Homework 3: Combinatorial & EM

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Question 3.1

Implement a random starts local search algorithm for minimizing the AIC for the baseball salary regression problem. Model your algorithm after Example 3.3.

• (a) Change the move strategy from steepest descent to immediate adoption of the first randomly selected downhill neighbor.

Code 1 Below is a snippet of code for finding k-Neighborhoods of a solution.

```
k Neighborhood <- function(sol, p, k=1) {</pre>
 1
 2
         # index of positions in solution
        positions <- 1:p
 3
         # candidates for the positions of changes
 4
 5
         candidates <- combn(positions, k)</pre>
         # init neighbors with padding zeros
 6
         neighbors <- matrix(0, ncol=p, nrow=ncol(candidates))</pre>
 7
         for (i in 1:ncol(candidates)){
 8
 9
           # init neighbor with the starting point
           neighbor <- c(sol)</pre>
1.0
11
           for (ind in candidates[,i]){
             # turn it to 1 if the change position is not in solution
13
             if (ind %in% sol){
14
               neighbor <- setdiff(neighbor, ind)</pre>
15
             }
16
             # turn it to 0 if the change position is in solution
17
18
               neighbor <- c(neighbor, ind)</pre>
19
             }
           }
21
           # do zero paddings for neighbor
22
           neighbors[i,] <- c(neighbor, rep(0, p - length(neighbor)))</pre>
23
         }
         return(neighbors)
24
25
```

```
1
      localSearchForLR <- function(</pre>
 2
          sol, x=baseballData[,2:28], y=baseballData[,1], k=1, n=1000){
 3
        # Start the clock!
 4
        ptm <- proc.time()</pre>
 5
        p < - ncol(x)
                                 # number of variables
 6
 7
        x$y <- y
                                  # add y to data
 8
               <- x[,sol]
                                       # init x data according to init solution
 9
                <- lm(y ~ ., data=X) # build linear regression model on
    filtered data
10
        lastRes <- AIC(lr) # calculate AIC for lr model</pre>
11
12
        iters <- c() # init iteration results of all AIC history
13
        for (j in 1:n){
          # get neighborhoods for the current solution
14
15
          neighbors <- k Neighborhood(sol, p, k=k)</pre>
16
17
          # Rule 1: Search all neighborhood
18
          # calculate lr for every neighborhood of current solution
19
          res <- c() # init results of AIC
20
          for (i in 1:nrow(neighbors)){
             neighbor <- neighbors[i,]</pre>
21
22
             neighbor <- neighbor[neighbor != 0] # k-neighborhood solution</pre>
23
             neighborX <- x[,neighbor]</pre>
24
            neighborX$y <- y</pre>
             lr <- lm(y ~ ., data=neighborX) # build linear regression model</pre>
25
26
            res <- c(res, AIC(lr))
                                                 # calculate AIC for lr model
27
          }
28
          # find better neighborhood in accordance with its AIC result
29
          minInd <- which.min(res)</pre>
          minRes <- res[minInd]</pre>
30
          sol <- neighbors[minInd,]</pre>
31
32
          sol
                 <- sol[sol != 0]
          # Stopping criterion
33
          if (minRes >= lastRes){
34
35
            # Stop the clock
36
            dt <- proc.time() - ptm</pre>
             result <- list("solution" = lastSol,
37
                                        = dt,
38
                            "time"
                            "iterations" = iters)
39
40
            return(result)
41
          }
42
43
          # Logging trace history of solutions
```

```
iters <- c(iters, minRes)
lastRes <- minRes
lastSol <- sol

stop("Exceeded allowed number of iterations")
}</pre>
```

Below is the results:

```
(Start from (1,2,3,4))
$solution [1] 3 4 13 14 8 10 27 15 7
$time user system elapsed 0.435 0.017 0.483
$iterations [1] 5486.195 5441.047 5405.131 5389.995 5384.965 5383.118 5381.728 5379.813
5378.474
```

Code 3 Below is a snippet of code for local searching Via immediate adoption of the first randomly selected downhill neighbor.

```
1
      localSearchForLR <- function(</pre>
 2
           sol, x=baseballData[,2:28], y=baseballData[,1], k=1, n=1000){
 3
        # Start the clock!
 4
        ptm <- proc.time()</pre>
 5
                                  # number of variables
 6
        p < - ncol(x)
 7
        x$y <- y
                                  # add y to data
 8
                 <- x[,sol]
                                        # init x data according to init solution
 9
                 <- lm(y ~ ., data=X) # build linear regression model on
    filtered data
10
        lastRes <- AIC(lr)</pre>
                                        # calculate AIC for lr model
11
12
        iters <- c() # init iteration results of all AIC history</pre>
13
        for (j in 1:n){
14
          # get neighborhoods for the current solution
           neighbors <- k_Neighborhood(sol, p, k=k)</pre>
15
16
17
           # Rule 2: Immediate adoption of the first randomly selected downhill
    neighbor
18
           # randomly pick neighborhood of current solution
           counter <- 0
19
20
           for (i in sample(1:nrow(neighbors))){
2.1
             neighbor <- neighbors[i,]</pre>
             neighbor <- neighbor[neighbor != 0] # k-neighborhood solution</pre>
22
             neighborX <- x[,neighbor]</pre>
23
24
             neighborX$y <- y</pre>
```

```
25
             lr <- lm(y ~ ., data=neighborX) # build linear regression model on</pre>
    filtered data
26
             res <- AIC(lr)
                                                  # calculate AIC for lr model
27
             # pick the first downhill neiborhood solution
28
             if (res < lastRes) {</pre>
               minRes <- res
29
30
               sol
                       <- neighbor
31
               break
32
             }
33
             counter <- counter + 1</pre>
34
           }
35
           # stopping criterion
36
           if (counter >= nrow(neighbors)){
37
             # Stop the clock
             dt <- proc.time() - ptm</pre>
             result <- list("solution" = lastSol,</pre>
39
                              "time"
40
                                           = dt,
                              "iterations" = iters)
41
42
             return(result)
43
           }
44
45
           # Logging trace history of solutions
46
           iters <- c(iters, minRes)</pre>
47
           lastRes <- minRes</pre>
           lastSol <- sol</pre>
48
49
         }
50
         stop("Exceeded allowed number of iterations")
51
       }
```

Below is the results:

```
(Start from (1,2,3,4))
$solution [1] 7 10 25 8 13 14 19 9
$time user system elapsed 0.331 0.003 0.358
```

\$iterations [1] 5575.563 5574.578 5562.569 5550.247 5549.765 5549.075 5547.291 5531.017 [9] 5529.764 5525.200 5518.767 5516.779 5515.913 5427.225 5381.288 5380.471 [17] 5378.790 5378.115 5377.333 5375.788 5375.674 5375.553 5375.400 5375.362

- (b) Change the algorithm to employ **2**-neighborhoods, and compare the results with those of previous runs.
 - Steepest descent

\$time user system elapsed 4.514 0.074 4.686 \$iterations [1] 5441.047 5389.995 5381.915 5378.460 5376.452 5375.708 5375.553 5375.362

• Imediate adoption

```
$solution [1] 3 8 13 14 10 16 4 18 12 15 17 25 11 19

$time user system elapsed 1.776 0.041 1.872

$iterations [1] 5559.430 5546.047 5453.730 5447.718 5446.832 5441.939 5441.937

5441.750 [9] 5441.290 5395.620 5393.999 5392.707 5390.283 5387.542 5387.400

5383.245 [17] 5383.071 5382.792 5381.700 5379.678 5379.004 5378.901 5378.856

5378.627 [25] 5376.532 5375.996 5375.850
```

Question 3.8

Thirteen chemical measurements were carried out on each of 178 wines from three regions of Italy. These data are available from the website for this book. Using one or more heuristic search methods from this chapter, partition the wines into three groups for which the total of the withingroup sum of squares is minimal. Comment on your work and the results. This is a search problem of size 3^p where p=178. If you have access to standard cluster analysis routines, check your results using a standard method like that of Hartigan and Wong.

Code 4 Below is a snippet of code for implementing k-means and visualization of the result via t-SNE

```
# Load data
    wineDataPath <- paste(rootPath, "datasets/wine.dat", sep="/")</pre>
 2
    wineData
<- read.table(wineDataPath, header=TRUE)</pre>
 3
   # Using K-Means (Hartigan and Wong) as a benchmark
 5
    set.seed(20)
    wineCluster <- kmeans(wineData[, 2:14], 3, nstart = 20)</pre>
    # Visualize the result via t-SNE
 7
 8
    library(caret)
9
    library(Rtsne)
    colorbar <- c("blue", "yellow", "red")</pre>
10
11
    tsneModel <- Rtsne(</pre>
12
     as.matrix(wineData[, 2:14]),
     check_duplicates=FALSE, pca=TRUE, perplexity=30, theta=0.5, dims=2)
13
14
    tsneEmbeddings
                           <- as.data.frame(tsneModel$Y)</pre>
15
    tsneEmbeddings$cluster <- apply(as.matrix(wineCluster$cluster), 1,
16
                                     function(x) colorbar[x])
17
    # Plot scatterring graph
    ggplot(tsneEmbeddings, aes(x=V1, y=V2, color=cluster)) +
18
19
      geom point(size=2.) +
20
      guides(colour=guide_legend(override.aes=list(size=6))) +
```

```
theme_light(base_size=10) +
theme(axis.text.x=element_blank(),
axis.text.y=element_blank()) +
scale_colour_brewer(palette = "Set2")
```

Below is the output of k-means in R.

K-means clustering with 3 clusters of sizes 51, 65, 62

Cluster means:

x1 x2 x3 x4 x5 x6 x7

1 0.1643137 0.8698039 0.1862745 0.5223529 -0.07333333 -0.97568627 -1.2111765 2 -0.9236923 -0.3927692 -0.4932308 0.1690769 -0.48830769 -0.07476923 0.0200000 3 0.8329032 -0.3030645 0.3637097 -0.6103226 0.57774194 0.88500000 0.9732258

x8 x9 x10 x11 x12 x13

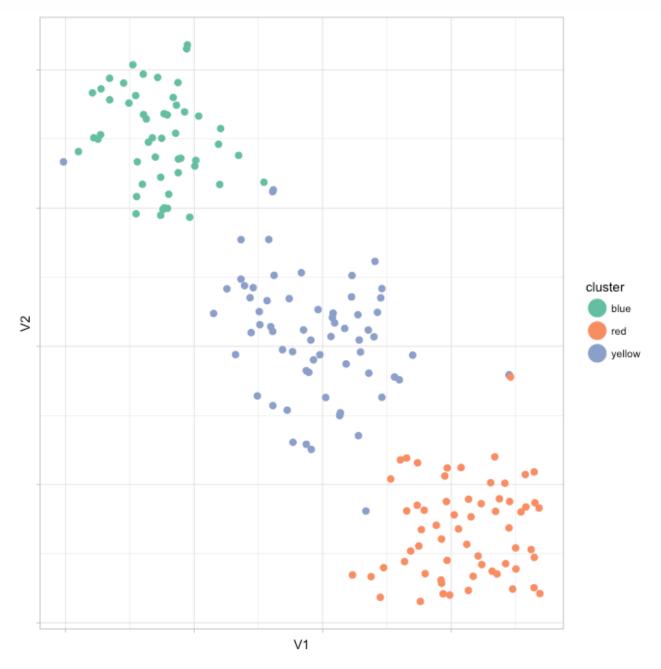
1 0.72372549 -0.77764706 0.9390196 -1.1627451 -1.2886275 -0.4062745 2 -0.03338462 0.05830769 -0.8990769 0.4596923 0.2695385 -0.7515385 3 -0.56177419 0.57822581 0.1703226 0.4717742 0.7772581 1.1214516

Within cluster sum of squares by cluster: [1] 326.4147 558.8050 385.7191 (between_SS / total_SS = 44.8 %)

Available components:

[1] "cluster" "centers" "totss" "withinss" "tot.withinss" [6] "betweenss" "size" "iter" "ifault"

We also visualize the output of k-means by applying t-SNE to project points to a 2-D space.



code 5 define how to calculate cost function

```
# cost = group rss
 2
    groupRSS <- function(data, cluster, K=3) {</pre>
 3
         for (k in 1:K) {
 4
             # get indices of data entries which belongs to a same cluster
 5
             indices <- which(cluster %in% k)</pre>
             # calculate mean value for each of attributes in a specific cluster
 6
 7
                     <- colMeans(data[indices,], dim=1)</pre>
             mean
8
             # get differences between original entries and mean value
9
             data[indices,] <- sweep(data[indices,], 2, mean)</pre>
10
         }
11
        return(sum(data^2))
12
    }
```

code 6 define how to find communicated neighborhoods for current solution

```
# get neighborhood of current solution
 2
    neighborhood <- function(sol){</pre>
 3
        # init neighbors with padding zeros
 4
        neighbors <- matrix(0, ncol=length(sol), nrow=length(sol)*2)</pre>
        # search all neighbors in distance 1.
 5
 6
        j <- 1
 7
        for (i in 1:length(sol)){
 8
             originVal <- sol[i]</pre>
                                                         # original value of
    candidate position
             candVals <- setdiff(c(1,2,3), originVal) # candidate values for</pre>
    this position
10
            for (val in candVals){
                neighbor
                                           # init as original solution
11
                              <- sol
12
                 neighbor[i] <- val # make change at specific position</pre>
                 neighbors[j,] <- neighbor # add this neighbor to matrix</pre>
13
                 j <- j + 1
14
15
             }
16
        }
17
        return(neighbors)
18
```

code 7 below is a snippet of code for Simulated Annealing

```
# Simulated Annealing
simulatedAnnealing <- function(sol, data=wineData[,2:13], n=10000,
step=0.1) {

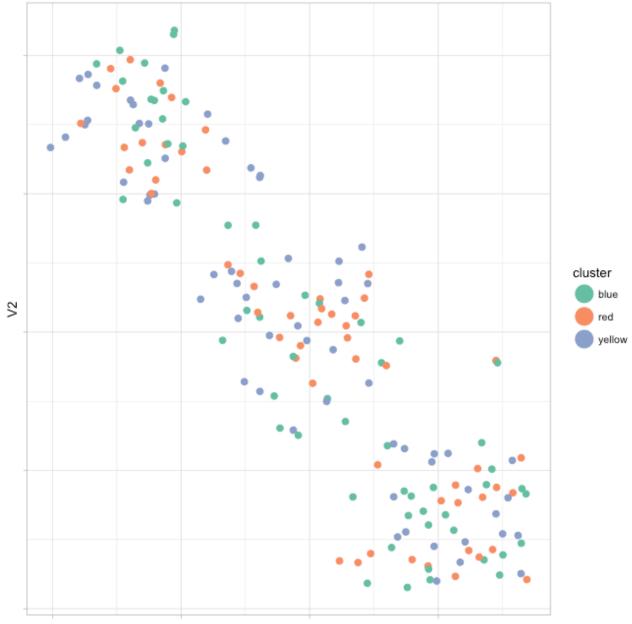
# Configuration
alpha <- 0.01  # cooling rate
beta <- 2  # stage rate</pre>
```

```
7
       ptm
             <- proc.time() # Start the clock!</pre>
 8
 9
       temp <- 1
                      # temperature
10
       stage <- 1
                     # length of stage m
            <- nrow(data) # number of variables
11
12
      cost <- groupRSS(data, sol, K=3)</pre>
13
14
       iters <- c() # init iteration results of cost</pre>
15
       for (j in 1:n){
16
         for (m in 1:stage){
17
           # get neighborhoods for the current solution
18
           neighbors
                            <- neighborhood(sol)</pre>
19
                             <- c() # init results for cost
           res
20
           neighborIndices <- c() # init candidates for neighbor</pre>
21
           for (i in 1:nrow(neighbors)){
                           <- neighbors[i,]</pre>
22
             neighbor
23
             neighborCost <- groupRSS(data, neighbor, K=3) # calculate cost for</pre>
    each neighbor
24
             if (neighborCost < cost){</pre>
25
                                 <- c(res, neighborCost)</pre>
26
               neighborIndices <- c(neighborIndices, i)</pre>
2.7
             }
28
           }
29
           # stop criterion
30
           if (length(res) <= 0){</pre>
31
             # Stop the clock
32
             dt <- proc.time() - ptm</pre>
             result <- list("solution"</pre>
33
                                            = sol,
                              "time"
34
                                            = dt,
35
                              "iterations" = iters)
36
             return(result)
37
           # randomly pick a neighbor from candidates
38
                         <- sample(1:length(res), 1)
39
           candInd
           candNeighbor <- neighbors[neighborIndices[candInd],]</pre>
40
41
           candCost
                         <- res[candInd]</pre>
           # accept this solution by accept rate
42
43
           acceptRate <- min(1, exp((cost - candCost)/temp))</pre>
44
           print(acceptRate)
45
           if (sample(c(TRUE,FALSE), size=1, replace=TRUE,
46
                       prob=c(acceptRate, 1-acceptRate))){
47
             sol
                    <- candNeighbor</pre>
48
             cost <- candCost</pre>
             iters <- c(iters, cost)</pre>
49
50
           }
51
         }
```

```
# update temperature and stage
temp <- temp/(1+alpha*temp)
stage <- stage * beta
}</pre>
```

Below is thee solution:

And the visualization of Simulated Annealing by t-SNE:



Question 4.1

Recall the peppered moth analysis introduced in Example 4.2. In the field, it is quite difficult to distinguish the *insularia* or *typica* phenotypes due to variations in wing color and mottle. In addition to the 662 moths mentioned in the example, suppose the sample collected by the researchers actually included $n_U = 578$ more moths that were known to be *insularia* or *typica* but whose exact phenotypes could not be determined.

• (a) Derive the EM algorithm for maximum likelihood estimation of p_C , p_I , and p_I for this modified problem having observed data n_C , n_I , n_T , and n_U as given above.

The observed data are $\mathbf{x} = (n_C, n_I, n_T, n_U)$ and

the complete data are $\mathbf{y} = (n_{CC}, n_{CI}, n_{CT}, n_{dII}, n_{dIT}, n_{dIT}, n_{nII}, n_{nIT}, n_{nTT})$,

where n_{dII} , n_{dIT} , n_{dTT} denote the numbers of moth whose phenotypes are determined, and n_{nII} , n_{nIT} , n_{nTT} denote the numbers of moth whose phenotypes could not be determined.

The mapping from the complete data to the observed data is:

$$egin{aligned} n_{C} &= n_{CC} + n_{CI} + n_{CT}, \ n_{I} &= n_{dII} + n_{dIT}, \ n_{T} &= n_{dTT}, \ n_{U} &= n_{nII} + n_{nIT} + n_{nTT} \end{aligned}$$

According to the question, we are going to estimate the allele probabilities, p_C , p_I , and p_T . The parameters for this problem is $\mathbf{p}=(p_C,p_I)$, similarly for notational brevity we refer to p_T in what follows.

The complete data log likelihood function is multinomial:

$$log f\mathbf{Y}(\mathbf{y}|\mathbf{p}) = n_{CC}log(p_C^2) + n_{CI}log(2p_Cp_I) + n_{CT}log(2p_Cp_T) + n_{II}log(p_I^2) + n_{IT}log(2p_Ip_T) + n_{TT}log(p_T^2) + log \binom{n}{n_{CC} n_{CI} n_{CT} n_{II} n_{IT} n_{TT}}$$

$$(2)$$

Let $\mathbf{Y}=(N_{CC},N_{CI},N_{CT},N_{II},N_{IT},N_{TT})$, and $n_{II}=n_{dII}+n_{nII}$, $n_{IT}=n_{dIT}+n_{nIT}$, $n_{TT}=n_{dTT}+n_{nTT}$. none of these frequencies can be observed directly.

The expected values of the random parts of Eq. (2) are

$$E(N_{CC}|n_C,n_I,n_T,n_U,\mathbf{p}^{(t)}) = n_{CC}^{(t)} = rac{n_C(p_C^{(t)})^2}{(p_C^{(t)})^2 + 2p_C^{(t)}p_I^{(t)} + 2p_C^{(t)}p_T^{(t)}}$$
 (3)

$$E(N_{CI}|n_C,n_I,n_T,n_U,\mathbf{p}^{(t)}) = n_{CI}^{(t)} = rac{2n_C p_C^{(t)} p_I^{(t)}}{(p_C^{(t)})^2 + 2p_C^{(t)} p_I^{(t)} + 2p_C^{(t)} p_T^{(t)}}$$
 (4

$$E(N_{CT}|n_C,n_I,n_T,n_U,\mathbf{p}^{(t)}) = n_{CT}^{(t)} = rac{2n_C p_C^{(t)} p_T^{(t)}}{(p_C^{(t)})^2 + 2p_C^{(t)} p_I^{(t)} + 2p_C^{(t)} p_T^{(t)}}$$
 (5

$$E(N_{II}|n_C, n_I, n_T, n_U, \mathbf{p}^{(t)}) = n_{dII}^{(t)} + n_{nII}^{(t)} = rac{n_I(p_I^{(t)})^2}{(p_I^{(t)})^2 + 2p_I^{(t)}p_T^{(t)}} + rac{n_U(p_I^{(t)})^2}{(p_I^{(t)})^2 + 2p_I^{(t)}p_T^{(t)} + (p_T^{(t)})^2}$$

$$(6)$$

$$E(N_{IT}|n_C, n_I, n_T, n_U, \mathbf{p}^{(t)}) = n_{dIT}^{(t)} + n_{nIT}^{(t)} = rac{2n_I p_I^{(t)} p_T^{(t)}}{(p_I^{(t)})^2 + 2p_I^{(t)} p_T^{(t)}} + rac{2n_U p_I^{(t)} p_T^{(t)}}{(p_I^{(t)})^2 + 2p_I^{(t)} p_T^{(t)} + (p_T^{(t)})^2}$$
 (7

$$E(N_{TT}|n_C,n_I,n_T,n_U,\mathbf{p}^{(t)}) = n_{dTT}^{(t)} + n_{nTT}^{(t)} = rac{n_U(p_T^{(t)})^2}{(p_I^{(t)})^2 + 2p_I^{(t)}p_T^{(t)} + (p_T^{(t)})^2} + n_T$$
 (8)

Then differentiating with respect to p_{C} and p_{I} yields

$$\frac{dQ(\mathbf{p}|\mathbf{p}^{(t)})}{dp_C} = \frac{2n_{CC}^{(t)} + n_{CI}^{(t)} + n_{CT}^{(t)}}{p_C} - \frac{2n_{TT}^{(t)} + n_{CT}^{(t)} + n_{IT}^{(t)}}{1 - p_C - p_I}$$
(9)

$$\frac{dQ(\mathbf{p}|\mathbf{p}^{(t)})}{dp_I} = \frac{2n_{II}^{(t)} + n_{IT}^{(t)} + n_{CI}^{(t)}}{p_I} - \frac{2n_{TT}^{(t)} + n_{CT}^{(t)} + n_{IT}^{(t)}}{1 - p_C - p_I}$$
(10)

Setting these derivatives equal to zero and solving for p_C and p_I completes the M step, yielding

$$p_C^{(t+1)} = \frac{2n_{CC}^{(t)} + n_{CI}^{(t)} + n_{CT}^{(t)}}{2n} \tag{11}$$

$$p_I^{(t+1)} = \frac{2n_{II}^{(t)} + n_{IT}^{(t)} + n_{CI}^{(t)}}{2n} \tag{12}$$

$$p_T^{(t+1)} = \frac{2n_{TT}^{(t)} + n_{CT}^{(t)} + n_{IT}^{(t)}}{2n} \tag{13}$$

• (b) Apply the algorithm to find the MLEs.

```
niters <- 1000
      2 # raw data
     3 nC <- 85
      4 nI <- 196
      5 nT <- 341
      6 nU <- 578
                   n < - nC + nI + nT + nU
      7
     9 # init value of p
10 pC <- 0.1
11 pI <- 0.1
12 pT <- 0.8
13
14
                  # standard EM
15
                   lastpC <- 0
16
                   lastpI <- 0
                   lastpT <- 1
17
18
                   for (i in 1:niters){
19
                            # E (Estimation) step
20
                            nCC \leftarrow (nC*pC^2) / (pC^2 + 2*pC*pI + 2*pC*pT)
                           nCI \leftarrow (2*nC*pC*pI) / (pC^2 + 2*pC*pI + 2*pC*pT)
21
22
                              nCT \leftarrow (2*nC*pC*pT) / (pC^2 + 2*pC*pI + 2*pC*pT)
                               nII \leftarrow (nI*pI^2) / (pI^2 + 2*pI*pT) + (nU*pI^2) / (pI^2 + 2*pI*pT + 2*pI*pT) + (nU*pI^2) / (pI^2 + 2*pI*pT) + (nU*pI^2) / 
23
                       pT^2)
                                nIT \leftarrow (2*nI*pI*pT) / (pI^2 + 2*pI*pT) + (2*nU*pI*pT) / (pI^2 + 2*pI*pT) / (pI^2 + 2*pI*
24
                      2*pI*pT + pT^2
                            nTT \leftarrow nT + (nU*pT^2) / (pI^2 + 2*pI*pT + pT^2)
25
                            # M (Maximization) step
26
27
                            pC \leftarrow (2*nCC + nCI + nCT) / (2*n)
28
                            pI \leftarrow (2*nII + nIT + nCI) / (2*n)
29
                              pT \leftarrow (2*nTT + nCT + nIT) / (2*n)
30
                              # stop criterion
                               if (((lastpC - pC)^2 + (lastpI - pI)^2 + (lastpT - pT)^2) < 10e-5){
31
32
                                           break
                                }
33
                               lastpC <- pC</pre>
34
35
                                lastpI <- pI
                                lastpT <- pT</pre>
36
37 }
```

The result is $p_C=0.03606708$, $p_I=0.1896198$, $p_T=0.7743131$.

• (c) Estimate the standard errors and pairwise correlations for $\hat{p_C}$, $\hat{p_I}$ and $\hat{p_I}$ using the SEM algorithm.

```
# init value
 2
           <- c(85, 196, 341, 578)
 3
    n
          \leftarrow rep(0,6)
 4
    itr <- 40
 5
         \leftarrow c(0.07, 0.19, 0.74)
    р
    p.em <- p
 7
    theta \leftarrow matrix(0,3,3)
    psi \leftarrow rep(0,3)
 8
9
         <- matrix(0,3,3)
    r
10
11
    # E step
12
    allele.e <- function(x,p){</pre>
       n.cc \leftarrow (x[1]*(p[1]^2))/((p[1]^2)+2*p[1]*p[2]+2*p[1]*p[3])
13
14
      \text{n.ci} \leftarrow (2*x[1]*p[1]*p[2])/((p[1]^2)+2*p[1]*p[2]+2*p[1]*p[3])
15
      n.ct \leftarrow (2*x[1]*p[1]*p[3])/((p[1]^2)+2*p[1]*p[2]+2*p[1]*p[3])
16
      \text{n.ii} \leftarrow (x[2]*p[2]^2) / (p[2]^2 + 2*p[2]*p[3]) + (x[4]*p[2]^2) /
     (p[2]^2 + 2*p[2]*p[3] + p[3]^2)
17
      n.it \leftarrow (2*x[2]*p[2]*p[3]) / (p[2]^2 + 2*p[2]*p[3]) +
     (2*x[4]*p[2]*p[3]) / (p[2]^2 + 2*p[2]*p[3] + p[3]^2)
18
      n.tt < -x[3] + (x[4]*p[3]^2) / (p[2]^2 + 2*p[2]*p[3] + p[3]^2)
19
      n \leftarrow c(n.cc, n.ci, n.ct, n.ii, n.it, n.tt)
20
      return(n)
21
22
23
    # M step
24
    allele.m <- function(x,n){</pre>
25
      p.c \leftarrow (2*n[1]+n[2]+n[3])/(2*sum(x))
2.6
      p.i \leftarrow (2*n[4]+n[5]+n[2])/(2*sum(x))
27
      p.t \leftarrow (2*n[6]+n[3]+n[5])/(2*sum(x))
28
      p <- c(p.c,p.i,p.t)
29
      return(p)
30
31
32
    # compute em computation
33
    for(i in 1:itr){
34
      n.em <- allele.e(x,p.em)</pre>
      p.em \leftarrow allele.m(x,n.em)
35
36
37
38
    # init theta
39
    for(j in 1:length(p)){
40
      theta[,j] <- p.em
41
      theta[j,j] <- p[j]
42
43
44 # main
```

```
45
    for(t in 1:5){
46
       n \leftarrow allele.e(x,p)
47
      p.hat <- allele.m(x,n)
48
       for(j in 1:length(p)){
49
         theta[j,j] <- p.hat[j]</pre>
         n <- allele.e(x,theta[,j])</pre>
50
        psi \leftarrow allele.m(x,n)
         for(i in 1:length(p)){
53
           r[i,j] \leftarrow (psi[i]-p.em[i])/(theta[j,j]-p.em[j])
         }
54
55
      }
56
      p <- p.hat
57
58
59
    # complete information
    iy.hat=matrix(0,2,2)
61
    iy.hat[1,1] <- ((2*n.em[1]+n.em[2]+n.em[3])/(p.em[1]^2) +
62
                       (2*n.em[6]+n.em[3]+n.em[5])/(p.em[3]^2))
63
    iy.hat[2,2] \leftarrow ((2*n.em[4]+n.em[5]+n.em[2])/(p.em[2]^2) +
64
                       (2*n.em[6]+n.em[3]+n.em[5])/(p.em[3]^2))
65
    iy.hat[1,2] \leftarrow iy.hat[2,1] \leftarrow (2*n.em[6]+n.em[3]+n.em[5])/(p.em[3]^2)
66
67
    # compute standard errors and correlations
    var.hat <- solve(iy.hat) %*%(diag(2)+t(r[-3,-3]) %*%solve(diag(2)-
    t(r[-3,-3]))
    sd.hat <- c(sqrt(var.hat[1,1]),sqrt(var.hat[2,2]),sqrt(sum(var.hat)))</pre>
69
70
    cor.hat <- c(var.hat[1,2]/(sd.hat[1]*sd.hat[2]),</pre>
71
                  (-var.hat[1,1]-var.hat[1,2])/(sd.hat[1]*sd.hat[3]),
72
                  (-var.hat[2,2]-var.hat[1,2])/(sd.hat[2]*sd.hat[3]))
```

> var.hat

```
[,1] [,2]
[1,] 1.475087e-05 -5.748342e-06
[2,] -3.078801e-06 1.235657e-04
> sd.hat
[1] 0.003840686 0.011116012 0.011379343
> cor.hat
[1] -0.1346433 -0.2059864 -0.9314149
```

• (d) Estimate the standard errors and pairwise correlations for $\hat{p_C}$, $\hat{p_I}$ and $\hat{p_I}$ by bootstrapping.

```
# init values
 2
           <- c(85, 196, 341, 578)
 3
          \leftarrow rep(0,6)
          \leftarrow rep(1/3,3)
 4
    p
 5
    itr <- 40
    theta <- matrix(0,3,10000)
 7
    set.seed(0)
 8
9
    # E step
10
    allele.e <- function(x,p){
      n.cc \leftarrow (x[1]*(p[1]^2))/((p[1]^2)+2*p[1]*p[2]+2*p[1]*p[3])
11
      n.ci \leftarrow (2*x[1]*p[1]*p[2])/((p[1]^2)+2*p[1]*p[2]+2*p[1]*p[3])
12
13
      n.ct < (2*x[1]*p[1]*p[3])/((p[1]^2)+2*p[1]*p[2]+2*p[1]*p[3])
14
      \text{n.ii} \leftarrow (x[2]*p[2]^2) / (p[2]^2 + 2*p[2]*p[3]) + (x[4]*p[2]^2) /
     (p[2]^2 + 2*p[2]*p[3] + p[3]^2)
15
      n.it \leftarrow (2*x[2]*p[2]*p[3]) / (p[2]^2 + 2*p[2]*p[3]) +
     (2*x[4]*p[2]*p[3]) / (p[2]^2 + 2*p[2]*p[3] + p[3]^2)
16
      n.tt < x[3] + (x[4]*p[3]^2) / (p[2]^2 + 2*p[2]*p[3] + p[3]^2)
17
      n \leftarrow c(n.cc, n.ci, n.ct, n.ii, n.it, n.tt)
18
      return(n)
19
20
21 # M step
    allele.m <- function(x,n){</pre>
22
23
      p.c \leftarrow (2*n[1]+n[2]+n[3])/(2*sum(x))
24
      p.i \leftarrow (2*n[4]+n[5]+n[2])/(2*sum(x))
25
      p.t \leftarrow (2*n[6]+n[3]+n[5])/(2*sum(x))
2.6
      p \leftarrow c(p.c, p.i, p.t)
27
      return(p)
28
29
30 # main
31 for(i in 1:itr){
32
     n \leftarrow allele.e(x,p)
33
      p \leftarrow allele.m(x,n)
34
35
36
    theta[,1] <- p
37
    for(j in 2:10000){
38
      n.c \leftarrow rbinom(1, sum(x), x[1]/sum(x))
39
      n.i \leftarrow rbinom(1, sum(x) - n.c, x[2]/(sum(x)-x[1]))
40
      n.t < -rbinom(1, sum(x) - n.c - n.i, x[2]/(sum(x)-x[1]-x[2]))
41
      n.u \leftarrow sum(x) - n.c - n.i - n.t
42
      x.new \leftarrow c(n.c, n.i, n.t, n.u)
43
      n < - rep(0,6)
      p \le rep(1/3,3)
44
```

```
45
       for(i in 1:itr){
46
         n <- allele.e(x.new,p)</pre>
47
         p <- allele.m(x.new,n)</pre>
48
       }
49
      theta[,j] \leftarrow p
50
51
    sd.hat \leftarrow c(sd(theta[1,]), sd(theta[2,]), sd(theta[3,]))
52
53
    cor.hat <- c(cor(theta[1,],theta[2,]), cor(theta[1,],theta[3,]),</pre>
54
                  cor(theta[2,],theta[3,]))
```

> sd.hat

[1] 0.003843569 0.017248652 0.017413335

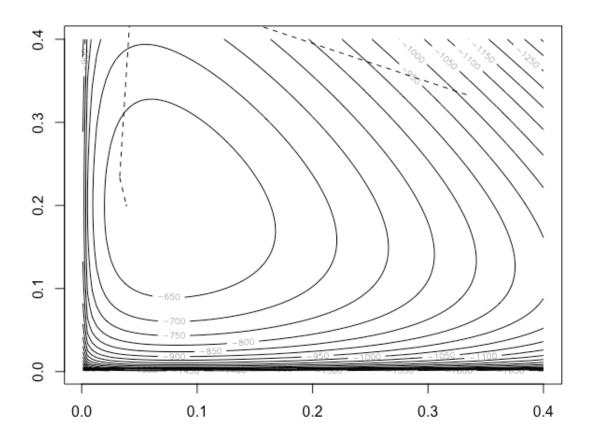
> cor.hat

[1] -0.06836572 -0.15300647 -0.97545267

• (e) Implement the EM gradient algorithm for these data. Experiment with step halving to ensure ascent and with other step scalings that may speed convergence.

```
# init values
   x < -c(85, 196, 341, 578)
 3 n < -rep(0,6)
   p < - rep(1/3,3)
 4
 5 itr <- 40
 6 prob.values <- matrix(0,3,itr+1)
 7
   prob.values[,1] <- p</pre>
   alpha.default <- 2
 8
10
   # E step
11
   allele.e <- function(x,p){
12
      n.cc < -(x[1]*(p[1]^2))/((p[1]^2)+2*p[1]*p[2]+2*p[1]*p[3])
13
     \text{n.ci} \leftarrow (2*x[1]*p[1]*p[2])/((p[1]^2)+2*p[1]*p[2]+2*p[1]*p[3])
14
      n.ct \le (2*x[1]*p[1]*p[3])/((p[1]^2)+2*p[1]*p[2]+2*p[1]*p[3])
      \text{n.ii} \leftarrow (x[2]*p[2]^2) / (p[2]^2 + 2*p[2]*p[3]) + (x[4]*p[2]^2) /
15
    (p[2]^2 + 2*p[2]*p[3] + p[3]^2)
16
      n.it \leftarrow (2*x[2]*p[2]*p[3]) / (p[2]^2 + 2*p[2]*p[3]) +
    (2*x[4]*p[2]*p[3]) / (p[2]^2 + 2*p[2]*p[3] + p[3]^2)
17
      n.tt < x[3] + (x[4]*p[3]^2) / (p[2]^2 + 2*p[2]*p[3] + p[3]^2)
18
      n \leftarrow c(n.cc, n.ci, n.ct, n.ii, n.it, n.tt)
19
      return(n)
20
    }
21
22 allele.l <- function(x,p){</pre>
```

```
23
      1 < (x[1]*log(2*p[1] - p[1]^2) + x[2]*log(p[2]^2 + 2*p[2]*p[3]) +
24
               2*x[3]*log(p[3]))
25
      return(1)
26
27
    # gradient estimation
28
29
    Q.prime <- function(n,p){</pre>
30
      da \leftarrow (2*n[1]+n[2]+n[3])/(p[1]) - (2*n[6]+n[3]+n[5])/(p[3])
31
      db \leftarrow (2*n[4]+n[5]+n[2])/(p[2]) - (2*n[6]+n[3]+n[5])/(p[3])
32
      dQ \leftarrow c(da,db)
33
      return(dQ)
34
35
36
    Q.2prime <- function(n,p){
37
      da2 \leftarrow -(2*n[1]+n[2]+n[3])/(p[1]^2) - (2*n[6]+n[3]+n[5])/(p[3]^2)
38
      db2 < -(2*n[4]+n[5]+n[2])/(p[2]^2) - (2*n[6]+n[3]+n[5])/(p[3]^2)
39
      dab <- -(2*n[6]+n[3]+n[5])/(p[3]^2)
      d2Q <- matrix(c(da2,dab,dab,db2), nrow=2, byrow=TRUE)</pre>
40
41
      return(d2Q)
42
    }
43
44
   # main
45
    1.old \leftarrow allele.l(x,p)
46
    for(i in 1:itr){
47
      alpha <- alpha.default</pre>
48
      n \leftarrow allele.e(x,p)
49
      p.new \leftarrow p[1:2] - alpha*solve(Q.2prime(n,p))%*%Q.prime(n,p)
50
      p.new[3] <- 1 - p.new[1] - p.new[2]</pre>
      if(p.new > 0 && p.new < 1){l.new <- allele.l(x,p.new)}
51
52
      # REDUCE ALPHA UNTIL A CORRECT STEP IS REACHED
      while(p.new < 0 | p.new > 1 | l.new < l.old){
53
54
        alpha <- alpha/2
55
        p.new \leftarrow p[1:2] - alpha*solve(Q.2prime(n,p))%*%Q.prime(n,p)
        p.new[3] <- 1 - p.new[1] - p.new[2]</pre>
56
57
        if(p.new > 0 && p.new < 1){l.new <- allele.l(x,p.new)}
58
      }
59
      p <- p.new
60
      prob.values[,i+1] <- p</pre>
      1.old <- 1.new
61
62
   }
```

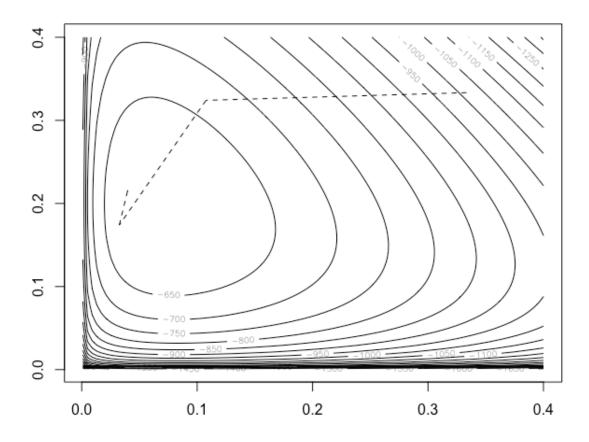


• (f) Implement Aitken accelerated EM for these data. Use step halving.

```
# init values
 2
    x < -c(85, 196, 341, 578)
   n < - rep(0,6)
   p \leftarrow rep(1/3,3)
 4
    itr <- 40
    prob.values <- matrix(0,3,itr+1)</pre>
 7
    prob.values[,1] <- p</pre>
    alpha.default <- 2
 8
 9
10
    # E step
    allele.e <- function(x,p){
11
12
      n.cc \leftarrow (x[1]*(p[1]^2))/((p[1]^2)+2*p[1]*p[2]+2*p[1]*p[3])
13
      n.ci \leftarrow (2*x[1]*p[1]*p[2])/((p[1]^2)+2*p[1]*p[2]+2*p[1]*p[3])
14
      n.ct \leftarrow (2*x[1]*p[1]*p[3])/((p[1]^2)+2*p[1]*p[2]+2*p[1]*p[3])
15
      \text{n.ii} \leftarrow (x[2]*p[2]^2) / (p[2]^2 + 2*p[2]*p[3]) + (x[4]*p[2]^2) /
    (p[2]^2 + 2*p[2]*p[3] + p[3]^2)
16
       n.it \leftarrow (2*x[2]*p[2]*p[3]) / (p[2]^2 + 2*p[2]*p[3]) +
    (2*x[4]*p[2]*p[3]) / (p[2]^2 + 2*p[2]*p[3] + p[3]^2)
```

```
17
       n.tt \leftarrow x[3] + (x[4]*p[3]^2) / (p[2]^2 + 2*p[2]*p[3] + p[3]^2)
18
       n \leftarrow c(n.cc, n.ci, n.ct, n.ii, n.it, n.tt)
19
       return(n)
20
21
22
    # M step
    allele.m <- function(x,n){</pre>
23
24
       p.c \leftarrow (2*n[1]+n[2]+n[3])/(2*sum(x))
25
       p.i \leftarrow (2*n[4]+n[5]+n[2])/(2*sum(x))
26
       p.t \leftarrow (2*n[6]+n[3]+n[5])/(2*sum(x))
27
       p \leftarrow c(p.c,p.i,p.t)
28
       return(p)
29
30
    allele.l <- function(x,p){</pre>
31
32
       1 < (x[1]*log(2*p[1] - p[1]^2) + x[2]*log(p[2]^2 + 2*p[2]*p[3]) +
33
                2*x[3]*log(p[3]))
34
       return(1)
35
36
37
    allele.iy <- function(n,p){</pre>
38
       iy.hat < -matrix(0,2,2)
39
       iy.hat[1,1] \leftarrow ((2*n[1]+n[2]+n[3])/(p[1]^2) +
40
                           (2*n[6]+n[3]+n[5])/(p[3]^2)
41
       iy.hat[2,2] \leftarrow ((2*n[4]+n[5]+n[2])/(p[2]^2) +
42
                           (2*n[6]+n[3]+n[5])/(p[3]^2)
43
       iy.hat[1,2] \leftarrow iy.hat[2,1] \leftarrow (2*n[6]+n[3]+n[5])/(p[3]^2)
       return(iy.hat)
44
45
46
47
    allele.l.2prime <- function(x,p){</pre>
48
       1.2prime <- matrix(0,2,2)
       1.2 \text{prime}[1,1] \leftarrow ((-x[1]*(2-2*p[1])^2)/((2*p[1]-p[1]^2)^2) -
49
50
                              2*x[1]/(2*p[1]-p[1]^2) -
51
                              (4*x[2])/((-2*p[1]-p[2]+2)^2) -
52
                              2*x[3]/(p[3]^2))
53
       1.2 \text{prime}[2,2] \leftarrow ((-4 \times [2] \times [3]^2)/((p[2]^2 + 2 \times [2] \times [3])^2) -
54
                              2*x[2]/(p[2]^2 + 2*p[2]*p[3]) -
55
                              2*x[3]/(p[3]^2))
56
       1.2prime[1,2] <-((-2*x[2])/((-2*p[1]-p[2]+2)^2) -
57
                             2*x[3]/(p[3]^2)
58
       1.2prime[2,1] <- 1.2prime[1,2]
59
       return(1.2prime)
60
61
62
    # main
```

```
1.old <- allele.l(x,p)</pre>
63
64
    for(i in 1:itr){
65
       alpha <- alpha.default</pre>
66
       n \leftarrow allele.e(x,p)
       p.em \leftarrow allele.m(x,n)
67
68
       p.new <- (p[1:2] - alpha*solve(allele.l.2prime(x,p))%*%</pre>
69
                   allele.iy(n,p)%*%(p.em[1:2]-p[1:2]))
70
       p.new[3] <- 1 - p.new[1] - p.new[2]</pre>
71
       if(p.new > 0 && p.new < 1) \{1.\text{new} \leftarrow \text{allele.l}(x,p.\text{new})\}
       # REDUCE ALPHA UNTIL A CORRECT STEP IS REACHED
72
       while(p.new < 0 || p.new > 1 || l.new < l.old){
73
         alpha <- alpha/2</pre>
74
75
         p.new \leftarrow (p[1:2] - alpha*solve(allele.1.2prime(x,p))%*%
76
                      allele.iy(n,p)%*%(p.em[1:2]-p[1:2]))
77
         p.new[3] <- 1 - p.new[1] - p.new[2]</pre>
78
         if(p.new > 0 && p.new < 1){l.new <- allele.l(x,p.new)}
       }
79
80
       p <- p.new
81
       prob.values[,i+1] <- p</pre>
       1.old <- 1.new
82
83 }
```

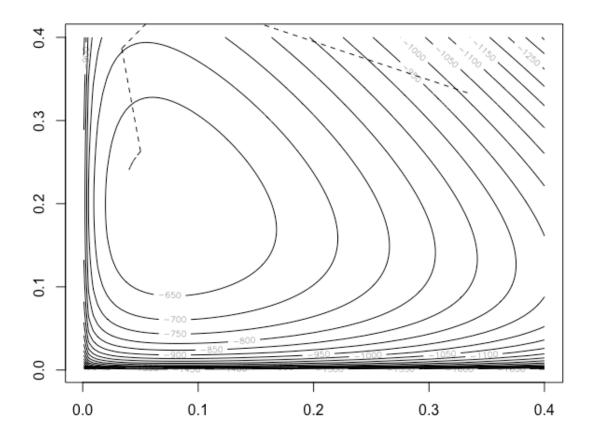


• (g) Implement quasi-Newton EM for these data. Compare performance with and without step halving.

```
# init values
    x <- c(85, 196, 341, 578)
 2
 3
   n < - rep(0,6)
    p \leftarrow rep(1/3,3)
 4
    itr <- 20
 5
    m <- matrix(0,2,2)
 7
    b <- matrix(0,2,2)
    prob.values <- matrix(0,3,itr+1)</pre>
 8
    prob.values[,1] <- p</pre>
    alpha.default <- 2</pre>
10
11
12
    # E step
13
    allele.e <- function(x,p){</pre>
       n.cc \leftarrow (x[1]*(p[1]^2))/((p[1]^2)+2*p[1]*p[2]+2*p[1]*p[3])
14
15
       \text{n.ci} \leftarrow (2*x[1]*p[1]*p[2])/((p[1]^2)+2*p[1]*p[2]+2*p[1]*p[3])
16
       n.ct \leftarrow (2*x[1]*p[1]*p[3])/((p[1]^2)+2*p[1]*p[2]+2*p[1]*p[3])
```

```
17
      \text{n.ii} \leftarrow (x[2]*p[2]^2) / (p[2]^2 + 2*p[2]*p[3]) + (x[4]*p[2]^2) /
    (p[2]^2 + 2*p[2]*p[3] + p[3]^2)
      \text{n.it} \leftarrow (2*x[2]*p[2]*p[3]) / (p[2]^2 + 2*p[2]*p[3]) +
18
    (2*x[4]*p[2]*p[3]) / (p[2]^2 + 2*p[2]*p[3] + p[3]^2)
19
      n.tt < -x[3] + (x[4]*p[3]^2) / (p[2]^2 + 2*p[2]*p[3] + p[3]^2)
20
      n \leftarrow c(n.cc, n.ci, n.ct, n.ii, n.it, n.tt)
21
      return(n)
22
23
    allele.1 <- function(x,p){</pre>
24
       1 \leftarrow (x[1]*log(2*p[1] - p[1]^2) + x[2]*log(p[2]^2 + 2*p[2]*p[3]) +
25
26
                 2*x[3]*log(p[3]))
27
      return(1)
28
29
30
    # gradient estimation
31
    Q.prime <- function(n,p){
      da \leftarrow (2*n[1]+n[2]+n[3])/(p[1]) - (2*n[6]+n[3]+n[5])/(p[3])
32
33
      db \leftarrow (2*n[4]+n[5]+n[2])/(p[2]) - (2*n[6]+n[3]+n[5])/(p[3])
34
      dQ \leftarrow c(da,db)
35
      return(dQ)
36
    }
37
38
    Q.2prime <- function(n,p){
39
      da2 <- -(2*n[1]+n[2]+n[3])/(p[1]^2) - (2*n[6]+n[3]+n[5])/(p[3]^2)
40
      db2 < -(2*n[4]+n[5]+n[2])/(p[2]^2) - (2*n[6]+n[3]+n[5])/(p[3]^2)
41
      dab <-(2*n[6]+n[3]+n[5])/(p[3]^2)
42
      d2Q <- matrix(c(da2,dab,dab,db2), nrow=2, byrow=TRUE)</pre>
43
      return(d2Q)
44
    }
45
46
    # main
    1.old \leftarrow allele.l(x,p)
47
    for(i in 1:itr){
48
49
      alpha <- alpha.default</pre>
      n \leftarrow allele.e(x,p)
50
51
      m \leftarrow Q.2prime(n,p) - b
52
      p.new \leftarrow p[1:2] - alpha*solve(m)%*%Q.prime(n,p)
      p.new[3] <- 1 - p.new[1] - p.new[2]</pre>
53
54
      if (p.new > 0 \& p.new < 1) \{1.new <- allele.l(x,p.new)\}
55
      # REDUCE ALPHA UNTIL A CORRECT STEP IS REACHED
56
      while(p.new < 0 | p.new > 1 | l.new < l.old){
57
         alpha <- alpha/2
58
         p.new \leftarrow p[1:2] - alpha*solve(m)%*%Q.prime(n,p)
59
         p.new[3] \leftarrow 1 - p.new[1] - p.new[2]
60
         if(p.new > 0 && p.new < 1) {l.new <- allele.l(x,p.new)}
```

```
61
62
       at <- p.new[1:2]-p[1:2]
63
       n <- allele.e(x,p.new)</pre>
64
       bt <- Q.prime(n,p)-Q.prime(n,p.new)</pre>
      vt <- bt - b%*%at
65
66
       ct <- as.numeric(1/(t(vt)%*%at))
67
       b <- b + ct*vt***t(vt)
68
       p <- p.new
69
       prob.values[,i+1] <- p</pre>
70
       1.old <- 1.new
71
   }
```



• (h) Compare the effectiveness and efficiency of the standard EM algorithm and the three variants in (e), (f), and (g). Use step halving to ensure ascent with the three variants. Base your comparison on a variety of starting points. Create a graph analogous to Figure 4.3.

Please the details in each subsection of this question.

Question 4.5

• (a) Show the following algorithms can be used to calculate $\alpha(i,h)$ and $\beta(i,h)$.

$$\alpha(0,h) = P(O_0 = o_0, H_0 = h)$$

$$= P(O_0 = o_0 | H_0 = h) \cdot P(H_0 = h)$$

$$= \pi(h)e(h, o_0)$$
(14)

$$\alpha(i+1,h) = P(\mathbf{O}_{\leq i+1} = \mathbf{o}_{\leq i+1}, H_{i+1} = h)$$

$$= \sum_{h^* \in H} P(\mathbf{O}_{\leq i} = \mathbf{o}_{\leq i}, H = h^*) \cdot P(O_{i+1} = o_{i+1} | H_{i+1} = h) \cdot P(H_{i+1} = h | H_i = h^*)$$

$$= \sum_{h^* \in H} \alpha(i,h^*)e(h,o_{i+1})p(h^*,h)$$
(15)

$$\beta(i-1,h) = P(\mathbf{O}_{>i-1} = \mathbf{o}_{>i-1}|H_{i-1} = h)$$

$$= \sum_{h^* \in H} P(\mathbf{O}_{>i} = \mathbf{o}_{>i}|H = h^*) \cdot P(O_i = o_i|H_i = h) \cdot P(H_i = h|H_i = h^*)$$

$$= \sum_{h^* \in H} \beta(i,h^*)e(h^*,o_i)p(h,h^*)$$
(16)

• (b) Prove that these random variables have the following expectations.

$$E_{Q}(N(h)|\mathbf{O} = \mathbf{o}) = P(H_{0} = h|\mathbf{O} = \mathbf{o}, \theta)$$

$$= \frac{P(\mathbf{O}_{>0} = \mathbf{o}, O_{0} = o_{0}|H_{o} = h, \theta) \cdot P(H_{o} = h|Q)}{P(\mathbf{O} = \mathbf{o}|\theta)}$$

$$= \frac{\beta(0, h)e(h, o_{0})\pi(h)}{P(\mathbf{O} = \mathbf{o}|\theta)}$$

$$= \frac{\alpha(0, h)\beta(0, h)}{P(\mathbf{O} = \mathbf{o}|\theta)}$$

$$(17)$$

$$E_{Q}(N(h, h^{*})|\mathbf{O} = \mathbf{o}) = E_{Q}(\sum_{i=0}^{n-1} \mathbb{I}(H_{i} = h, H_{i+1} = h^{*})|\mathbf{O} = \mathbf{o})$$

$$= \sum_{i=0}^{n-1} E_{Q}(\mathbb{I}(H_{i} = h, H_{i+1} = h^{*})|\mathbf{O} = \mathbf{o})$$

$$= \sum_{i=0}^{n-1} \frac{P(H_{i} = h, H_{i+1} = h^{*}, \mathbf{O} = \mathbf{o}|\theta)}{P(\mathbf{O} = \mathbf{o}|\theta)}$$

$$= \sum_{i=0}^{n-1} \frac{P(H_{i} = h, H_{i+1} = h^{*}, \mathbf{O}_{\leq i} = \mathbf{o}_{\leq i}, O_{i+1} = o_{i+1}, \mathbf{O}_{>i+1} = \mathbf{o}_{>i+1}|\theta)}{P(\mathbf{O} = \mathbf{o}|\theta)}$$

$$= \sum_{i=0}^{n-1} \frac{\alpha(i, h)e(h^{*}, o_{i+1})\beta(i+1, h^{*})P(h, h^{*}))}{P(\mathbf{O} = \mathbf{o}|\theta)}$$

$$= \sum_{i=0}^{n-1} \frac{\alpha(i, h)e(h^{*}, o_{i+1})\beta(i+1, h^{*})P(h, h^{*}))}{P(\mathbf{O} = \mathbf{o}|\theta)}$$

$$E_{Q}(N(h,o)|\mathbf{O} = \mathbf{o}) = E_{Q}(\sum_{i=0}^{n-1} \mathbb{I}(H_{i} = h, O_{i} = o)|\mathbf{O} = \mathbf{o})$$

$$= \sum_{i \in O_{i} = o} E_{Q}(\mathbb{I}(H_{i} = h)|\mathbf{O} = \mathbf{o})$$

$$= \sum_{i \in O_{i} = o} \frac{P(H_{i} = h, \mathbf{O}_{\leq i} = \mathbf{o}_{\leq i}, \mathbf{O}_{>i} = \mathbf{o}_{>i}|\theta)}{P(\mathbf{O} = \mathbf{o}|\theta)}$$

$$= \sum_{i \in O_{i} = o} \frac{\sum_{h \in H} P(\mathbf{O}_{>i} = \mathbf{o}_{>i}|H_{i} = h, \mathbf{O}_{\leq i} = \mathbf{o}_{\leq i}, \theta)\alpha(i, h)}{P(\mathbf{O} = \mathbf{o}|\theta)}$$

$$= \sum_{i \in O_{i} = o} \frac{\alpha(i, h)\beta(i, h)}{P(\mathbf{O} = \mathbf{o}|\theta)}$$
(19)

• (c) Prove that the Baum-Welch algorithm is an EM algorithm.

Take one component of π as an example.

$$max_{\pi} \sum E(N(h)|\theta^{(t)}, \mathbf{O})log \,\pi(h)$$
 (20)

$$s.t. \sum_{h \in H^*} \pi(h) = 1$$
 (21)

We apply Lagrangian Multiplier.

$$Lang(\pi, \lambda) = \sum_{h \in H} E(N(h)|Q^{(t)}, \mathbf{O})log \ \pi(h) + \lambda(\sum_{h \in H} \pi(h) - 1)$$
 (22)

And solve $0=rac{\partial}{\partial\pi(h)}Lang(\pi,\lambda)$, we can get

$$\pi(h) = \frac{E(N(h)|Q^{(t)}, \mathbf{O})}{\sum_{h \in H} E(N(h)|Q^{(t)}, \mathbf{O})}$$
(23)

$$\lambda = -\sum_{h \in H} E(N(h)|Q^{(t)}, \mathbf{O})$$
 (24)

• (d) Use the Baum-Welch algorithm to estimate p, d, and s.

```
1    require(HMM)
2    hmm1 = initHMM(c('dim', "penny"), c("tail", "Head"), c(0.5,0.5),
    matrix(c(0.25,0.75,0.75,0.25),2),
3         matrix(c(0.25,0.5,0.75,0.5),2))
4    O = read.table('coin.dat', header = TRUE)$outcome
5    observation = O
6    observation[O == 1] = 'Head'
```

```
observation[0 == 2] = 'tail'
    B1 = exp(backward(hmm1,observation))
8
   A1 =exp(forward(hmm1, observation))
10
   baumWelch(hmm1, observation, maxIterations=100, delta=1E-9, pseudoCount
    = 0)
11
12
    hmm2 = initHMM(c('dim', "penny"), c("tail", "Head"), c(0.5,0.5),
    matrix(c(0.5,0.5,0.5,0.5),2),
13
                   matrix(c(0.5,0.5,0.5,0.5),2))
    baumWelch(hmm2, observation, maxIterations=100, delta=1E-9, pseudoCount
14
    = 0)
15
    hmm3 = initHMM(c('dim', "penny"), c("tail", "Head"), c(0.5,0.5),
16
    matrix(c(0.1,0.9,0.9,0.1),2),
17
                   matrix(c(0.1,0.1,0.9,0.9),2))
    baumWelch(hmm3, observation, maxIterations=100, delta=1E-9, pseudoCount
18
    = 0)
19
20
   hmm4 = initHMM(c('dim', "penny"), c("tail", "Head"), c(0.5,0.5),
    matrix(c(1/4,2/3,3/4,1/3),2),
21
                   matrix(c(1/4,2/3,3/4,1/3),2))
22
   baumWelch(hmm3, observation, maxIterations=100, delta=1E-9, pseudoCount
    = 0)
```

Below is the results:

```
hmmStates [1] "dim" "penny"
hmmSymbols [1] "tail" "Head"
hmmstartProbs dim penny 0.5 0.5
hmmtransProbs
from dim penny dim 0.1 0.9 penny 0.9 0.1
hmmemissionProbs
states tail Head dim 0.45 0.55 penny 0.45 0.55
$difference [1] 7.000000e-01 1.353259e-14
```