Homework11

Jun Rao

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Segmentation model selection and evaluation

The goals of this homework are to explore how a subtrain/validation split can be used to select the segmentation model size parameter. compare segmentation models in terms of label error rates and ROC curves

```
library(ggplot2)
library(data.table)
data(neuroblastoma, package="neuroblastoma")
```

1.For data sequence profile.id=79, chromosome=2 in the neuroblastoma data, assign observations to 50% subtrain 50% validation sets. How many observations are in each set? Hint: use table(set)

```
pro.dt <- data.table(neuroblastoma$profiles)[profile.id=="79" & chromosome=="
2"]
pro.dt[, set := rep(rep(c("subtrain","validation"), each=2), l=.N)]
pro.dt[, index := 1:.N]

subtrain.dt <- pro.dt[set=="subtrain"]
validation.dt <- pro.dt[set== "validation"]

str(subtrain.dt)
```

```
## Classes 'data.table' and 'data.frame':   98 obs. of  6 variables:
##  $ profile.id: Factor w/ 575 levels "1","2","4","5",..: 76 76 76 76 76 76
76 76 76 76 ...
##  $ chromosome: Factor w/ 24 levels "1","2","3","4",..: 2 2 2 2 2 2 2 2 2 2
 ...
##  $ position  : int  18094 2063049 8107742 8179390 11607188 11885382 156479
03 15998838 17554158 18160714 ...
##  $ logratio  : num  0.2 0.506 0.474 0.43 0.455 ...
##  $ set       : chr  "subtrain" "subtrain" "subtrain" "subtrain" ...
##  $ index     : int  1 2 5 6 9 10 13 14 17 18 ...
##  - attr(*, ".internal.selfref")=<externalptr>
```

We total have 196 observations.

In our set, each set have 98 observations, because I use each = 2 at here. It will equally split the original data.

2.Use binsegRcpp::binseg_normal to compute models from 1 to 10 segments on the subtrain data, then compute one data table with predicted changepoint positions

```
subtrain.binseg.models <- binsegRcpp::binseg_normal(subtrain.dt$logratio, 10)
subtrain.binseg.dt <- coef(subtrain.binseg.models)

subtrain.getPos <- function(subtrain.index){
    orig.index <- subtrain.dt$index[ subtrain.index ]
    pro.dt$position[ orig.index ]
}



subtrain.binseg.dt[, start_in_all_data := subtrain.getPos(subtrain.binseg.dt$
start)]
subtrain.binseg.dt[, end_in_all_data := subtrain.getPos(subtrain.binseg.dt$en
d)]
subtrain.binseg.dt[, type := rep("subtrain", l=.N)]
head(subtrain.binseg.dt)
```

```
##    segments start end       mean start_in_all_data end_in_all_data     typ
e
## 1:        1     1  98 0.14558115             18094       240618997 subtrai
n
## 2:        2     1   8 1.30763500             18094        15998838 subtrai
n
## 3:        2     9  98 0.04228748          17554158       240618997 subtrai
n
## 4:        3     1   6 0.40969361             18094        11885382 subtrai
n
## 5:        3     7   8 4.00145916          15647903        15998838 subtrai
n
## 6:        3     9  98 0.04228748          17554158       240618997 subtrai
n
```

and another data table with segment start/end values (in terms of the full data indices/positions, not just the subtrain set).

```
validation.binseg.models <- binsegRcpp::binseg_normal(validation.dt$logratio,
 10)
validation.binseg.dt <- coef(validation.binseg.models)

validation.getPos <- function(validation.index){
    orig.index <- validation.dt$index[ validation.index ]
    pro.dt$position[orig.index ]
}



validation.binseg.dt[, start_in_all_data := validation.getPos(validation.bins
eg.dt$start)]
validation.binseg.dt[, end_in_all_data := validation.getPos(validation.binseg
```

```
.dt$end)]
validation.binseg.dt[, type := rep("validation", l=.N)]
head(validation.binseg.dt)
```

```
##    segments start end       mean start_in_all_data end_in_all_data       t
ype
## 1:        1     1  98 0.14231781           3098882       242801018 validat
ion
## 2:        2     1   7 1.36618893           3098882        16084178 validat
ion
## 3:        2     8  98 0.04817387          16498022       242801018 validat
ion
## 4:        3     1   5 0.39228628           3098882        12173642 validat
ion
## 5:        3     6   7 3.80094555          15291502        16084178 validat
ion
## 6:        3     8  98 0.04817387          16498022       242801018 validat
ion
```

Plot these models on top of the data (use points with different color/fill for different sets, black=subtrain, red=validation), and use facet_grid(segments ~ .) to draw each model size in a different panel. After how many segments does the model appear to overfit?

```
total.dt <- rbind(subtrain.binseg.dt,validation.binseg.dt)

for(col.name in c("start_in_all_data", "end_in_all_data")){
  col.value <- total.dt[[col.name]]
  set(total.dt, j=paste0(col.name, ".pos"),
  value=pro.dt$position[col.value])
}

total.dt[, end.before := c(NA, end_in_all_data[-.N]), by=.(type, segments) ]
change.dt <- data.table(pro.dt, total.dt[1 < start_in_all_data])
```

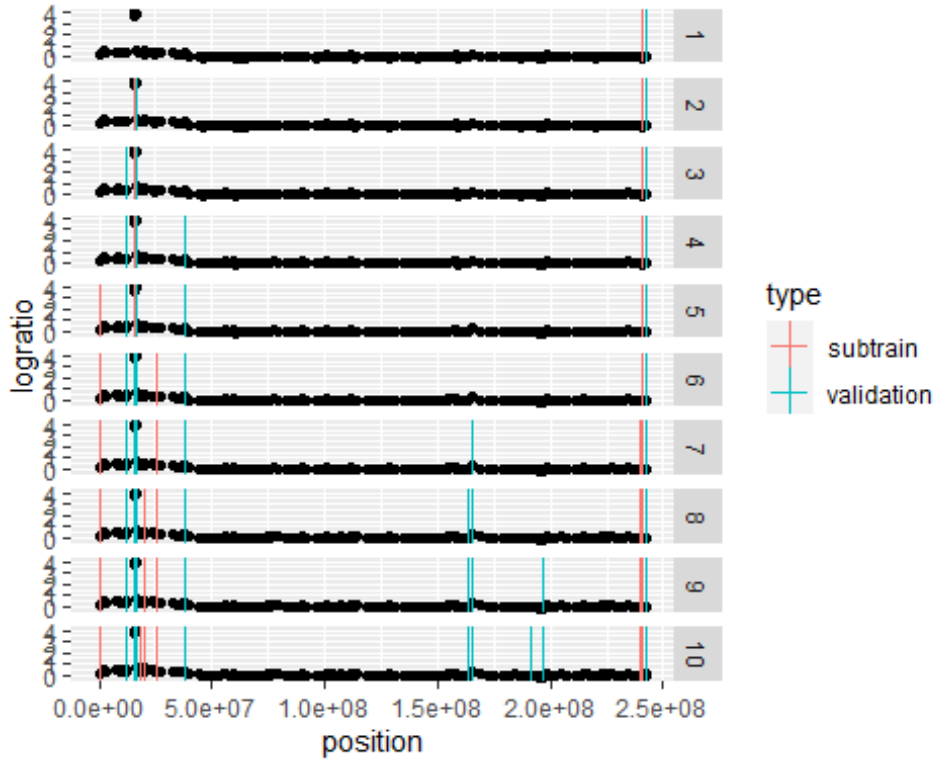
```
## Warning in as.data.table.list(x, keep.rownames = keep.rownames, check.name
s
## = check.names, : Item 2 has 110 rows but longest item has 196; recycled wi
th
## remainder.
```

```
change.dt[, changepoint := (start_in_all_data+end.before)/2]


gg <- ggplot(aes(x=position, y=logratio), data=pro.dt)+geom_point()

(gg+ facet_grid(segments ~ .)+
  geom_segment(aes(
    x=start, y=mean,
    xend=end, yend=mean,
    color=type),
```

```
    data=total.dt) +
  geom_vline(aes(
    xintercept=end_in_all_data,
    color=type),
    data=change.dt)+
  scale_size_manual(values=c(subtrain=2, validation=1))
)
```



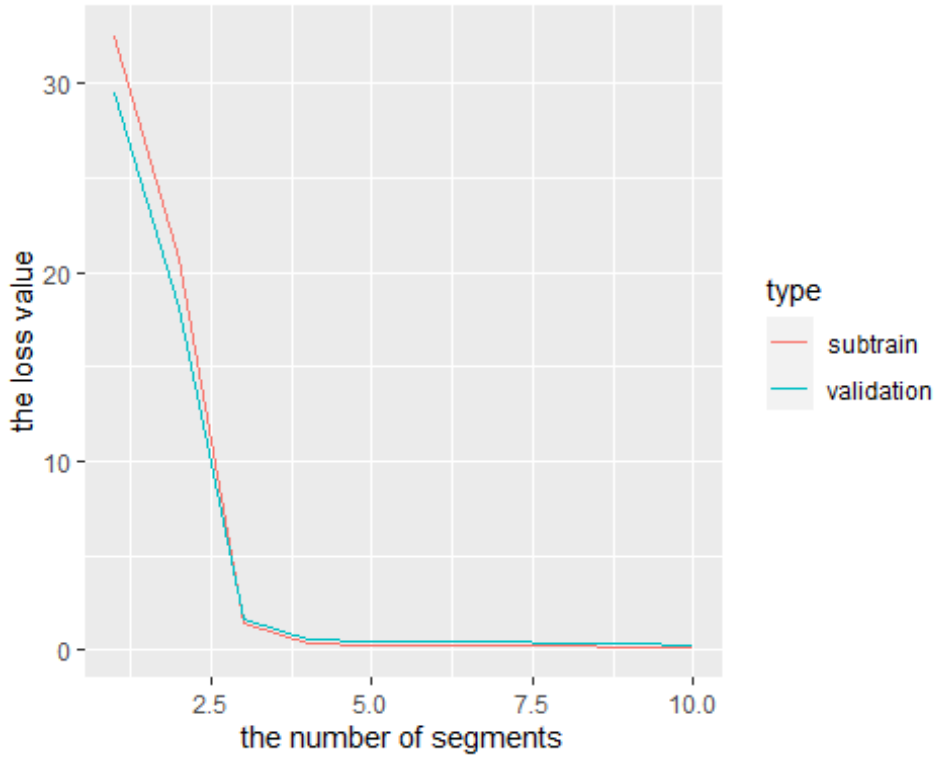
In our result, it looks like after 3 segments, the model appears to overfit

3.Compute the square loss for each model size and set, and store these numbers in a data table with columns segments, set,loss. Plot the loss as a function of the number of segments, with different sets in different colors (black=subtrain, red=validation). Based on the loss values/plot, what is the number of segments you should select?

```
subtrain.loss.dt<- data.table()
validation.loss.dt <- data.table()
subtrain.loss.dt[, loss := subtrain.binseg.models$loss]
subtrain.loss.dt[, segments := subtrain.binseg.models$segments]
subtrain.loss.dt[, type := "subtrain"]
validation.loss.dt[, loss := validation.binseg.models$loss]
validation.loss.dt[, segments := validation.binseg.models$segments]
validation.loss.dt[, type := "validation"]
loss.dt <- rbind(subtrain.loss.dt,validation.loss.dt)


ggplot()+
```

```
  geom_line(aes(
    segments, loss, color=type),
    data=loss.dt)+
  xlab("the number of segments") + ylab("the loss value")
```



Based on the picture, I will choose segments = 3.

4.Compute model selection criteria = loss + penalty*segments, for penalty=2 (AIC) and penalty=log(N.data) (BIC). Save these numbers in a single data table with columns segments, crit.name(AIC/BIC), crit.value(numeric value defined in equation above). Then plot them using different colors for different penalties (e.g., AIC=blue, BIC=orange). Do the two criteria select the same number of segments?

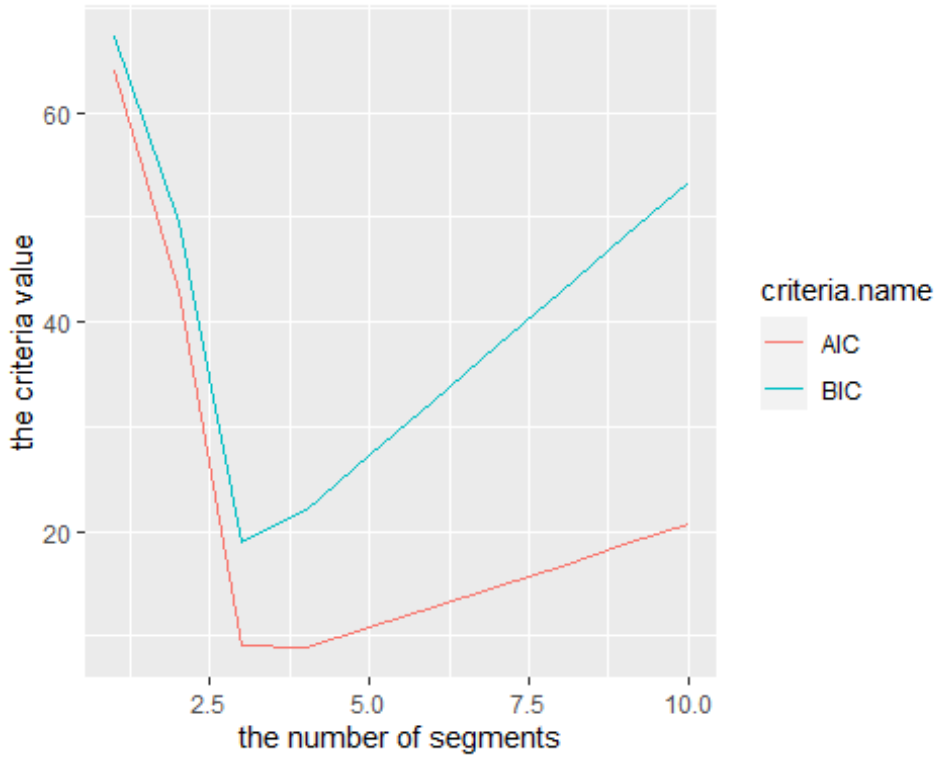
```
binseg.models <- binsegRcpp::binseg_normal(pro.dt$logratio, 10)
AIC.criteria.dt<- data.table()
BIC.criteria.dt <- data.table()

AIC.criteria.dt[, criteria.value := binseg.models$loss + 2 * binseg.models$se
gments]
AIC.criteria.dt[, segments := binseg.models$segments]
AIC.criteria.dt[, criteria.name := "AIC"]

BIC.criteria.dt[, criteria.value := binseg.models$loss + log(length(pro.dt$lo
gratio)) * binseg.models$segments]
BIC.criteria.dt[, segments := binseg.models$segments]
BIC.criteria.dt[, criteria.name := "BIC"]
```

```
criteria.dt <- rbind(AIC.criteria.dt,BIC.criteria.dt)


ggplot()+
  geom_line(aes(
    segments, criteria.value, color=criteria.name),
    data=criteria.dt)+
  xlab("the number of segments") + ylab("the criteria value")
```



Yes. The two criteria select the same number of segments which is 3.

The goal is to run binsegRcpp::binseg_normal on ALL labeled neuroblastoma data sequences, and compare two model selection criteria (AIC/BIC) in terms of label error rates and ROC curves. You should have a for loop over rows of the "annotations" data table, since there is only one label/row per data sequence. For each sequence (unique value of profile.id, chromosome) you should run binary segmentation up to 20 segments. Use penaltyLearning::modelSelection to compute a data table representing the model selection function (which maps penalty values to model sizes).

```
AIC.loss.dt.list <- list()
BIC.loss.dt.list <- list()
change.dt.list <- list()

all.profiles <- data.table(neuroblastoma$profiles)
all.labels <- data.table(neuroblastoma$annotations)
label.i.todo <- 1:nrow(all.labels)
```

```
# label.i.done <- as.integer(unique(sub(" .*", "", names(loss.dt.list))))
# label.i.new <- label.i.todo[! label.i.todo %in% label.i.done]

max.segments <- 10

for (label.i in label.i.todo) {
  # cat(sprintf("label.i=%d\n", label.i))
  one.label <- all.labels[label.i]
  select.dt <- one.label[, .(profile.id, chromosome)]
  pro.dt <- all.profiles[select.dt, on=names(select.dt)]


  this.max <- if(nrow(pro.dt) < max.segments){
    nrow(pro.dt)
  }else{
    max.segments
  }

  binseg.models <- binsegRcpp::binseg_normal(pro.dt$logratio,  this.max)

  segs.dt.list <- list()

  for (n.segs in 1:this.max) {
    end <- binseg.models$end[1:n.segs]
    start <- c(1, end[-length(end)]+1)
    segs.dt.list[[paste(n.segs)]] <- data.table(start, end)[, .(
      segments=n.segs,
      mean=mean(pro.dt$logratio[start:end]),
      algorithm="DP"
    ), by=.(start, end)]
  }

  segs.dt <- do.call(rbind, segs.dt.list)

  for(col.name in c("start", "end")){
    col.value <- segs.dt[[col.name]]
    set(segs.dt, j=paste0(col.name, ".pos"),
        value=pro.dt$position[col.value])
  }

  segs.dt[, end.before := c(NA, end.pos[-.N]), by=.(segments) ]
  change.dt <- data.table(select.dt, segs.dt[1 < start])
  change.dt[, changepoint := (start.pos+end.before)/2]
  AIC.this.loss.dt <- data.table(
    segments=1:this.max,
    loss=binseg.models$loss)

  BIC.this.loss.dt <- data.table(
```

```
    segments=1:this.max,
    loss=binseg.models$loss)

  penalty <- 0.12
  AIC.this.loss.dt[, crit.value := loss + penalty*segments]
  BIC.this.loss.dt[, crit.value := loss + log10(length(pro.dt$logratio))*segm
ents]
  AIC.this.loss.dt[, criteria.name := "AIC"]
  BIC.this.loss.dt[, criteria.name := "BIC"]
  AIC.loss.dt.list[[paste(label.i)]] <- data.table(
    select.dt, AIC.this.loss.dt)
  change.dt.list[[paste(label.i)]] <- change.dt[, data.table(
    select.dt, changepoint, segments)]


  BIC.loss.dt.list[[paste(label.i)]] <- data.table(
    select.dt, BIC.this.loss.dt)
  change.dt.list[[paste(label.i)]] <- change.dt[, data.table(
    select.dt, changepoint, segments)]

}

change.dt <- do.call(rbind, change.dt.list)
AIC.loss.dt <- do.call(rbind, AIC.loss.dt.list)
BIC.loss.dt <- do.call(rbind, BIC.loss.dt.list)



## Compute model selection function, which maps penalty (lambda)
## values to model complexity (segments) values.
AIC.all.model.selection <- AIC.loss.dt[, penaltyLearning::modelSelection(
  .SD, "loss", "segments"),
  by=.(profile.id, chromosome)]
pred.penalty.dt <- AIC.loss.dt[, data.table(
  pred.log.lambda=log(10)
), by=.(profile.id, chromosome)]



## Compute label error, fp/fn for each selected model.
AIC.error.list <- penaltyLearning::labelError(
  models=AIC.all.model.selection,
  labels=all.labels[label.i.todo],
  changes=change.dt,
  problem.vars=c("profile.id", "chromosome"),
  change.var="changepoint",
  model.vars="segments")
AIC.error.list$label.errors[, .(
  profile.id, chromosome, min.lambda, max.lambda, segments, fp, fn)]
```

```
##        profile.id chromosome min.lambda max.lambda segments fp fn
##     1:          1          1 0.00000000 0.10981858       10  1  0
##     2:          1          1 0.10981858 0.14642178        7  1  0
##     3:          1          1 0.14642178 0.27946950        5  1  0
##     4:          1          1 0.27946950 1.23652855        4  0  0
##     5:          1          1 1.23652855 1.83184494        3  0  0
##    ---
## 20062:        603         17 0.06763515 0.07307963        7  0  0
## 20063:        603         17 0.07307963 0.11831418        6  0  0
## 20064:        603         17 0.11831418 0.17108867        5  0  0
## 20065:        603         17 0.17108867 2.10773718        2  0  1
## 20066:        603         17 2.10773718        Inf        1  0  1
```

```
## Compute ROC curve, FPR/TPR for every prediction threshold (default
## prediction threshold is zero).
AIC.roc.list <- penaltyLearning::ROChange(
  AIC.error.list$model.errors,
  pred.penalty.dt,
  problem.vars=c("profile.id", "chromosome"))

AIC.roc.list$roc[, .(min.thresh, max.thresh, FPR, TPR, errors)]
```

```
##       min.thresh max.thresh       FPR         TPR errors
##    1:       -Inf  -7.526805 0.9785589 1.000000000   2784
##    2:  -7.526805  -7.475998 0.9782074 1.000000000   2783
##    3:  -7.475998  -7.366749 0.9778559 1.000000000   2782
##    4:  -7.366749  -7.362607 0.9775044 1.000000000   2781
##    5:  -7.362607  -7.337930 0.9771529 1.000000000   2780
##   ---
## 3321:   1.943780   2.099433 0.0000000 0.006980803    569
## 3322:   2.099433   2.121908 0.0000000 0.005235602    570
## 3323:   2.121908   2.338209 0.0000000 0.003490401    571
## 3324:   2.338209   2.491455 0.0000000 0.001745201    572
## 3325:   2.491455        Inf 0.0000000 0.000000000    573
```

```
## Compute model selection function, which maps penalty (lambda)
## values to model complexity (segments) values.
BIC.all.model.selection <- BIC.loss.dt[, penaltyLearning::modelSelection(
  .SD, "loss", "segments"),
  by=.(profile.id, chromosome)]
pred.penalty.dt <- BIC.loss.dt[, data.table(
  pred.log.lambda=log(10)
), by=.(profile.id, chromosome)]



## Compute label error, fp/fn for each selected model.
BIC.error.list <- penaltyLearning::labelError(
  models=BIC.all.model.selection,
  labels=all.labels[label.i.todo],
```

```
  changes=change.dt,
  problem.vars=c("profile.id", "chromosome"),
  change.var="changepoint",
  model.vars="segments")
BIC.error.list$model.errors[, .(
  profile.id, chromosome, min.lambda, max.lambda, segments, fp, fn)]
```

```
##        profile.id chromosome min.lambda max.lambda segments fp fn
##     1:          1          1 0.00000000 0.10981858       10  1  0
##     2:          1          1 0.10981858 0.14642178        7  1  0
##     3:          1          1 0.14642178 0.27946950        5  1  0
##     4:          1          1 0.27946950 1.23652855        4  0  0
##     5:          1          1 1.23652855 1.83184494        3  0  0
##    ---
## 20062:        603         17 0.06763515 0.07307963        7  0  0
## 20063:        603         17 0.07307963 0.11831418        6  0  0
## 20064:        603         17 0.11831418 0.17108867        5  0  0
## 20065:        603         17 0.17108867 2.10773718        2  0  1
## 20066:        603         17 2.10773718        Inf        1  0  1
```

```
## Compute ROC curve, FPR/TPR for every prediction threshold (default
## prediction threshold is zero).
BIC.roc.list <- penaltyLearning::ROChange(
  BIC.error.list$model.errors,
  pred.penalty.dt,
  problem.vars=c("profile.id", "chromosome"))
BIC.roc.list$roc[, .(min.thresh, max.thresh, FPR, TPR, errors)]
```

```
##       min.thresh max.thresh       FPR         TPR errors
##    1:       -Inf  -7.526805 0.9785589 1.000000000   2784
##    2:  -7.526805  -7.475998 0.9782074 1.000000000   2783
##    3:  -7.475998  -7.366749 0.9778559 1.000000000   2782
##    4:  -7.366749  -7.362607 0.9775044 1.000000000   2781
##    5:  -7.362607  -7.337930 0.9771529 1.000000000   2780
##   ---
## 3321:   1.943780   2.099433 0.0000000 0.006980803    569
## 3322:   2.099433   2.121908 0.0000000 0.005235602    570
## 3323:   2.121908   2.338209 0.0000000 0.003490401    571
## 3324:   2.338209   2.491455 0.0000000 0.001745201    572
## 3325:   2.491455        Inf 0.0000000 0.000000000    573
```

Then use the model selection data table as input to penaltyLearning::labelError, which computes the number of incorrectly predicted labels as a function of the penalty/lambda. Also compute a data table of predicted penalty values for AIC/BIC with two rows and columns sequenceID,crit.name,pred.log.lambda. Hint: for reference/example see http://members.cbio.mines-paristech.fr/~thocking/change-tutorial/Supervised.html

```
head(BIC.error.list$label.errors)
```

```
##    profile.id chromosome segments min       max pred.changes min.lambda
## 1:          1          1       10   0 125000000            4  0.0000000
```

```
## 2:          1          1        7   0 125000000            3  0.1098186
## 3:          1          1        5   0 125000000            1  0.1464218
## 4:          1          1        4   0 125000000            0  0.2794695
## 5:          1          1        3   0 125000000            0  1.2365286
## 6:          1          1        2   0 125000000            0  1.8318449
##    max.lambda min.log.lambda max.log.lambda cum.iterations     loss crit.v
alue
## 1:  0.1098186           -Inf     -2.2089256             12 3.434715   30.1
9250
## 2:  0.1464218     -2.2089256     -1.9212639              7 3.764170   22.4
9462
## 3:  0.2794695     -1.9212639     -1.2748621              4 4.057014   17.4
3591
## 4:  1.2365286     -1.2748621      0.2123079              3 4.336483   15.0
3960
## 5:  1.8318449      0.2123079      0.6053236              2 5.573012   13.6
0035
## 6:  8.5101305      0.6053236      2.1412573              1 7.404857   12.7
5641
##    criteria.name annotation min.changes max.changes   color possible.fn
## 1:           BIC     normal           0           0 #f6f4bf           0
## 2:           BIC     normal           0           0 #f6f4bf           0
## 3:           BIC     normal           0           0 #f6f4bf           0
## 4:           BIC     normal           0           0 #f6f4bf           0
## 5:           BIC     normal           0           0 #f6f4bf           0
## 6:           BIC     normal           0           0 #f6f4bf           0
##    possible.fp weight fp fn         status
## 1:           1      1  1  0 false positive
## 2:           1      1  1  0 false positive
## 3:           1      1  1  0 false positive
## 4:           1      1  0  0        correct
## 5:           1      1  0  0        correct
## 6:           1      1  0  0        correct
```

```
head(AIC.error.list$label.errors)
```

```
##    profile.id chromosome segments min       max pred.changes min.lambda
## 1:          1          1       10   0 125000000            4  0.0000000
## 2:          1          1        7   0 125000000            3  0.1098186
## 3:          1          1        5   0 125000000            1  0.1464218
## 4:          1          1        4   0 125000000            0  0.2794695
## 5:          1          1        3   0 125000000            0  1.2365286
## 6:          1          1        2   0 125000000            0  1.8318449
##    max.lambda min.log.lambda max.log.lambda cum.iterations     loss crit.v
alue
## 1:  0.1098186           -Inf     -2.2089256             12 3.434715   4.63
4715
## 2:  0.1464218     -2.2089256     -1.9212639              7 3.764170   4.60
4170
## 3:  0.2794695     -1.9212639     -1.2748621              4 4.057014   4.65
```

```
7014
## 4:  1.2365286     -1.2748621      0.2123079             3 4.336483   4.81
6483
## 5:  1.8318449      0.2123079      0.6053236             2 5.573012   5.93
3012
## 6:  8.5101305      0.6053236      2.1412573             1 7.404857   7.64
4857
##    criteria.name annotation min.changes max.changes   color possible.fn
## 1:           AIC     normal           0           0 #f6f4bf           0
## 2:           AIC     normal           0           0 #f6f4bf           0
## 3:           AIC     normal           0           0 #f6f4bf           0
## 4:           AIC     normal           0           0 #f6f4bf           0
## 5:           AIC     normal           0           0 #f6f4bf           0
## 6:           AIC     normal           0           0 #f6f4bf           0
##    possible.fp weight fp fn         status
## 1:           1      1  1  0 false positive
## 2:           1      1  1  0 false positive
## 3:           1      1  1  0 false positive
## 4:           1      1  0  0        correct
## 5:           1      1  0  0        correct
## 6:           1      1  0  0        correct
```

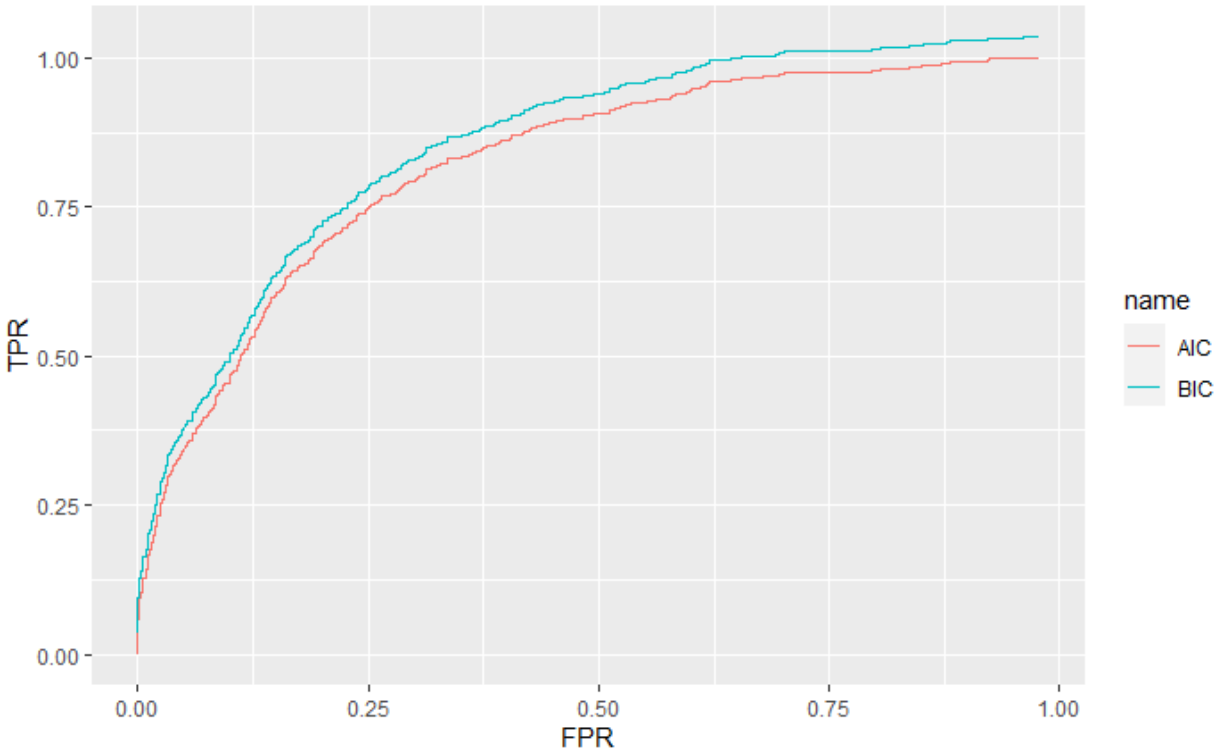
Also inspect the thresholds element of the ROChange result in order to see the number of label errors per model. Which model has a smaller number of predicted label errors?

```
AIC.list.dt <- data.table()
AIC.list.dt[, FPR := AIC.roc.list$roc$FPR]
AIC.list.dt[, TPR := AIC.roc.list$roc$TPR]
AIC.list.dt[, name := 'AIC']
BIC.list.dt <- data.table()
BIC.list.dt[, FPR := BIC.roc.list$roc$FPR]
BIC.list.dt[, TPR := BIC.roc.list$roc$TPR]
BIC.list.dt[, name := 'BIC']

roc.list.dt <- data.table()


roc.list.dt <- rbind(AIC.list.dt,BIC.list.dt)


ggplot()+
  geom_path(aes(
    FPR, TPR, color=name),
    data=roc.list.dt)
```



Based on the result, BIC model has a larger area under the curve

Based on the result, AIC model has a smaller number of predicted label errors