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.

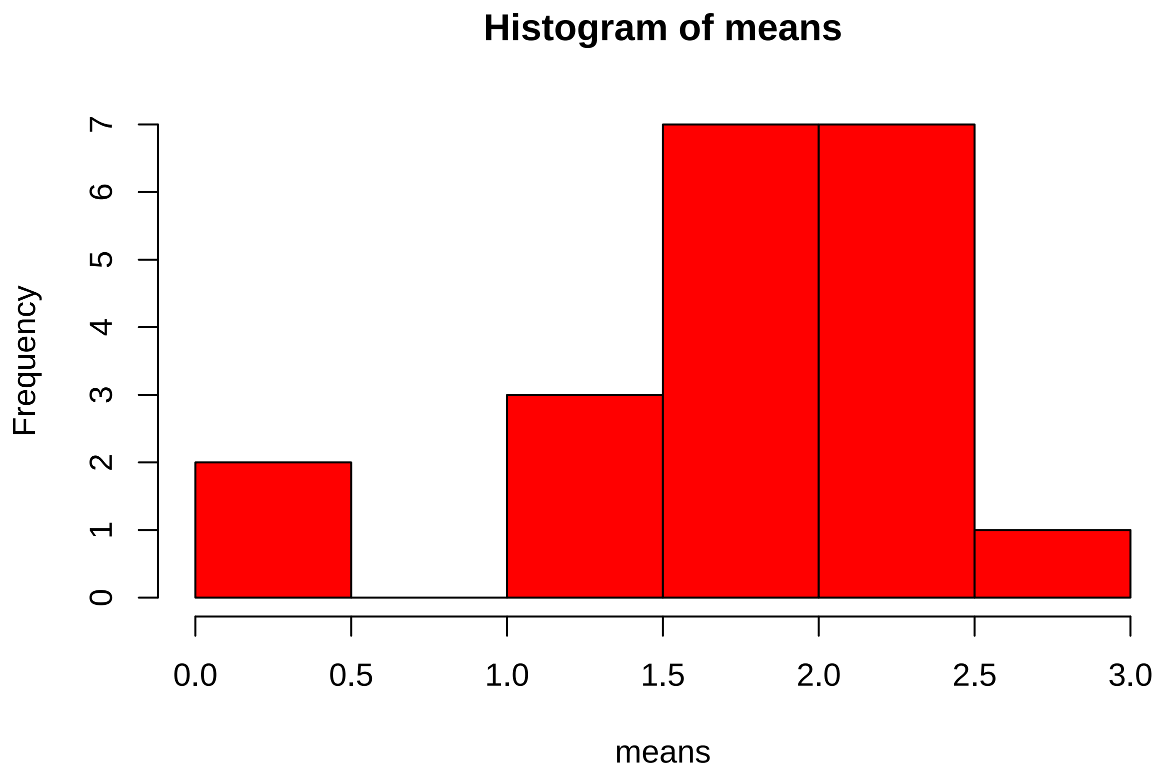
```r
# sample 100 datapoints
n_data_100 <- rnorm(100, mean = 2, sd = sqrt(8))
cat("Mean is", mean(n_data_100))
```

```
## Mean is 2.024138
```

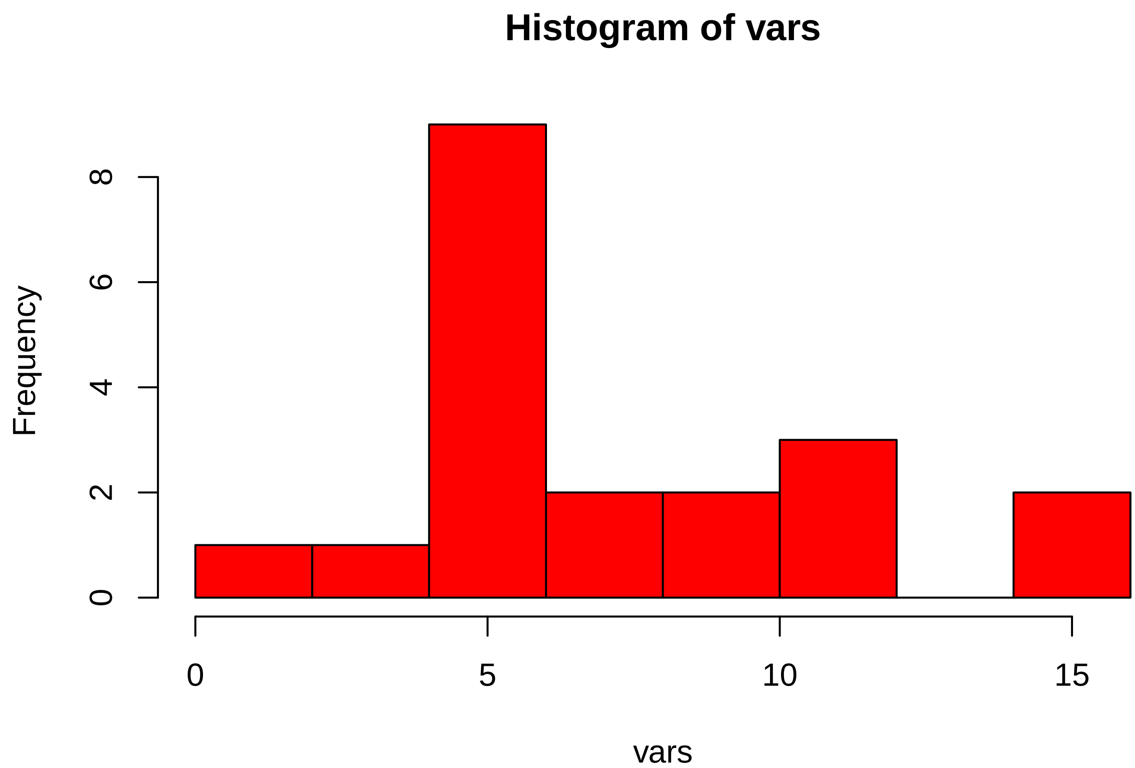
```r
cat("Var is", var(n_data_100))
```

```
## Var is 8.714753
```

```r
means <- c()
vars <- c()
N <- 20
k <- 10
for (i in 1:N) {
    this <- sample(n_data_100, k, replace = T)
    # print(this)
    means <- c(means, mean(this))
    vars <- c(vars, var(this))
}

hist(means, col = c("Red"))
```




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




```r
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

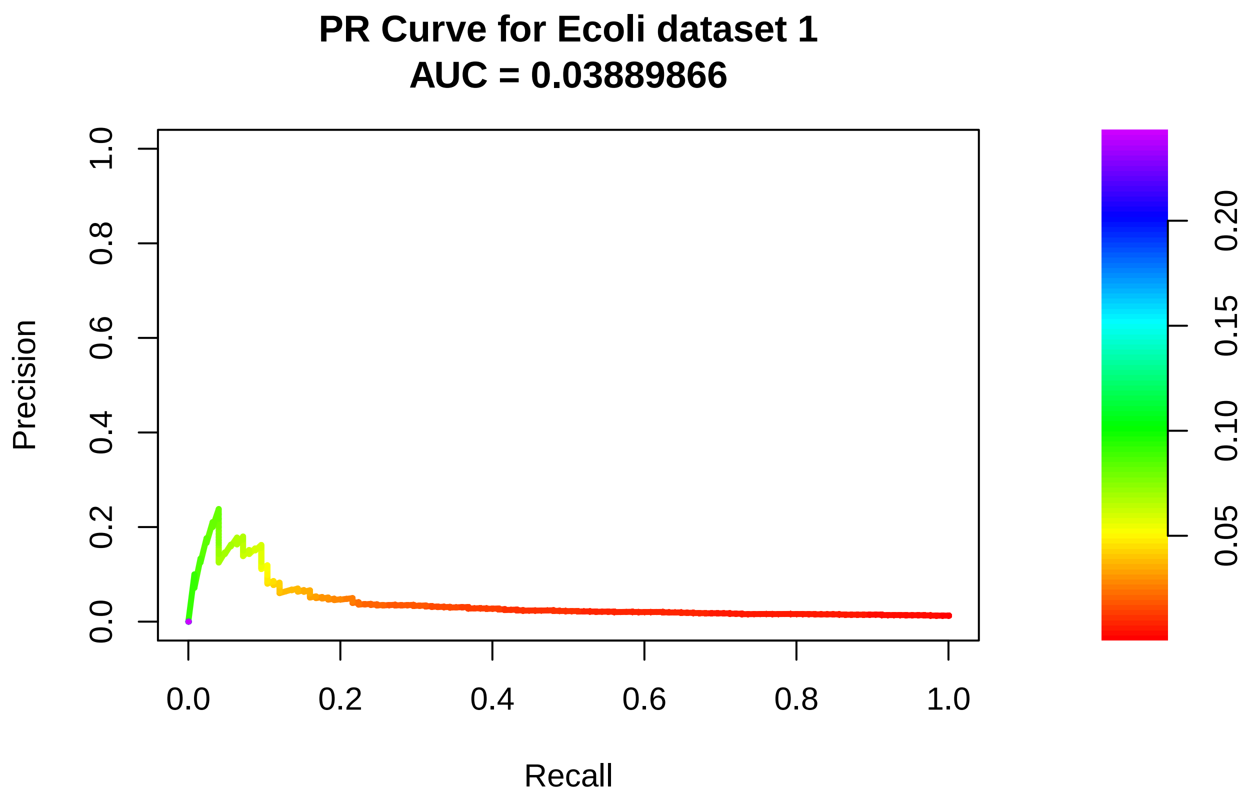
A novel association method

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.

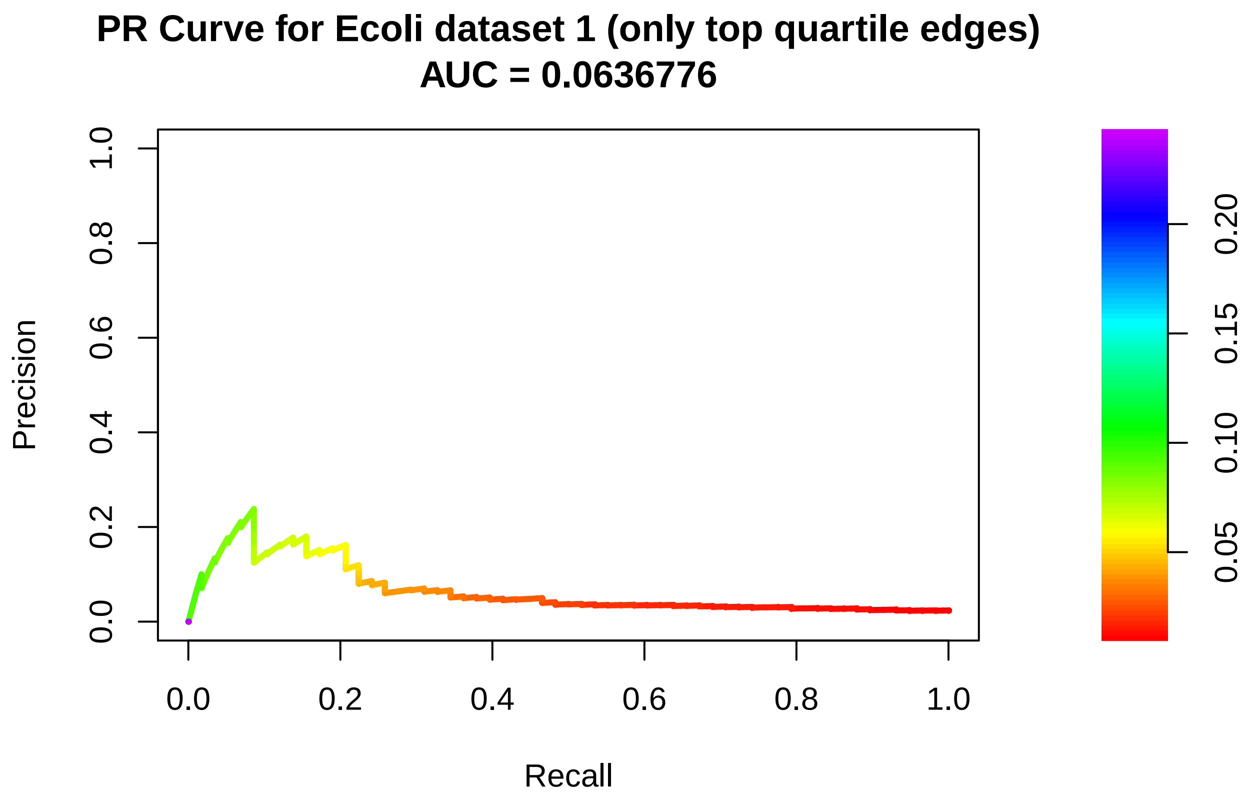
Solution 4

```
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 = "")
colnames(expmat) <- paste("Samp", 1:966, sep = "")

res1 <- GENIE3(expmat, nCores = 6, nTrees = 100)
linkList <- getLinkList(res1)
names(linkList) <- c("RG", "TG", "Weight")
names(trueEcoli1) <- c("RG", "TG", "Label")

q4thresh <- quantile(linkList$Weight, 0.75)
# q4thresh<-0.1
linkList_q4 <- linkList[linkList$Weight >= q4thresh, ]
names(linkList_q4) <- c("RG", "TG", "Weight")
joined_data <- plyr::join(linkList, trueEcoli1)
joined_data_q4 <- plyr::join(linkList_q4, trueEcoli1)
pr1 <- pr.curve(scores.class0 = joined_data$Weight, weights.class0 = joined_data$Label,
```

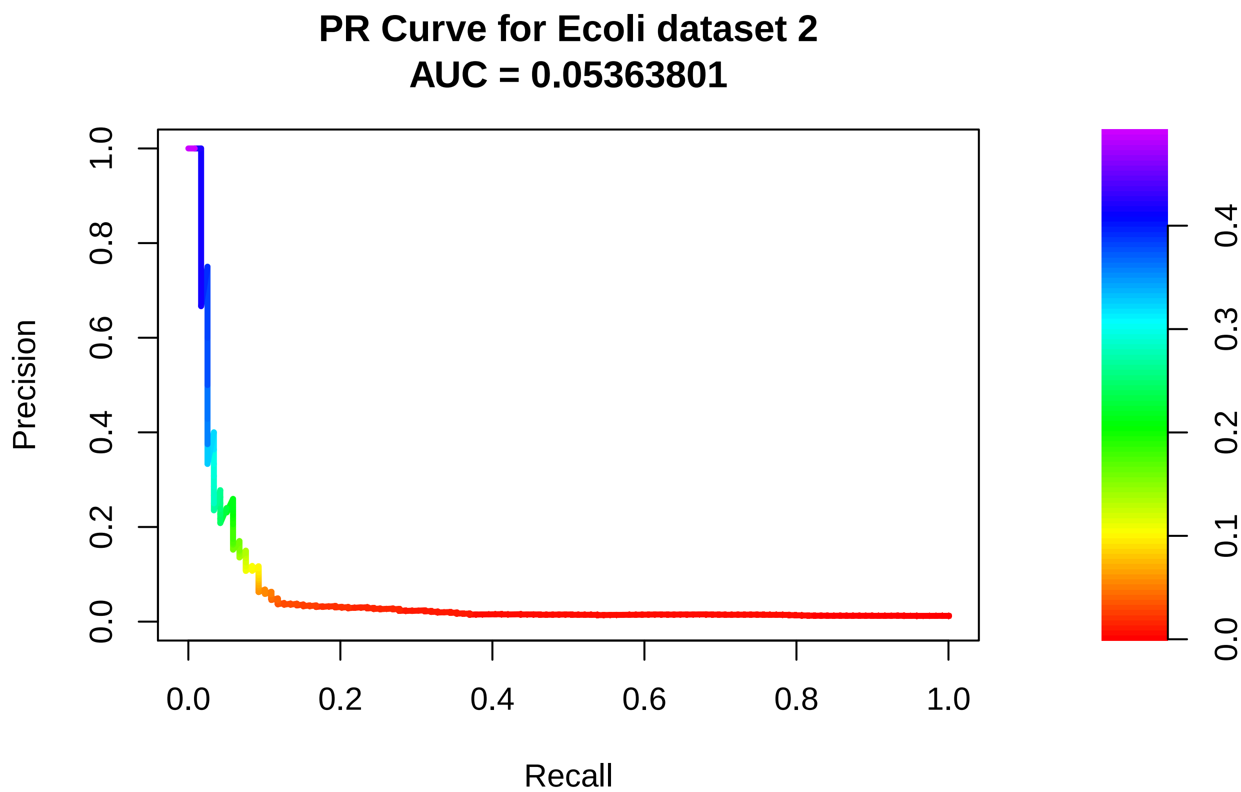
```
    curve = T)
plot(pr1, main = "PR Curve for Ecoli dataset 1")
```



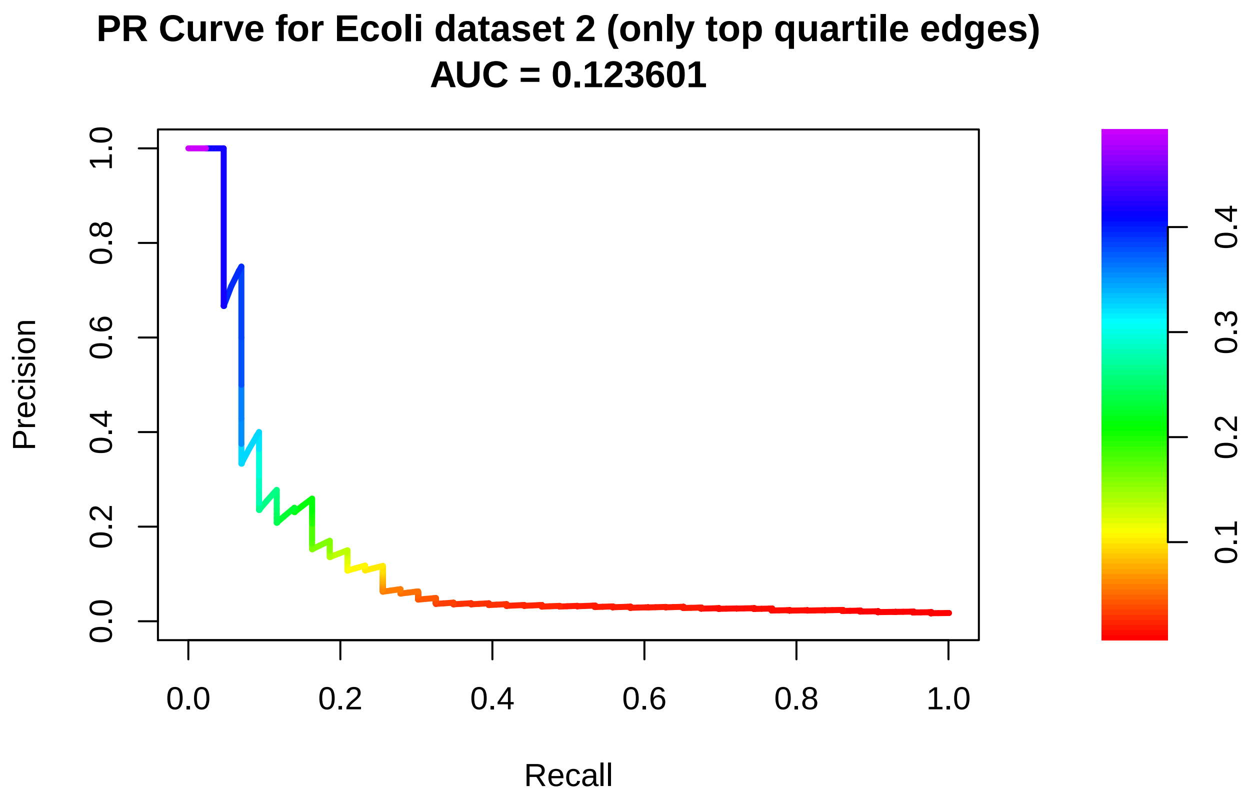

```
pr1_1 <- pr.curve(scores.class0 = joined_data_q4$Weight, weights.class0 = joined_data_q4$Label,
    curve = T)
plot(pr1_1, main = "PR Curve for Ecoli dataset 1 (only top quartile edges)")
```




```r
# 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)
expmat2 <- as.matrix(adata2[2:101, 1:966])
rownames(expmat2) <- paste("G", 1:100, sep = "")
colnames(expmat2) <- paste("Samp", 1:966, sep = "")

res2 <- GENIE3(expmat2, nCores = 6, K = "all", nTrees = 100)
linkList2 <- getLinkList(res2)
names(linkList2) <- c("RG", "TG", "Weight")

names(trueEcoli2) <- c("RG", "TG", "Label")
q4thresh2 <- quantile(linkList2$Weight, 0.75)
linkList2_q4 <- linkList2[linkList2$Weight >= q4thresh2, ]
names(linkList2_q4) <- c("RG", "TG", "Weight")
joined_data2 <- plyr::join(linkList2, trueEcoli2)
joined_data2_q4 <- plyr::join(linkList2_q4, trueEcoli2)
pr2 <- pr.curve(scores.class0 = joined_data2$Weight, weights.class0 = joined_data2$Label,
    curve = T)
plot(pr2, main = "PR Curve for Ecoli dataset 2")
```




```r
pr2_1 <- pr.curve(scores.class0 = joined_data2_q4$Weight, weights.class0 = joined_data2_q4$Label,
    curve = T)
plot(pr2_1, main = "PR Curve for Ecoli dataset 2 (only top quartile edges)")
```




```r
# 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")
```

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   G36 G34 0.05256332 0.009601923
## 30   G23 G21 0.05243834 0.011945607
## 31   G16  G9 0.05236794 0.040137635
## 32    G5 G49 0.05168572 0.022957553
## 33   G17  G5 0.05078428 0.009215007
## 34   G18 G59 0.04987122 0.009471102
## 35   G51 G87 0.04965906 0.011863316
## 36   G63 G64 0.04945444 0.171017427
## 37   G16 G80 0.04938229 0.019806393
## 38   G28 G98 0.04801344 0.010306426
## 39   G82 G83 0.04671165 0.417102096
## 40   G47 G50 0.04428631 0.009279675
## 41   G51  G8 0.04387378 0.044331969
```

```
## 42   G61  G59 0.04380656 0.009579306
## 43   G61  G64 0.04361619 0.019268455
## 44   G39  G38 0.04357242 0.015530803
## 45   G32  G59 0.04262978 0.018944100
## 46   G68  G55 0.04177970 0.011411278
## 47   G50  G47 0.04176139 0.010402571
## 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   G51  G40 0.04012734 0.019246157
## 54   G68  G70 0.04011311 0.013675525
## 55   G49   G5 0.03998728 0.012354642
## 56   G41   G2 0.03975259 0.016928342
## 57   G39  G93 0.03972749 0.011024929
## 58   G97   G2 0.03968363 0.041735961
## 59   G16  G20 0.03955842 0.011896984
## 60   G17   G8 0.03920944 0.010039812
## 61   G41  G16 0.03914060 0.010129431
## 62   G35  G26 0.03912696 0.016311448
## 63   G80   G9 0.03889456 0.011233662
## 64   G21  G79 0.03876957 0.011618636
## 65    G9  G23 0.03849022 0.010621985
## 66   G49  G31 0.03808134 0.012153970
## 67   G64  G41 0.03797340 0.023641587
## 68   G34  G36 0.03792750 0.010155900
## 69   G60  G57 0.03790503 0.095877730
## 70   G40  G80 0.03786658 0.034194037
## 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
## 75   G16  G32 0.03689561 0.016269992
## 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   G23  G59 0.03605691 0.010950341
## 82   G93  G41 0.03603287 0.061618257
## 83   G17   G6 0.03581804 0.020602758
## 84   G93  G40 0.03560491 0.117911092
## 85   G80  G40 0.03547144 0.011042922
## 86   G64  G59 0.03542134 0.009930045
## 87   G96  G49 0.03534876 0.030223350
## 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    G3  G75 0.03469260 0.024129155
## 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
## 98    G2  G95 0.03353169 0.022873042
## 99   G47  G92 0.03340733 0.014101340
## 100  G64  G61 0.03318244 0.024101959
## 101  G92  G44 0.03308052 0.013338764
## 102   G6  G94 0.03297438 0.019151756
## 103  G72  G73 0.03273757 0.023934662
## 104  G81  G23 0.03215453 0.036361903
## 105  G37  G61 0.03204300 0.053511280
## 106  G81   G2 0.03199372 0.016084251
## 107  G55  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
## 114  G18  G88 0.03067207 0.016998158
## 115  G46  G79 0.03061646 0.009568428
## 116  G79  G88 0.03058667 0.014618820
## 117  G16  G79 0.03045550 0.037622101
## 118  G37   G2 0.03045396 0.009204104
## 119  G25  G26 0.03039506 0.016177434
## 120   G5  G79 0.03018807 0.010922002
## 121   G8  G46 0.03013462 0.016400182
## 122  G39  G97 0.02995462 0.020425977
## 123  G37  G41 0.02990516 0.011930989
## 124  G51  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
## 138  G18  G80 0.02813341 0.011304061
## 139  G37  G48 0.02812036 0.017863032
## 140  G16  G23 0.02796637 0.009208941
## 141  G69  G78 0.02790849 0.015470520
## 142  G86   G8 0.02783405 0.010243700
## 143  G58  G45 0.02773012 0.014003509
## 144  G32   G4 0.02772748 0.012981682
## 145  G39   G2 0.02757343 0.009158128
## 146  G76  G46 0.02743362 0.057231123
## 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
## 155  G40  G24 0.02673968 0.043076456
## 156  G86  G46 0.02666464 0.013304635
## 157   G9  G27 0.02665807 0.023369549
## 158  G23  G20 0.02658056 0.020575826
## 159  G67  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
## 166  G99  G11 0.02595309 0.157582516
## 167  G38   G1 0.02584902 0.015432025
## 168   G8  G51 0.02582904 0.010972166
## 169   G6  G40 0.02578767 0.082968102
## 170  G57  G44 0.02565458 0.009182807
## 171  G23  G30 0.02564940 0.012160931
## 172  G81  G14 0.02553622 0.028191590
## 173  G88  G16 0.02545079 0.024796099
## 174  G99  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
## 178  G32  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
## 183  G24   G7 0.02487888 0.024935121
## 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
## 193  G59  G32 0.02413861 0.014546624
## 194  G42  G18 0.02411510 0.010119378
## 195  G42  G17 0.02401998 0.026920027
## 196  G69  G55 0.02401403 0.010038204
## 197  G43  G30 0.02382991 0.019871617
## 198  G76   G8 0.02374562 0.010659387
## 199   G4  G21 0.02366010 0.021214416
## 200  G88  G99 0.02340800 0.009097908
## 201  G94  G27 0.02328728 0.009612790
## 202  G61  G96 0.02315969 0.011370099
## 203  G90  G37 0.02297018 0.010455004
```

```
## 204   G19   G1 0.02292810 0.009300770
## 205   G86  G81 0.02291787 0.027262685
## 206   G22  G98 0.02273926 0.019581942
## 207   G32  G97 0.02266802 0.012611230
## 208    G5   G2 0.02263099 0.022866569
## 209   G32  G14 0.02251653 0.009154635
## 210   G12  G82 0.02241730 0.018755391
## 211   G79   G9 0.02241616 0.010028960
## 212 G100  G26 0.02236407 0.010134460
## 213   G19  G34 0.02222290 0.011776330
## 214   G20  G33 0.02207739 0.043474912
## 215   G98  G22 0.02195363 0.012131420
## 216    G4  G97 0.02182152 0.015194895
## 217   G13  G58 0.02165284 0.013805584
## 218   G72  G30 0.02162316 0.019717225
## 219   G17   G9 0.02154795 0.012761838
## 220   G87  G26 0.02144717 0.011536872
## 221   G65  G99 0.02142142 0.009535085
## 222   G16  G21 0.02138926 0.016677566
## 223   G77  G90 0.02130657 0.011046409
## 224   G14   G4 0.02124634 0.010807627
## 225   G22  G33 0.02115101 0.021117472
## 226   G39  G82 0.02105678 0.012661378
## 227   G64  G88 0.02105601 0.024356623
## 228   G57  G61 0.02104253 0.067656961
## 229   G30  G45 0.02098128 0.009771188
## 230   G16  G82 0.02096476 0.012933254
## 231   G49  G86 0.02095358 0.009139450
## 232   G39  G30 0.02093603 0.009215716
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## 255   G96  G37 0.01961407 0.022752283
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## 613  G25  G68 0.01108526 0.009981104
## 614   G8  G86 0.01107934 0.024254381
## 615  G53  G19 0.01104490 0.015081495
## 616  G52  G54 0.01103989 0.209010834
## 617  G76  G28 0.01102084 0.219401489
## 618  G13  G22 0.01101281 0.020753609
## 619  G55  G95 0.01101129 0.017296392
## 620  G82  G61 0.01099485 0.009630219
## 621  G81  G79 0.01096874 0.014678699
## 622  G85  G44 0.01095537 0.018304924
## 623   G5  G90 0.01094671 0.011904048
## 624  G68  G77 0.01091604 0.015218679
## 625  G55  G62 0.01091348 0.014241262
## 626  G27  G16 0.01091042 0.038545102
## 627  G12   G6 0.01090995 0.044843712
## 628  G27  G33 0.01090853 0.011222186
## 629  G76  G73 0.01090572 0.017546840
## 630  G90 G100 0.01087339 0.011563191
## 631  G69   G6 0.01087143 0.083811480
## 632  G33  G17 0.01083549 0.012155122
## 633  G13  G98 0.01082936 0.009583639
## 634  G51   G9 0.01082820 0.009158000
## 635  G26  G10 0.01080367 0.015016506
```

```
## 636   G4  G75 0.01079443 0.022248927
## 637  G58  G27 0.01078080 0.013631046
## 638  G38  G27 0.01077737 0.010191054
## 639  G21  G88 0.01076828 0.119563008
## 640  G55  G26 0.01076706 0.010049733
## 641  G80  G26 0.01076270 0.009355551
## 642  G32   G1 0.01075956 0.102490372
## 643  G22   G4 0.01075588 0.009092789
```

Q3) We have MC $X \rightarrow Y \rightarrow Z$

Where $X \perp Z \mid Y$ then $I(X,Y) \geq I(X,Z)$ [to Prove]

We know, $H(X,Y) \leq H(X) + H(Y)$

$\Rightarrow H((X, Y)|Z) \leq H(X|Z) + H(Y|Z)$

$\Rightarrow H(X|Z) \geq H((X,Y)|Z) - H(Y|Z)$

$\Rightarrow H(X|Z) \geq H(X, Y|Z)$ $[\because H(Y|Z) \geq 0]$

$\Rightarrow H(X|Z) \geq H(X|Y)$ $[\because X \perp Z \mid Y \Rightarrow H(X, Y|Z) = H(X|Y)$

$\Rightarrow H(X) - H(X|Z) \leq H(X) - H(X|Y)$

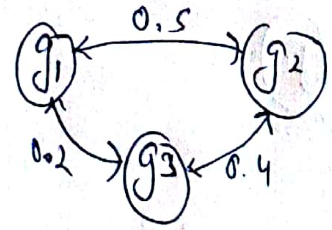
or $I(X,Z) \leq I(X,Y)$

3b) Data processing inequality (DPI): if we have $A \leftarrow B \leftrightarrow C$

then $I(A,C) \leq \min[I(A,B) ; I(B,C)]$

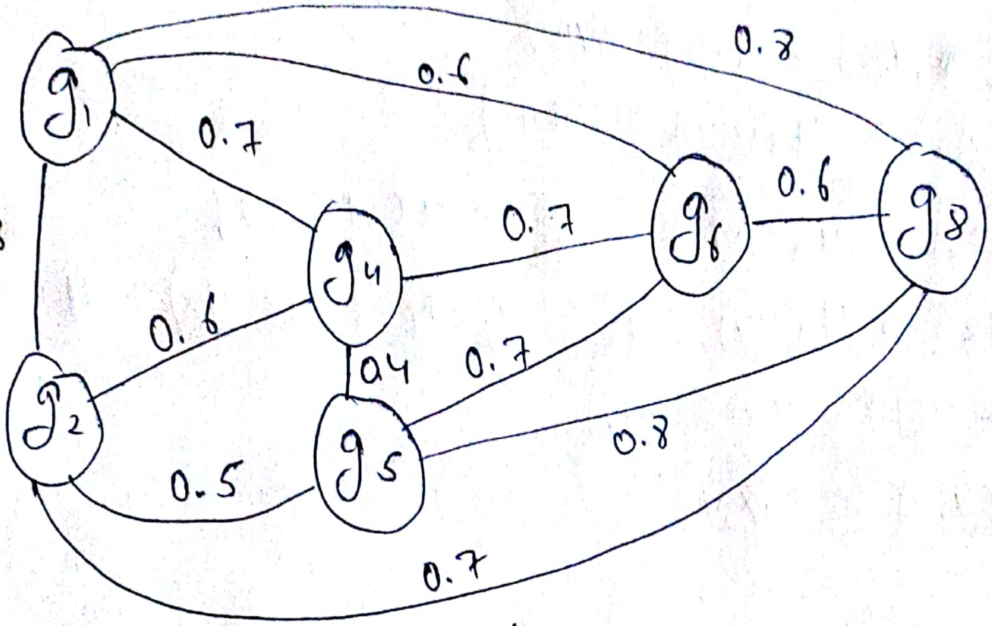
Using DPI we can remove links with smallest I in triangles.

e.g.

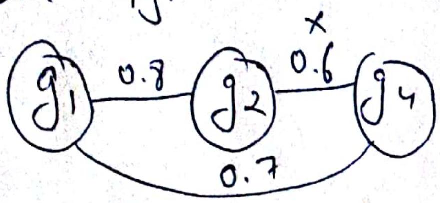


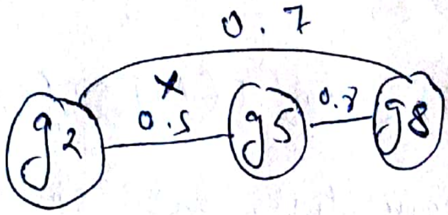
Using DPI we can remove link b/w g_1 and g_3 and simplify to $g_1 \overset{0.5}{\longleftrightarrow} g_2 \overset{0.4}{\longleftarrow} g_3$. This way we can simplify our network by removing low information edges.

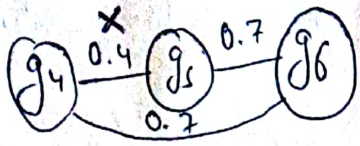
3c)

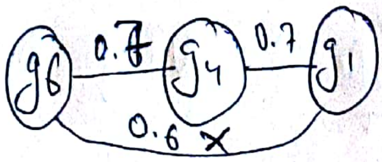


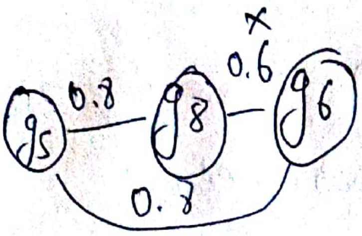
Starting at g_1 we find triangles and ~~remove~~ remove edges with lowest ~~ent~~ entropy.

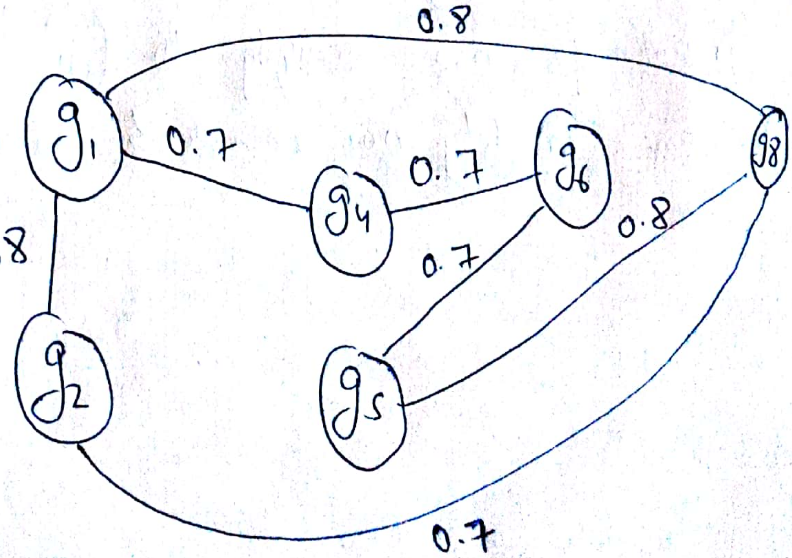












After Simplification