test sd_AUC_test train_fraction
##            <dbl>        <dbl>         <dbl>       <dbl>          <dbl>
## 1          0.964       0.0129         0.968     0.00224            0.2
## # … with 1 more variable: replicates <dbl>
```

```
# redo with a different model
formula2 <- outcome ~ clump_thickness + normal_nucleoli + marg_adhesion
subsample_validate(biopsy, formula2, train_fraction, replicates)
```

```
## # A tibble: 1 x 6
##   mean_AUC_train sd_AUC_train mean_AUC_test sd_AUC_test train_fraction
##            <dbl>        <dbl>         <dbl>       <dbl>          <dbl>
## 1          0.985      0.00850         0.984     0.00362            0.2
## # … with 1 more variable: replicates <dbl>
```