Beck Paper1 PCA DryAlmond and Pistachio

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Import Data:

(3 Reps each of Dry Pistacio and Dry Almond for Days 0,1,3,7)

```
dat1 <- read.csv("DataFormattedV2.csv", header=T, row.names=1,)
dat1[1:6,1:4]  # look at the first few rows
```

```
##                           DPD0R1    DPD0R2    DPD0R3    DPD1R1
## 5.043/1006.89338235294  12968378  12109546  12889863  13547220
## 5.303/1019.92814171123 179715111 168716306 172987382 182432571
## 5.377/1023.63803475936 220476339 206818874 222438879 225979379
## 6.112/1060.48629679144  39431412  35468909  36930073  40293315
## 6.182/1063.99565508021         0         0         0         0
## 6.471/1078.48429144385         0         0         0         0
```

Replace zeroes with a small value:

```
# This function will find the minimum value greater than zero
# and divide that value by two
replacezero = function(x) "[<-"(x, !x | is.na(x), min(x[x > 0], na.rm = TRUE) / 2)

# Apply function across rows
dat2 <- as.data.frame(t(apply(dat1, 1, replacezero)))
dat2[1:6,1:4]  # look at the first few rows
```

```
##                           DPD0R1    DPD0R2    DPD0R3    DPD1R1
## 5.043/1006.89338235294  12968378  12109546  12889863  13547220
## 5.303/1019.92814171123 179715111 168716306 172987382 182432571
## 5.377/1023.63803475936 220476339 206818874 222438879 225979379
## 6.112/1060.48629679144  39431412  35468909  36930073  40293315
## 6.182/1063.99565508021     77132     77132     77132     77132
## 6.471/1078.48429144385     79838     79838     79838     79838
```

```
# Log transform the data (base 2 log)
logdata <- log(dat2, 2)

# Function for pareto scaling
paretoscale <- function(z) {
  rowmean <- apply(z, 1, mean) # row means
  rowsd <- apply(z, 1, sd)  # row standard deviation
  rowsqrtsd <- sqrt(rowsd) # sqrt of sd
  rv <- sweep(z, 1, rowmean,"-")  # mean center
  rv <- sweep(rv, 1, rowsqrtsd, "/")  # dividing by sqrtsd
  return(rv)
}

# Pareto scale log transformed data
logdata.pareto <- paretoscale(logdata)

# Run PCA (note use of "t" to transpose matrix)
pca <- prcomp(t(logdata.pareto), center=F, scale=F)
```

```
# Create a container called "results" for PCA results
results <- summary(pca)

results$importance  # summary table of explained variance
```

```
##                             PC1      PC2      PC3       PC4       PC5       PC6
## Standard deviation     8.448571 1.953589 1.149988 0.9472375 0.8267369 0.6979051
## Proportion of Variance 0.878650 0.046980 0.016280 0.0110500 0.0084100 0.0060000
## Cumulative Proportion  0.878650 0.925630 0.941910 0.9529600 0.9613700 0.9673700
##                             PC7       PC8       PC9      PC10      PC11
## Standard deviation     0.632231 0.5563639 0.5415805 0.5189232 0.4884143
## Proportion of Variance 0.004920 0.0038100 0.0036100 0.0033100 0.0029400
## Cumulative Proportion  0.972290 0.9761000 0.9797100 0.9830200 0.9859600
##                             PC12      PC13      PC14     PC15      PC16
## Standard deviation     0.4383678 0.4297771 0.3994069 0.360467 0.3435429
## Proportion of Variance 0.0023700 0.0022700 0.0019600 0.001600 0.0014500
## Cumulative Proportion  0.9883200 0.9906000 0.9925600 0.994160 0.9956100
##                             PC17      PC18      PC19      PC20      PC21
## Standard deviation     0.3190758 0.2626712 0.2389219 0.2012406 0.1906502
## Proportion of Variance 0.0012500 0.0008500 0.0007000 0.0005000 0.0004500
## Cumulative Proportion  0.9968700 0.9977200 0.9984200 0.9989200 0.9993600
##                             PC22      PC23        PC24
## Standard deviation     0.1780675 0.1410183 8.59615e-15
## Proportion of Variance 0.0003900 0.0002400 0.00000e+00
## Cumulative Proportion  0.9997600 1.0000000 1.00000e+00
```

```
results$x          # scores matrix
```

```
##              PC1        PC2         PC3          PC4          PC5         PC6
## DPD0R1  -6.477680 -4.1787440  0.27687443 -0.056756200 -1.113121049  0.02932134
## DPD0R2  -5.502525 -4.2580468  0.01333411  0.097865238 -1.115301451 -0.04881901
## DPD0R3  -6.263230 -4.0026285  0.49406542  0.185894919 -0.707972684  0.13709898
## DPD1R1  -8.875632 -1.0334763  0.26948693 -0.153722315  1.518073224 -0.25277207
## DPD1R2  -7.984104 -0.9637881  0.21446055 -0.050377868  1.695093213 -0.02644602
## DPD1R3  -7.886679 -0.6593741  0.27183137 -0.068227059  2.158856992  0.06033400
## DPD3R1 -10.147961  2.0474627 -0.02471014 -0.255258694  0.238408196 -0.06134058
## DPD3R2  -8.246734  1.3859866 -0.21630463  0.004463907 -0.097950038  0.09842351
## DPD3R3  -8.562518  0.8733620 -0.03375991  0.026726657 -0.065596922  0.10501314
## DPD7R1 -10.323879  2.6622186 -0.08207349  0.011773321 -1.091426972 -0.07583191
## DPD7R2  -9.168648  2.1368543 -0.14717912  0.125161702 -0.592007544 -0.01652720
## DPD7R3  -9.027081  3.5442396 -0.69045212  0.064899713 -1.013289751  0.04407047
## DAD0R1   7.930649 -0.4289846 -2.88132198  0.436899865  0.188067804 -0.37088029
## DAD0R2   7.526477 -0.8608231 -2.96413032  0.478806114 -0.003577976 -0.42990718
## DAD0R3   8.502702  0.1277276 -1.74492752  0.191226992  0.368714661  0.15044010
## DAD1R1   8.394591  0.2623536  0.25651495 -1.655763681 -0.119743755 -0.03654745
## DAD1R2   8.676173  0.2281222  0.88256303 -3.250499181 -0.226020181 -0.71236414
## DAD1R3   8.204982  0.2264660  0.14944458 -1.099995431  0.045142451  1.19150923
## DAD3R1   8.533326  0.6243563  1.54055026  0.995859416  0.015874543 -0.88727703
## DAD3R2   8.196290  0.4837437  0.61824199  0.193403525  0.012348953 -0.77558148
## DAD3R3   7.950754  0.2459457 -0.23055958  0.194148339  0.056747330  1.05016738
## DAD7R1   8.203658  0.5105451  1.45695486  1.485921810 -0.117965827 -1.60843478
## DAD7R2   8.317901  0.6832509  1.52342130  1.158825943  0.011436376  0.60180364
## DAD7R3   8.029168  0.3432306  1.04767502  0.938722970 -0.044789593  1.83454735
##                PC7         PC8         PC9         PC10         PC11
## DPD0R1  0.0673728008  0.19514744  0.61707022 -0.33925927  1.06005274
## DPD0R2 -0.4753353631 -0.21107629 -0.32991561  0.50662729  0.03700842
## DPD0R3  0.4904485595 -0.18038511 -0.24947587 -0.52842026 -0.89719703
## DPD1R1  0.0002369267  0.43295232  0.19461007  0.53075734  0.12570308
## DPD1R2 -0.5607101109  0.21814995  0.12487497 -0.19290549 -0.66635648
## DPD1R3 -0.5305838015 -0.14561155  0.25104887 -0.32939244  0.70286117
## DPD3R1  1.5880430063 -0.51503342 -0.58713986  0.42753793  0.51054719
## DPD3R2  0.3678427771 -0.60590110 -0.62077198  0.19111473  0.05895691
## DPD3R3  0.0824693279 -0.68273256 -0.80912140 -0.09219305 -0.86560675
## DPD7R1  0.6762940189  0.63179767  0.46082823  0.06078261  0.35133579
## DPD7R2 -0.0377382680  1.49559565  0.80446276  0.29611736 -0.77087651
## DPD7R3 -1.8548812266 -0.74837218  0.11498053 -0.64492647  0.32277652
## DAD0R1  0.1044626030  0.10562493 -0.04276408  0.22479467  0.02888483
## DAD0R2 -0.4610521560 -0.01465900 -0.19017497  0.67991591 -0.04552944
## DAD0R3  0.8952971275 -0.23832789  0.62127073 -0.54983697  0.14347414
## DAD1R1 -0.4630724589  1.31635523 -1.59760683 -0.17025207  0.36475366
## DAD1R2 -0.1046300018 -0.72498358  0.82377425  0.71679443 -0.26160123
## DAD1R3  0.2328628127 -0.09760955  0.15487417 -0.62163147 -0.04172698
## DAD3R1  0.1491564695  0.05086618 -0.20251621 -0.27327431  0.53014463
## DAD3R2  0.2249186851  0.06591666  0.04176474 -0.96130835 -0.24042225
## DAD3R3  0.2067192031  0.01751816  0.19311374 -0.61592106 -0.33073688
## DAD7R1 -0.1343881762 -0.26272533  0.15713050  0.26452229 -0.28089508
## DAD7R2 -0.1387028235  0.08268815 -0.09588256  0.41121285  0.07660118
## DAD7R3 -0.3250299316 -0.18519479  0.16556560  1.00914382  0.08784836
##               PC12         PC13        PC14        PC15         PC16
## DPD0R1  0.66523510 -0.305803578  0.14899955 -0.35964429  0.583011844
## DPD0R2 -1.02589533  0.448869670 -0.04525016 -0.17426671  0.032474129
```

```
## DPD0R3  0.37054007 -0.197258468 -0.10743332  0.67218281 -0.780176843
## DPD1R1 -0.84225122  0.358837513 -0.75426341  0.14563412  0.097136367
## DPD1R2  0.71537181 -0.037097724 -0.23895630 -0.21833398  0.270459733
## DPD1R3 -0.06499801 -0.287675580  0.67690235  0.23284841 -0.354768271
## DPD3R1  0.02297251 -0.086411954 -0.06470708  0.00894897  0.128278470
## DPD3R2 -0.13417974 -0.093696362  0.93856195 -0.16987047 -0.227310402
## DPD3R3  0.38163863  0.184959972 -0.30087844 -0.44464897  0.562224396
## DPD7R1 -0.05502779 -0.136920174 -0.27675024  0.47732429 -0.059163212
## DPD7R2  0.02385033  0.172283209  0.48149025 -0.40006200 -0.166868989
## DPD7R3 -0.05663770  0.006259720 -0.41520007  0.19440080 -0.135357017
## DAD0R1  0.27079976  0.082837756 -0.01024591  0.30112611 -0.006068772
## DAD0R2  0.15660943  0.101731942  0.38170241 -0.09838991 -0.017958804
## DAD0R3  0.01676062 -0.172473406 -0.72261788 -0.13400894 -0.124485280
## DAD1R1  0.10119690 -0.465672469 -0.22838462  0.07854916 -0.039516721
## DAD1R2  0.25031175  0.124390703  0.07817285  0.18913386 -0.030066490
## DAD1R3 -0.43752185 -0.102557083  0.04670191 -0.70472267 -0.221913063
## DAD3R1  0.44478000  1.155732045 -0.15376943 -0.49157843 -0.628647024
## DAD3R2 -0.34793687  0.594372493  0.51061044  0.57039292  0.677951735
## DAD3R3 -0.63914738 -0.141688053  0.21098188  0.00437589  0.170246628
## DAD7R1 -0.37716331 -1.264838936 -0.11540344 -0.32321096 -0.044535503
## DAD7R2  0.24975614  0.062218986  0.08288806  0.50349190  0.402020217
## DAD7R3  0.31093617 -0.000400221 -0.12315137  0.14032809 -0.086967128
##                PC17         PC18         PC19         PC20         PC21
## DPD0R1 -0.056046543  0.004638255 -0.02955344  0.196097033 -0.148211699
## DPD0R2  0.284858670 -0.012143768  0.12293014 -0.309099355  0.264145111
## DPD0R3 -0.114658196 -0.146108298  0.02549834  0.113776345 -0.070706895
## DPD1R1 -0.143470124  0.126036867 -0.08645313  0.406941727 -0.229251727
## DPD1R2 -0.359258266  0.347034886  0.46842674 -0.192075521  0.210995587
## DPD1R3  0.281819113 -0.279389897 -0.37420164 -0.242394779  0.040355095
## DPD3R1 -0.239416100 -0.599569565  0.41205865 -0.049390280  0.018771083
## DPD3R2  0.271671872  0.742975123  0.16013018  0.281146820 -0.047025166
## DPD3R3  0.250044654 -0.098680319 -0.63130482 -0.071529982 -0.090275758
## DPD7R1 -0.419897193  0.464654501 -0.35789643 -0.358533213  0.142366429
## DPD7R2  0.400468642 -0.354098350  0.09695486  0.087424985 -0.033640402
## DPD7R3 -0.024593821 -0.171632693  0.21372855  0.141010400 -0.029293050
## DAD0R1  0.006217721 -0.041360265 -0.20554407  0.266799421  0.156150567
## DAD0R2 -0.504717941 -0.085343823  0.02189118 -0.167777721 -0.102781804
## DAD0R3  0.856107854  0.169992808  0.18474288 -0.127373519  0.016753122
## DAD1R1  0.205935586  0.026980450  0.04866138 -0.037993778 -0.081046412
## DAD1R2  0.039673569  0.008031905 -0.05467479  0.024381848  0.005596649
## DAD1R3 -0.408643246 -0.071779579 -0.06377961  0.053232618  0.246144032
## DAD3R1 -0.168050004  0.041339482 -0.08904086  0.007150664 -0.019395391
## DAD3R2  0.080234728  0.002094377  0.19857296 -0.168750992 -0.219601452
## DAD3R3 -0.446434196 -0.026368940 -0.09333623  0.099924697 -0.129583683
## DAD7R1 -0.081660918 -0.020271467 -0.02015968 -0.012112084 -0.040897798
## DAD7R2  0.182659096 -0.091027050 -0.03740499  0.274265103  0.532946262
## DAD7R3  0.107155044  0.063995360  0.08975384 -0.215120437 -0.392512701
##                PC22         PC23         PC24
## DPD0R1 -0.012558782 -0.007161070 8.451573e-15
## DPD0R2  0.161186241 -0.011622200 8.715251e-15
## DPD0R3 -0.115551904  0.012971869 8.715251e-15
## DPD1R1 -0.166348637  0.033874939 9.089951e-15
## DPD1R2  0.144556214 -0.006508562 8.854029e-15
## DPD1R3  0.012300320 -0.018163619 8.507084e-15
```

```
## DPD3R1  0.078191666 -0.008623002 9.159340e-15
## DPD3R2 -0.022719744 -0.004284545 8.257284e-15
## DPD3R3 -0.041955945 -0.007711880 8.867906e-15
## DPD7R1 -0.020934541  0.015160609 8.645862e-15
## DPD7R2  0.010235946 -0.006994437 8.798517e-15
## DPD7R3 -0.007961345  0.003454763 8.437695e-15
## DAD0R1  0.445736065  0.261918460 8.239937e-15
## DAD0R2 -0.422789613 -0.139641615 8.083811e-15
## DAD0R3 -0.138839951 -0.124947432 8.368306e-15
## DAD1R1  0.018658966 -0.043424580 8.396062e-15
## DAD1R2  0.057849304 -0.081913900 8.493206e-15
## DAD1R3 -0.214754445  0.309845810 8.520962e-15
## DAD3R1  0.093181103 -0.089132964 8.396062e-15
## DAD3R2 -0.092784579  0.200518744 8.132384e-15
## DAD3R3  0.327548468 -0.391688814 8.160139e-15
## DAD7R1  0.041933462  0.063115766 8.576473e-15
## DAD7R2 -0.225542574 -0.121571456 7.993606e-15
## DAD7R3  0.091364305  0.162529115 8.465451e-15
```

```
results$rotation    # loadings matrix
```

```
##                               PC1           PC2           PC3           PC4
## 5.043/1006.89338235294  -0.08845888 -0.0355775573  2.038417e-02 -9.357645e-03
## 5.303/1019.92814171123  -0.24936209 -0.1167348158  6.262671e-02  1.252895e-02
## 5.377/1023.63803475936  -0.25030428 -0.1175009609  5.333553e-02 -7.037384e-02
## 6.112/1060.48629679144  -0.08811077 -0.0343223677  1.890489e-02 -9.728073e-03
## 6.182/1063.99565508021   0.08048505  0.0711408259  4.231779e-01 -1.531799e-01
## 6.471/1078.48429144385   0.01131770  0.0066152356  1.866600e-02 -1.775847e-01
## 7.058/1106.0608         -0.08837345 -0.0353210968  1.964699e-02 -8.945860e-03
## 7.379/1118.3872         -0.09086866 -0.0512464646  2.509138e-02 -8.642286e-03
## 7.643/1128.5248         -0.08978261 -0.0279161229  1.828893e-02 -7.259922e-03
## 7.791/1134.208          -0.10577537  0.0775527201 -5.319538e-03 -1.246902e-02
## 8.088/1145.6128         -0.08733653 -0.0402839844  2.080505e-02 -7.622861e-03
## 8.483/1160.7808         -0.09010638 -0.0449654007  2.459273e-02 -8.305169e-03
## 8.896/1176.64           -0.09179048 -0.0445912982  2.495271e-02 -1.093943e-02
## 9.435/1197.3376         -0.22160293 -0.1026255386  4.146794e-02 -2.080990e-02
## 9.679/1205.86545278161  -0.09381509 -0.0052034964  1.256674e-02 -8.651886e-03
## 10.384/1229.53994253946 -0.16201517  0.0914015678  6.065197e-02  1.775306e-01
## 10.505/1233.60322376031 -0.09446998 -0.0168296826  1.275339e-02 -5.720509e-03
## 10.797/1243.4088280288  -0.08963538 -0.0388580998  1.887311e-02 -4.341104e-03
## 10.924/1247.67359426887  0.10785289  0.0554629989  1.056992e-02 -1.187825e-01
## 10.987/1249.78918697064 -0.09264268 -0.0418190382  2.384062e-02 -6.084569e-03
## 11.073/1252.67713891273 -0.09744654 -0.0891495138  3.941017e-02 -6.388905e-03
## 11.503/1267.11689862319 -0.08766678 -0.0288930931  1.750889e-02 -7.690867e-03
## 11.912/1280.85146076639 -0.23041310 -0.1036322699  4.534021e-02 -9.113576e-05
## 13.327/1327.1729807005  -0.12389701  0.0467427427  8.557701e-03 -1.641854e-02
## 14.185/1354.77126518942  0.01106028  0.0128733762  1.060193e-01  1.593687e-01
## 15.299/1390.60400285919 -0.09980876 -0.0431664471  3.546139e-02 -1.544735e-02
## 15.314/1391.08649035025  0.11892037  0.0523596300 -9.140270e-02  2.768278e-02
## 16.191/1419.68598681524 -0.10972513 -0.0998832145  4.394927e-02 -1.522885e-02
## 16.259/1421.91747856018 -0.12502291  0.0262948077  4.778575e-03 -2.440024e-02
## 16.602/1433.17338545009 -0.09909973  0.0387475007  1.615296e-03 -8.480805e-03
## 16.724/1437.17694416895 -0.09233465 -0.0253339385  1.834796e-02 -9.242603e-03
## 16.908/1443.21509830232 -0.12729375 -0.2176308629  7.670120e-02 -2.116202e-02
## 17.155/1451.32066390526  0.05217636  0.3217630674  1.675739e-01  5.957312e-02
## 17.292/1455.81646345021 -0.10729698 -0.0639415705  4.331677e-02 -2.578574e-02
## 17.351/1457.75261069949  0.10608888  0.0448152595 -9.046613e-02  1.854077e-01
## 17.578/1465.00495887054 -0.10159717  0.0425332308  3.246157e-03 -1.336905e-02
## 18.073/1481.44580246193 -0.08742928  0.2417375694 -3.621955e-02 -2.987976e-02
## 18.481/1494.83475293157 -0.08115631  0.1934089643 -2.292268e-02 -3.566921e-02
## 18.545/1496.93498045622  0.05935228  0.0640227179  4.273073e-01  2.386696e-02
## 18.959/1510.7521008806  -0.14149450 -0.1314772714  7.059602e-02 -8.939927e-03
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## 19.858/1540.90225275726  0.09326273  0.0453570196 -1.194473e-02  1.113639e-01
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## 21.633/1600.45331372332 -0.11717192  0.0552261435 -1.355440e-02 -2.067591e-03
## 21.645/1600.87640653175  0.09379697  0.0475139150  1.824249e-02 -9.644033e-02
## 22.124/1617.7648611349  -0.11321788  0.1112857062 -1.565531e-02 -1.277811e-02
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## 22.437/1628.8005318881  -0.09074293 -0.0237420040  1.471417e-02 -6.795403e-03
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## 23.492/1665.99744129587  0.03157057  0.0165586643  1.064517e-01 -6.774315e-01
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## 23.746/1674.95290574097 -0.07835609  0.2021226169 -3.323635e-02 -2.345562e-02
## 23.877/1679.57166889966 -0.10302284 -0.0999527767  3.258420e-02 -1.258862e-02
## 24.102/1687.50465905771 -0.09576110  0.0216328020  1.637987e-03 -1.050056e-02
## 24.278/1693.71002024801  0.10295972  0.0494064894 -7.205291e-02  8.511475e-02
## 24.301/1694.52094813084 -0.06702651  0.3122062094 -9.320829e-02  3.393143e-03
## 24.399/1697.97620606634 -0.12175011  0.1451600911 -2.532239e-02 -1.930557e-02
## 24.495/1701.40537391684 -0.10520618  0.0325345669  7.671600e-03 -1.711560e-02
## 24.592/1704.9370130343  -0.08583485  0.2228773926 -3.530611e-02 -1.830048e-02
## 25.163/1725.72635258137 -0.11062260  0.0614739714 -7.836664e-03 -1.019532e-02
## 25.273/1729.73130415787 -0.10993675  0.0753276059 -1.615017e-02 -1.344823e-02
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## 27.512/1811.78220086937  0.01169733  0.0057520927  6.422208e-02 -3.486240e-01
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## 28.435/1846.97628307786 -0.09618243  0.0206624098  6.121439e-05 -9.120552e-03
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## 34.508/2091.7501473188   0.16455233  0.1243291305  4.677275e-01 -7.879952e-02
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## 5.303/1019.92814171123  -0.0449608566  0.0406168138 -0.049454460 -0.077297320
## 5.377/1023.63803475936  -0.0501625079 -0.0130144397 -0.043032745 -0.095671500
## 6.112/1060.48629679144  -0.0149194319 -0.0074289077  0.047483669 -0.002876969
## 6.182/1063.99565508021  -0.0465191588  0.3481687566 -0.113396369 -0.012813999
## 6.471/1078.48429144385  -0.0168594405 -0.0072208661 -0.111486517  0.409241940
## 7.058/1106.0608         -0.0200507754 -0.0070021012  0.056308477  0.003399530
## 7.379/1118.3872         -0.0216116347 -0.0059728294  0.072659810  0.006485353
## 7.643/1128.5248         -0.0361227407 -0.0068030787  0.051701119  0.016094709
## 7.791/1134.208          -0.0020316432 -0.0138780254  0.032506644  0.074868784
## 8.088/1145.6128         -0.0083413927 -0.0034710652  0.035365265 -0.018122494
## 8.483/1160.7808          0.0113100056 -0.0032806999  0.036514603 -0.020056605
## 8.896/1176.64            0.0269585913 -0.0064325036  0.051006579 -0.020447740
## 9.435/1197.3376         -0.0352750530  0.0734794909 -0.047912351 -0.083442944
## 9.679/1205.86545278161   0.0010017990 -0.0159045689 -0.052853024  0.090490033
## 10.384/1229.53994253946 -0.0794083352 -0.0820167623 -0.113693944  0.165187337
## 10.505/1233.60322376031 -0.0223482181 -0.0154950606 -0.089147098  0.127957815
## 10.797/1243.4088280288  -0.0540792479 -0.0014324792 -0.005679584 -0.007856649
## 10.924/1247.67359426887  0.0206433174  0.0118529455  0.058845797  0.140405718
## 10.987/1249.78918697064  0.0053413612 -0.0042360601 -0.010132783  0.026359196
## 11.073/1252.67713891273  0.0629854985 -0.0048967132 -0.031526394  0.043536711
## 11.503/1267.11689862319  0.0008648284 -0.0066964796  0.019273287  0.019094242
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## 14.185/1354.77126518942 -0.0166091154 -0.3177866568 -0.032354482 -0.081678730
## 15.299/1390.60400285919 -0.0298079468 -0.0213645605  0.240317181  0.156296737
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## 16.191/1419.68598681524  0.0112560774 -0.0210777669  0.178624747  0.087786760
## 16.259/1421.91747856018 -0.0836147513 -0.0277673092  0.182435990  0.102810723
## 16.602/1433.17338545009 -0.0511388986 -0.0074059069  0.029022279  0.045601005
## 16.724/1437.17694416895 -0.0668529384 -0.0032597680  0.094981134  0.049407518
## 16.908/1443.21509830232  0.1227558155 -0.0075844703  0.141803805 -0.211936261
## 17.155/1451.32066390526  0.1175712211  0.1340710436  0.336083384 -0.039055341
## 17.292/1455.81646345021  0.2685945481  0.0050640298  0.167848341 -0.303067329
## 17.351/1457.75261069949  0.0368399904  0.0055307016  0.013371195  0.037594547
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## 18.073/1481.44580246193  0.1525371111 -0.0278896570  0.166031401  0.058882518
## 18.481/1494.83475293157  0.3232301763 -0.0159810830  0.127309244 -0.142223363
## 18.545/1496.93498045622 -0.0479583001 -0.7547353274 -0.038347933 -0.016747567
## 18.959/1510.7521008806   0.0491541171 -0.0191056398  0.341420366  0.316741585
## 19.117/1516.05101522599 -0.0137285469  0.0615259806 -0.087209333 -0.075278568
## 19.858/1540.90225275726  0.0251726325 -0.0062035626  0.042590534  0.025329835
## 20.097/1548.91769914048 -0.0357208192  0.0079020601  0.167142881  0.154189569
## 20.544/1563.9089314974   0.0529617226 -0.0052346593  0.164008401  0.075056575
## 20.574/1564.91505447437 -0.0122973535  0.0003376958 -0.068711927 -0.124737916
## 20.758/1571.08594206648  0.0338442633 -0.0135012444 -0.035271938  0.060736798
## 20.954/1577.65927884938  0.0232230057  0.0597404491  0.076221870  0.027423095
## 20.982/1578.59832696122  0.0454908974 -0.0091948657  0.002696735 -0.003448796
## 21.413/1593.05296039708  0.1137805390 -0.0194698027 -0.072907108 -0.058332348
## 21.633/1600.45331372332 -0.2220220317  0.0013208067 -0.020559580 -0.034988642
## 21.645/1600.87640653175  0.0140152092  0.0215743488  0.040913852  0.102023792
## 22.124/1617.7648611349  -0.0020179148 -0.0103484496 -0.054782191  0.032578218
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## 22.813/1642.05743988556  0.0114671030 -0.0098922230 -0.016057703 -0.006463485
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## 23.492/1665.99744129587 -0.0517108658 -0.0441277840 -0.090077285  0.022686469
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## 24.592/1704.9370130343   0.2230251405 -0.0200808686 -0.089530046  0.172792309
## 25.163/1725.72635258137 -0.0161626054 -0.0153362632 -0.185528702  0.198317359
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## 25.295/1730.53229447317  0.0932053844 -0.0103411159  0.020266655  0.014711281
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##                                   PC9           PC10          PC11          PC12
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## 5.303/1019.92814171123   0.0104093197 -0.0877208883 -0.0130960360 -0.0249715584
## 5.377/1023.63803475936   0.0327962998 -0.0916475264 -0.0472192046 -0.0588990018
## 6.112/1060.48629679144   0.0004487349  0.0021158120  0.0404425420  0.0126566621
## 6.182/1063.99565508021   0.0149747768  0.2087486681 -0.0729332355 -0.0672097874
## 6.471/1078.48429144385  -0.5241659084 -0.0608430789  0.1471458275  0.0506774753
## 7.058/1106.0608          0.0020365290  0.0029412813  0.0378783750  0.0041202024
## 7.379/1118.3872          0.0013965877 -0.0047396511  0.0283256158  0.0253903598
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## 7.791/1134.208           0.0293138244  0.0509026184 -0.0415636693 -0.0123418006
## 8.088/1145.6128         -0.0101719248 -0.0193056011  0.0125576248  0.0213013164
## 8.483/1160.7808         -0.0070979702 -0.0362578723  0.0077621180  0.0477735472
## 8.896/1176.64           -0.0138918677 -0.0169293783  0.0153827173  0.0508666973
## 9.435/1197.3376          0.0153756547 -0.0846598843 -0.0337520479 -0.0271302526
## 9.679/1205.86545278161   0.0961106671 -0.0185640501 -0.0015867820  0.0178000783
## 10.384/1229.53994253946 -0.0314492124  0.0081270916 -0.2644848423 -0.1962357897
## 10.505/1233.60322376031  0.1222272458 -0.0152387735 -0.0318887240  0.0264437698
## 10.797/1243.4088280288   0.0137759832 -0.0588950947 -0.0157947205  0.0704960861
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## 17.292/1455.81646345021 -0.2817066613 -0.0094259088 -0.0114755025  0.0905060765
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## 18.959/1510.7521008806   0.0214425954  0.1764642539 -0.3993170685  0.0514370106
## 19.117/1516.05101522599  0.0032330296  0.4210913216  0.1707988225  0.3101426295
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## 23.476/1665.4333175513  -0.0869488139  0.0351330644  0.0695891032  0.0313672348
## 23.492/1665.99744129587 -0.0457825519  0.1477508399 -0.0276760848  0.0699050523
## 23.646/1671.42713233739  0.0005223156  0.0013650618  0.1441861015 -0.0954889098
## 23.746/1674.95290574097  0.0271115230  0.0123593020  0.1048275791 -0.0662482910
## 23.877/1679.57166889966  0.0276383094 -0.0300542446  0.2514139231 -0.1009710189
## 24.102/1687.50465905771  0.0553718236 -0.0241342716  0.1080117838 -0.0093480232
## 24.278/1693.71002024801  0.2103737432 -0.1291212462 -0.0177597981 -0.0437419256
## 24.301/1694.52094813084  0.0231919860  0.0048125976  0.0060802437 -0.0005644231
## 24.399/1697.97620606634  0.1086860809  0.0968816010  0.3075179939 -0.3453621166
## 24.495/1701.40537391684  0.0442118999  0.0090099865  0.0828360465  0.0164318635
## 24.592/1704.9370130343   0.1284567990  0.0613717003 -0.0420091303 -0.0122684801
## 25.163/1725.72635258137  0.2846833013 -0.0673057799  0.2133297063  0.0186351012
## 25.273/1729.73130415787  0.0244388720 -0.0719170147  0.0884773414 -0.0057273912
## 25.295/1730.53229447317  0.0036463452  0.0407135546  0.0448027856  0.0067118623
## 25.922/1753.36051845919 -0.0426318489 -0.0234280844  0.1255985558  0.0533338719
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## 26.581/1777.35381926746 -0.0333713930 -0.0058234220 -0.1377847120 -0.0271572785
## 27.512/1811.78220086937  0.2702757439  0.2561612314 -0.1055329505  0.1253513466
## 27.667/1817.692366354    0.0242871612 -0.0281508328 -0.0226701358  0.0713528208
## 28.086/1833.66887821246  0.0223560456 -0.0341733924  0.0361786711  0.1484400097
## 28.435/1846.97628307786  0.0285015223 -0.0196344963  0.1321131441  0.0218550712
## 30.206/1915.20019180053 -0.2515800930  0.0420638279 -0.0154220677  0.0633644612
## 32.534/2008.66234531526 -0.2194582501 -0.0552561681 -0.0251617071  0.0489041726
## 34.508/2091.7501473188   0.2004422412 -0.2272102323 -0.0277834120 -0.2591017742
##                                 PC13          PC14          PC15         PC16
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## 5.303/1019.92814171123   0.0572083789  0.0580662451 -0.0561960429 -0.058282442
## 5.377/1023.63803475936  -0.0735968957  0.0002617753 -0.1471208502 -0.141797723
## 6.112/1060.48629679144  -0.0022509650 -0.0421958433  0.0027697470  0.030889546
## 6.182/1063.99565508021  -0.0572977552  0.1602329670  0.2680541976  0.289359760
## 6.471/1078.48429144385  -0.2426157268 -0.1377719344  0.0581748908 -0.032221361
## 7.058/1106.0608         -0.0060756041 -0.0313314309  0.0291196956 -0.001580528
## 7.379/1118.3872         -0.0135647310 -0.0348669331  0.0373697081 -0.003978476
## 7.643/1128.5248          0.0005996481 -0.0708302320  0.0613477615 -0.027635445
## 7.791/1134.208           0.0375392116 -0.0390752334 -0.0542776668  0.047319795
## 8.088/1145.6128         -0.0105047626 -0.0204579756  0.0342110237 -0.026527897
## 8.483/1160.7808         -0.0218944546 -0.0424660209  0.0564157739 -0.023573303
## 8.896/1176.64           -0.0169448664 -0.0507209804  0.0245935065  0.016827365
## 9.435/1197.3376         -0.0009220253  0.0192029210 -0.0695397623 -0.087994345
## 9.679/1205.86545278161   0.0257669540 -0.1849213865  0.0191578851  0.075227765
## 10.384/1229.53994253946 -0.0858840831  0.0342780882  0.2708220607 -0.039798476
## 10.505/1233.60322376031  0.0467955575 -0.1698674340 -0.0666898755  0.145244099
## 10.797/1243.4088280288  -0.0069584233 -0.0982005021  0.0205685823  0.045235676
## 10.924/1247.67359426887  0.0846186622 -0.0887353445  0.1159736918  0.021078307
## 10.987/1249.78918697064 -0.0271685924 -0.0546384960  0.1088848226 -0.086448246
## 11.073/1252.67713891273 -0.0212685829 -0.0992256663  0.0793205026 -0.044851604
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## 14.185/1354.77126518942 -0.6589820916 -0.0696165764 -0.2393757214 -0.036313603
## 15.299/1390.60400285919 -0.0395276830 -0.1353571203  0.1669045771 -0.032823311
## 15.314/1391.08649035025  0.0417442583 -0.0113428244 -0.0180742992  0.057430878
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## 16.259/1421.91747856018  0.0665367840  0.0406591535 -0.2658822604  0.351640151
## 16.602/1433.17338545009  0.0055399450 -0.0555749618  0.0234227293 -0.039037236
## 16.724/1437.17694416895 -0.0380038796 -0.0027279223 -0.0586034004  0.095142919
## 16.908/1443.21509830232 -0.0499478370 -0.1227934627  0.1263850107  0.092745946
## 17.155/1451.32066390526 -0.1143663795  0.0204052009  0.1569757274 -0.145456879
## 17.292/1455.81646345021 -0.0545986931  0.1025036370 -0.0015418721 -0.030471195
## 17.351/1457.75261069949 -0.3615068746 -0.2313230898  0.1677427625  0.050371031
## 17.578/1465.00495887054  0.0086146739  0.0092403592 -0.0386802984  0.012004808
## 18.073/1481.44580246193  0.0513433521 -0.0821868733 -0.1091872135  0.138939652
## 18.481/1494.83475293157 -0.0643241122  0.2415091482  0.0117414299 -0.058422185
## 18.545/1496.93498045622  0.2302261663  0.1253716201  0.1188642831  0.091699790
## 18.959/1510.7521008806   0.0925851511  0.0090162727 -0.1346649234 -0.023278437
## 19.117/1516.05101522599  0.1230893548 -0.1617708975 -0.1128724546 -0.307713578
## 19.858/1540.90225275726  0.0133434379 -0.0326376913  0.0837418516  0.061899752
## 20.097/1548.91769914048 -0.2353597820  0.2808740697  0.0105915189 -0.034061027
## 20.544/1563.9089314974  -0.0031176371  0.0402947547  0.0189093522 -0.062576805
## 20.574/1564.91505447437  0.0096134118 -0.1459762759  0.0376822886 -0.023549411
## 20.758/1571.08594206648 -0.0158305220 -0.1313120493  0.0649237523 -0.015076581
## 20.954/1577.65927884938  0.1952519496 -0.0807145599 -0.1648528688 -0.159635019
## 20.982/1578.59832696122  0.0073315342 -0.0467807574 -0.0323394618  0.059941034
## 21.413/1593.05296039708  0.0720272285 -0.2353911603 -0.0861118936  0.188024458
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## 22.124/1617.7648611349   0.0075342345 -0.0330788950 -0.0052635285  0.001170416
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## 24.399/1697.97620606634  0.0285346835  0.1140916865  0.1329941630 -0.215845721
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## 24.592/1704.9370130343  -0.0004716622  0.1660290107 -0.0422748111 -0.114625747
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## 25.295/1730.53229447317  0.0173969499  0.0671993377 -0.1542852395  0.121770365
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## 30.206/1915.20019180053 -0.0200658851  0.1154341476 -0.0790157345  0.085600565
## 32.534/2008.66234531526  0.0646082359  0.1674005843  0.1453604550  0.220164376
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## 5.303/1019.92814171123   0.138776398  0.0541917702  0.048053676  0.043946161
## 5.377/1023.63803475936   0.147372172  0.0764000860  0.036883730 -0.026133976
## 6.112/1060.48629679144  -0.022181900  0.0346261565  0.052742359  0.042915110
## 6.182/1063.99565508021  -0.219669044 -0.0825077589  0.002921574  0.089552036
## 6.471/1078.48429144385   0.194656393  0.0376312926  0.082034649 -0.090283069
## 7.058/1106.0608         -0.025694377  0.0381235246  0.039284291 -0.026217986
## 7.379/1118.3872         -0.031651939  0.0183960804  0.018802906 -0.034584300
## 7.643/1128.5248         -0.034309033 -0.0291371717 -0.016731997 -0.099272990
## 7.791/1134.208           0.010022368  0.0564089799 -0.047497825 -0.062183511
## 8.088/1145.6128          0.004009289 -0.0049161760  0.006938979 -0.010278299
## 8.483/1160.7808         -0.017593254  0.0160205044 -0.067430270  0.006026090
## 8.896/1176.64           -0.047773703  0.1006526354  0.046432174  0.123217814
## 9.435/1197.3376          0.165886779  0.0458808093  0.056017003 -0.034344045
## 9.679/1205.86545278161  -0.098666245  0.1227914140 -0.020347973 -0.029189565
## 10.384/1229.53994253946 -0.134040199  0.0903696224 -0.120307757 -0.033608436
## 10.505/1233.60322376031 -0.048077664  0.2648693540 -0.077263493  0.032436775
## 10.797/1243.4088280288  -0.006398694  0.0749601142 -0.201089123  0.016575851
## 10.924/1247.67359426887  0.069191952  0.0085459118 -0.094423569  0.229442423
## 10.987/1249.78918697064 -0.018584262 -0.0602906451 -0.096059906 -0.088321318
## 11.073/1252.67713891273 -0.024672521 -0.0883988860 -0.093638628 -0.066548256
## 11.503/1267.11689862319  0.036418797  0.0272585198  0.004999221 -0.018170540
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## 17.155/1451.32066390526  0.059242479 -0.0635434552 -0.217546310  0.099385029
## 17.292/1455.81646345021  0.080040396 -0.2249860391  0.058998152  0.252288696
## 17.351/1457.75261069949  0.272002223 -0.0127645928 -0.047554111  0.226631970
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## 18.073/1481.44580246193 -0.125512786 -0.1767663516  0.193839967 -0.012865872
## 18.481/1494.83475293157 -0.054047160  0.1916791775  0.253217463  0.015078303
## 18.545/1496.93498045622  0.045345161 -0.0149423248  0.047240958  0.007892995
## 18.959/1510.7521008806   0.073083843 -0.0023126354  0.046867917  0.133246250
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## 20.097/1548.91769914048 -0.114818143  0.0370475606  0.109759619 -0.051560591
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## 20.954/1577.65927884938 -0.112280219  0.0159251369 -0.052264694 -0.018589777
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## 21.645/1600.87640653175 -0.096646529 -0.0105426306 -0.078086989  0.105149716
## 22.124/1617.7648611349   0.033201417  0.0012268793 -0.133111784  0.024011596
## 22.135/1618.15269620929  0.142610265  0.0935428740  0.032749817 -0.115928510
## 22.263/1622.66568616587 -0.026867202 -0.0859047725  0.107451480  0.101641610
## 22.437/1628.8005318881   0.025966379 -0.0594354245  0.022241585  0.133138679
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## 23.877/1679.57166889966 -0.156452480  0.1252852402  0.165343841 -0.008899633
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## 24.495/1701.40537391684 -0.047112797  0.0130533211  0.015636719  0.133999481
## 24.592/1704.9370130343   0.008490474  0.2923199915  0.167422662 -0.040582479
## 25.163/1725.72635258137  0.060829654  0.0117325489  0.034384009  0.222513971
## 25.273/1729.73130415787  0.104761450 -0.1974734215  0.030511531  0.165145919
## 25.295/1730.53229447317  0.133917118 -0.1399940876 -0.112989840  0.035990690
## 25.922/1753.36051845919  0.019902589 -0.0343059253 -0.012410455  0.059883419
## 26.436/1771.85611301245 -0.071709899 -0.3283022990  0.170272936 -0.338113388
## 26.581/1777.35381926746  0.116464157  0.0796056995 -0.279780768 -0.028004875
## 27.512/1811.78220086937  0.037500628  0.0112025912 -0.092172220  0.057937594
## 27.667/1817.692366354    0.037496096  0.0402927679 -0.194948229  0.029664912
## 28.086/1833.66887821246 -0.095597648  0.0681794534  0.123912944  0.126466575
## 28.435/1846.97628307786  0.010581715 -0.0174447377 -0.014761563  0.066674309
## 30.206/1915.20019180053  0.044392064  0.2947206873 -0.246190403 -0.048863971
## 32.534/2008.66234531526  0.218288189  0.0029786300  0.025082356 -0.014116982
## 34.508/2091.7501473188   0.182347055  0.0844598527  0.197247502 -0.127498700
##                                 PC21         PC22          PC23          PC24
## 5.043/1006.89338235294   0.041652323  0.007304408  2.739410e-03  1.385331e-01
## 5.303/1019.92814171123   0.168039468  0.144589578  1.489436e-01  1.915036e-02
## 5.377/1023.63803475936   0.022227965  0.234785931 -1.907673e-01 -2.166220e-03
## 6.112/1060.48629679144   0.004213493  0.006994802 -9.250496e-04  3.239921e-02
## 6.182/1063.99565508021  -0.118701071  0.133868031 -3.763592e-03 -3.792378e-02
## 6.471/1078.48429144385  -0.214577597  0.056629561 -2.101404e-01 -3.632002e-02
## 7.058/1106.0608          0.045433735  0.017787116 -1.795272e-03 -7.171075e-02
## 7.379/1118.3872          0.037886836  0.009993502 -2.377933e-03  8.212264e-02
## 7.643/1128.5248          0.065464189  0.007397405  2.513284e-03  1.357643e-01
## 7.791/1134.208           0.045091832  0.010343566  2.048721e-03 -1.533780e-01
## 8.088/1145.6128          0.023714950  0.003546831 -6.462392e-03  1.220845e-01
## 8.483/1160.7808         -0.015033391 -0.038414716  5.474302e-05  1.956622e-01
## 8.896/1176.64           -0.046509185 -0.038859029  6.499804e-03  1.527635e-01
## 9.435/1197.3376          0.073972545  0.044552031 -9.840210e-02  9.306091e-02
## 9.679/1205.86545278161   0.041781474 -0.016676531  2.533733e-02  1.524136e-01
## 10.384/1229.53994253946 -0.236024286  0.289886725 -2.278086e-01  1.595626e-02
## 10.505/1233.60322376031  0.023656986 -0.019234398  2.445994e-02 -9.018131e-02
## 10.797/1243.4088280288  -0.046224634 -0.070156931  6.772117e-03  1.566889e-02
## 10.924/1247.67359426887  0.085592894  0.607941175  3.955032e-01 -7.008451e-02
## 10.987/1249.78918697064  0.030573222 -0.034461055  1.853667e-03 -2.035401e-01
```
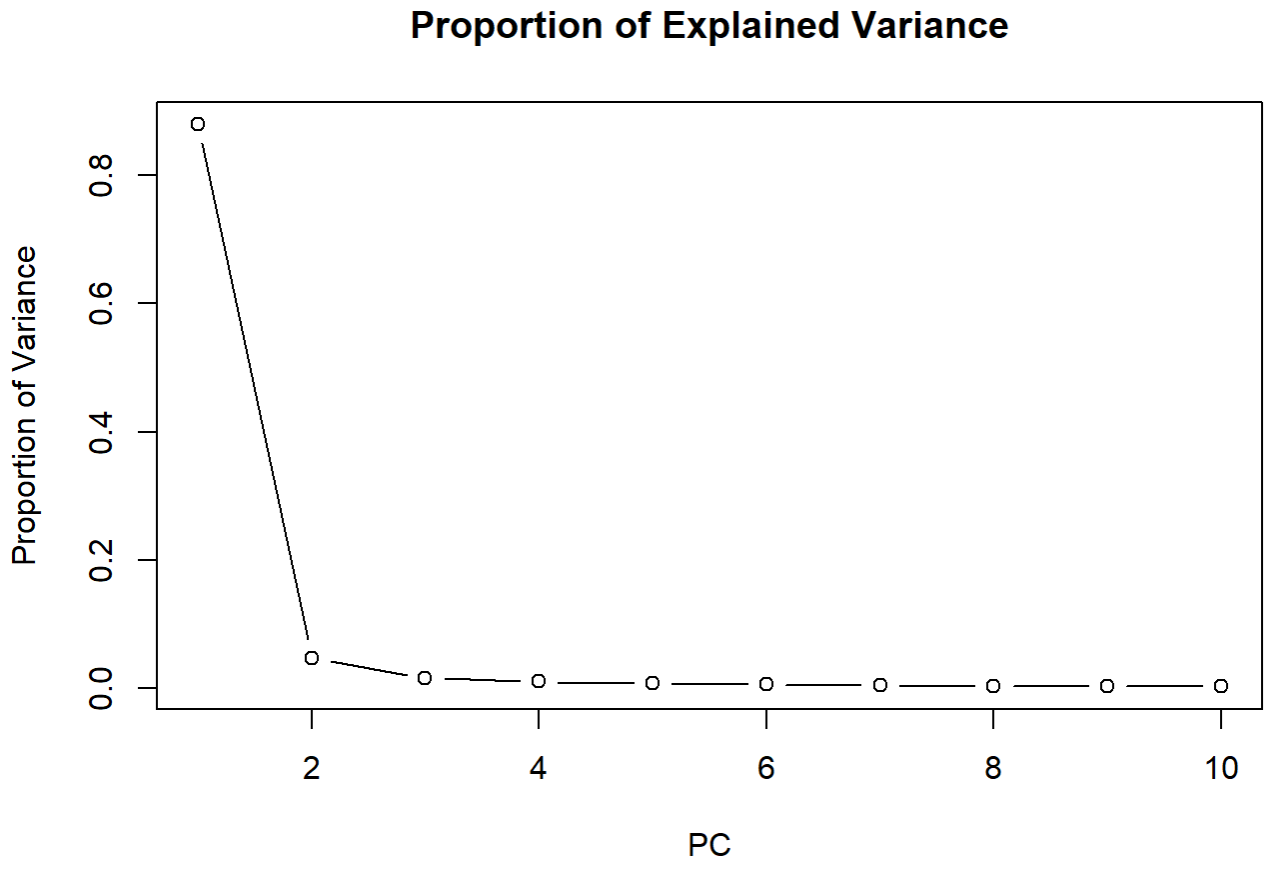
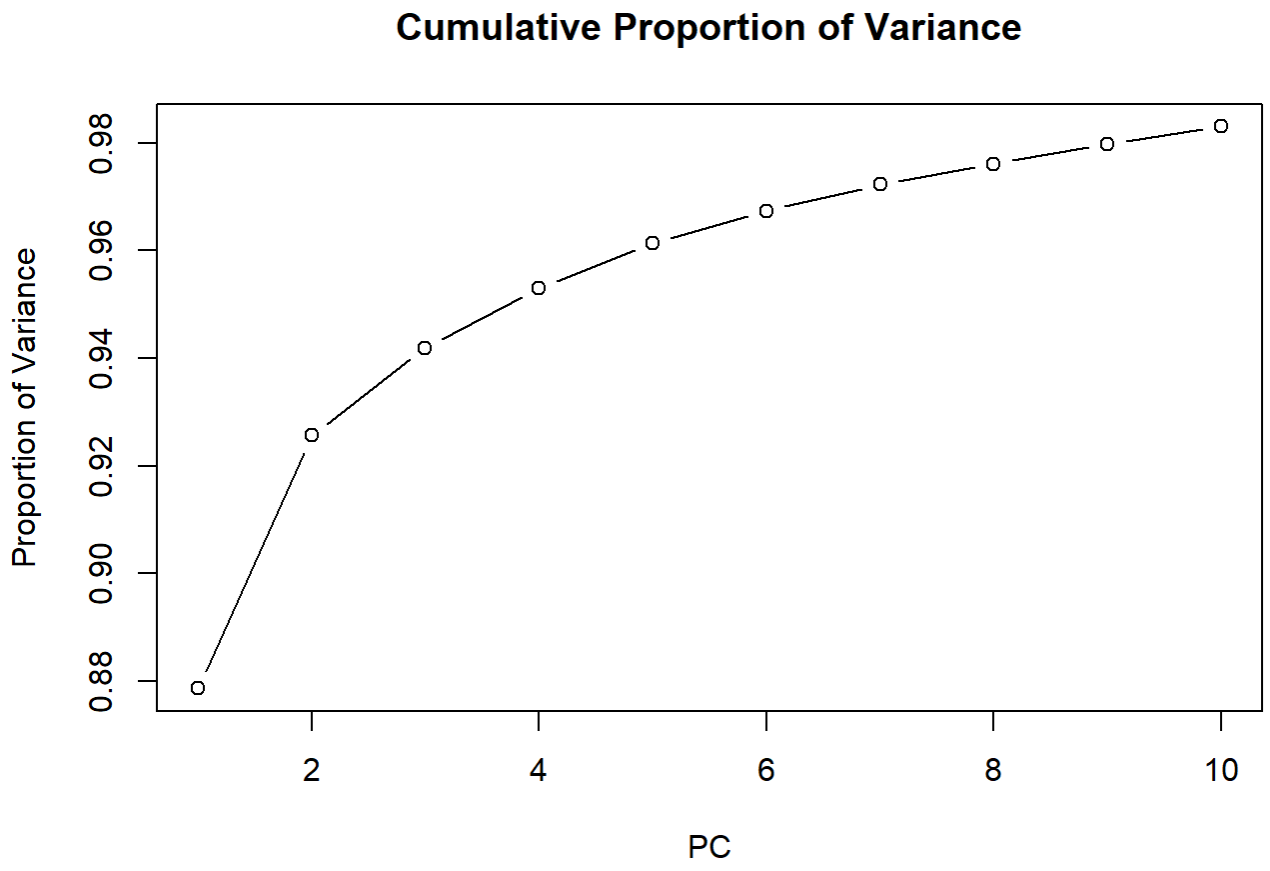

```
## 11.073/1252.67713891273  0.013758234 -0.031586556  2.418391e-04 -4.465045e-02
## 11.503/1267.11689862319  0.043924078  0.020030965 -7.100573e-03 -2.670893e-01
## 11.912/1280.85146076639 -0.030396777  0.153937495  2.274014e-02  1.150674e-01
## 13.327/1327.1729807005   0.089004214 -0.025292555  4.497930e-02  8.360298e-02
## 14.185/1354.77126518942 -0.108280564  0.127267151  3.054301e-01 -3.106496e-02
## 15.299/1390.60400285919 -0.074913376 -0.115796931  4.327714e-02  3.328121e-02
## 15.314/1391.08649035025  0.192122912 -0.042649162 -1.379337e-01 -2.314539e-02
## 16.191/1419.68598681524  0.116017990  0.065573127 -1.223699e-02 -1.387279e-01
## 16.259/1421.91747856018 -0.027773873  0.100983447 -2.596530e-02 -3.270227e-02
## 16.602/1433.17338545009  0.008981648 -0.004892006 -2.709941e-04 -5.372623e-03
## 16.724/1437.17694416895  0.022120405  0.059687296 -2.272066e-02 -2.266003e-01
## 16.908/1443.21509830232  0.098982168  0.053143992 -1.350096e-02  8.379075e-02
## 17.155/1451.32066390526 -0.004523896  0.008454848  8.608512e-02  1.152783e-01
## 17.292/1455.81646345021 -0.194296138 -0.039725407 -4.596829e-02 -1.833756e-01
## 17.351/1457.75261069949  0.419804228 -0.096847976 -2.480530e-01 -1.590809e-02
## 17.578/1465.00495887054  0.014202976  0.017533567 -1.400264e-02  2.979819e-02
## 18.073/1481.44580246193 -0.024256850  0.033589429  9.018851e-03  1.700041e-01
## 18.481/1494.83475293157  0.037732149  0.067556330 -2.705571e-02 -6.500504e-02
## 18.545/1496.93498045622  0.049433868 -0.077953477 -2.390462e-03  2.029687e-02
## 18.959/1510.7521008806  -0.040951724 -0.059399607  1.578026e-02  7.568210e-02
## 19.117/1516.05101522599 -0.069404719  0.098780730  1.305881e-01  5.577031e-02
## 19.858/1540.90225275726 -0.010340228  0.114239038 -2.519367e-01  5.922656e-02
## 20.097/1548.91769914048 -0.021758574  0.027407193 -4.892266e-02  9.084073e-02
## 20.544/1563.9089314974   0.075672886 -0.009105895 -1.001819e-02 -2.196278e-01
## 20.574/1564.91505447437  0.008918227 -0.003246672 -8.493374e-03 -7.277938e-02
## 20.758/1571.08594206648 -0.024347066 -0.049360941  1.477331e-02 -4.581109e-02
## 20.954/1577.65927884938 -0.049777978  0.050511695  4.660355e-02 -7.866456e-02
## 20.982/1578.59832696122 -0.007056705 -0.001252335 -6.900049e-03  2.208617e-01
## 21.413/1593.05296039708 -0.060879911 -0.058969368  3.084127e-02 -1.875032e-01
## 21.633/1600.45331372332 -0.065817712 -0.017224514  3.422870e-03 -1.289840e-03
## 21.645/1600.87640653175  0.071221377  0.145512574 -1.980755e-01  2.244916e-01
## 22.124/1617.7648611349  -0.043406382 -0.056308391  3.011702e-03  7.503450e-02
## 22.135/1618.15269620929 -0.170817077  0.095726266 -1.419872e-01 -4.358453e-02
## 22.263/1622.66568616587  0.013380472 -0.077053048  2.993204e-02 -2.311658e-01
## 22.437/1628.8005318881  -0.067886959 -0.044820057  7.451958e-04  3.604789e-02
## 22.813/1642.05743988556 -0.079002572 -0.069224026  9.638880e-03 -6.803941e-04
## 23.324/1660.07414197786 -0.350423127 -0.035224186  2.569959e-01  7.287268e-02
## 23.476/1665.4333175513   0.091143680  0.033305726 -2.321111e-03  3.008933e-02
## 23.492/1665.99744129587  0.248243525 -0.128632452  2.399219e-01  6.122864e-02
## 23.646/1671.42713233739 -0.048838412 -0.063016648  2.954242e-02  4.892399e-03
## 23.746/1674.95290574097  0.026370484 -0.049138190  2.371862e-02  1.081365e-01
## 23.877/1679.57166889966  0.092240768  0.013067594  2.354958e-02 -1.573681e-02
## 24.102/1687.50465905771 -0.004967437  0.001674724  1.264680e-03 -1.760932e-01
## 24.278/1693.71002024801  0.206550524  0.239001508 -2.098854e-02 -7.003814e-02
## 24.301/1694.52094813084  0.035493278  0.003952147 -3.876496e-03  3.571415e-02
## 24.399/1697.97620606634 -0.081357533 -0.105553702  9.478157e-03  1.372445e-02
## 24.495/1701.40537391684 -0.086773368 -0.048619777  9.372374e-03 -5.413001e-02
## 24.592/1704.9370130343   0.116107092  0.039541712 -3.876608e-04 -8.526276e-02
## 25.163/1725.72635258137 -0.105803961 -0.049438562  3.540195e-04 -1.784059e-01
## 25.273/1729.73130415787 -0.084902125  0.015075617 -2.159485e-02  2.210963e-01
## 25.295/1730.53229447317 -0.067985409  0.029260133 -3.507272e-02  5.007221e-02
## 25.922/1753.36051845919 -0.050669994  0.057056559 -3.197360e-02  5.755017e-02
## 26.436/1771.85611301245  0.185382923  0.179868249 -3.704776e-02 -1.774828e-02
## 26.581/1777.35381926746 -0.023243994 -0.086658097 -2.052641e-03  1.113288e-01
```

```
## 27.512/1811.78220086937  0.014817627  0.175571390 -3.963981e-01 -4.543623e-02
## 27.667/1817.692366354   -0.079626424 -0.100199689 -4.301089e-03 -1.583642e-01
## 28.086/1833.66887821246 -0.056104399 -0.021849587 -4.087681e-04 -1.522730e-01
## 28.435/1846.97628307786 -0.043320209 -0.013790584 -7.986493e-03 -7.259997e-06
## 30.206/1915.20019180053 -0.023268209 -0.037240203 -1.811414e-02 -4.563615e-02
## 32.534/2008.66234531526  0.306961308 -0.181545271  1.702378e-01  6.795407e-03
## 34.508/2091.7501473188  -0.017502211 -0.182328920 -1.532517e-01 -5.189435e-02
```

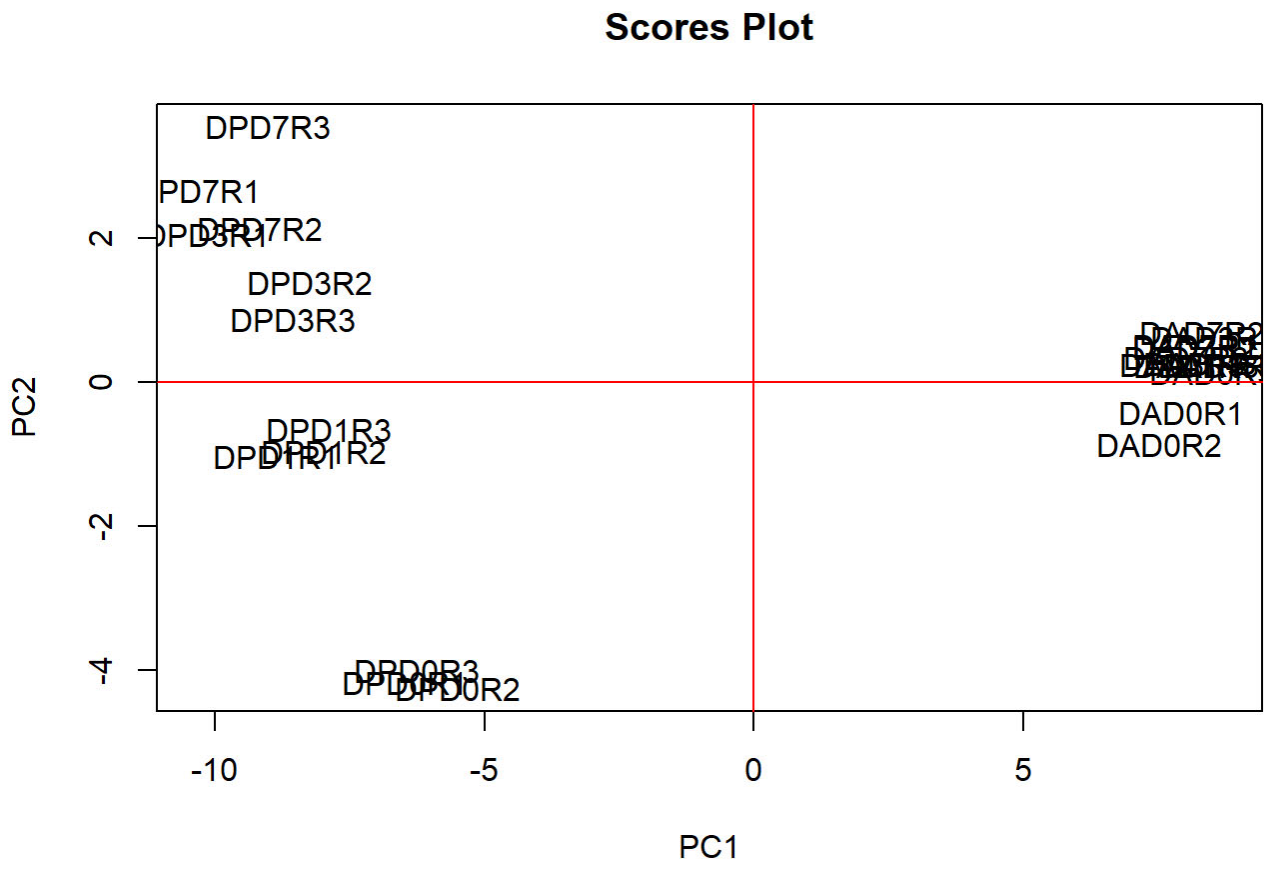
```
# Make a simple scree plot
plot(results$importance[2,1:10], type="b",
     main="Proportion of Explained Variance",
     xlab="PC", ylab="Proportion of Variance")
```



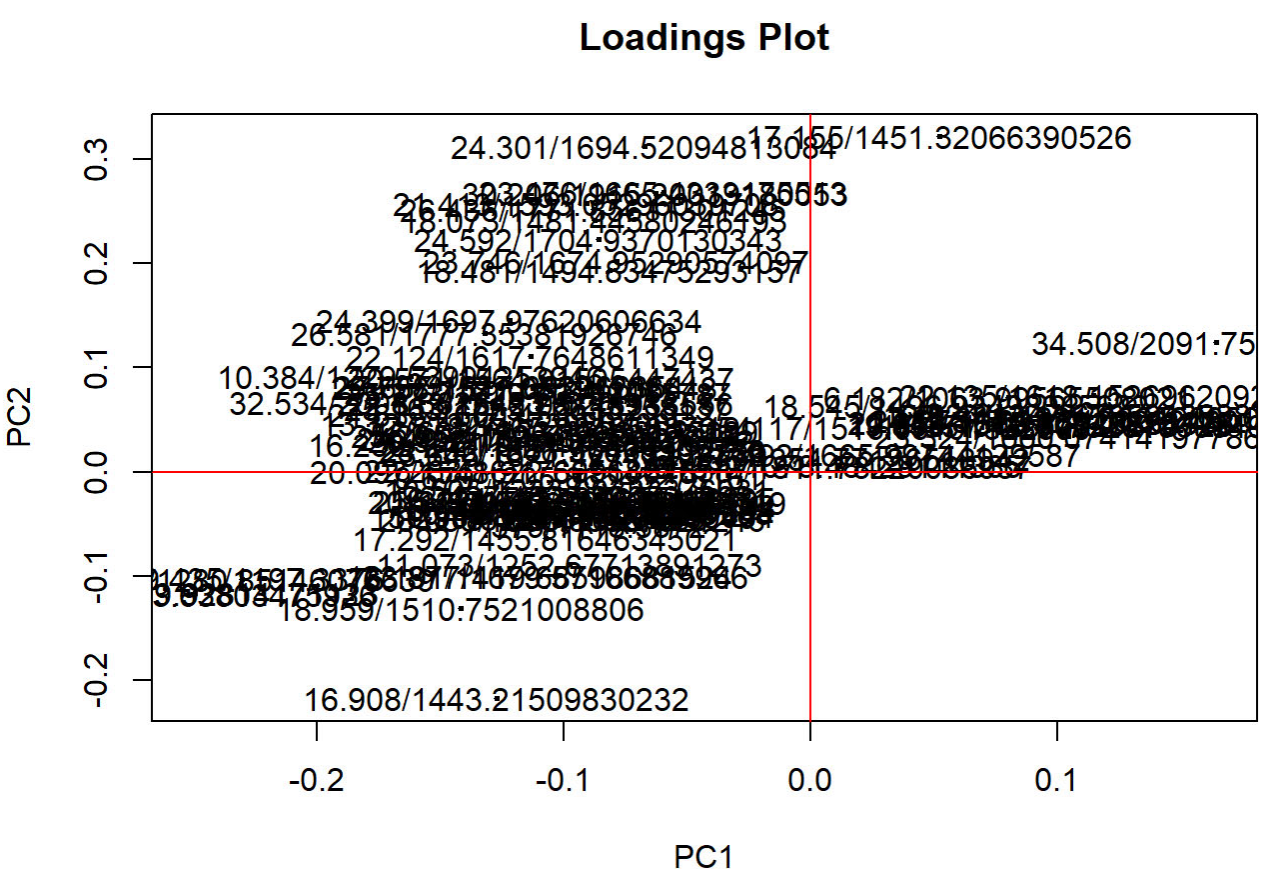

```
# Plot the cumulative proportion of variance
plot(results$importance[3,1:10], type="b",
     main="Cumulative Proportion of Variance",
     xlab="PC", ylab="Proportion of Variance")
```



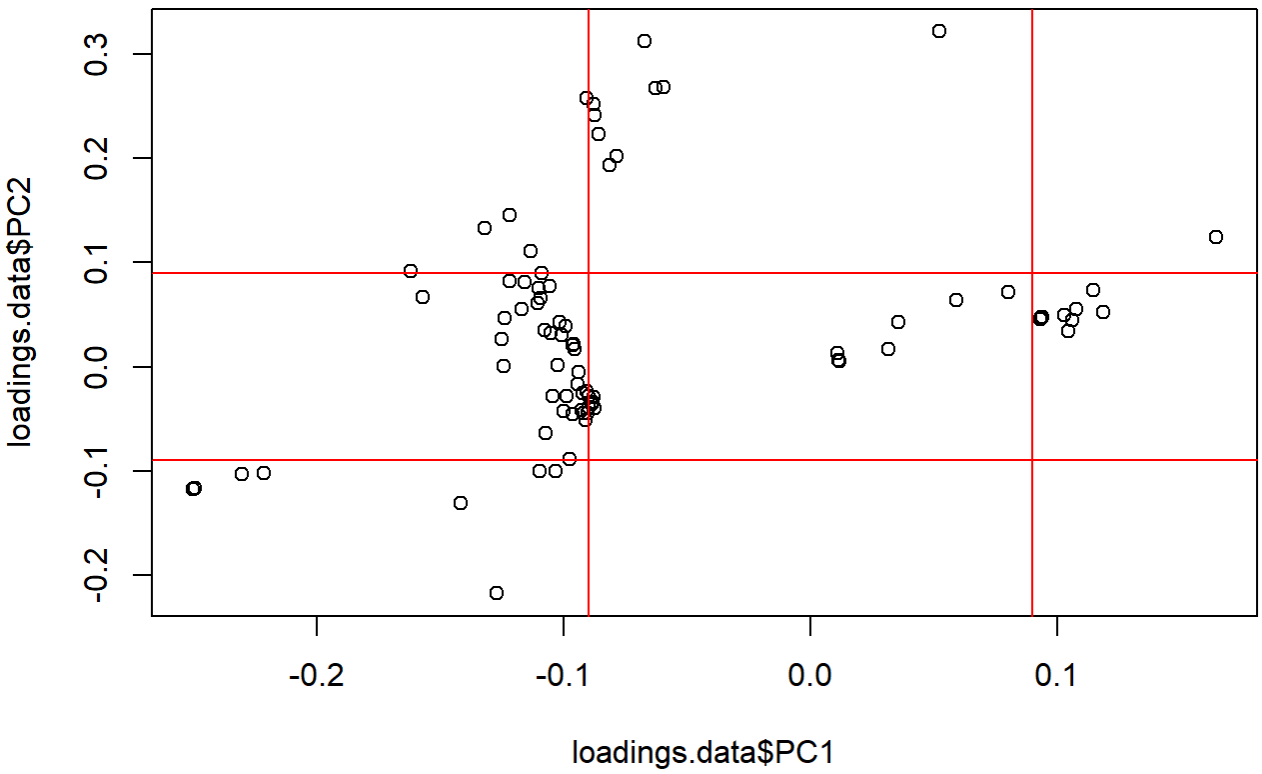

```
# Make a simple scores plot
plot(pca$x[,1], pca$x[,2], type='p', cex=0, pch=20,
     main="Scores Plot", xlab="PC1", ylab="PC2")

# add text labels to data points
text(pca$x[,1], pca$x[,2], labels=rownames(pca$x), cex=1.0)
abline(h=0, v=0, col="red")
```




```
# Make a simple loadings plot (variance among variables)
plot(pca$rotation[,1], pca$rotation[,2], type='p', cex=0.5, pch=20,
     main="Loadings Plot", xlab="PC1", ylab="PC2")

# add text labels for data points
text(pca$rotation[,1], pca$rotation[,2], labels=rownames(pca$rotation), cex=1.0)
abline(h=0, v=0, col="red")
```



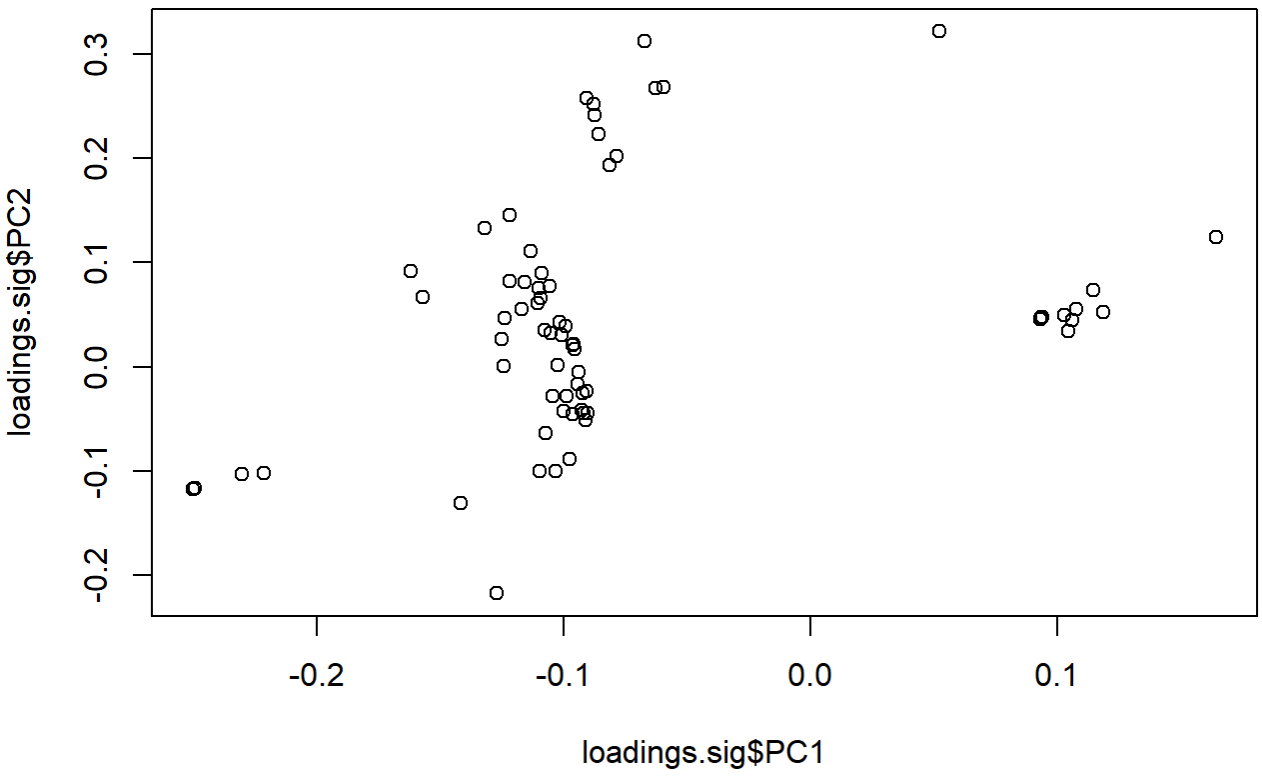

```
# Extract PCA results into data frames

scree.data <- as.data.frame(results$importance)
score.data <- as.data.frame(results$x)
loadings.data <- as.data.frame(results$rotation)

# Save PCA results to file (we'll use later)
write.csv(scree.data, "pca_scree.csv")
write.csv(score.data, "pca_scores.csv")
write.csv(loadings.data, "pca_loadings.csv")

# Find important variables (Loadings)

plot(loadings.data$PC1, loadings.data$PC2)
abline(v=0.09, col="red")
abline(v=-0.09, col="red")
abline(h=0.09, col="red")
abline(h=-0.09, col="red")
```




```
# Make a new data frame with PC1, PC2, and PC3 loadings
loadings.PC1.PC2 <- loadings.data[,1:3]
loadings.PC1.PC2[1:6,1:3]  # look at the first few rows
```

```
##                                PC1          PC2        PC3
## 5.043/1006.89338235294 -0.08845888 -0.035577557 0.02038417
## 5.303/1019.92814171123 -0.24936209 -0.116734816 0.06262671
## 5.377/1023.63803475936 -0.25030428 -0.117500961 0.05333553
## 6.112/1060.48629679144 -0.08811077 -0.034322368 0.01890489
## 6.182/1063.99565508021  0.08048505  0.071140826 0.42317786
## 6.471/1078.48429144385  0.01131770  0.006615236 0.01866600
```

```
# subset significant loadings
loadings.sig <- subset(loadings.PC1.PC2,
                       PC1 > 0.09 | PC1 < -0.09 |
                         PC2 > 0.09 | PC2 < -0.09)

# sanity check - plot the results
plot(loadings.sig$PC1, loadings.sig$PC2)
```




```
# Use the "ifelse" function to mark high loadings

# PC1 loadings
loadings.sig$pc1.change <-
  ifelse(loadings.sig$PC1 > 0.09,"UP",
         ifelse(loadings.sig$PC1 < -0.09,"DOWN",
                "none"))

# PC2 loadings
loadings.sig$pc2.change <-
  ifelse(loadings.sig$PC2 > 0.09,"UP",
         ifelse(loadings.sig$PC2 < -0.09,"DOWN",
                "none"))

# Number of signficant PC1 loadings
length(which(loadings.sig$pc1.change=="UP"))
```

```
## [1] 10
```

```
length(which(loadings.sig$pc1.change=="DOWN"))
```

```
## [1] 48
```

```
length(which(loadings.sig$pc1.change=="none"))
```

```
## [1] 9
```

```
# Number of signficant PC2 loadings
length(which(loadings.sig$pc2.change=="UP"))
```

```
## [1] 16
```

```
length(which(loadings.sig$pc2.change=="DOWN"))
```

```
## [1] 8
```

```
length(which(loadings.sig$pc2.change=="none"))
```

```
## [1] 43
```

```
# Write significant loadings to file for later use.
write.csv(loadings.sig, "sig_loadings.csv")

# Merge significant PC1 and PC2 loadings with raw data
# Note: use missing values corrected data
pca.sig.vars <- merge(dat2, loadings.sig, by="row.names")


# use the "arrange" function in the plyr package to order
library(plyr)
pca.sig.vars <- arrange(pca.sig.vars, pc1.change, pc2.change)

# Re-assign row names and delete "Row.names" column
row.names(pca.sig.vars) <- pca.sig.vars$Row.names
pca.sig.vars$Row.names <- NULL

# Write the results to file for later use.
write.csv(pca.sig.vars, "dat_sig_loadings.csv")
```

###Plots with Ellipses

```
# import scores matrix
data <- read.csv("pca_scores.csv", header=T)

# subset to include only PC1 to PC3 scores
data <- data[, c(1:4)]

# look at first few rows
data[1:6,1:4]
```

```
##        X       PC1        PC2        PC3
## 1 DPD0R1 -6.477680 -4.1787440 0.27687443
## 2 DPD0R2 -5.502525 -4.2580468 0.01333411
## 3 DPD0R3 -6.263230 -4.0026285 0.49406542
## 4 DPD1R1 -8.875632 -1.0334763 0.26948693
## 5 DPD1R2 -7.984104 -0.9637881 0.21446055
## 6 DPD1R3 -7.886679 -0.6593741 0.27183137
```

```
# Get variance percentages for first 3 PC's
screedat <- read.csv("pca_scree.csv", header=T)
var1 <- round(screedat[2,2:4] * 100, 1)

# Change "X" column to "Sample"
colnames(data)[colnames(data)=="X"] <- "Sample"

# Add Group label to the data frame
Group <- c(rep("DryPistachio", 12),
           rep("DryAlmond", 12))


data <- cbind(data, Group)

# install ggplot2 (can skip if already installed)
#install.packages("ggplot2")

# load ggplot2
library(ggplot2)

# Make custom theme for ggplot
my.theme <- theme(axis.text = element_text(colour="black", size=15),
                  text = element_text(size=16),
                  title = element_text(size=18, face="bold", vjust=2),
                  panel.background = element_rect(fill = 'gray99',
                                                  colour = "black",
                                                  size=0.5),
                  axis.title.x=  element_text(vjust=-0.45),
                  axis.title.y = element_text(vjust=1.2),
                  axis.ticks = element_line(colour="black"),
                  axis.line = element_line(),
                  panel.grid.major = element_line(colour = "gray40", linetype="dotted"),
                  panel.grid.minor = element_line(colour = "gray40", linetype="dashed"),
                  legend.justification=c(1,1),
                  legend.position=c(1,1),
                  legend.title=element_blank(),
                  legend.text = element_text(size = 14))

# check variances for PC1 and PC2
var1
```

```
##    PC1 PC2 PC3
## 2 87.9 4.7 1.6
```

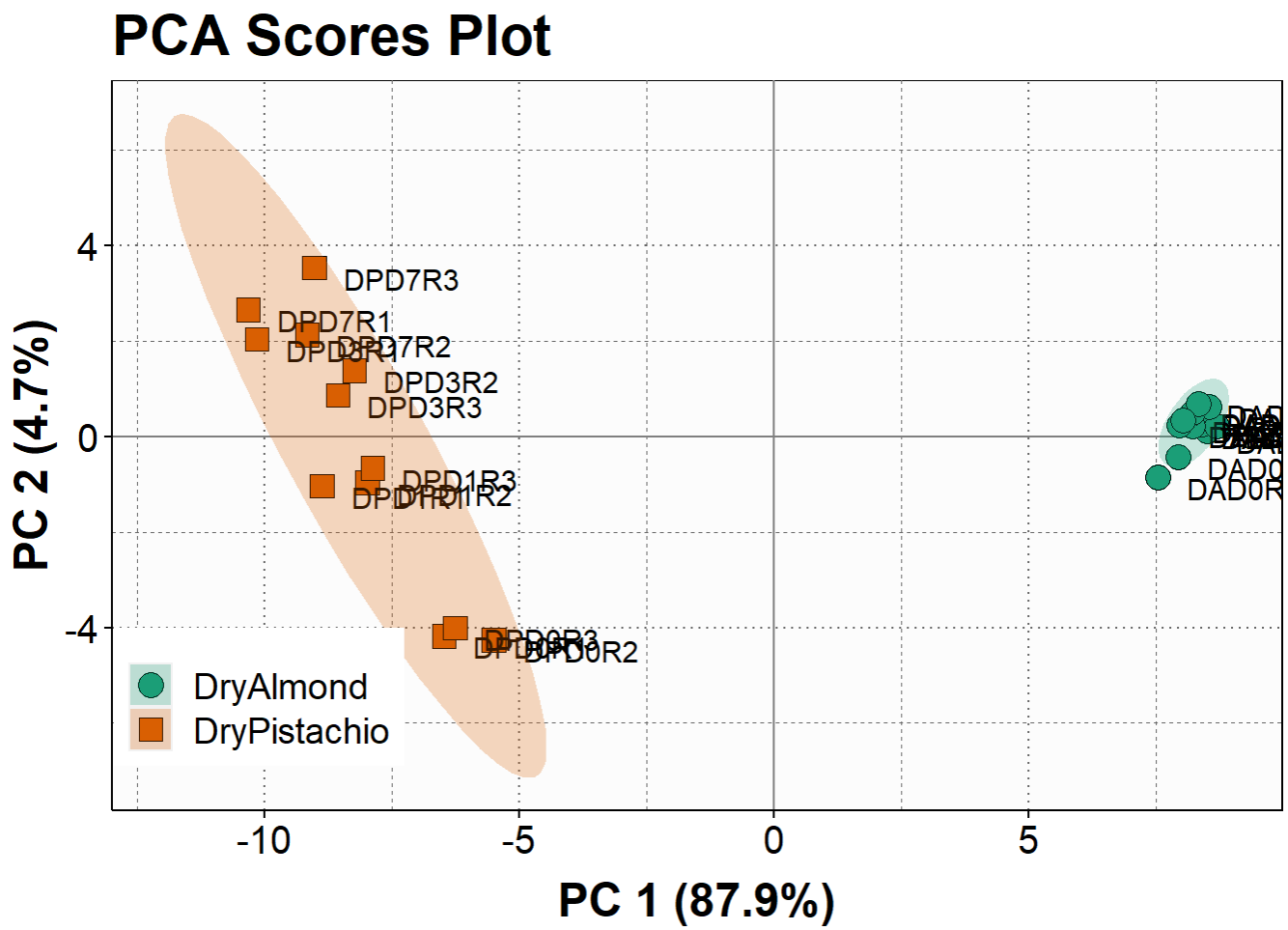
```
# Calculate 95% ellipse values for PC1,PC2
library(ellipse)
```

```
##
## Attaching package: 'ellipse'
```

```
## The following object is masked from 'package:graphics':
##
##     pairs
```

```
centroids <- aggregate(cbind(PC1,PC2)~Group,data,mean)
#---------this section did not work remove
# conf.rgn1  <- do.call(rbind,lapply(unique(data$Group),function(t)# no function (T)
#   data.frame(Group=as.character(t),
#              ellipse(cov(data[data$Group==t,2:3]),
#                      centre=as.matrix(centroids[t,2:3]),
#                      level=0.95),
#              stringsAsFactors=FALSE)))

# make plot for PC1 vs. PC2
g1 <-
  ggplot(data, aes(PC1, PC2)) +
  geom_hline(yintercept = 0, colour = "gray50") +
  geom_vline(xintercept = 0, colour = "gray50") +
  # geom_polygon(data=conf.rgn1,  # this did not work
  #              aes(fill=Group), colour="black", alpha = 0.2,
  #              linetype="blank", show.legend=FALSE) +
  geom_point(aes(shape=Group, bg=Group), colour="black", size=4.5) +
  geom_text(aes(label=data$Sample), colour="black",
            size=4, hjust=-0.25, vjust=1) +
  #this is the correct way to apply geom polygon in line 88
  stat_ellipse(geom = "polygon",
               aes(fill = Group),
               alpha = 0.25)+


  scale_fill_brewer(palette = "Dark2") +
  scale_shape_manual(values=c(21,22,23,24)) +
  ggtitle("PCA Scores Plot") +
  xlab("PC 1 (87.9%)") + #from var1 above
  ylab("PC 2 (4.7%)") +
  my.theme +
  theme(legend.position=c(0.25,0.25))

# draw scores plot
g1
```

```
## Warning: Use of `data$Sample` is discouraged. Use `Sample` instead.
```




```
# save as png file
png(file="scores.plot.png", height=2400, width=2800, res=350)
g1
```

```
## Warning: Use of `data$Sample` is discouraged. Use `Sample` instead.
```

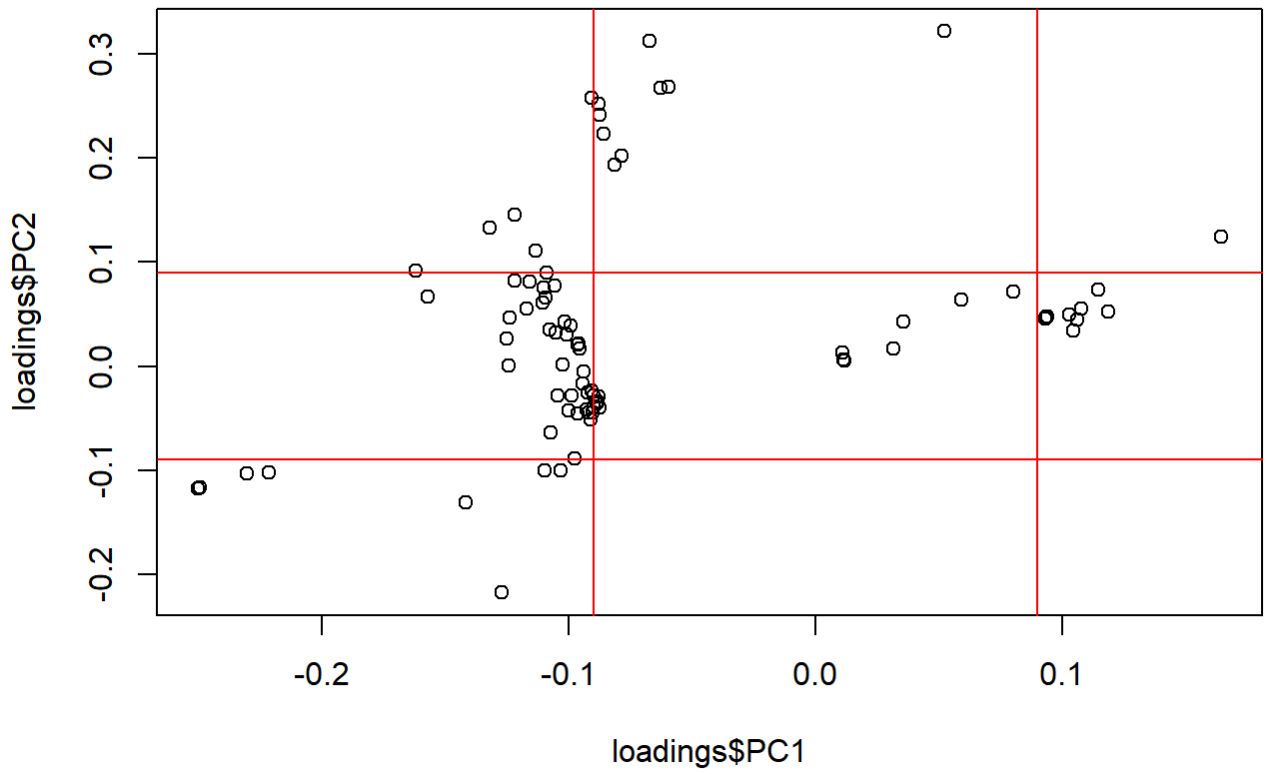
```
dev.off()
```

```
## png
##   2
```

```
######################
# Loadings plot
######################

# Import loadings matrix
loadings <- read.csv("pca_loadings.csv", header=T)

# subset to include only PC1 to PC3 loadings
loadings <- loadings[, c(1:4)]

# look at first few rows
loadings[1:6,1:4]
```

```
##                         X         PC1          PC2        PC3
## 1 5.043/1006.89338235294 -0.08845888 -0.035577557 0.02038417
## 2 5.303/1019.92814171123 -0.24936209 -0.116734816 0.06262671
## 3 5.377/1023.63803475936 -0.25030428 -0.117500961 0.05333553
## 4 6.112/1060.48629679144 -0.08811077 -0.034322368 0.01890489
## 5 6.182/1063.99565508021  0.08048505  0.071140826 0.42317786
## 6 6.471/1078.48429144385  0.01131770  0.006615236 0.01866600
```

```
# Change "X" column to "Variable"
colnames(loadings)[colnames(loadings)=="X"] <- "Variable"

# make a quick loadings plot
plot(loadings$PC1, loadings$PC2)

# add lines for cutoff values
abline(v=0.09, col="red")
abline(v=-0.09, col="red")
abline(h=0.09, col="red")
abline(h=-0.09, col="red")
```



```
# Create new column based on PC1 loadings
loadings$pc1.change <-
  ifelse(loadings$PC1 > 0.09,"UP",
         ifelse(loadings$PC1 < -0.09,"DOWN",
                "zeit"))

# Create new column based on PC2 loadings
loadings$pc2.change <-
  ifelse(loadings$PC2 > 0.09,"UP",
         ifelse(loadings$PC2 < -0.09,"DOWN",
                "zeit"))

# Create label column for PC1 loadings
loadings$pc1.label <-
  ifelse(loadings$PC1 > 0.09, as.character(loadings$Variable),
         ifelse(loadings$PC1 < -0.09, as.character(loadings$Variable),
                "null"))

# Create label column for PC2 loadings
loadings$pc2.label <-
  ifelse(loadings$PC2 > 0.09, as.character(loadings$Variable),
         ifelse(loadings$PC2 < -0.09, as.character(loadings$Variable),
                "null"))

# subset significant loadings
loadings.sig <- subset(loadings,
                       PC1 > 0.09 | PC1 < -0.09 |
                         PC2 > 0.09 | PC2 < -0.09)

library(plyr)

# use the "arrange" function in the plyr package to sort
loadings.sig <- arrange(loadings.sig, pc1.change, pc2.change)

# Write the results to file
write.csv(loadings.sig, "significant_loadings.csv", row.names=F)

# make loadings plot
g2 <-
  ggplot(loadings, aes(PC1, PC2)) +
  geom_hline(yintercept = 0, colour = "gray40") +
  geom_vline(xintercept = 0, colour = "gray40") +
  geom_point(size=2.5, pch=21, color="gray20", bg="khaki1") +
  stat_ellipse(level=0.15, colour="gray40", linetype="dashed", type="euclid") +
  geom_point(data=subset(loadings, pc1.change=="UP"),
             size=4, pch=21, color="black", bg="blue") +
  geom_point(data=subset(loadings, pc1.change=="DOWN"),
             size=4, pch=22, color="black", bg="orange") +
  geom_point(data=subset(loadings, pc2.change=="UP"),
             size=4, pch=23, color="black", bg="green") +
  geom_point(data=subset(loadings, pc2.change=="DOWN"),
             size=4, pch=24, color="black", bg="red") +
  scale_x_continuous(limits = c(-0.18, 0.16)) +
```

```
  scale_y_continuous(limits = c(-0.16, 0.16)) +
  ggtitle("PCA Loadings Plot") +
  my.theme

# draw loadings plot
g2
```

```
## Warning: Removed 16 rows containing non-finite values (stat_ellipse).
```

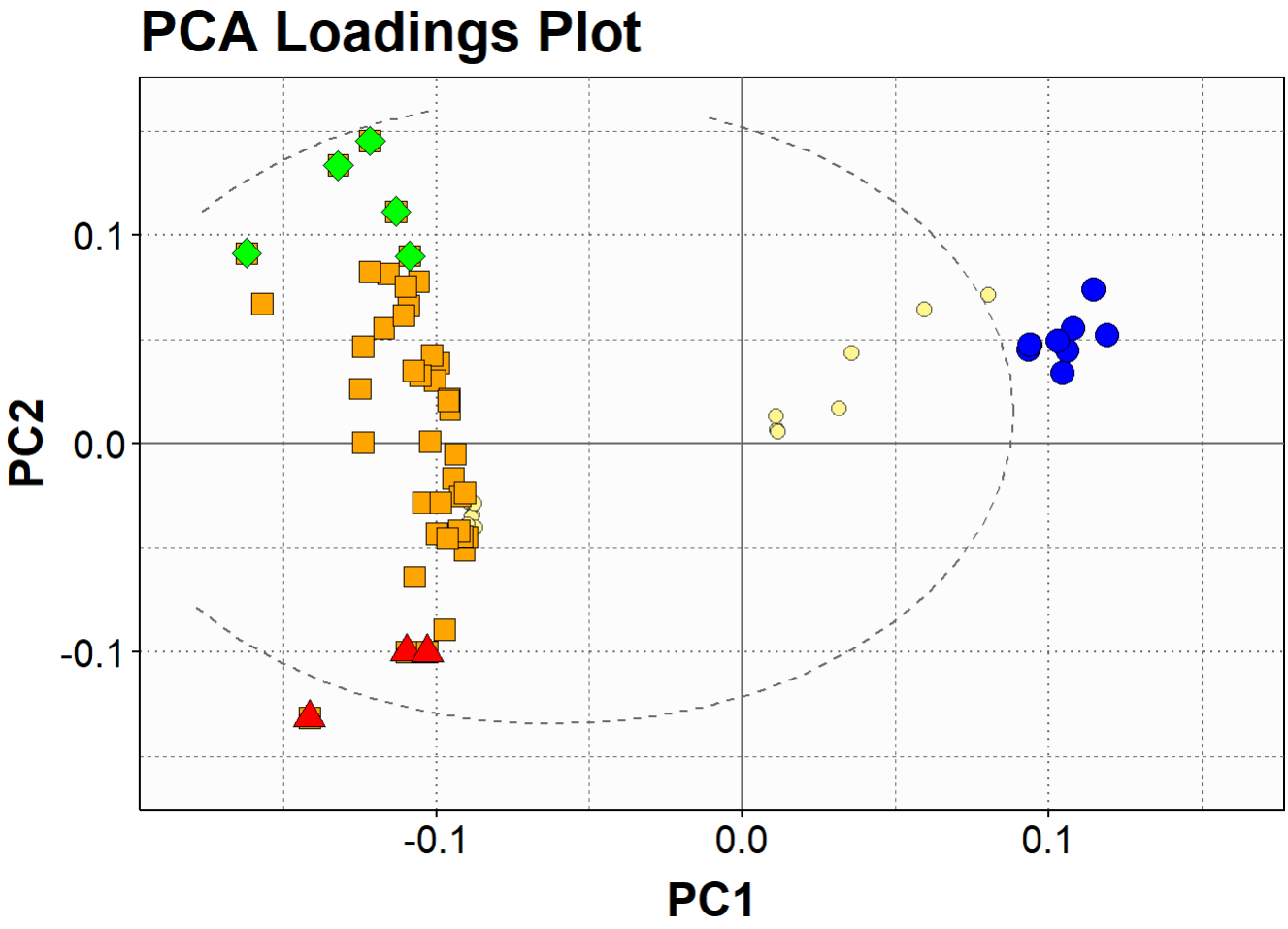
```
## Warning: Removed 16 rows containing missing values (geom_point).
```

```
## Warning: Removed 1 rows containing missing values (geom_point).
```

```
## Warning: Removed 6 rows containing missing values (geom_point).
```

```
## Warning: Removed 11 rows containing missing values (geom_point).
```

```
## Warning: Removed 5 rows containing missing values (geom_point).
```



```
# add text annotations using the grid package
library(grid)

PC1.pos <- grobTree(textGrob("Positively \n correlated \n with PC1",
                             x=0.82, y=0.22, gp=gpar(col="blue", fontsize=14, fontface="bold")))
PC1.neg <- grobTree(textGrob("Negatively \n correlated \n with PC1",
                             x=0.15, y=0.7, gp=gpar(col="orange", fontsize=14, fontface="bold"
)))
PC2.pos <- grobTree(textGrob("Positively \n correlated \n with PC2",
                             x=0.63, y=0.88, gp=gpar(col="green", fontsize=14, fontface="bold"
)))
PC2.neg <- grobTree(textGrob("Negatively \n correlated \n with PC2",
                             x=0.17, y=0.1, gp=gpar(col="red", fontsize=14, fontface="bold")))

g2a <-
  g2 +
  annotation_custom(PC1.pos) +
  annotation_custom(PC1.neg) +
  annotation_custom(PC2.pos) +
  annotation_custom(PC2.neg)

g2a
```

```
## Warning: Removed 16 rows containing non-finite values (stat_ellipse).
```

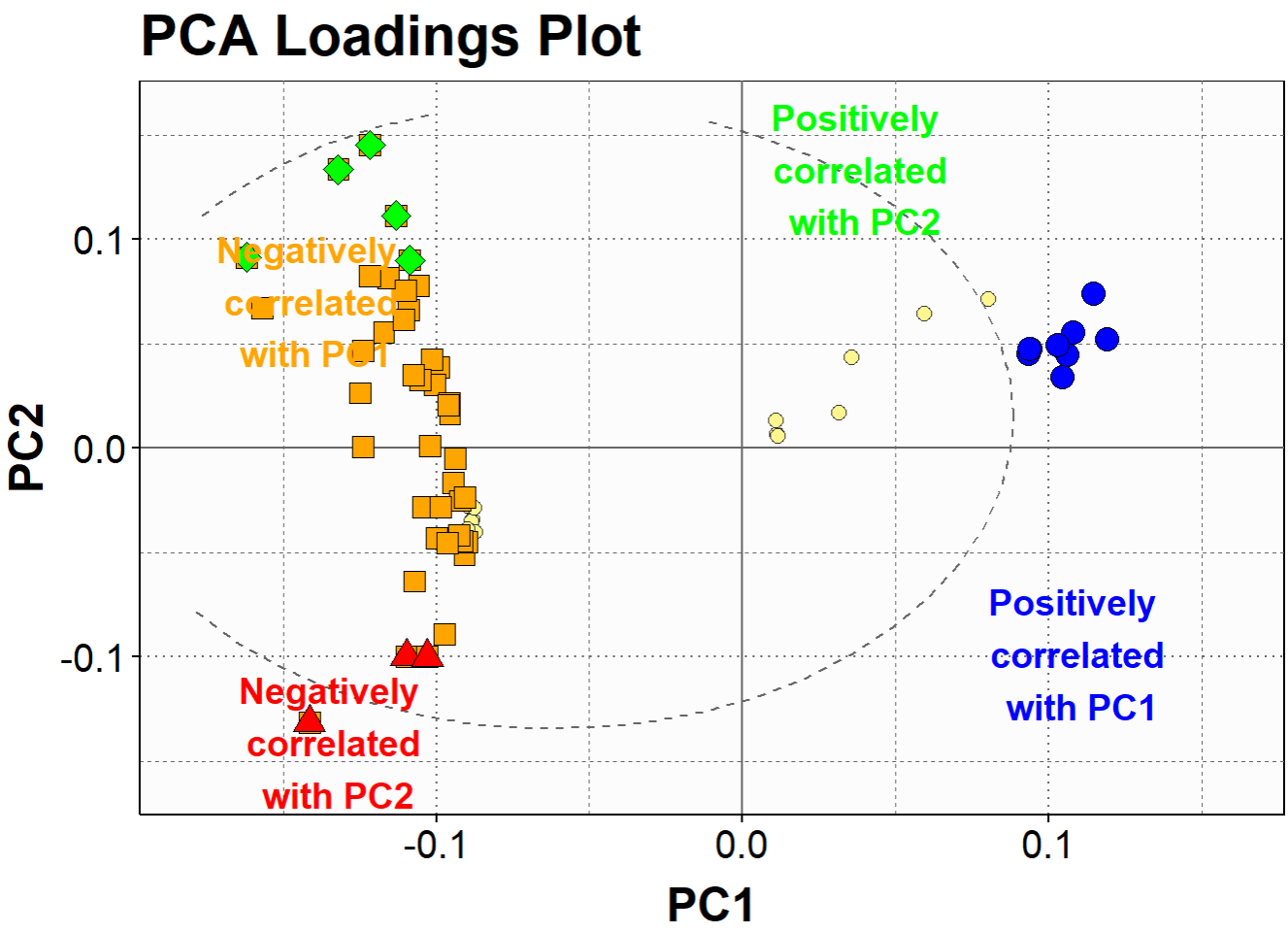
```
## Warning: Removed 16 rows containing missing values (geom_point).
```

```
## Warning: Removed 1 rows containing missing values (geom_point).
```

```
## Warning: Removed 6 rows containing missing values (geom_point).
```

```
## Warning: Removed 11 rows containing missing values (geom_point).
```

```
## Warning: Removed 5 rows containing missing values (geom_point).
```




```
# save as png file
png(file="loadings.plot.png", height=2400, width=2800, res=350)
g2a
```

```
## Warning: Removed 16 rows containing non-finite values (stat_ellipse).
```

```
## Warning: Removed 16 rows containing missing values (geom_point).
```

```
## Warning: Removed 1 rows containing missing values (geom_point).
```

```
## Warning: Removed 6 rows containing missing values (geom_point).
```

```
## Warning: Removed 11 rows containing missing values (geom_point).
```

```
## Warning: Removed 5 rows containing missing values (geom_point).
```

```
dev.off()
```

```
## png
##   2
```