Classification: Data Preparation

CITS4009 Computational Data Analysis

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KDD Cup 2009 Data

The KDD Cup 2009 provided a dataset about customer relationship management.

- The contest supplied 230 facts (features) about 50,000 credit card accounts.
- The goal was to predict
  - account cancellation (called *churn*),
  - the innate tendency to use new products and services (called *appetency*), and
  - willingness to respond favorably to marketing pitches (called *upselling*)

Data Available at:

https://github.com/WinVector/zmPDSwR

Why Three-way splitting

This problem has

- a large number of variables, many of which have a large number of possible levels.
- The competition's AUC (*area under curve*) measure, isn't particularly resistant to *overfitting* (not having built-in model complexity or chance corrections).

Because of this concern, we'll split our data into three sets: training, calibration, and test.

- Use the training set for most of our work, and we'll never look at the test set (we'll reserve it for our final report of model performance).
- The calibration set is used to simulate the unseen test set during modeling-
  - performance on the calibration set is used to estimate overfitting.

KDD2009 Data Pre-processing

```
path <- '../../data_v2/KDD2009/'
d <- read.table(paste0(path, 'orange_small_train.data.gz'),
                header=T, sep='\t', na.strings=c('NA',''))

churn <- read.table(
  paste0(path,'orange_small_train_churn.labels.txt'),
  header=F,sep='\t')
d$churn <- churn$V1                #___churn___
appetency <- read.table(
  paste0(path,'orange_small_train_appetency.labels.txt'),
  header=F,sep='\t')
d$appetency <- appetency$V1     # ___appetency___
upselling <- read.table(
  paste0(path,'orange_small_train_upselling.labels.txt'),
  header=F,sep='\t')
d$upselling <- upselling$V1     # ___upselling___

# d - data frame having 5000 rows and 233 (=230+3) columns;
# churn, appetency, upselling - all having 5000 rows and 1 column.
```

KDD2009 Data Pre-processing (Cont.)

```
# do a 90/10 split to form the training and test sets.
set.seed(729375)
d$rgroup <- runif(dim(d)[1])
dTrainAll <- subset(d, rgroup<=0.9)
dTest <- subset(d, rgroup>0.9)
outcomes <- c('churn', 'appetency', 'upselling')
# names of columns that are categorical type and numerical type
vars <- setdiff(colnames(dTrainAll),  c(outcomes, 'rgroup'))
catVars <- vars[sapply(dTrainAll[, vars], class) %in%
                  c('factor', 'character')]
numericVars <- vars[sapply(dTrainAll[, vars], class) %in%
                      c('numeric', 'integer')]
# remove the original tables
rm(list=c('d', 'churn', 'appetency', 'upselling'))

# split dTrainAll into a training set and a validation (or calibration) set
useForCal <- rbinom(n=dim(dTrainAll)[1], size=1, prob=0.1)>0
dCal <- subset(dTrainAll, useForCal)
dTrain <- subset(dTrainAll, !useForCal)
```

References

- **Practical Data Science with R**, *Nina Zumel, John Mount*, Manning, 2nd Ed., 2020 (Section 8.1-8.2)
- See https://github.com/WinVector/PDSwR2 for all the datasets provided by the authors Zumel et al for the book above.
- See https://github.com/WinVector/PDSwR2/raw/master/CodeExamples.zip for all the R code that produces all the results and almost all the plots in the book above.

Single Variable Classification – Categorical

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Classification and Scoring methods in data science

- The simplest classification method is one that always returns the majority category (a typical Null model)
- The simplest scoring (regression) method is one that always returns the average value of a subset of the original training data (a typical Null model)
- Other simpler methods (can be used for classification or scoring) include:
  - the single variable method (similar to the analyst's pivot table)
  - the nearest neighbor method
  - the Naïve Bayes method.

Section 1

Building Single Variable Models - Categorical

Single categorical variable model using `table()`

A single-variable model based on categorical features is easiest to describe as a table.

- Business analysts use what's called a *pivot table* (which promotes values or levels of a feature to be families of new columns) and
- statisticians use what's called a *contingency table* (where each possibility is given a column name).

In either case, the R command to produce a table is `table()`.

Single categorical variable model – example

```
outcome <- 'churn'  # We can also try the 'appetency' and 'upselling' columns.
pos <- '1'          # We are interested in when 'churn' is positive. We need
                    # to put quotes around number 1 as it is the column name
                    # of the table created.
# Column 'Var218' is a categorical column containing 'cJvF' and 'UYBR'.
table218 <- table(Var218=dTrain[,'Var218'], churn=dTrain[,outcome], useNA='ifany')
kable(table218)
```

	-1	1
cJvF	19245	1220
UYBR	17860	1618
NA	423	152

```
print(table218[,2] / (table218[,1] + table218[,2]))
##       cJvF       UYBR       <NA>
## 0.05961398 0.08306808 0.26434783
```

What does this mean when we use Var218 to predict the outcome churn? — if the value of Var218 is equal to cJvF then the predictor has 0.0596 probability of outputting a 1.

Function to repeat model building

```
# outCol: vector holding the values (known in the training step) of the
#         output column that we want to predict, e.g., the 'churn' column.
# varCol: the single variable column that is of interest. Can we use this
#         column alone to predict outCol?
# appCol: after building the model, we can apply it to this column (same
#         as varCol but may come from the calibration or test set).
mkPredC <- function(outCol, varCol, appCol) {
  pPos <- sum(outCol == pos) / length(outCol)
  naTab <- table(as.factor(outCol[is.na(varCol)]))
  pPosWna <- (naTab/sum(naTab))[pos]
  vTab <- table(as.factor(outCol), varCol)
  pPosWv <- (vTab[pos, ] + 1.0e-3*pPos) / (colSums(vTab) + 1.0e-3)
  pred <- pPosWv[appCol]
  pred[is.na(appCol)] <- pPosWna
  pred[is.na(pred)] <- pPos
  pred
}
```

Code with annotation

```
mkPredC <- function(outCol,varCol,appCol) {
    pPos <- sum(outCol==pos)/length(outCol)
    naTab <- table(as.factor(outCol[is.na(varCol)]))
    pPosWna <- (naTab/sum(naTab))[pos]
    vTab <- table(as.factor(outCol),varCol)
    pPosWv <- (vTab[pos,]+1.0e-3*pPos)/(colSums(vTab)+1.0e-3)
    pred <- pPosWv[appCol]
    pred[is.na(appCol)] <- pPosWna
    pred[is.na(pred)] <- pPos
    pred
}
```

Given a vector of training outcomes (outCol), a categorical training variable (varCol), and a prediction variable (appCol), use outCol and varCol to build a single-variable model and then apply the model to appCol to get new predictions.

Get stats on how often outcome is positive during training.

Get stats on how often outcome is positive for NA values of variable during training.

Get stats on how often outcome is positive, conditioned on levels of training variable.

Make predictions by looking up levels of appCol.

Add in predictions for NA levels of appCol.

Add in predictions for levels of appCol that weren't known during training.

Return vector of predictions.

Predict for all categorical variables

```
# call the mkPredC() function for all the categorical columns
for(v in catVars) {
  pi <- paste('pred', v, sep='')
  dTrain[,pi] <- mkPredC(dTrain[,outcome], dTrain[,v], dTrain[,v])
  dCal[,pi] <- mkPredC(dTrain[,outcome], dTrain[,v], dCal[,v])
  dTest[,pi] <- mkPredC(dTrain[,outcome], dTrain[,v], dTest[,v])
}
```

Recall that `outcome` was set to the value `churn` in an earlier slide. So we try to use each categorical column in `catVars` to predict when `churn` is positive (i.e., equal to `1`).

Predict for all categorical variables (cont.)

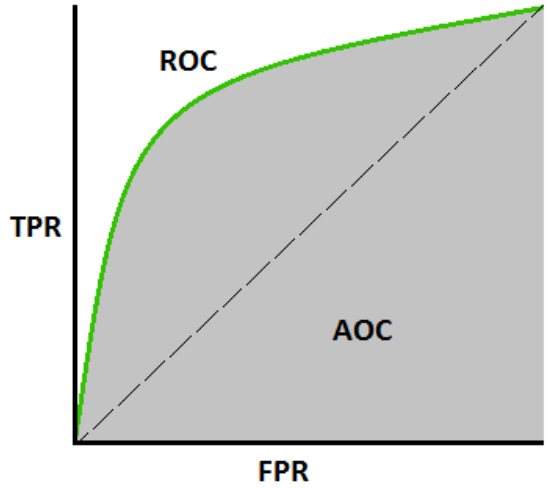
```
# We can inspect a few rows of the output column that has been added
# to dTrain for the categorical variable 'Var194'.
factor(dTrain[,"Var194"])["Levels"]  # how many levels are there?
## [1] <NA>
## Levels: CTUH lvza SEuy
```

```
rows <- c(620, 725, 9502, 40310)
dTrain[rows, c("Var194", "predVar194")]
##       Var194 predVar194
## 767     CTUH 0.06451643
## 895     lvza 0.06521745
## 11712   SEuy 0.06674519
## 49743   <NA> 0.07622426
```

```
rows <- c(842, 2885, 4507, 4510)
dCal[rows, c("Var194", "predVar194")]
##       Var194 predVar194
## 9040    CTUH 0.06451643
## 31804   lvza 0.06521745
## 49966   SEuy 0.06674519
## 49983   <NA> 0.07622426
```

What are the measures that we can use to evaluate the predictions above?

Area under ROC curve (AUC)



$$TPR/Recall/Sensitivity = \frac{TP}{TP + FN}$$

$$Specificity = \frac{TN}{TN + FP} \; Specificity \text{ is also known as } TNR)$$

$$FPR = 1 - Specificity = \frac{FP}{TN + FP}$$

Evaluate

Every classifier evaluation using ROCR starts with creating a prediction object created using the `prediction()` function.

The `performance()` function takes a prediction object and an evaluation metric to work out the relevant measurement.

```
library('ROCR')
calcAUC <- function(predcol,outcol) {
  perf <- performance(prediction(predcol,outcol==pos),'auc')
  as.numeric(perf@y.values)
}
```

Evaluate (cont.)

```
for(v in catVars) {
  pi <- paste('pred', v, sep='')
  aucTrain <- calcAUC(dTrain[,pi], dTrain[,outcome])
  if (aucTrain >= 0.8) {
    aucCal <- calcAUC(dCal[,pi], dCal[,outcome])
    print(sprintf(
      "%s: trainAUC: %4.3f; calibrationAUC: %4.3f",
      pi, aucTrain, aucCal))
  }
}
```

```
## [1] "predVar200: trainAUC: 0.830; calibrationAUC: 0.565"
## [1] "predVar202: trainAUC: 0.827; calibrationAUC: 0.525"
## [1] "predVar214: trainAUC: 0.830; calibrationAUC: 0.565"
## [1] "predVar217: trainAUC: 0.897; calibrationAUC: 0.553"
```

100-fold cross-validation

Let's inspect the AUC values of two example categorical columns a bit more.

```
vars <- c('Var200', 'Var217')

for (var in vars) {
  aucs <- rep(0,100)
  for (rep in 1:length(aucs)) {
    useForCalRep <- rbinom(n=nrow(dTrainAll), size=1, prob=0.1) > 0
    predRep <- mkPredC(dTrainAll[!useForCalRep, outcome],
                       dTrainAll[!useForCalRep, var],
                       dTrainAll[useForCalRep, var])
    aucs[rep] <- calcAUC(predRep, dTrainAll[useForCalRep, outcome])
  }
  print(sprintf("%s: mean: %4.3f; sd: %4.3f", var, mean(aucs), sd(aucs)))
}
## [1] "Var200: mean: 0.549; sd: 0.014"
## [1] "Var217: mean: 0.554; sd: 0.014"
```

Messages from the cross-validation

The 100-fold repeated estimates of the AUC give a mean of 0.549 for `Var200` and 0.554 for `Var217`, each has standard deviation: 0.014.

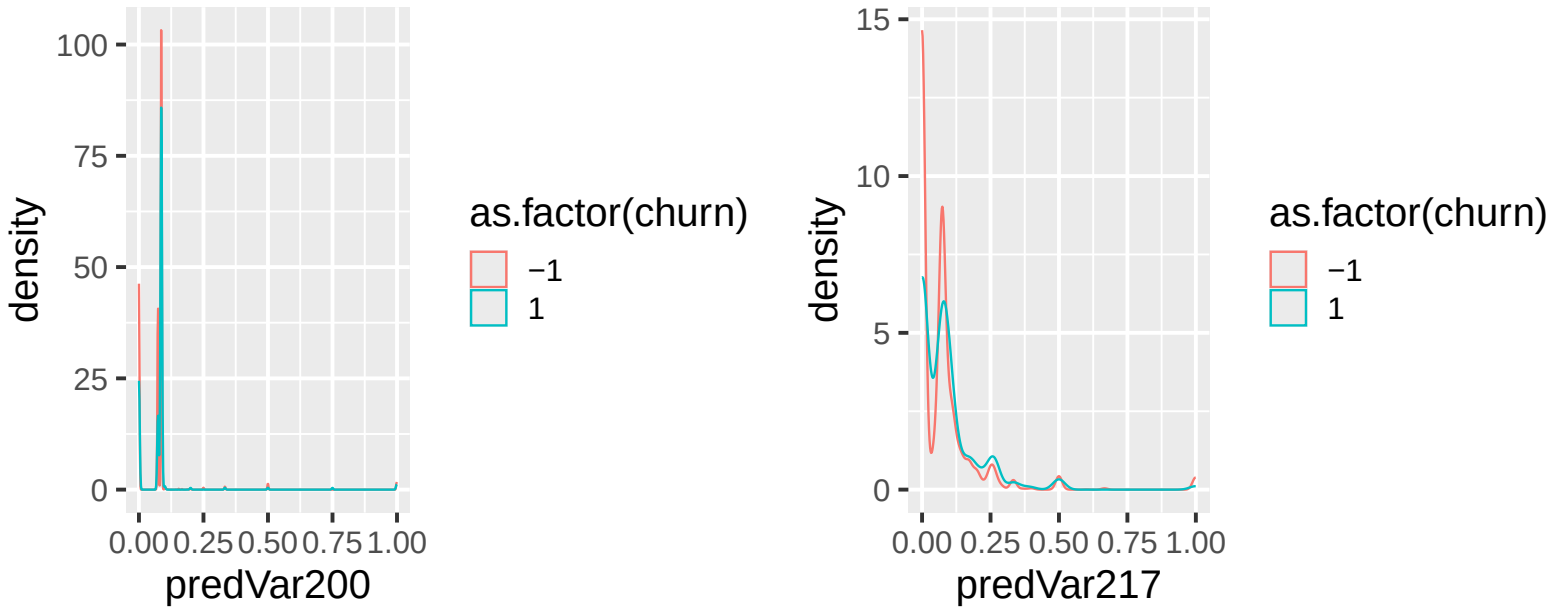
- So the original AUC estimate of 0.565 for `Var200` was a bit high, but our original AUC estimate of 0.553 for `Var217` was very good.
- In some modelling circumstances, training set estimations are good enough (linear regression is often such an example).
- In many other circumstances, estimations from a single calibration set are good enough.
- In extreme cases (such as fitting models with very many variables or level values), you're well advised to use replicated cross-validation estimates of variable utilities and model fits.
- It's critical to automate the modelling steps so that we can perform cross-validation studies.

Double density plot – useful for inspecting the predicted probabilities

```
str(factor(dTrain[,"Var200"]))
##  Factor w/ 13442 levels "_84etK_","_9bTOWp",..: NA NA 11937 NA 401 NA 13079 2702 2449 11820 ...
```

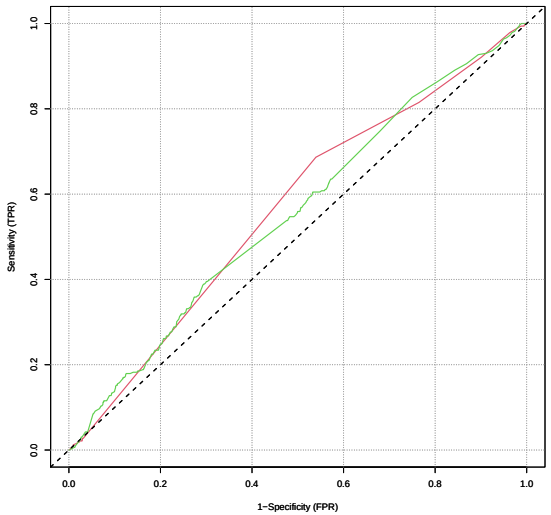
```
str(factor(dTrain[,"Var217"]))
##  Factor w/ 12481 levels "__VZ","_00E",..: 9492 NA 2784 4033 5109 2115 NA 2645 10407 11871 ...
```

```
fig1 <- ggplot(dCal) + geom_density(aes(x=predVar200, color=as.factor(churn)))
fig2 <- ggplot(dCal) + geom_density(aes(x=predVar217, color=as.factor(churn)))
grid.arrange(fig1, fig2, ncol=2)
```



Plotting the ROC curve

```
library(ROCit)
# colour_id 1-7 are: black,red,green,blue,cyan,purple,gold
plot_roc <- function(predcol, outcol, colour_id=2, overlaid=F) {
    ROCit_obj <- rocit(score=predcol, class=outcol==pos)
    par(new=overlaid)
    plot(ROCit_obj, col = c(colour_id, 1),
       legend = FALSE, YIndex = FALSE, values = FALSE)
}
plot_roc(dCal$predVar200, dCal[,outcome])  #red
plot_roc(dCal$predVar217, dCal[,outcome], colour_id=3, overlaid=T) # green
```



Interpret and choose the best single variable model

As expected, each variable's training AUC is inflated compared to its calibration AUC.

- This is because many of these variables have thousands of levels.
  - For example, `length(unique(dTrain$Var217))` is $12,434$
- A good trick to work around this is to sort the variables by their AUC score on the calibration set (not seen during training), which is a better estimate of the variable's true utility.
- In our case, the most promising variable is variable 206, which has both training and calibration AUCs of 0.59.
- The winning KDD entry, which was a model that combined evidence from multiple features, had a much larger AUC of 0.76.

References

- **Practical Data Science with R**, *Nina Zumel, John Mount*, Manning, 2nd Ed., 2020 (Section 8.1-8.2)
- See https://github.com/WinVector/PDSwR2 and e https://github.com/WinVector/PDSwR2/raw/master/CodeExamples.zip for all the datasets and code provided by the authors Zumel et al for the book above.

Single Variable Classification – Numerical

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Discretisation: Binning numeric into categorical

- Bin the numeric feature into a number of ranges and then use the range labels as a new categorical variable.
- R can do this quickly with its `quantile()` and `cut()` commands,
- Let's look at how `quantile()` and `cut()` work on two example numeric columns.

```
(q1 <- quantile(dTrain[,"Var1"], probs=seq(0, 1, 0.1), na.rm=T))
##   0%  10%  20%  30%  40%  50%  60%  70%  80%  90% 100%
##    0    0    0    0    0    0    8    8   16   24  680
```

```
(q6 <- quantile(dTrain[,"Var6"], probs=seq(0, 1, 0.1), na.rm=T))
##     0%    10%    20%    30%    40%    50%    60%    70%    80%    90%   100%
##      0    161    406    623    763    861   1008   1260   1659   2520 114079
```

```
# dis.Var1 and dis.Var6 are the discretised version of dTrain[,"Var1"] and dTrain[,"Var6"]
dis.Var1 <- cut(dTrain[,"Var1"], unique(q1))
dis.Var6 <- cut(dTrain[,"Var6"], unique(q6))

# inspect the number of levels
dis.Var1["Levels"]
## [1] <NA>
## Levels: (0,8] (8,16] (16,24] (24,680]
```

```
dis.Var6["Levels"]
## [1] <NA>
## 10 Levels: (0,161] (161,406] (406,623] (623,763] (763,861] (861,1.01e+03] (1.01e+03,1.26e+03] ... (2.52e+03,1
```

Discretisation: Binning numeric into categorical (cont.)

- Put all these operations into a function.

```
mkPredN <- function(outCol, varCol, appCol) {
  # compute the cuts
  cuts <- unique(
    quantile(varCol, probs=seq(0, 1, 0.1), na.rm=T))
  # discretize the numerical columns
  varC <- cut(varCol,cuts)
  appC <- cut(appCol,cuts)

  mkPredC(outCol,varC,appC)
}
```

Processing all numerical variables

```
for(v in numericVars) {
  pi <- paste('pred', v, sep='')
  dTrain[,pi] <- mkPredN(dTrain[,outcome], dTrain[,v], dTrain[,v])
  dCal[,pi] <- mkPredN(dTrain[,outcome], dTrain[,v], dCal[,v])
  dTest[,pi] <- mkPredN(dTrain[,outcome], dTrain[,v], dTest[,v])
  aucTrain <- calcAUC(dTrain[,pi], dTrain[,outcome])

  if(aucTrain >= 0.55) {
    aucCal <- calcAUC(dCal[,pi], dCal[,outcome])
    print(sprintf(
      "%s: trainAUC: %4.3f; calibrationAUC: %4.3f",
      pi, aucTrain, aucCal))
  }
}
## [1] "predVar6: trainAUC: 0.557; calibrationAUC: 0.554"
## [1] "predVar7: trainAUC: 0.555; calibrationAUC: 0.565"
## [1] "predVar13: trainAUC: 0.568; calibrationAUC: 0.553"
## [1] "predVar73: trainAUC: 0.608; calibrationAUC: 0.616"
## [1] "predVar74: trainAUC: 0.574; calibrationAUC: 0.566"
## [1] "predVar81: trainAUC: 0.558; calibrationAUC: 0.542"
```

100-fold cross-validation

Let's inspect the AUC values of two example numerical columns a bit more.

```
vars <- c('Var7', 'Var13', 'Var73')

for (var in vars) {
  aucs <- rep(0,100)
  for (rep in 1:length(aucs)) {
    useForCalRep <- rbinom(n=nrow(dTrainAll), size=1, prob=0.1) > 0
    predRep <- mkPredN(dTrainAll[!useForCalRep, outcome],
                       dTrainAll[!useForCalRep, var],
                       dTrainAll[useForCalRep, var])
    aucs[rep] <- calcAUC(predRep, dTrainAll[useForCalRep, outcome])
  }
  print(sprintf("%s: mean: %4.3f; sd: %4.3f", var, mean(aucs), sd(aucs)))
}
## [1] "Var7: mean: 0.555; sd: 0.015"
## [1] "Var13: mean: 0.563; sd: 0.016"
## [1] "Var73: mean: 0.605; sd: 0.015"
```

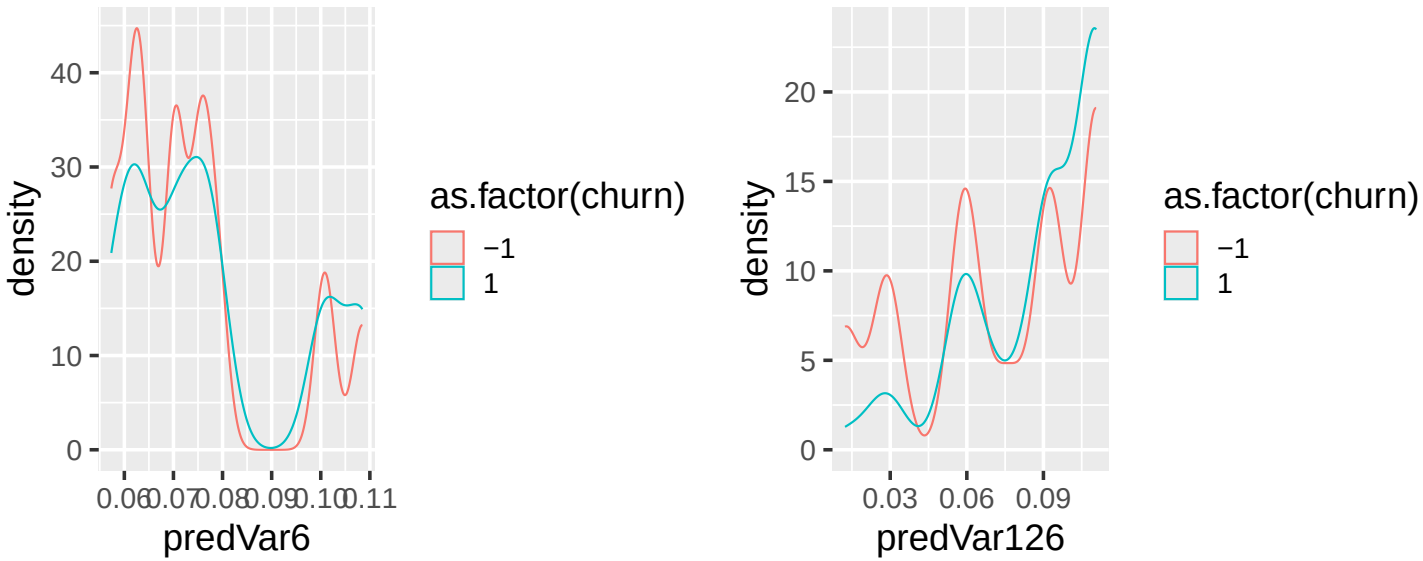
Messages from the cross-validation

- On slide 4/11, the predictions using `Var7` and `Var73` have slightly higher calibrationAUC values than the trainAUC values.
- The 100-fold repeated estimates of the AUC show that that happened simply by chance, as on slide 5/11, all the `calibrationAUC` values are slightly lower than the `trainAUC` values on slide 4/11.

Double density plot – useful for inspecting the predicted probabilities

```
calcAUC(dTrain[,"predVar126"], dTrain[,outcome]); calcAUC(dCal[,"predVar126"], dCal[,outcome])
## [1] 0.6349584
## [1] 0.6288453
```

```
fig1 <- ggplot(dCal) + geom_density(aes(x=predVar6, color=as.factor(churn)))
fig2 <- ggplot(dCal) + geom_density(aes(x=predVar126, color=as.factor(churn)))
grid.arrange(fig1, fig2, ncol=2)
```

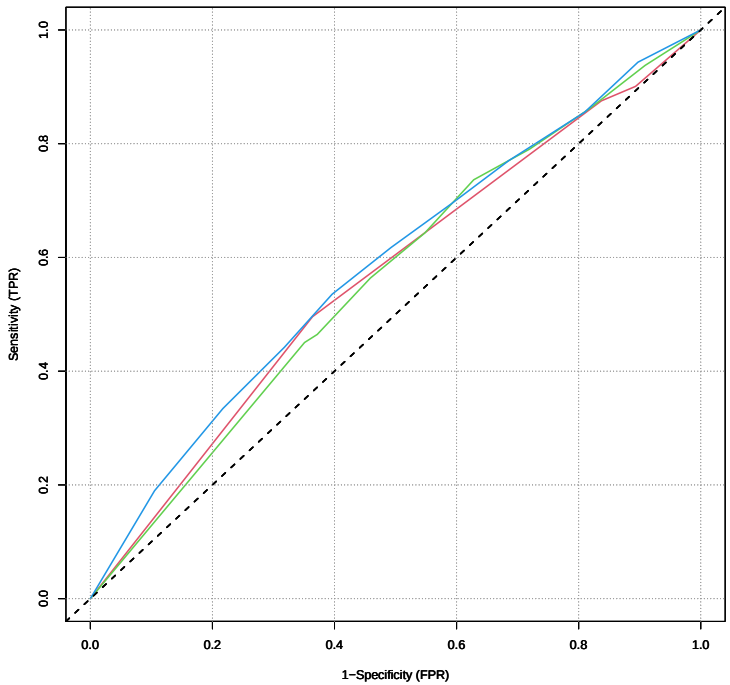


We can deduce that churning (i.e., `churn=1`) is unlikely when the value of `predVar126` is low (the graph is read by comparing the areas under the curves).

Comparing the ROC curves for the test set

```
# call calcAUC() to calculate the AUC of each variable (code omitted)
cat("Var7's AUC:", auc.predVar7, "; Var13's AUC:", auc.predVar13, "; Var73's AUC:",
## Var7's AUC: 0.5658961 ; Var13's AUC: 0.5636032 ; Var73's AUC: 0.5854976
```

```
plot_roc(dTest$predVar7, dTest[,outcome]) #red
plot_roc(dTest$predVar13, dTest[,outcome], colour_id=3, overlaid=T) #green
plot_roc(dTest$predVar73, dTest[,outcome], colour_id=4, overlaid=T) #blue
```



How about the Null model?

```
(Npos <- sum(dTrain[,outcome] == 1))
## [1] 2990
```

```
pred.Null <- Npos / nrow(dTrain)
cat("Proportion of outcome == 1 in dTrain:", pred.Null)
## Proportion of outcome == 1 in dTrain: 0.07379436
```

We have a classification task where `churn` takes on the value `1` or `−1`. The simplest Null model is to always output `pred.Null` as the predicted probability. How does this model perform on the calibration set?

```
TP <- 0; TN <- sum(dCal[,outcome] == -1); # using threshold 0.5
FP <- 0; FN <- sum(dCal[,outcome] == 1);  # using threshold 0.5
cat("nrow(dCal):", nrow(dCal), "TP:", TP, "TN:", TN, "FP:", FP, "FN:", FN)
## nrow(dCal): 4510 TP: 0 TN: 4181 FP: 0 FN: 329
```

```
(accuracy <- (TP + TN) / nrow(dCal))
## [1] 0.927051
```

```
(precision <- TP/(TP + FP))
## [1] NaN
```

```
(recall <- TP/(TP + FN))
## [1] 0
```

```
pred.Null <- rep(pred.Null, nrow(dCal))
```

Take home messages

- How to deal with categorical variables
- How to deal with numerical variables
- Single Variable Models
- How to select models based on AUC values

References

- **Practical Data Science with R**, *Nina Zumel, John Mount*, Manning, 2nd Ed., 2020 (Sections 8.1-8.2)
- **Decision Tree Algorithm:** https://medium.com/deep-math-machine-learning-ai/chapter-4-decision-trees-algorithms-b93975f7a1f1
- **Best Machine Learning Packages in R:** https://www.r-bloggers.com/what-are-the-best-machine-learning-packages-in-r/