BCB570 HW5

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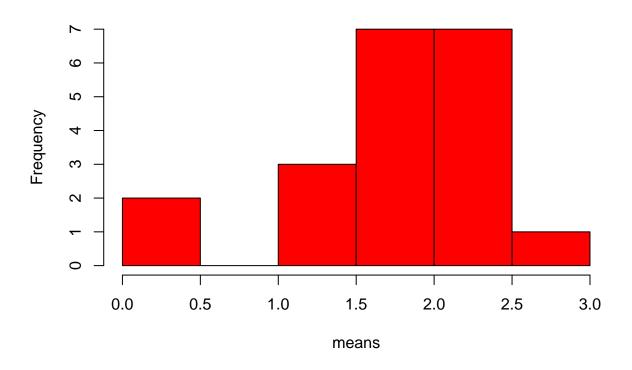
Solution 1

Bagging

Bagging is an ensembl method to improve stability of learning algorithms by reducing its variance. In general, given a dataset D with n datapoints (in any k-dimentional space), bagging generates m new datasets each of size n. It does so by doing sampling-with-replacement and samples n datapoints m times. If n is large enough, the 63.2% unique datapoints are expected to be in the m samples. A variation of bagging can have another parameter n' which is the dataset size of the sampled datasets. Here, bagging will generates m new datasets each of size n' by doing sampling-with-replacement.

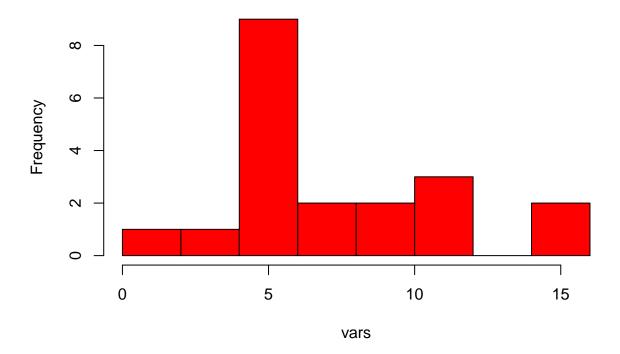
```
# sample 100 datapoints
n_data_100 <- rnorm(100, mean = 2, sd = sqrt(8))</pre>
cat("Mean is", mean(n_data_100))
## Mean is 2.024138
cat("Var is", var(n_data_100))
## Var is 8.714753
means \leftarrow c()
vars <- c()</pre>
N <- 20
k <- 10
for (i in 1:N) {
    this <- sample(n_data_100, k, replace = T)
    # print(this)
    means <- c(means, mean(this))</pre>
    vars <- c(vars, var(this))</pre>
}
hist(means, col = c("Red"))
```

Histogram of means



hist(vars, col = c("Red"))

Histogram of vars



```
e_mean <- mean(means)
e_var <- mean(vars)
```

From the histograms it is hard to estimate true parametes as we sampled very few datasets. From the sub samples the mean of means is 1.7435098 and mean of variances is 7.4471093. These are our best estimates from our sub-samples.

Solution 2

Creating association networks

To create any association network we need to go through following steps.

- 1. First we have to define a way that can "associate" datapoints or variables. If two points are associated we must connect them through an edge and in this way we can create a network. We have to define a mathematical function that can quantify association between two datapoints e.g. we can compute the correlation between two variables if it is greater than zero, we say the variables are accosiated.
- 2. We may choose an association function, depending on the type of network we want i.e directed, undirected, weighted or unweighted.E.g. if we want directed association graph our association function should not be always symmetrical.
- 3. After defining a function that can quantify association, we need to set a threshold such that we create edges between only the strongly associated nodes. E.g. if we define distance between two points to be our measure of association then we need to set a cut-off such that if the distance is more than a value, we do not count that as true association.

• 3a Depending on the data, sometimes it may be useful to scale all the association metrics computed to make all the association comparable with in the graph

A novel association method

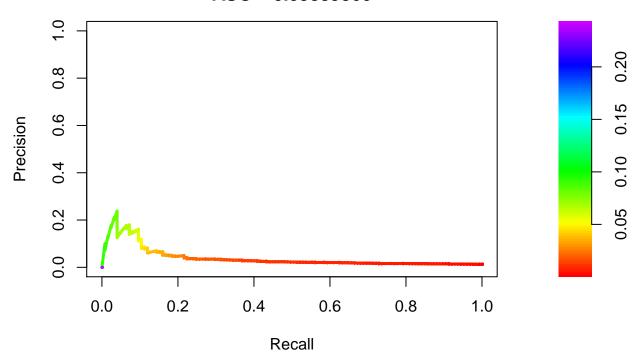
A method for creating association networks, not discussed in class, is using partial correlations. This method is not completely novel as it has been applied to study phenotypic networks (Chu et. al. 2014) but i am describing this in context of my data which may be novel. I am working with human transcript expression data and it would be interesting to create an association network using partial correlations. Partial correlation method finds the correlation between two variable while conditional all other variables. We can easily threshold this kind of network by calculating p-values as under the null, where all variables are independent, Hotelling is the null distribution. Using this we can test for significant partial correlations and filter the network. I can compare results of networks obtained from using correlation and partial correlation networks. A network based on partial correlation is expected to be more dense and may reveal interesting hidden links. So I will first select the transcript which are highly likely to interact using mutual information metric and filter some of the weekly interacting components. Then, on the remaining transcripts i'll use partial correlation measure to build an association network.

Solution 4

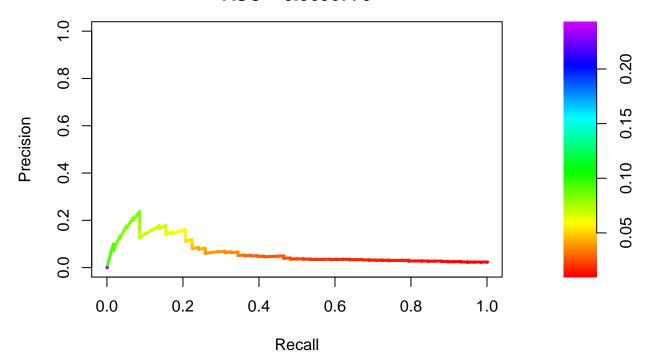
```
library(GENIE3)
library(readr)
library("doParallel", lib.loc = "~/R/win-library/3.4")
library("doRNG", lib.loc = "~/R/win-library/3.4")
library(plyr)
library(PRROC)
# read true labels
trueEcoli1 <- read.csv("NIHW in silico data/NIHW in silico data/Size100/DREAM3 gold standards/DREAM3Gol
    sep = "\t", header = F)
trueEcoli2 <- read.csv("NIHW in silico data/NIHW in silico data/Size100/DREAM3 gold standards/DREAM3Gol
    sep = "\t", header = F)
# do for ecoli data 1
adata <- read.csv("NIHW in silico data/NIHW in silico data/Size100/DREAM3 data/InSilicoSize100-Ecoli1-t
    sep = "\t")
adata <- t(adata)
expmat <- as.matrix(adata[2:101, 1:966])
rownames(expmat) <- paste("G", 1:100, sep = "")</pre>
colnames(expmat) <- paste("Samp", 1:966, sep = "")</pre>
res1 <- GENIE3(expmat, nCores = 6, nTrees = 100)
linkList <- getLinkList(res1)</pre>
names(linkList) <- c("RG", "TG", "Weight")</pre>
names(trueEcoli1) <- c("RG", "TG", "Label")</pre>
q4thresh <- quantile(linkList$Weight, 0.75)
# q4thresh<-0.1
linkList q4 <- linkList[linkList$Weight >= q4thresh, ]
names(linkList_q4) <- c("RG", "TG", "Weight")</pre>
joined_data <- plyr::join(linkList, trueEcoli1)</pre>
joined_data_q4 <- plyr::join(linkList_q4, trueEcoli1)</pre>
pr1 <- pr.curve(scores.class0 = joined_data$Weight, weights.class0 = joined_data$Label,
```

```
curve = T)
plot(pr1, main = "PR Curve for Ecoli dataset 1")
```

PR Curve for Ecoli dataset 1 AUC = 0.03889866

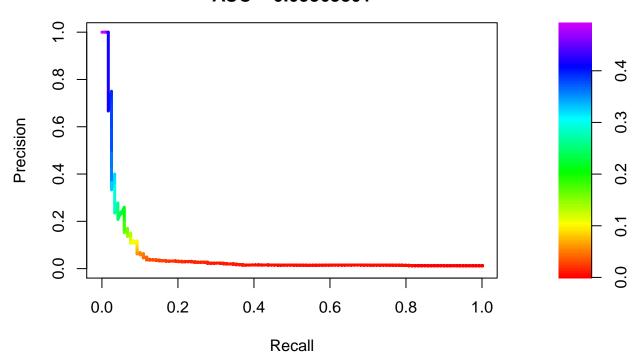


PR Curve for Ecoli dataset 1 (only top quartile edges) AUC = 0.0636776

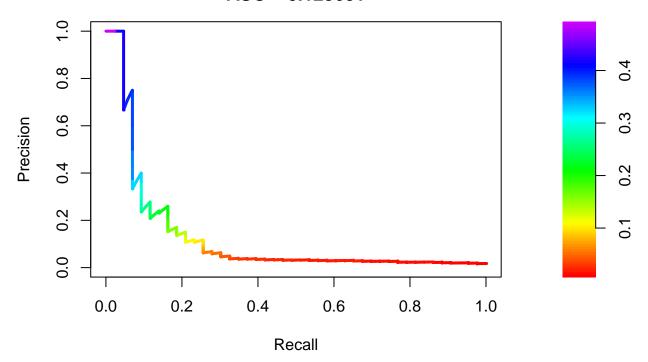


```
# do for ecoli data 2
adata2 <- read.csv("NIHW in silico data/NIHW in silico data/Size100/DREAM3 data/InSilicoSize100-Ecoli2-
    sep = "\t")
adata2 <- t(adata2)</pre>
expmat2 <- as.matrix(adata2[2:101, 1:966])</pre>
rownames(expmat2) <- paste("G", 1:100, sep = "")</pre>
colnames(expmat2) <- paste("Samp", 1:966, sep = "")</pre>
res2 <- GENIE3(expmat2, nCores = 6, K = "all", nTrees = 100)
linkList2 <- getLinkList(res2)</pre>
names(linkList2) <- c("RG", "TG", "Weight")</pre>
names(trueEcoli2) <- c("RG", "TG", "Label")</pre>
q4thresh2 <- quantile(linkList2$Weight, 0.75)
linkList2_q4 <- linkList2[linkList2$Weight >= q4thresh2, ]
names(linkList2_q4) <- c("RG", "TG", "Weight")</pre>
joined_data2 <- plyr::join(linkList2, trueEcoli2)</pre>
joined_data2_q4 <- plyr::join(linkList2_q4, trueEcoli2)</pre>
pr2 <- pr.curve(scores.class0 = joined_data2$Weight, weights.class0 = joined_data2$Label,</pre>
    curve = T)
plot(pr2, main = "PR Curve for Ecoli dataset 2")
```

PR Curve for Ecoli dataset 2 AUC = 0.05363801



PR Curve for Ecoli dataset 2 (only top quartile edges) AUC = 0.123601



```
# save results to file
write_tsv(linkList, "Ecoli1_results_all.tsv")
write_tsv(linkList_q4, "Ecoli1_results_topq.tsv")
write_tsv(linkList2, "Ecoli2_results_all.tsv")
write_tsv(linkList2_q4, "Ecoli2_results_topq.tsv")

# find best estimate intersection from linkList_q4 and linkList2_q4
temp_linkList_q4 <- linkList_q4
names(temp_linkList_q4) <- c("RG", "TG", "ecoli1")
temp_linkList2_q4 <- linkList2_q4
names(temp_linkList2_q4) <- c("RG", "TG", "ecoli2")
# common edges
common <- plyr::join(temp_linkList_q4, temp_linkList2_q4, type = "inner")
# save to file
write_tsv(common, "Ecoli_best_estimate.tsv")</pre>
```

 \mathbf{a}

GENIE3 is an algorithm for inferring gene regulatory networks from expression data. GENIE3 decomposes the prediction of a regulatory network between p genes into p different regression problems. In each of the regression problems, the expression pattern of one of the genes (target gene) is predicted from the expression patterns of all the other genes (input genes), using tree-based ensemble methods.

I ran GENEI3 with default parameters except I changed number of trees to 100 (to be faster). To threshold the network I took the top quartile values and selected the edges.

b

I ran GENEI3 for the two ecoli data sets on the trajectories file. Then I plotted the PR curve as shown in the attached figures. Then I filtered my networks by keeping only the edges which have weights in the top quartile. To come up with my best estimate about Ecoli network, I took the intersection of the two results i.e. if edge is present in the two networks. I saved these results to file "Ecoli_best_estimate.tsv".

c Best estimates for ecoli data sets

common				
##	RG	TG	ecoli1	ecoli2
## 1	G66	G68	0.09550842	0.033417604
## 2	G18	G16	0.08563683	0.011648596
## 3	G31	G30	0.08346623	0.040799943
## 4	G68	G66	0.08264686	0.016296007
## 5	G37	G93	0.07636189	0.064046040
## 6	G28	G45	0.07032582	0.015785393
## 7	G63	G60	0.06979220	0.022103001
## 8	G18	G32	0.06965476	0.016845274
## 9	G16	G18	0.06771008	0.010163507
## 10	G14	G93	0.06759043	0.020017658
## 11	G41	G45	0.06751179	0.009864705
## 12	G18	G46	0.06656073	0.024081322
## 13	G99	G5	0.06433153	0.010759347
## 14	G82	G43	0.06365858	0.019729160
## 15	G45	G28	0.06185529	0.019163994
## 16	G30	G31	0.06135637	0.030019798
## 17	G40	G5	0.06094871	0.016461434
## 18	G93	G37	0.06074766	0.098612802
## 19	G31	G36	0.06066831	0.011496761
## 20	G97	G39	0.05814637	0.009990772
## 21	G83	G38	0.05740563	0.036520452
## 22	G32	G18	0.05688047	0.012798603
## 23	G90	G60	0.05641278	0.010744575
## 24	G88	G36	0.05596317	0.009386102
## 25	G99	G2	0.05566076	0.041797108
## 26	G33	G20	0.05548770	0.033741731
## 27	G23	G81	0.05509880	0.016668972
## 28	G40	G17	0.05333692	0.030176309
## 29 ## 30	G36 G23	G34 G21	0.05256332 0.05243834	0.009601923 0.011945607
## 30 ## 31	G23	G21 G9	0.05243634	0.040137635
## 31 ## 32	G5	G49	0.05230794	0.040137633
## 32	G17	G5	0.05100372	0.0022937333
## 34	G18	G59	0.03078428	0.009213007
## 35	G51	G87		0.003471102
## 36	G63	G64		0.171017427
## 37	G16	G80		
## 38	G28	G98		0.010306426
## 39	G82	G83		
## 40	G47	G50		0.009279675
## 41	G51	G8		

```
## 42
        G61
             G59 0.04380656 0.009579306
##
             G64 0.04361619 0.019268455
  43
        G61
             G38 0.04357242 0.015530803
##
   44
        G39
##
        G32
             G59 0.04262978 0.018944100
   45
##
   46
        G68
             G55 0.04177970 0.011411278
             G47 0.04176139 0.010402571
##
   47
        G50
##
  48
        G43
             G97 0.04149473 0.014574427
## 49
         G5
             G85 0.04105565 0.009799214
##
   50
        G64
             G63 0.04093342 0.105197477
##
   51
        G14
             G45 0.04081945 0.011576487
##
   52
        G75
              G3 0.04020607 0.042214776
   53
             G40 0.04012734 0.019246157
##
        G51
##
   54
        G68
             G70 0.04011311 0.013675525
##
  55
        G49
              G5 0.03998728 0.012354642
##
  56
              G2 0.03975259 0.016928342
        G41
##
  57
        G39
             G93 0.03972749 0.011024929
              G2 0.03968363 0.041735961
##
   58
        G97
##
   59
             G20 0.03955842 0.011896984
        G16
##
              G8 0.03920944 0.010039812
   60
        G17
##
   61
        G41
             G16 0.03914060 0.010129431
##
  62
        G35
             G26 0.03912696 0.016311448
   63
              G9 0.03889456 0.011233662
##
        G80
## 64
             G79 0.03876957 0.011618636
        G21
             G23 0.03849022 0.010621985
##
   65
         G9
##
   66
        G49
             G31 0.03808134 0.012153970
##
   67
        G64
             G41 0.03797340 0.023641587
##
   68
             G36 0.03792750 0.010155900
        G34
##
   69
        G60
             G57 0.03790503 0.095877730
##
   70
             G80 0.03786658 0.034194037
        G40
##
  71
        G82
             G12 0.03776867 0.009234299
##
  72
        G99
             G63 0.03732218 0.010507367
##
   73
        G21
             G23 0.03703495 0.010749170
##
   74
        G41
             G47 0.03692703 0.030236280
##
             G32 0.03689561 0.016269992
  75
        G16
##
   76
        G49
             G96 0.03677504 0.009815624
##
  77
        G23
              G9 0.03674412 0.031960401
##
  78
        G28
             G30 0.03673785 0.017631801
## 79
        G37
             G18 0.03618648 0.013782284
##
   80
        G81
             G86 0.03616645 0.018829778
  81
             G59 0.03605691 0.010950341
##
        G23
             G41 0.03603287 0.061618257
##
   82
        G93
##
  83
              G6 0.03581804 0.020602758
        G17
             G40 0.03560491 0.117911092
##
   84
        G93
##
   85
        G80
             G40 0.03547144 0.011042922
##
   86
        G64
             G59 0.03542134 0.009930045
## 87
             G49 0.03534876 0.030223350
        G96
##
   88
        G14
             G86 0.03530097 0.011460183
##
   89
        G18
             G37 0.03527731 0.010415026
##
  90
        G34
             G19 0.03491836 0.020757611
##
  91
        G55
             G44 0.03477841 0.010134641
## 92
             G75 0.03469260 0.024129155
         G3
## 93
        G88
             G86 0.03431062 0.014521874
## 94
        G17
             G40 0.03421996 0.077210727
## 95
        G46
             G18 0.03365283 0.016662045
```

```
## 96
        G32
             G38 0.03359961 0.023757966
## 97
        G42
             G30 0.03359512 0.026147607
             G95 0.03353169 0.022873042
##
  98
##
  99
        G47
             G92 0.03340733 0.014101340
##
   100
        G64
             G61 0.03318244 0.024101959
        G92
             G44 0.03308052 0.013338764
##
  101
             G94 0.03297438 0.019151756
## 102
         G6
## 103
        G72
             G73 0.03273757 0.023934662
##
  104
        G81
             G23 0.03215453 0.036361903
        G37
## 105
             G61 0.03204300 0.053511280
  106
        G81
              G2 0.03199372 0.016084251
        G55
  107
             G89 0.03194773 0.014502308
##
##
  108
        G79
              G5 0.03165494 0.010691902
## 109
        G42
             G99 0.03151784 0.060846343
## 110
        G40
              G6 0.03151063 0.084998087
## 111
        G17
             G42 0.03147548 0.280873963
## 112
        G52
             G76 0.03142608 0.013721138
  113
        G13
             G42 0.03112532 0.011471305
        G18
             G88 0.03067207 0.016998158
##
  114
##
  115
        G46
             G79 0.03061646 0.009568428
## 116
        G79
             G88 0.03058667 0.014618820
## 117
        G16
             G79 0.03045550 0.037622101
        G37
              G2 0.03045396 0.009204104
## 118
        G25
             G26 0.03039506 0.016177434
##
  119
         G5
## 120
             G79 0.03018807 0.010922002
  121
         G8
             G46 0.03013462 0.016400182
  122
        G39
             G97 0.02995462 0.020425977
##
        G37
##
   123
             G41 0.02990516 0.011930989
        G51
## 124
             G13 0.02988311 0.017857681
## 125
        G11
             G29 0.02977565 0.009491852
## 126
        G80
             G60 0.02961760 0.019747560
##
  127
        G18
             G97 0.02949718 0.032383359
##
   128
        G58
             G13 0.02949252 0.009288736
  129
        G43
             G24 0.02948547 0.018347530
##
##
   130
        G96
             G44 0.02946444 0.010797919
##
  131
        G83
             G82 0.02941753 0.418905835
## 132
        G40
             G41 0.02913226 0.010459206
## 133
        G37
             G90 0.02890624 0.011492933
  134
        G42
             G20 0.02849433 0.018953389
##
##
  135
        G80
             G49 0.02846486 0.016948099
   136
        G41
             G93 0.02839658 0.038047106
  137
        G24
              G5 0.02818025 0.019503890
##
             G80 0.02813341 0.011304061
##
  138
        G18
        G37
##
  139
             G48 0.02812036 0.017863032
## 140
        G16
             G23 0.02796637 0.009208941
        G69
## 141
             G78 0.02790849 0.015470520
##
  142
        G86
              G8 0.02783405 0.010243700
        G58
##
  143
             G45 0.02773012 0.014003509
##
  144
        G32
              G4 0.02772748 0.012981682
##
   145
        G39
              G2 0.02757343 0.009158128
##
        G76
             G46 0.02743362 0.057231123
  146
## 147
        G99
             G42 0.02743241 0.010492830
## 148
        G60
             G90 0.02740925 0.014537633
## 149
        G18
             G41 0.02740297 0.012614910
```

```
## 150
        G40
             G51 0.02727947 0.012082339
## 151
        G86
             G90 0.02725303 0.011844617
   152
        G62
             G57 0.02722220 0.019749474
  153
        G79
             G16 0.02698078 0.031840512
##
##
   154
        G15
              G3 0.02684842 0.012039795
        G40
             G24 0.02673968 0.043076456
##
  155
             G46 0.02666464 0.013304635
## 156
        G86
## 157
             G27 0.02665807 0.023369549
         G9
##
  158
        G23
             G20 0.02658056 0.020575826
        G67
##
  159
             G22 0.02654312 0.014760255
  160
        G37
             G96 0.02650491 0.062020710
   161
        G55
             G68 0.02626418 0.023233419
##
##
   162
        G97
              G4 0.02620511 0.022084775
## 163
        G38
             G10 0.02618078 0.104777401
## 164
        G49
             G94 0.02610108 0.056201351
## 165
         G6
             G46 0.02598914 0.009401715
        G99
             G11 0.02595309 0.157582516
##
  166
##
   167
        G38
              G1 0.02584902 0.015432025
  168
             G51 0.02582904 0.010972166
##
         G8
##
   169
         G6
             G40 0.02578767 0.082968102
##
  170
        G57
             G44 0.02565458 0.009182807
        G23
             G30 0.02564940 0.012160931
## 171
        G81
             G14 0.02553622 0.028191590
## 172
        G88
             G16 0.02545079 0.024796099
##
  173
        G99
## 174
             G61 0.02542064 0.253702689
  175
        G87
             G85 0.02541927 0.023492212
  176
        G88
             G53 0.02538553 0.009763460
##
##
   177
        G57
             G68 0.02526282 0.010101693
        G32
## 178
             G16 0.02524275 0.019783422
## 179
        G46
             G89 0.02521256 0.056506941
## 180
        G95
             G76 0.02503465 0.016012124
##
   181
        G77
             G44 0.02499024 0.017505185
##
   182
        G14
             G97 0.02492174 0.018670561
              G7 0.02487888 0.024935121
  183
        G24
##
   184
       G100
             G35 0.02467739 0.018547887
##
##
  185
        G39
             G53 0.02455833 0.027538762
##
  186
        G47
             G83 0.02442998 0.016769833
## 187
        G62
             G15 0.02439291 0.009463404
   188
        G81
             G85 0.02435790 0.034181180
##
  189
        G61
             G37 0.02434209 0.119170130
##
   190
        G20
             G84 0.02432673 0.047375161
  191
        G83
             G24 0.02425830 0.017046953
##
##
  192
        G40
             G90 0.02416804 0.020720708
        G59
##
  193
             G32 0.02413861 0.014546624
        G42
## 194
             G18 0.02411510 0.010119378
        G42
## 195
             G17 0.02401998 0.026920027
        G69
##
  196
             G55 0.02401403 0.010038204
        G43
             G30 0.02382991 0.019871617
##
  197
##
  198
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