Analysis Frontier Final version

OC

23 January 2019

Contents

1 Data

In this data set, **three bioreactors** with similar performances were considered as replicates. Different parameters were measured accross time in the three bioreactors.

Performance data: Based on chemical measurement, the time course evolution of a set of parameters was measured (CH4, C02, acetate, propionate).

Metabolites data: The time course evolution of 20 selected metabolites was measured with GCMS.

Microbial data: DNA from samples taken across time was extracted and sequenced. (16S metabarcoding).

```
## Loading of the data
```

2 Data transformation

Performance data is not transformed.

Metabolites (GCMS) data are log transformed.

Microbial data

1) are filtered (only OTUs with at least 1% of abundance in at least 1 sample are kept = 51 OTUs).
2) a count of 1 sequence is added to each sample/OTU (to avoid 0 in the datamatrix)
3) relative abundance is calculated
4) obtain data is clr transformed

```
## Ther are 51 OTUs after 0.01 % filter
```

3 Spline smoothing

All the data are modelled with spline smoothing. After spline smoothing,

```
## Warning in lmmSpline(data = (GCMS_log), time =
## metadata_GCMS$Number_of_days, : The number of knots is automatically
## estimated
```

```
## Warning in lmmSpline(data = (clr_abundance), time =
## OTU_metadata$Number_of_days, : The number of knots is automatically
## estimated
```

```
## Warning in lmmSpline(data = cbind(melt_liq$acetate, melt_liq$propionate), :
## The number of knots is automatically estimated
```

```
## Warning in lmmSpline(data = cbind(melt_perf$CH4, melt_perf$CO2), time =
## melt_perf$time, : The number of knots is automatically estimated
```

4 Use of Antoine's filters

4.1 OTUs

```
## Warning: package 'tseries' was built under R version 3.5.2
```

```
## Warning: package 'lmtest' was built under R version 3.5.2
```

```
## Loading required package: zoo
```

```
## Warning: package 'zoo' was built under R version 3.5.2
```

```
##
## Attaching package: 'zoo'
```

```
## The following objects are masked from 'package:base':
##
##     as.Date, as.Date.numeric
```

```
## Warning: Column `molecule` joining factor and character vector, coercing
## into character vector
```

```
## Joining, by = c("time", "molecule")
```

```
## Joining, by = "molecule"
```

```
## Joining, by = c("time", "molecule")
```

```
## # A tibble: 102 x 3
## # Groups:   molecule [?]
##    molecule model_used     MSE
##    <chr>    <fct>        <dbl>
##  1 OTU_1    0           0.0750
##  2 OTU_1    <NA>       NA
##  3 OTU_10   1           0.0235
##  4 OTU_10   <NA>       NA
##  5 OTU_107  0           3.42
##  6 OTU_107  <NA>       NA
##  7 OTU_11   0           0.0553
##  8 OTU_11   <NA>       NA
##  9 OTU_13   1           0.0534
## 10 OTU_13   <NA>       NA
## # ... with 92 more rows
```

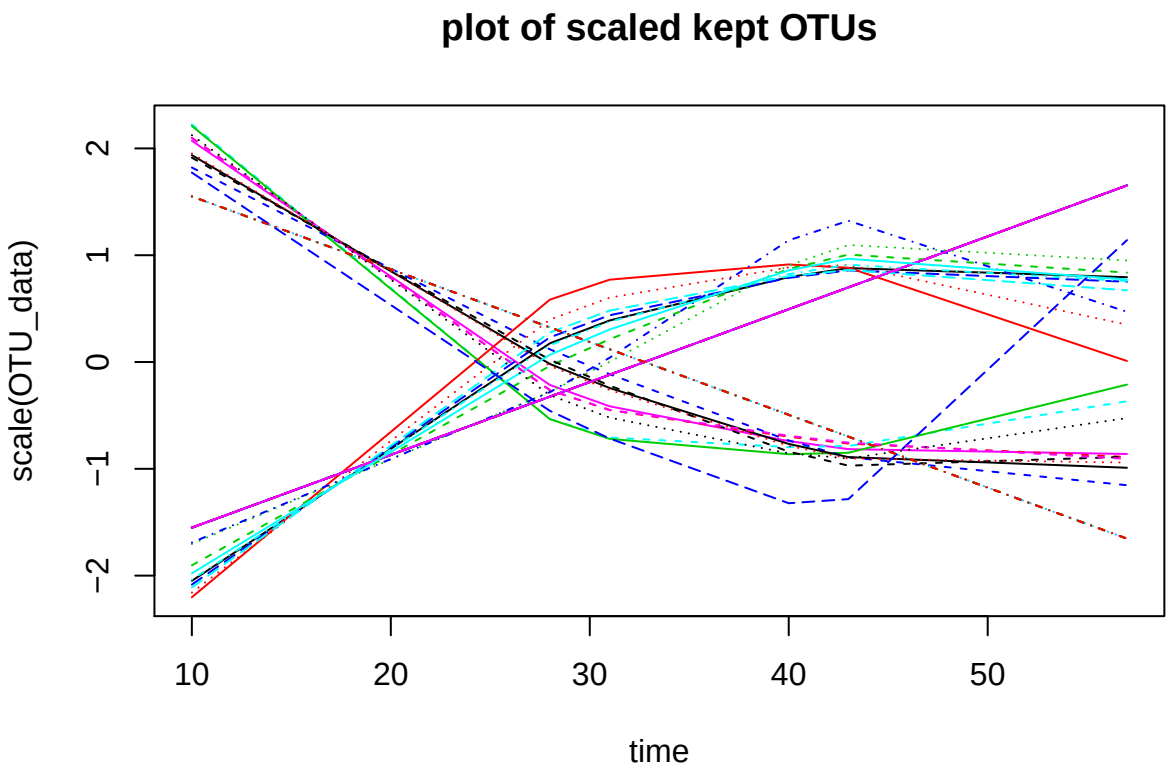
```
## [1] "res.filter" "to_keep"
```

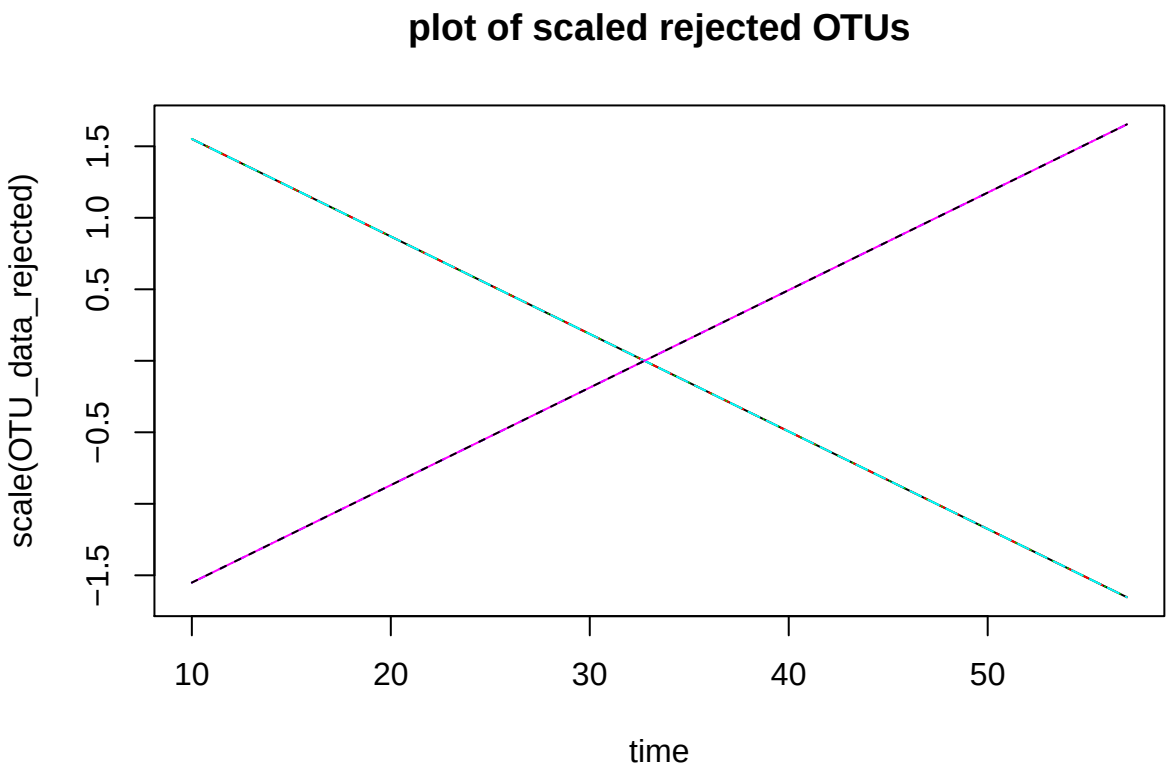
```
## character(0)
```

```
## # A tibble: 102 x 4
## # Groups:   molecule [?]
##    molecule MSE.filter modelsUsed BP.test
##    <chr>    <lgl>           <dbl> <lgl>
##  1 OTU_2    TRUE                1 TRUE
##  2 OTU_2    NA                  1 TRUE
##  3 OTU_1    TRUE                0 TRUE
##  4 OTU_1    NA                  0 TRUE
##  5 OTU_4    TRUE                0 TRUE
##  6 OTU_4    NA                  0 TRUE
##  7 OTU_5    TRUE                0 TRUE
##  8 OTU_5    NA                  0 TRUE
##  9 OTU_6    TRUE                0 TRUE
## 10 OTU_6    NA                  0 TRUE
## # ... with 92 more rows
```

```
##  MSE.filter       BP.test
##  Mode :logical   Mode :logical
##  FALSE:6         FALSE:2
##  TRUE :45        TRUE :100
##  NA's :51
```

```
##    molecule         MSE.filter        modelsUsed     BP.test
##  Length:51          Mode :logical   Min.   :0.000   Mode :logical
##  Class :character   FALSE:6         1st Qu.:0.000   FALSE:1
##  Mode  :character   TRUE :45        Median :0.000   TRUE :50
##                                     Mean   :0.451
##                                     3rd Qu.:1.000
##                                     Max.   :2.000
```


plot of scaled kept OTUs
scale(OTU_data)
2
1
0
−1
−2
10
20
30
40
50
time




```
## rejected OTUs are OTU_22 OTU_33 OTU_34 OTU_51 OTU_84 OTU_92 OTU_107
```

4.2 GCMS

```
## Warning: Column `molecule` joining character vector and factor, coercing
## into character vector

## Warning in function_list[[k]](value): NAs introduced by coercion

## Joining, by = c("time", "molecule")

## Warning in max(.): no non-missing arguments to max; returning -Inf

## Joining, by = "molecule"

## Warning in function_list[[k]](value): NAs introduced by coercion

## Joining, by = c("time", "molecule")

## # A tibble: 20 x 3
## # Groups:   molecule [?]
##    molecule  model_used   MSE
##    <chr>     <fct>      <dbl>
##  1 M106T894  <NA>          NA
##  2 M129T1196 <NA>          NA
##  3 M179T1018 <NA>          NA
##  4 M205T1473 <NA>          NA
##  5 M207T1196 <NA>          NA
##  6 M229T1227 <NA>          NA
```

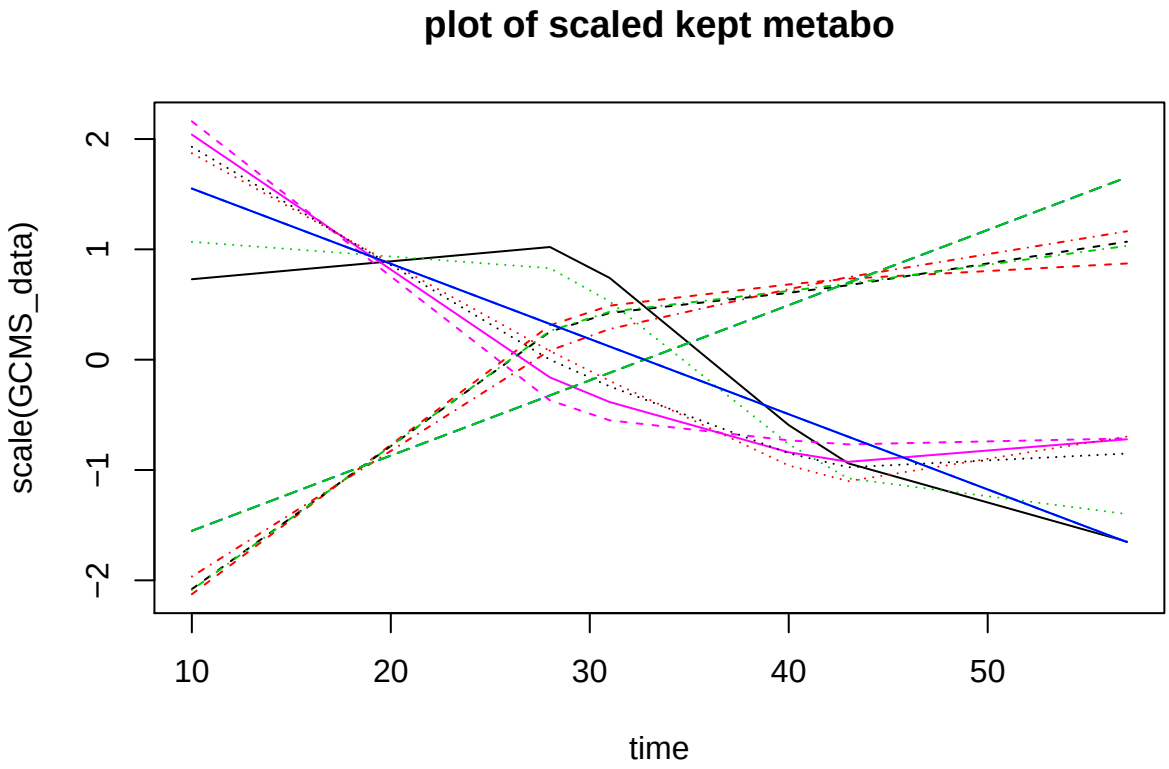
```
##  7 M266T1372 <NA>          NA
##  8 M271T1466 <NA>          NA
##  9 M285T1569 <NA>          NA
## 10 M290T1524 <NA>          NA
## 11 M291T1584 <NA>          NA
## 12 M292T1383 <NA>          NA
## 13 M299T1033 <NA>          NA
## 14 M308T1437 <NA>          NA
## 15 M310T1500 <NA>          NA
## 16 M357T2099 <NA>          NA
## 17 M369T1850 <NA>          NA
## 18 M379T1799 <NA>          NA
## 19 M398T1643 <NA>          NA
## 20 M415T2220 <NA>          NA
```

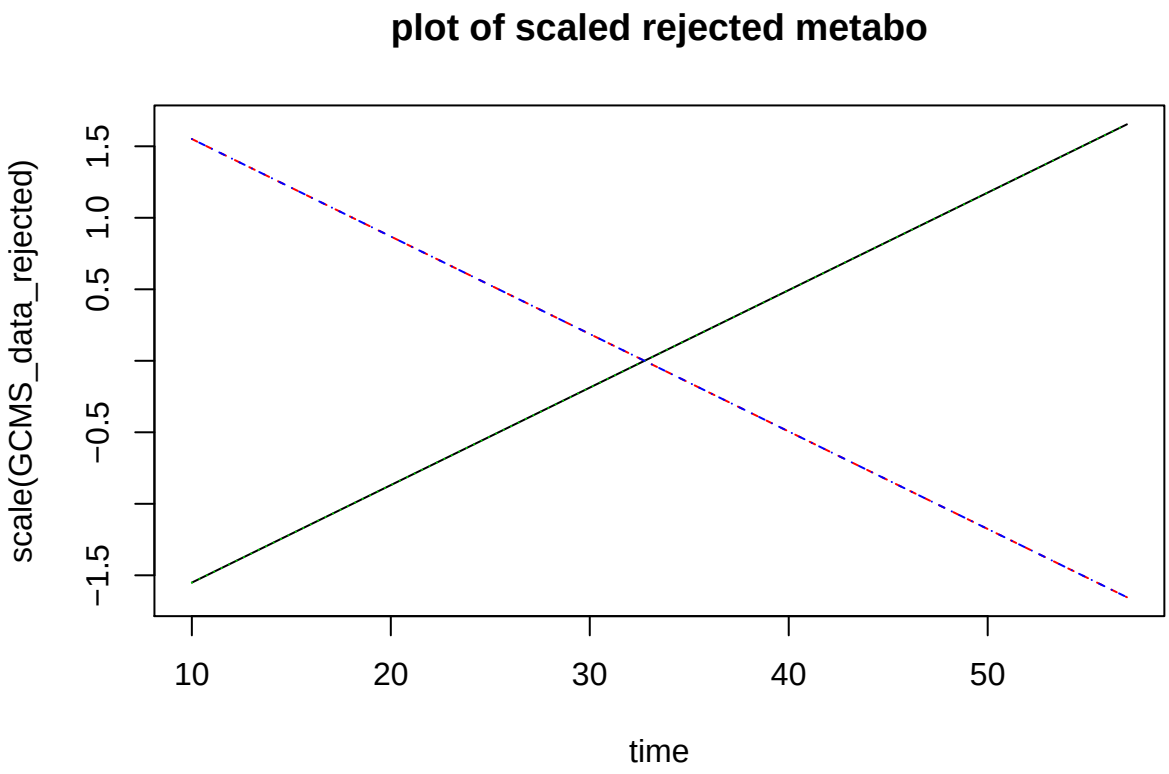
```
## [1] "res.filter" "to_keep"
```

```
## character(0)
```

```
## # A tibble: 20 x 5
## # Groups:   molecule [?]
##    molecule  MSE.filter ADF.test modelsUsed BP.test
##    <chr>     <lgl>      <lgl>         <dbl> <lgl>
##  1 M266T1372 NA         FALSE             0 FALSE
##  2 M271T1466 NA         FALSE             2 TRUE
##  3 M179T1018 NA         FALSE             2 TRUE
##  4 M129T1196 NA         FALSE             0 FALSE
##  5 M207T1196 NA         FALSE             3 TRUE
##  6 M106T894  NA         FALSE             0 TRUE
##  7 M308T1437 NA         FALSE             0 TRUE
##  8 M310T1500 NA         FALSE             2 TRUE
##  9 M290T1524 NA         FALSE             3 TRUE
## 10 M285T1569 NA         FALSE             2 TRUE
## 11 M379T1799 NA         FALSE             3 TRUE
## 12 M369T1850 NA         FALSE             0 FALSE
## 13 M357T2099 NA         FALSE             0 TRUE
## 14 M415T2220 NA         FALSE             0 TRUE
## 15 M229T1227 NA         FALSE             3 TRUE
## 16 M205T1473 NA         FALSE             3 TRUE
## 17 M292T1383 NA         FALSE             3 TRUE
## 18 M299T1033 NA         FALSE             0 FALSE
## 19 M291T1584 NA         FALSE             0 TRUE
## 20 M398T1643 NA         FALSE             0 TRUE
```

```
##   ADF.test        BP.test
##  Mode :logical   Mode :logical
##  FALSE:20        FALSE:4
##                  TRUE :16
```


plot of scaled kept metabo
scale(GCMS_data)
2
1
0
−1
−2
10
20
30
40
50
time



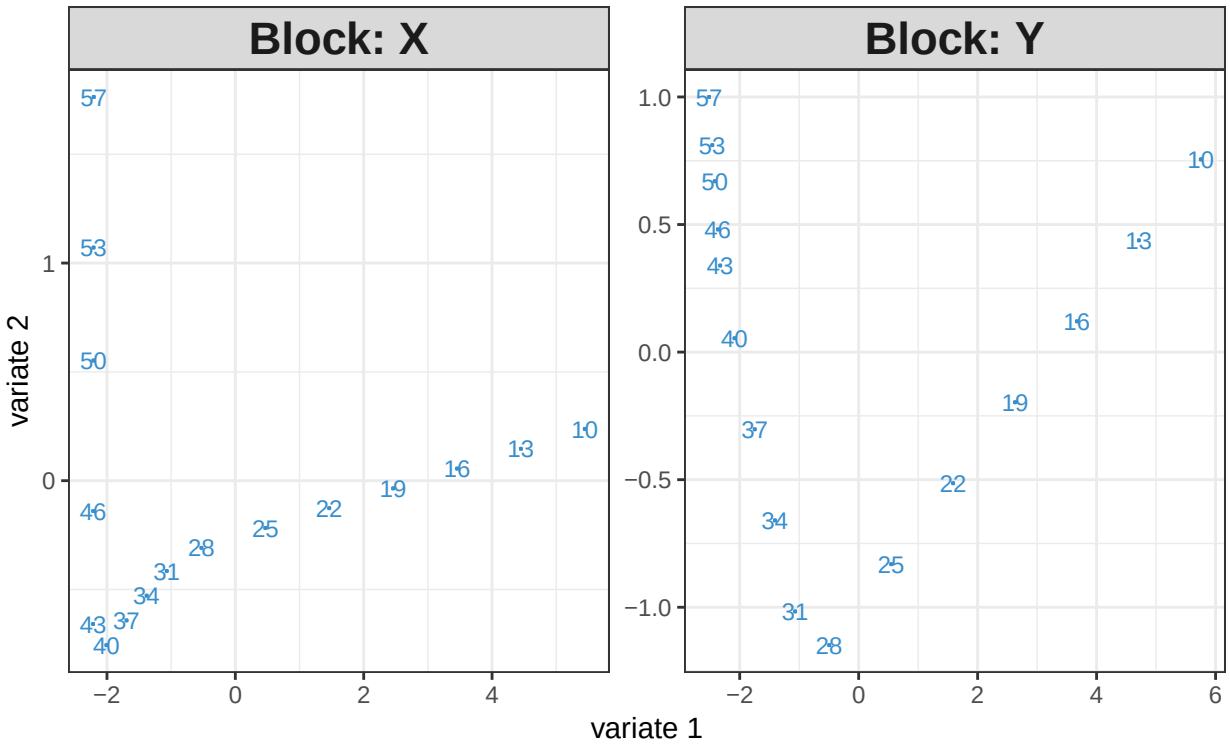

```
## rejected OTUs are M266T1372 M129T1196 M369T1850 M299T1033
```

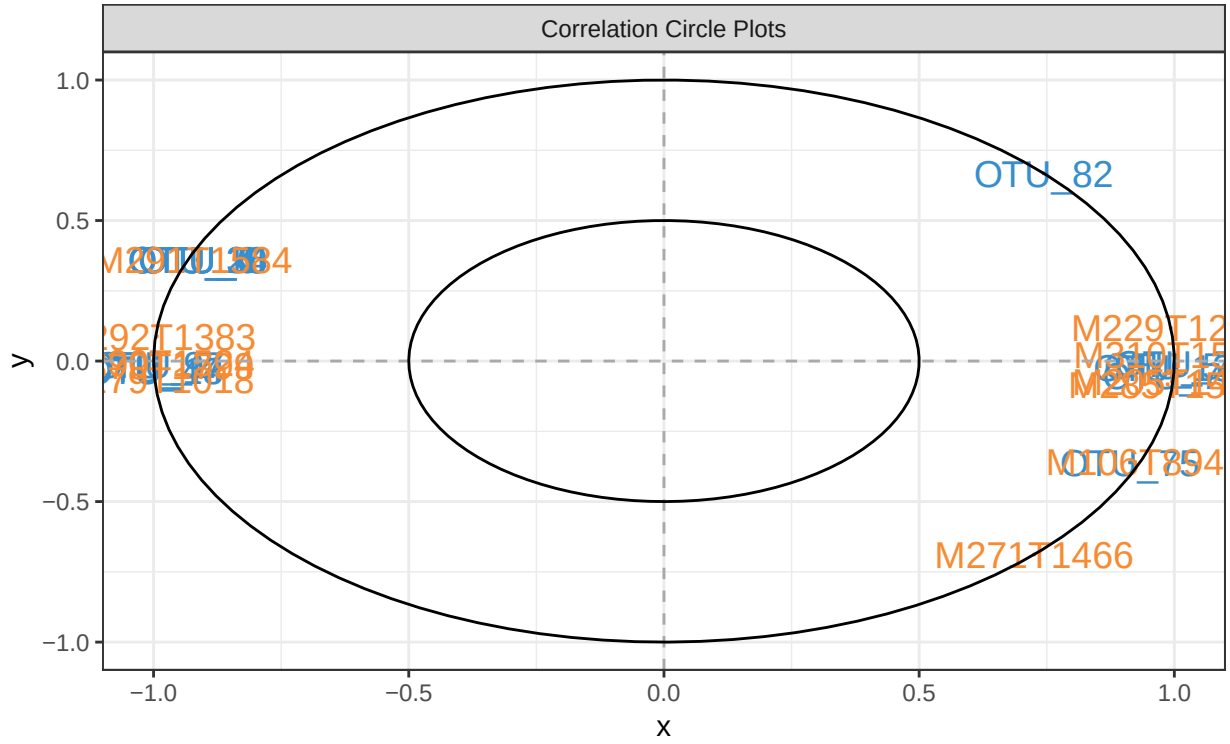
5 Data integration with PLS/sPLS

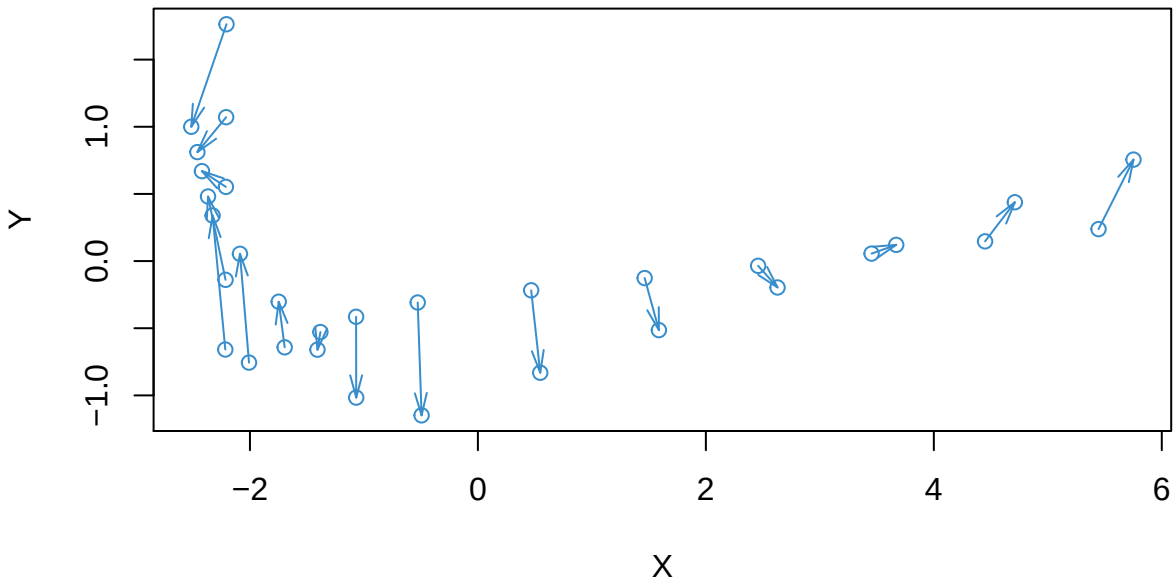
5.1 sPLS

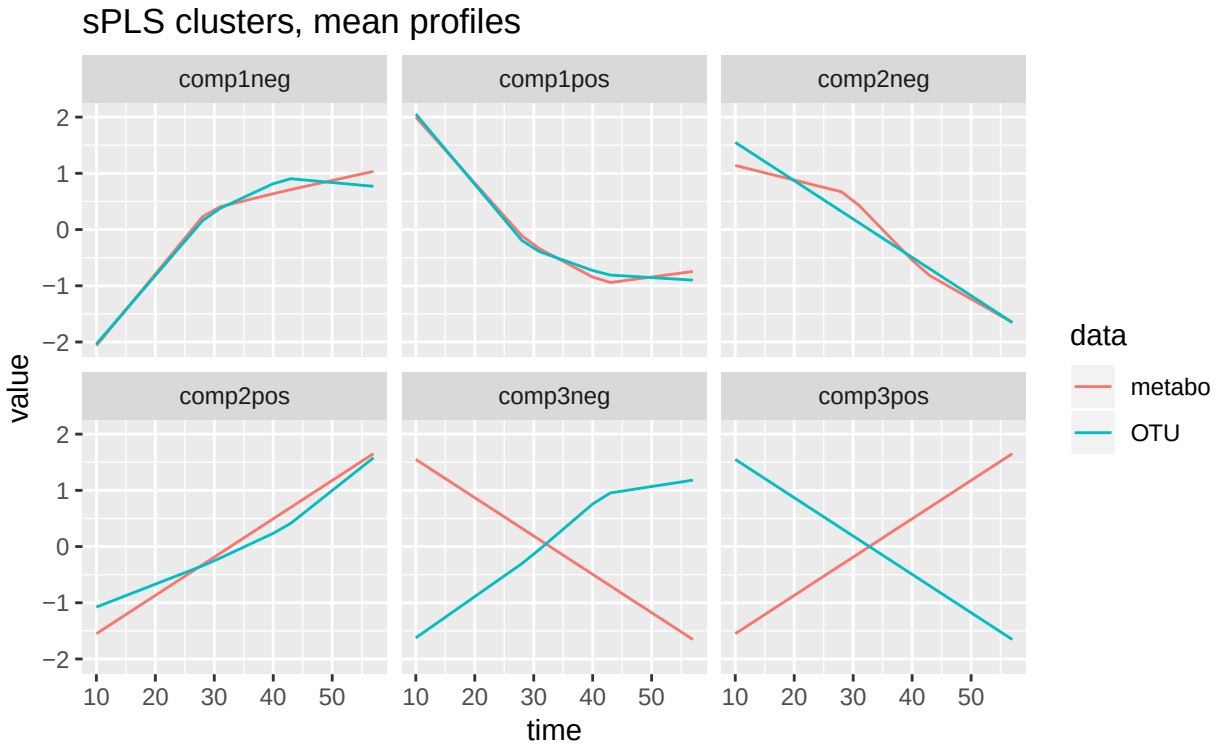
5.1.1 OTUs versus 20 metabolites

5.1.1.1 canonical

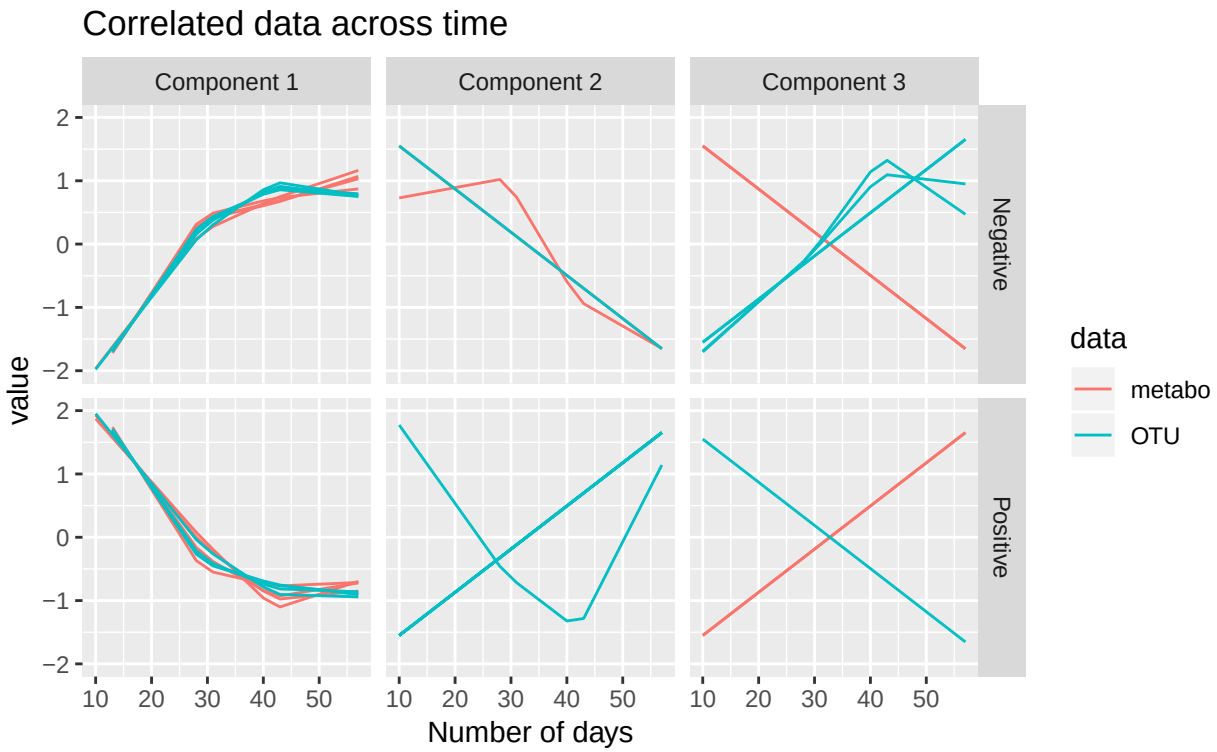

Block: X
Block: Y
variate 2
variate 1
57
53
50
46
43
40
37
34
31
28
25
22
19
16
13
10


Correlation Circle Plots
OTU_82
M271T1466
y
x

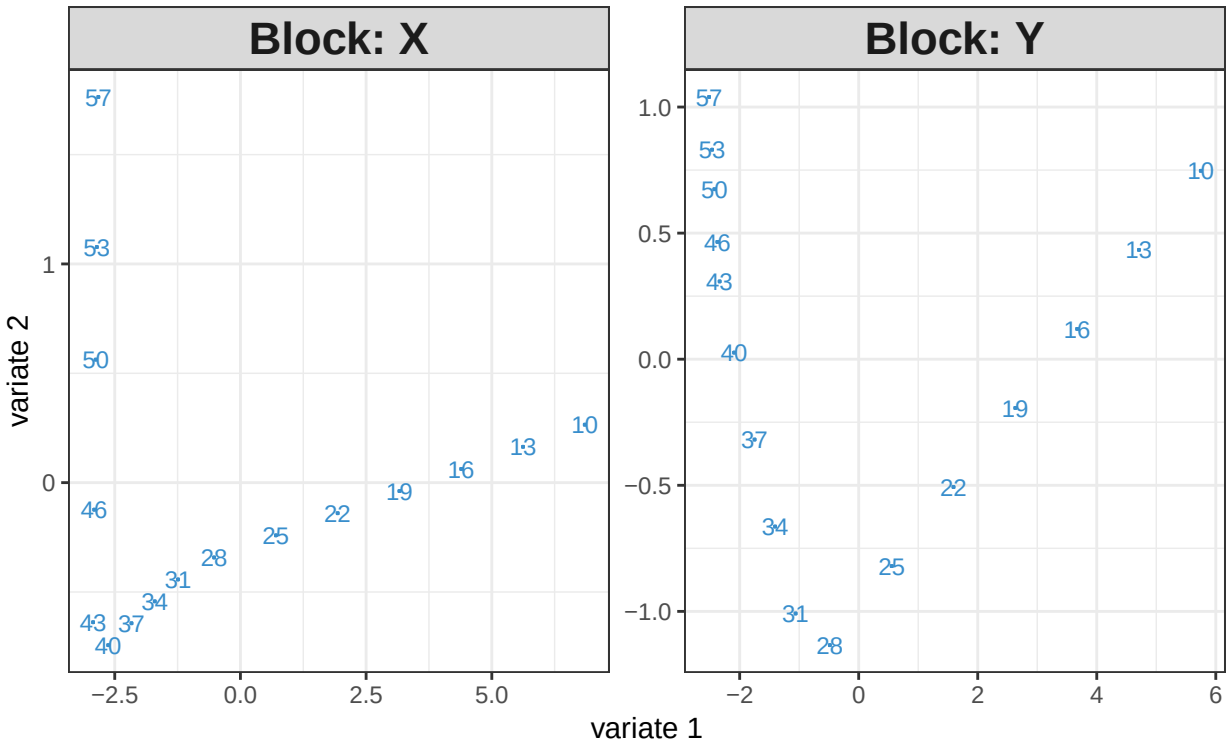


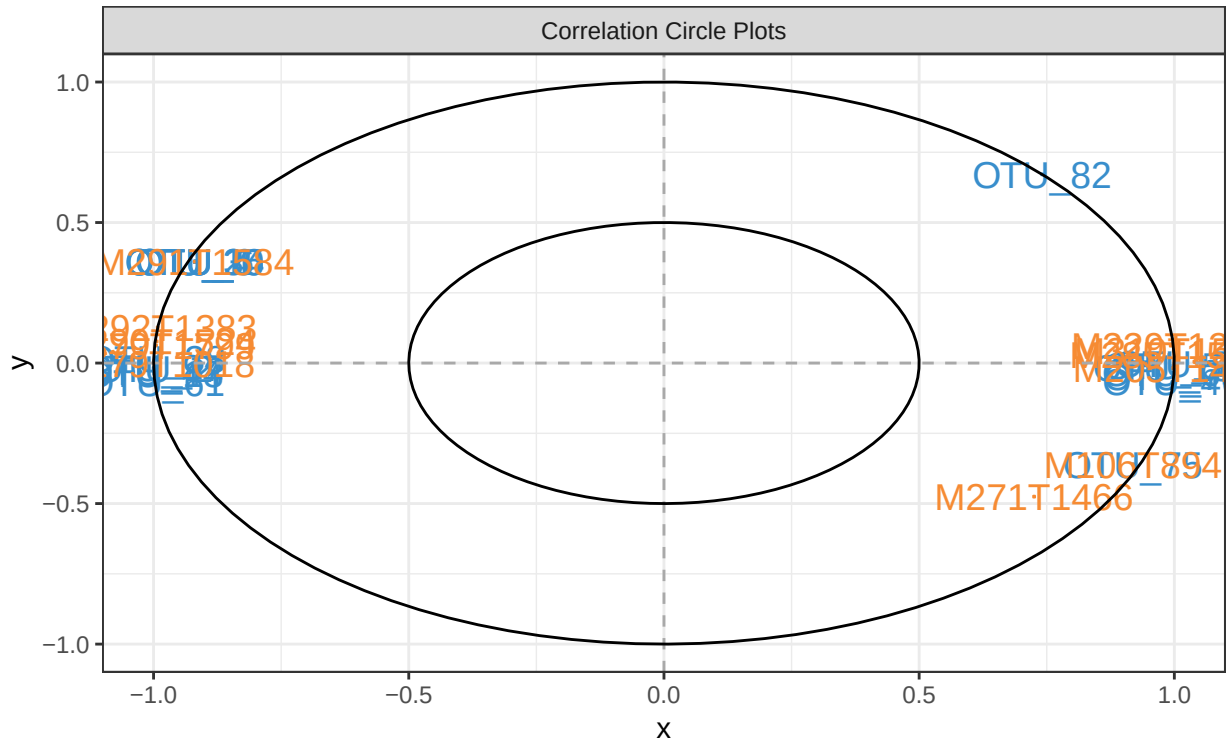


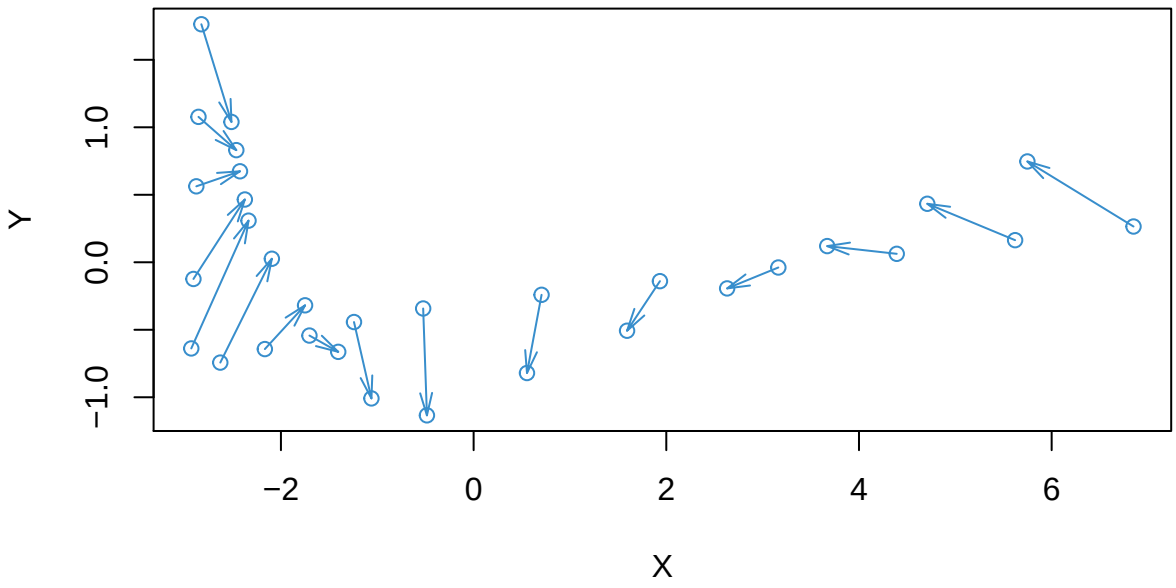

```
## Warning: Removed 11 rows containing missing values (geom_path).
```



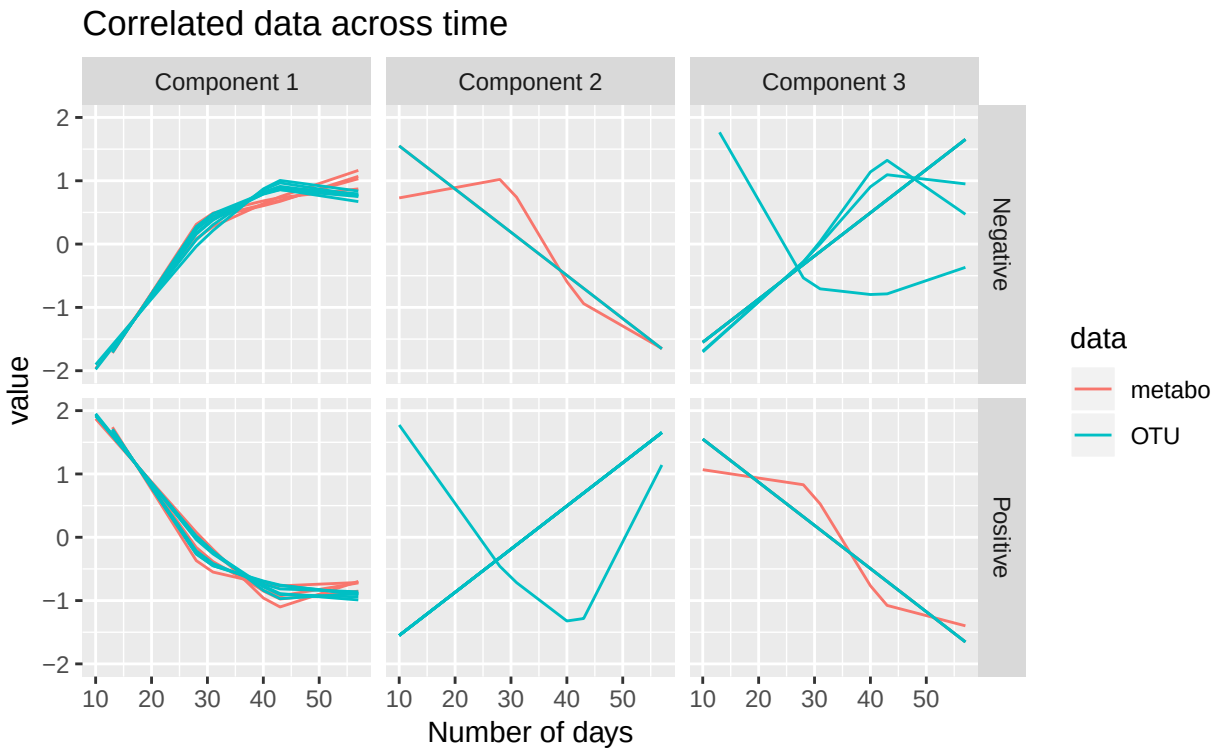
5.1.1.2 regression


Block: X
Block: Y
variate 2
variate 1
57
53
50
46
43
40
37
34
31
28
25
22
19
16
13
10


Correlation Circle Plots
OTU_82
M271T1466
x
y

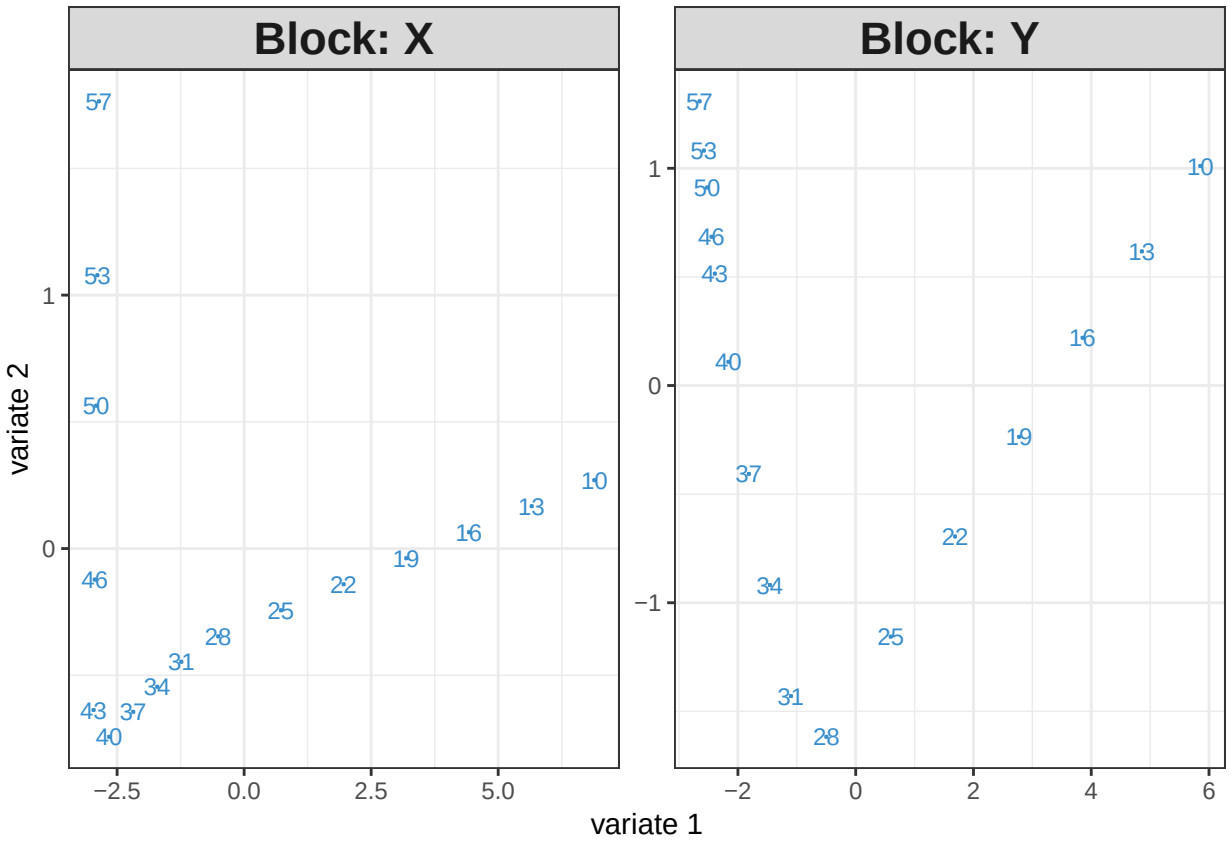


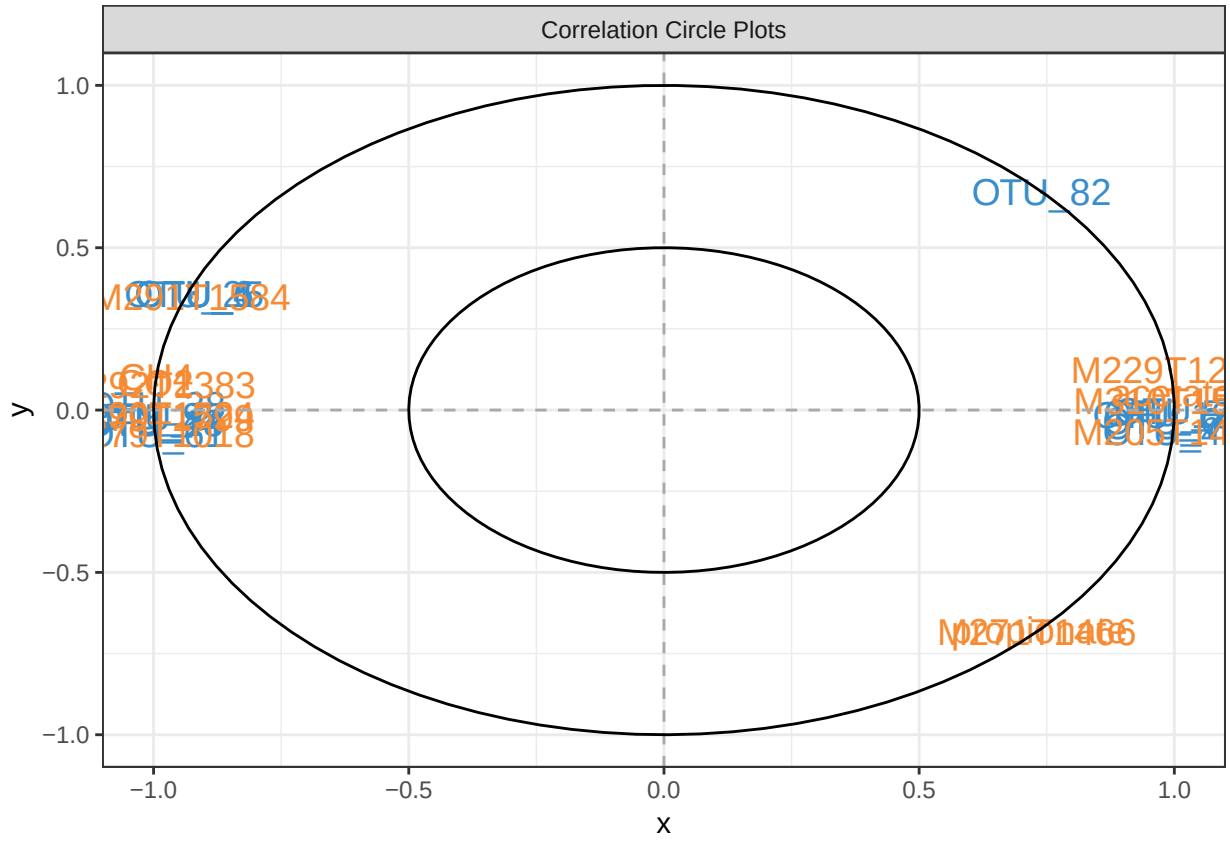

```
## Warning: Removed 13 rows containing missing values (geom_path).
```

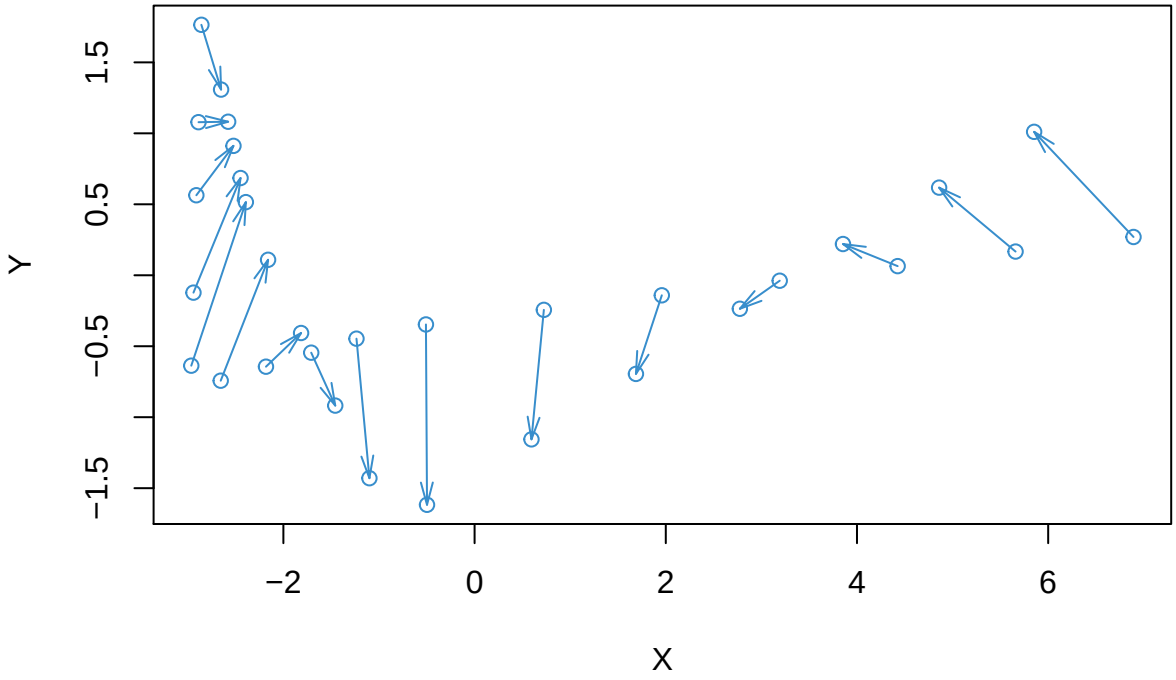


5.1.2 OTUs versus CH4-C02-acetate-propionate-20 metabolites

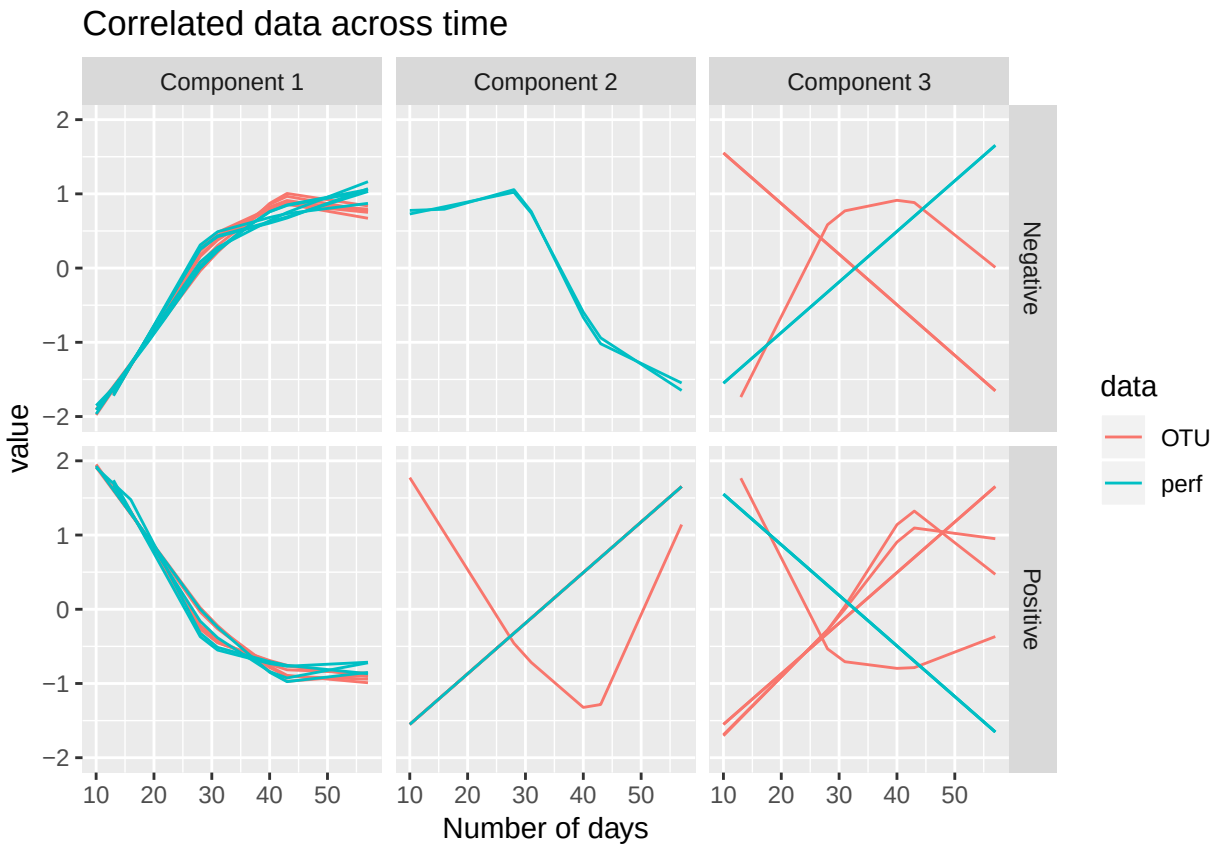
5.1.2.1 canonical


Block: X
Block: Y
variate 2
variate 1
57
53
50
46
43
40
37
34
31
28
25
22
19
16
13
10

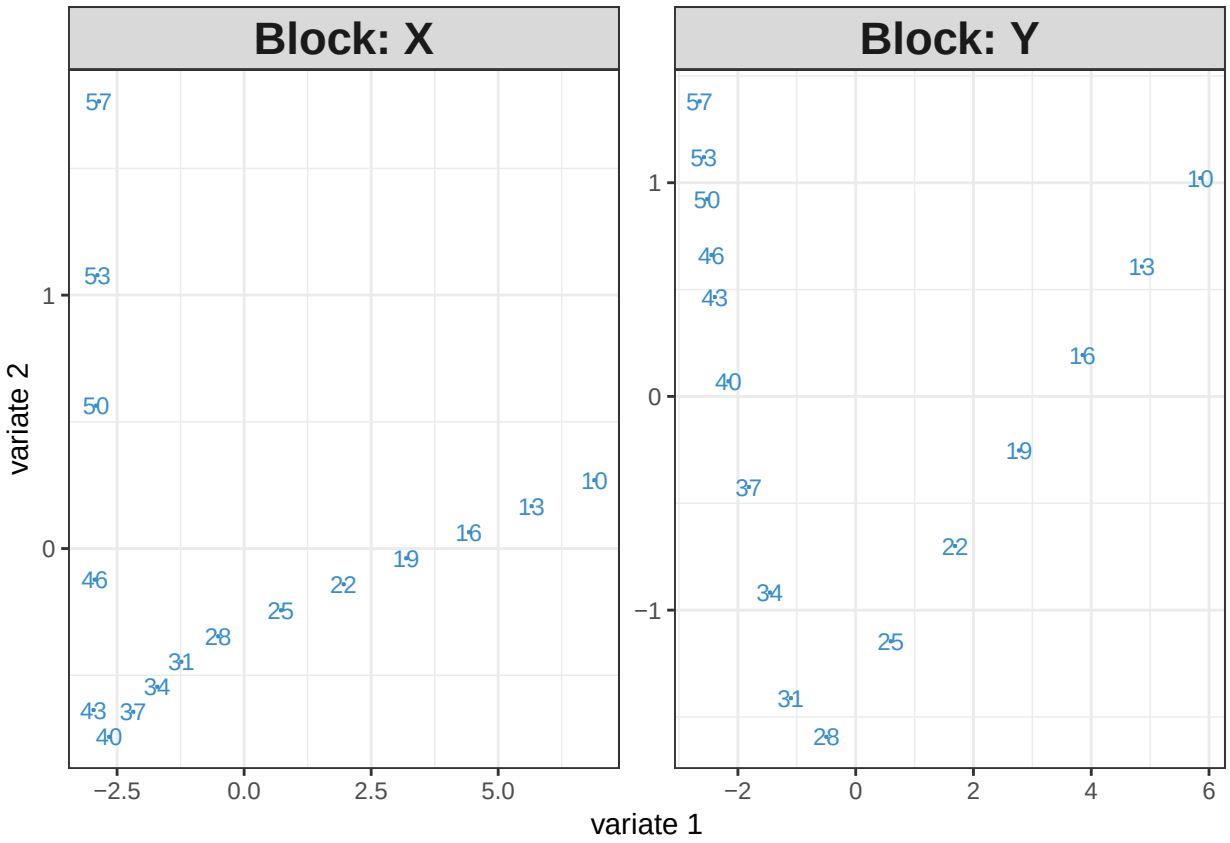

Correlation Circle Plots
OTU_82
x
y

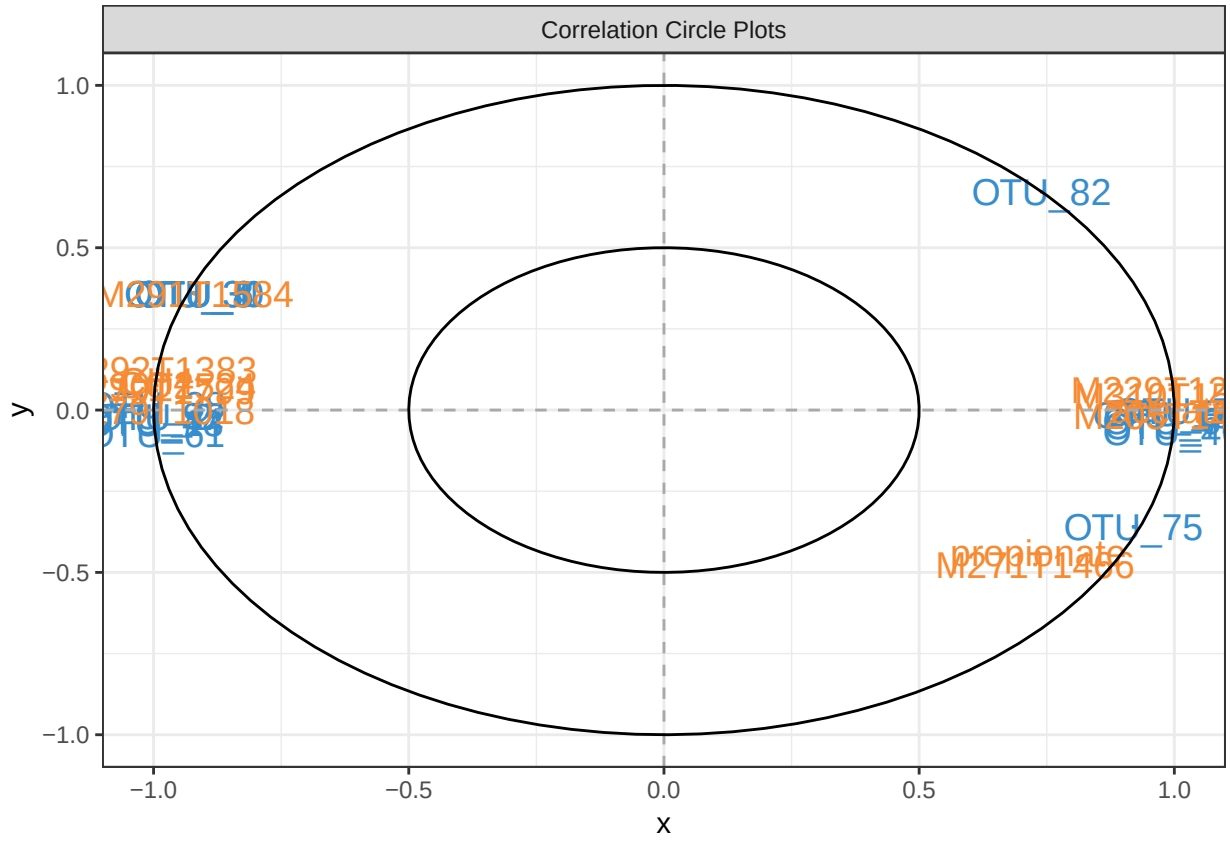

Y
1.5
0.5
−0.5
−1.5
−2
0
2
4
6
X

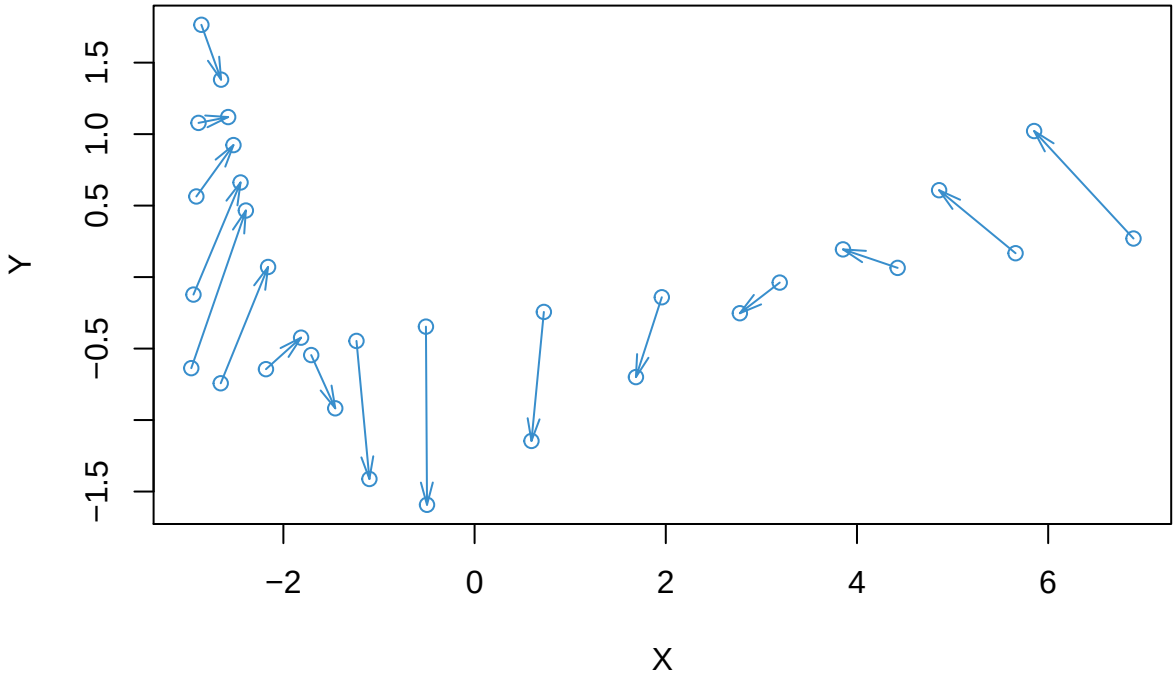

```
## Warning: Removed 14 rows containing missing values (geom_path).
```

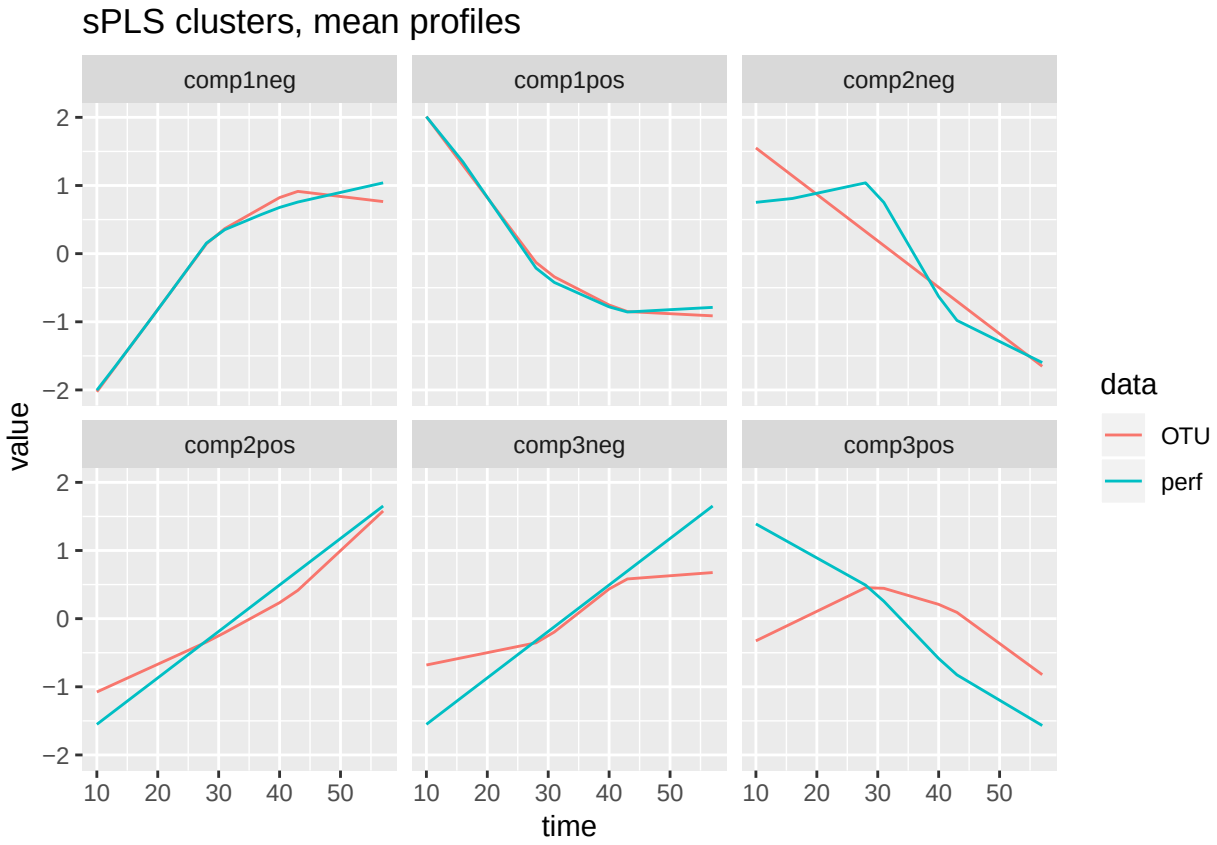


5.1.2.2 regression

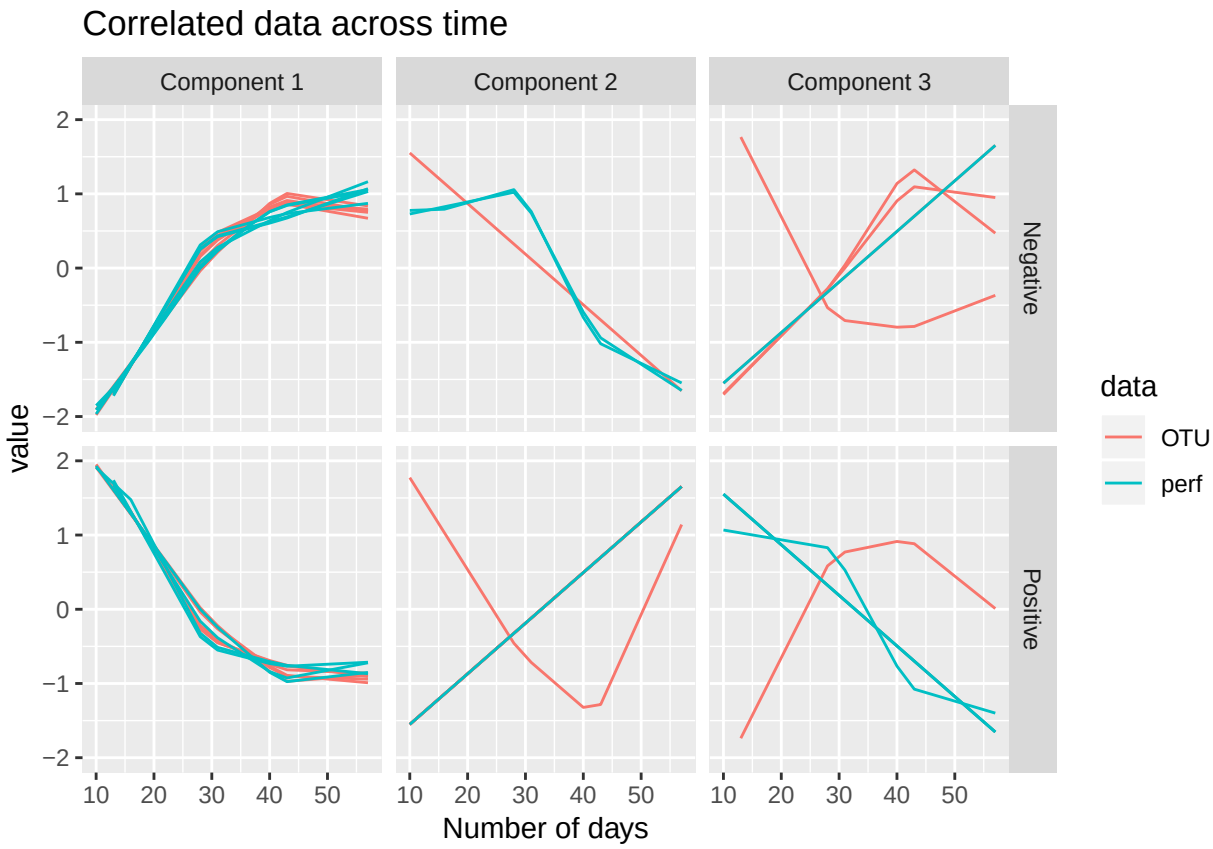

Block: X
Block: Y
variate 2
variate 1
57
53
50
46
43
40
37
34
31
28
25
22
19
16
13
10


Correlation Circle Plots
OTU_82
OTU_75
propionate
M2711466
y
x


Y
1.5
1.0
0.5
−0.5
−1.5
−2
0
2
4
6
X

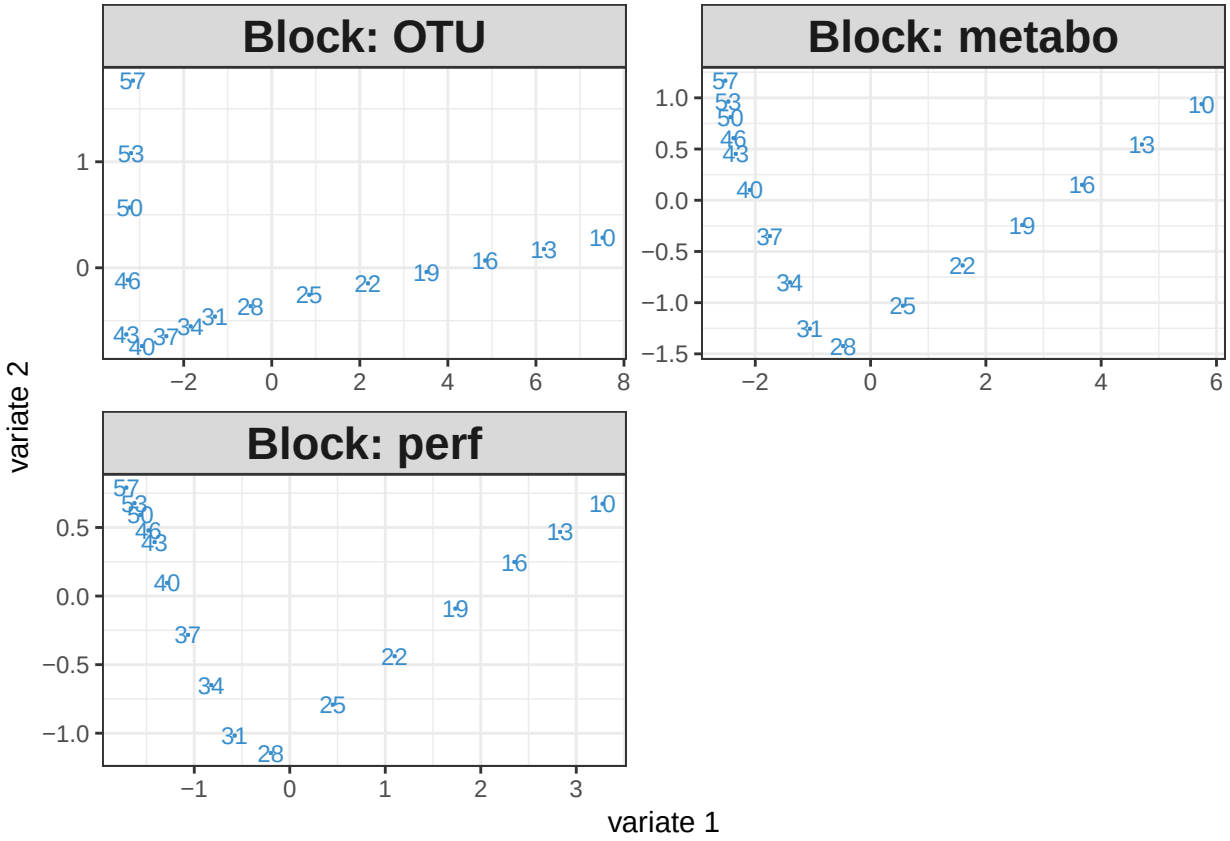


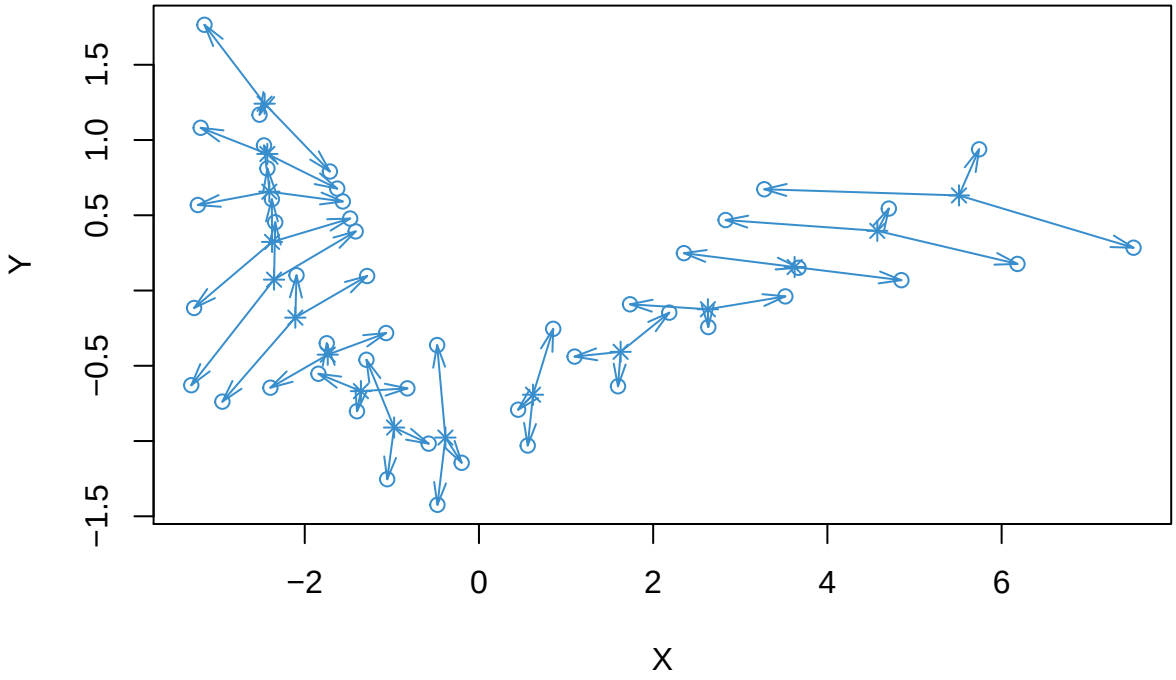

```
## Warning: Removed 14 rows containing missing values (geom_path).
```

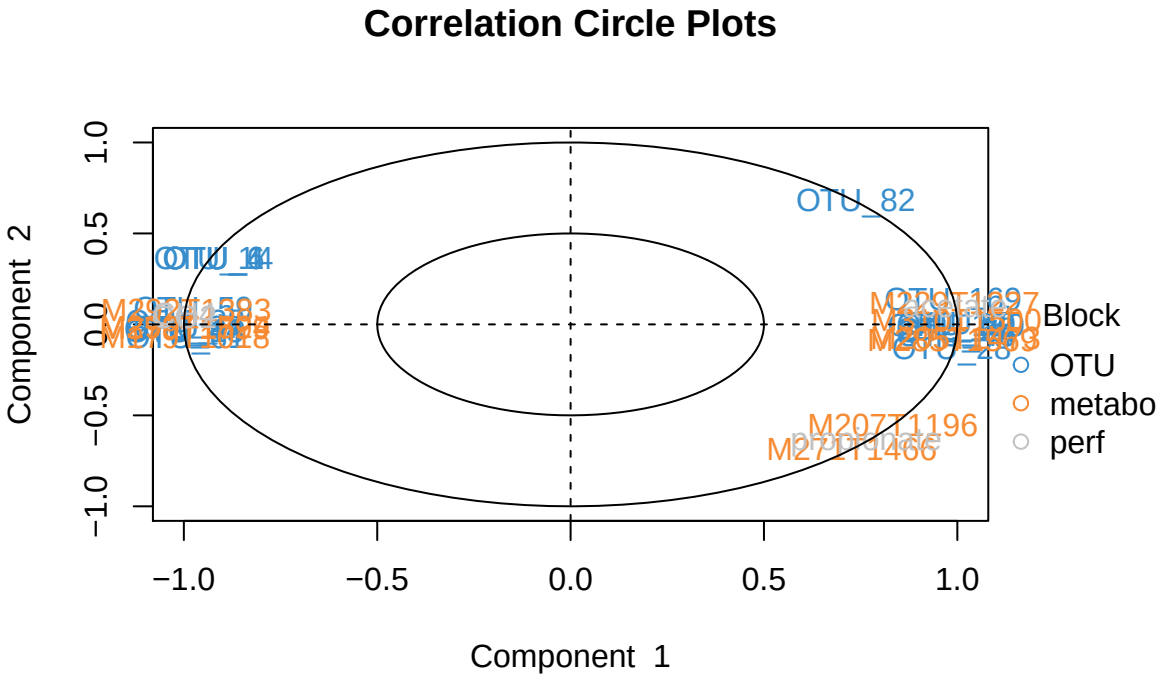

Correlated data across time
Component 1
Component 2
Component 3
Negative
Positive
value
Number of days
data
OTU
perf

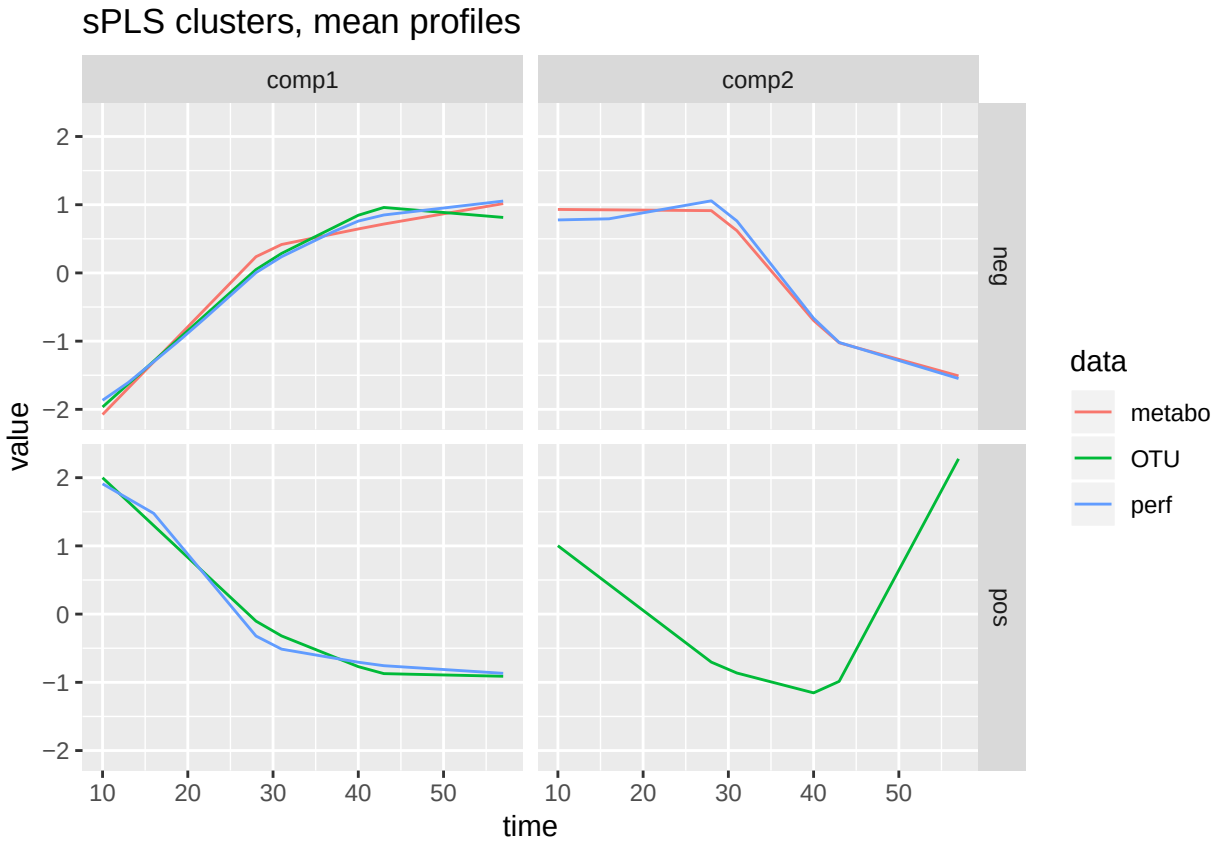
6 rGCCA

6.1 canonical

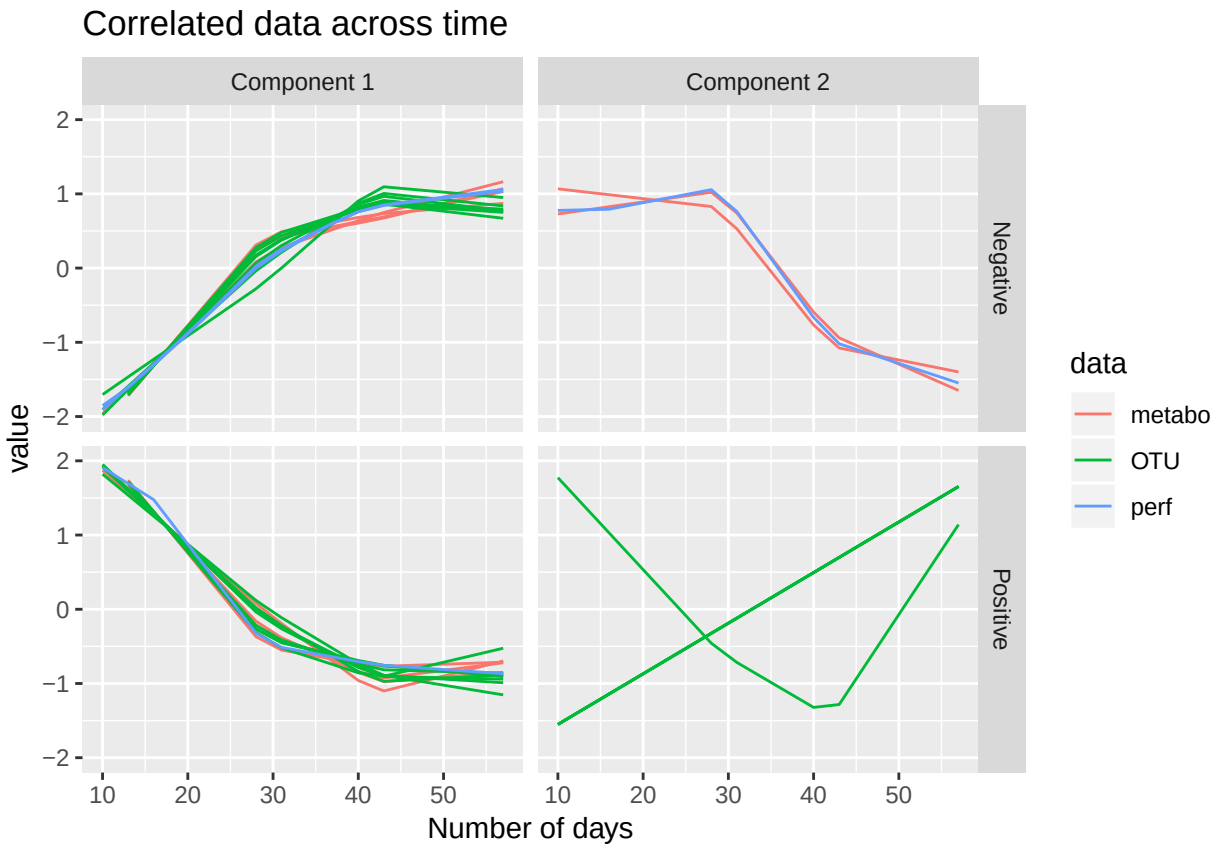



Y
1.5
1.0
0.5
−0.5
−1.5
−2
0
2
4
6
X

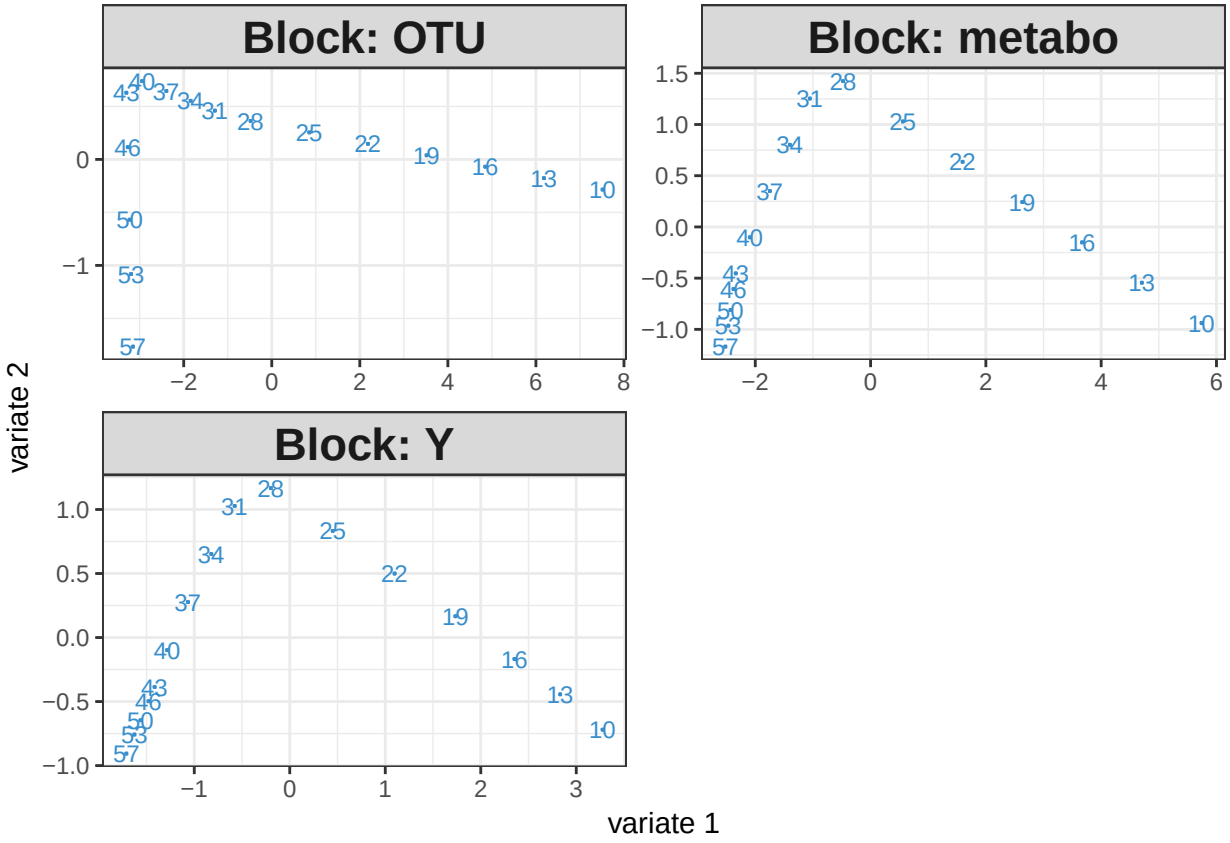

Correlation Circle Plots
Component 2
Component 1
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0
OTU_82
M207T1196
Block
OTU
metabo
perf

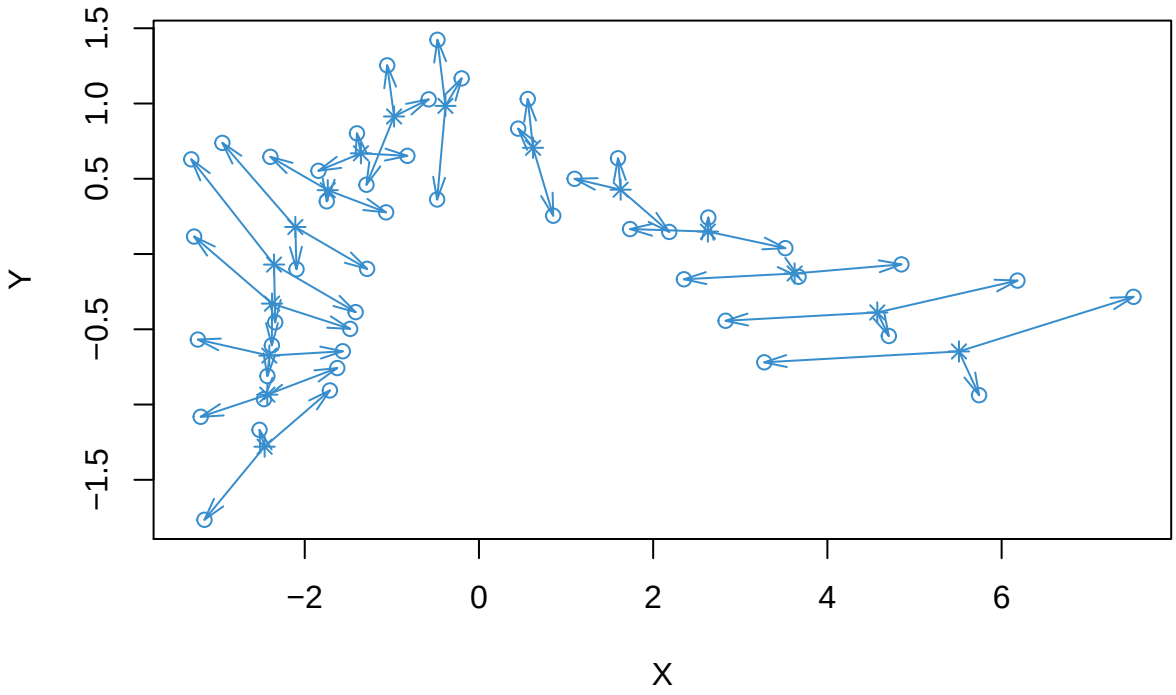


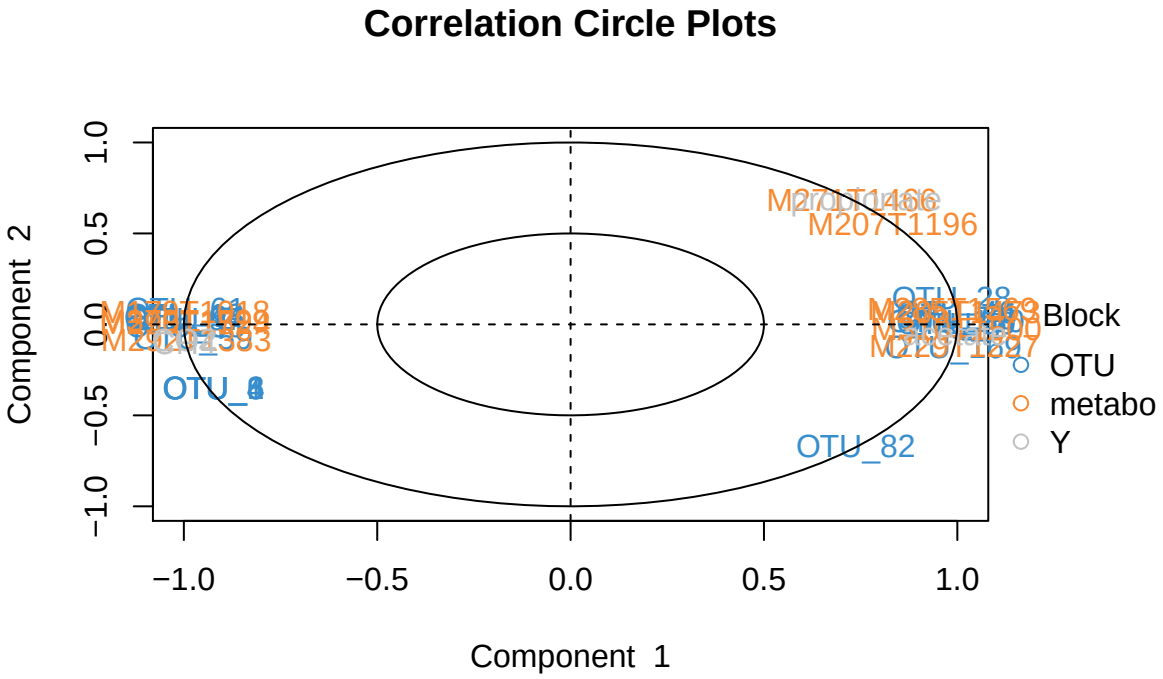

```
## Warning: Removed 13 rows containing missing values (geom_path).
```

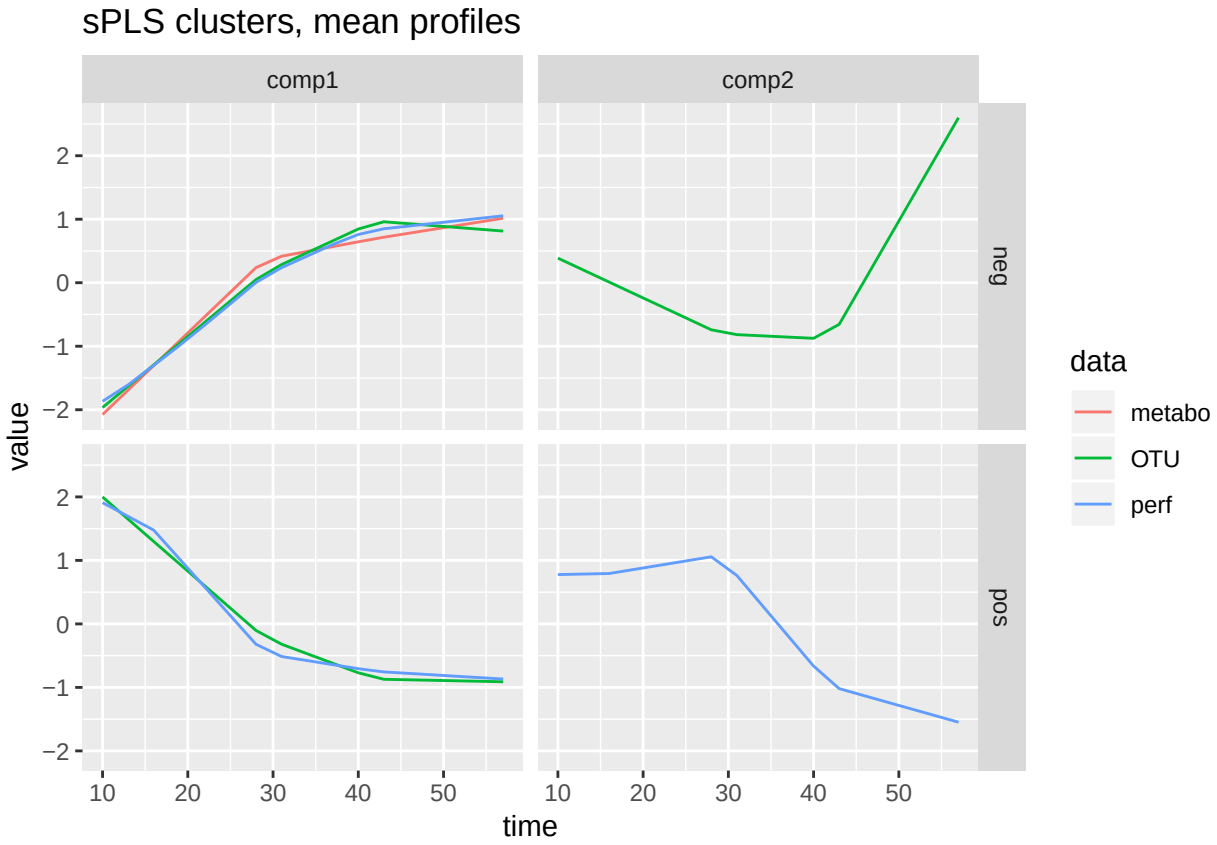

Correlated data across time
Component 1
Component 2
Negative
Positive
value
Number of days
data
metabo
OTU
perf

6.2 regression (Y= perf)

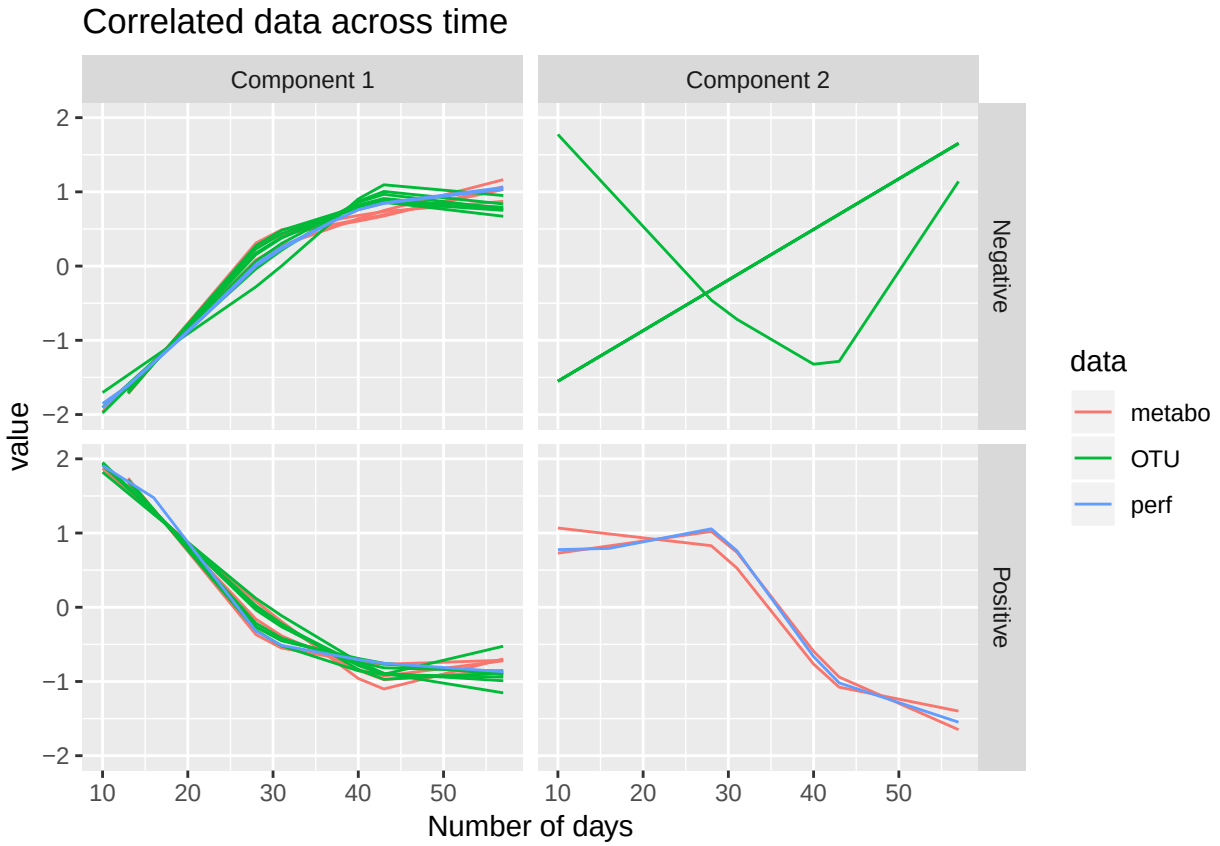



Y
1.5
1.0
0.5
−0.5
−1.5
−2
0
2
4
6
X


Correlation Circle Plots
Component 2
Component 1
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0
M207T1196
OTU_82
Block
OTU
metabo
Y




```
## Warning: Removed 13 rows containing missing values (geom_path).
```



7 timeomics

I try to find delays between the omics and perf data. Perf data: CH4 or propionate (CO2 and acetate are correlated to CH4, I do not use them). To start with, I look at delays between OTUs and CH4/propionate on one side and metabolites and CH4/propionate on another side.

** NEXT STEP: 1) SIMPLIFY THE PLOTS SHOWING THE DELAYS (USE OF source('Code/plot.associations-method2.R') - plot.associations2() FUNCTION ->KIM-ANH PLEASE SEND ME THE CORRESPONDING CODE I COULD NOT FIND IT 2) LOOK FOR POTENTIAL DELAYS BETWEEN METABOLITES AND OTUS 3) INTEGRATE THE DATA TAKING INTO ACCOUNT THE DELAYS, IF NECESSARY. -> I NEED TO CHECK HOW MANY PROFILES WERE 'CORRECTED' AND WERE NOT ALREADY CORRELATED TO SOMETHING**

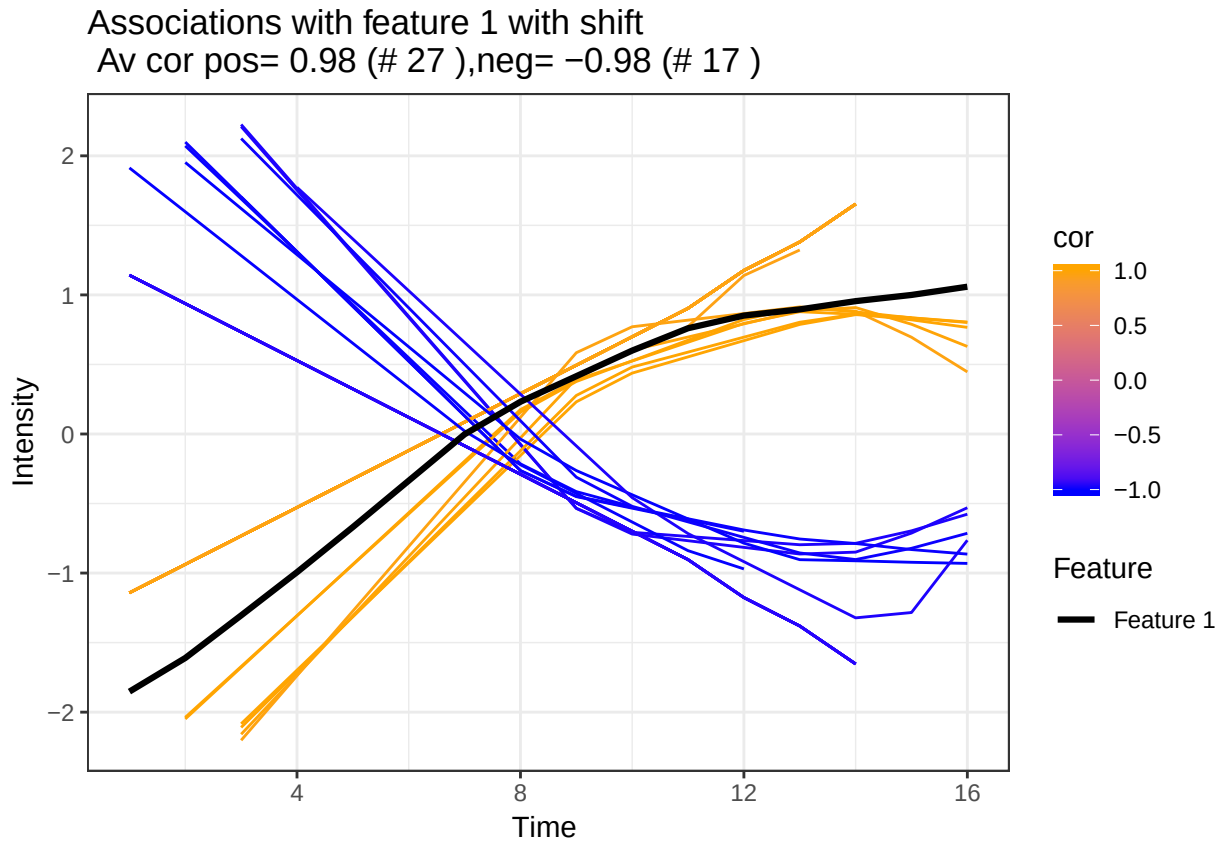
7.1 OTUs versus CH4

```
## reference is methane production.
```

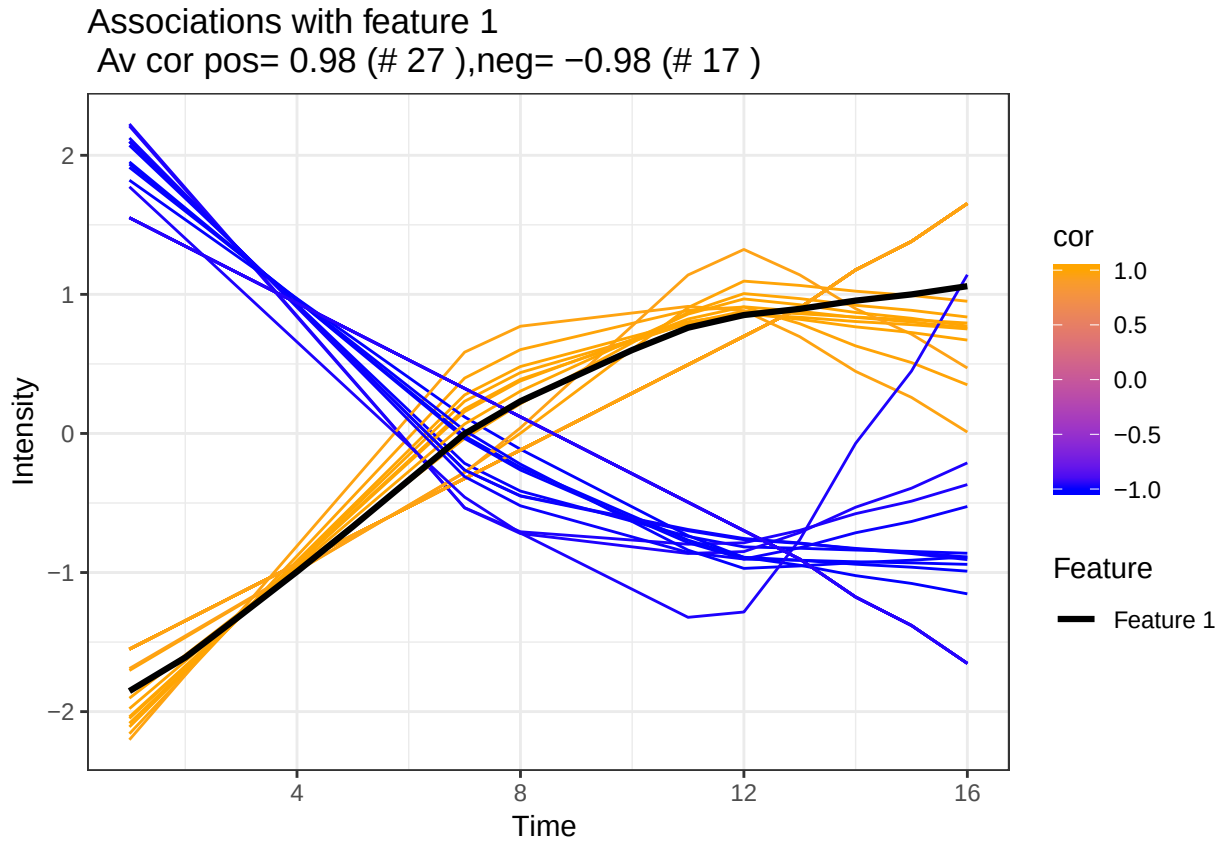
```
##
##
## Table: Example of output from dynOmics time delay detection
##
##  Feature1  Feature2    delay     pBefore   pAfter    corBefore     corAfter
## ---------  ---------  ------  ----------  -------  -----------  -----------
##         1  OTU_2           1   0.0000000        0    0.9910371    0.9973565
```

```
##         1  OTU_1          -2   0.0000000        0    0.9565143    0.9707634
##         1  OTU_4          -2   0.0000000        0    0.9565143    0.9707634
##         1  OTU_5          -2   0.0000000        0    0.9565143    0.9707634
##         1  OTU_6          -2   0.0000000        0    0.9565143    0.9707634
##         1  OTU_7           1   0.0000000        0   -0.9907413   -0.9970082
##         1  OTU_8          -2   0.0000000        0    0.9565143    0.9707634
##         1  OTU_10          2   0.0000000        0    0.9481432    0.9898479
##         1  OTU_11         -2   0.0000000        0    0.9565143    0.9707634
##         1  OTU_13          2   0.0000000        0    0.9864877    0.9975544
##         1  OTU_14         -2   0.0000000        0    0.9565143    0.9707634
##         1  OTU_15         -2   0.0000000        0    0.9565143    0.9707634
##         1  OTU_16         -2   0.0000000        0    0.9565143    0.9707634
##         1  OTU_17         -2   0.0000000        0   -0.9565143   -0.9707634
##         1  OTU_18         -2   0.0000000        0    0.9565143    0.9707634
##         1  OTU_19         -2   0.0000000        0    0.9565143    0.9707634
##         1  OTU_20          2   0.0000001        0   -0.9331336   -0.9812939
##         1  OTU_21         -2   0.0000000        0   -0.9565143   -0.9707634
##         1  OTU_24         -2   0.0000000        0   -0.9565143   -0.9707634
##         1  OTU_25         -2   0.0000000        0    0.9565143    0.9707634
##         1  OTU_26          2   0.0000005        0   -0.9188645   -0.9799382
##         1  OTU_28         -1   0.0000000        0   -0.9973186   -0.9990726
##         1  OTU_29         -2   0.0000000        0   -0.9565143   -0.9707634
##         1  OTU_30         -2   0.0000000        0    0.9565143    0.9707634
##         1  OTU_31         -2   0.0000000        0    0.9565143    0.9707634
##         1  OTU_35          2   0.0000041        0    0.8890857    0.9732323
##         1  OTU_38          0   0.0000000        0    0.9962075    0.9962075
##         1  OTU_41         -2   0.0000000        0    0.9565143    0.9707634
##         1  OTU_44          1   0.0000000        0    0.9906073    0.9971317
##         1  OTU_45         -2   0.0000000        0    0.9565143    0.9707634
##         1  OTU_46          0   0.0000000        0   -0.9993447   -0.9993447
##         1  OTU_50          1   0.0000000        0   -0.9879706   -0.9951466
##         1  OTU_59         -1   0.0000000        0    0.9881575    0.9918399
##         1  OTU_60          1   0.0000000        0    0.9633617    0.9650104
##         1  OTU_61          2   0.0000000        0    0.9800194    0.9964702
##         1  OTU_65         -2   0.0000000        0    0.9565143    0.9707634
##         1  OTU_68          0   0.0000000        0   -0.9977189   -0.9977189
##         1  OTU_74          1   0.0000000        0   -0.9986184   -0.9987703
##         1  OTU_75         -2   0.0000000        0   -0.9565143   -0.9707634
##         1  OTU_82          3   0.0041705        0   -0.6743315   -0.9816714
##         1  OTU_97          1   0.0000000        0    0.9937034    0.9973144
##         1  OTU_130         1   0.0000000        0   -0.9883070   -0.9952384
##         1  OTU_169         2   0.0000000        0   -0.9692590   -0.9945581
##         1  OTU_304        -2   0.0000000        0   -0.9565143   -0.9707634
## Identifying associations between time profiles using fast Fourier transform.
##
##  Significant associations <0.05 found with shift and without shift:
##                      object$pBefore < 0.05
## object$pAfter < 0.05 TRUE
##                 TRUE   44
##
##  Predicted delays:
##
## -2 -1  0  1  2  3
```

```
## 23  2  3  8  7  1
## number of delays with a correlation > 0.9 once reshifted
## [1] 44
## Warning: Removed 105 rows containing missing values (geom_path).
```




```
## without shift
```

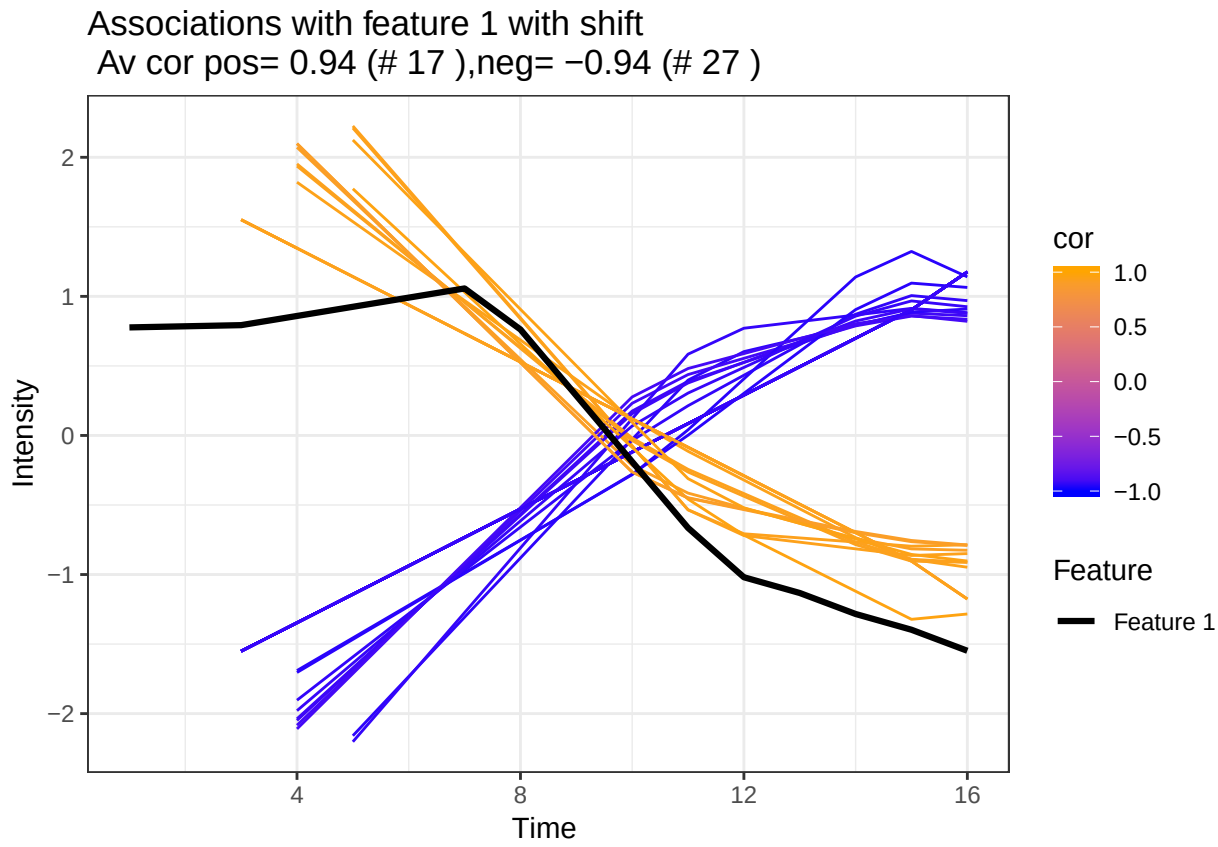


7.2 OTUs versus propionate

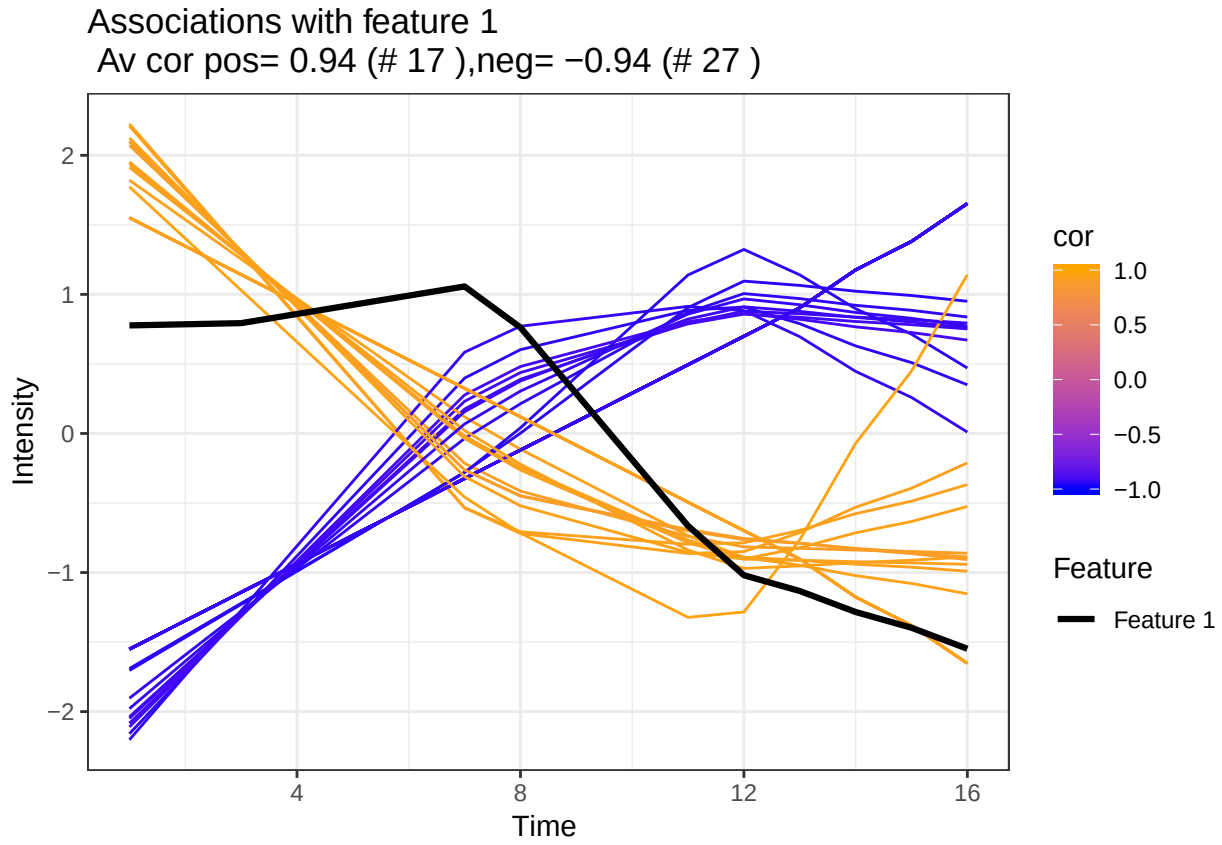
```
## reference is methane production.
```

```
##
##
## Table: Example of output from dynOmics time delay detection
##
##  Feature1  Feature2    delay      pBefore      pAfter    corBefore     corAfter
## ---------  ---------  ------  -----------  ---------  -----------  -----------
##         1  OTU_2           3   0.0016419   5.90e-06   -0.7204872   -0.9250810
##         1  OTU_1           2   0.0000008   4.00e-07   -0.9133549   -0.9442819
##         1  OTU_4           2   0.0000008   4.00e-07   -0.9133549   -0.9442819
##         1  OTU_5           2   0.0000008   4.00e-07   -0.9133549   -0.9442819
##         1  OTU_6           2   0.0000008   4.00e-07   -0.9133549   -0.9442819
##         1  OTU_7           3   0.0018589   1.08e-05    0.7148020    0.9162098
##         1  OTU_8           2   0.0000008   4.00e-07   -0.9133549   -0.9442819
##         1  OTU_10          4   0.0166011   8.00e-07   -0.5879682   -0.9592194
##         1  OTU_11          2   0.0000008   4.00e-07   -0.9133549   -0.9442819
##         1  OTU_13          3   0.0026614   1.03e-05   -0.6976001   -0.9169537
##         1  OTU_14          2   0.0000008   4.00e-07   -0.9133549   -0.9442819
##         1  OTU_15          2   0.0000008   4.00e-07   -0.9133549   -0.9442819
##         1  OTU_16          2   0.0000008   4.00e-07   -0.9133549   -0.9442819
##         1  OTU_17          2   0.0000008   4.00e-07    0.9133549    0.9442819
##         1  OTU_18          2   0.0000008   4.00e-07   -0.9133549   -0.9442819
```

```
##         1  OTU_19          2   0.0000008   4.00e-07   -0.9133549   -0.9442819
##         1  OTU_20          4   0.0308078   4.20e-06    0.5400705    0.9432113
##         1  OTU_21          2   0.0000008   4.00e-07    0.9133549    0.9442819
##         1  OTU_24          2   0.0000008   4.00e-07    0.9133549    0.9442819
##         1  OTU_25          2   0.0000008   4.00e-07   -0.9133549   -0.9442819
##         1  OTU_26          4   0.0407556   2.90e-06    0.5159884    0.9475889
##         1  OTU_28          3   0.0000464   4.00e-07    0.8401447    0.9546864
##         1  OTU_29          2   0.0000008   4.00e-07    0.9133549    0.9442819
##         1  OTU_30          2   0.0000008   4.00e-07   -0.9133549   -0.9442819
##         1  OTU_31          2   0.0000008   4.00e-07   -0.9133549   -0.9442819
##         1  OTU_35          4   0.0707072   3.10e-06   -0.4632985   -0.9468088
##         1  OTU_38          3   0.0002854   6.00e-07   -0.7883632   -0.9517014
##         1  OTU_41          2   0.0000008   4.00e-07   -0.9133549   -0.9442819
##         1  OTU_44          3   0.0015721   4.50e-06   -0.7224443   -0.9290238
##         1  OTU_45          2   0.0000008   4.00e-07   -0.9133549   -0.9442819
##         1  OTU_46          3   0.0002867   1.40e-06    0.7882109    0.9427268
##         1  OTU_50          3   0.0024658   1.99e-05    0.7013585    0.9060202
##         1  OTU_59          3   0.0000180   1.00e-07   -0.8615800   -0.9656696
##         1  OTU_60          3   0.0001781   1.00e-07   -0.8033613   -0.9661047
##         1  OTU_61          3   0.0042737   1.46e-05   -0.6730064   -0.9113797
##         1  OTU_65          2   0.0000008   4.00e-07   -0.9133549   -0.9442819
##         1  OTU_68          3   0.0002756   7.00e-07    0.7895070    0.9493597
##         1  OTU_74          3   0.0003836   1.60e-06    0.7783112    0.9415105
##         1  OTU_75          2   0.0000008   4.00e-07    0.9133549    0.9442819
##         1  OTU_82          4   0.3556572   1.00e-07    0.2473664    0.9731347
##         1  OTU_97          3   0.0007957   1.60e-06   -0.7511841   -0.9410882
##         1  OTU_130         3   0.0023656   2.06e-05    0.7033766    0.9054480
##         1  OTU_169         4   0.0072010   5.00e-07    0.6431090    0.9634644
##         1  OTU_304         2   0.0000008   4.00e-07    0.9133549    0.9442819

## Identifying associations between time profiles using fast Fourier transform.
##
##  Significant associations <0.05 found with shift and without shift:
##                      object$pBefore < 0.05
## object$pAfter < 0.05 FALSE TRUE
##                TRUE     2   42
##
##  Predicted delays:
##
##  2  3  4
## 23 15  6

## number of delays with a correlation > 0.9 once reshifted

## [1] 44

## Warning: Removed 146 rows containing missing values (geom_path).
```




```
## without shift
```



7.3 metabolites versus CH4

```
## reference is methane production.
```

```
##
##
## Table: Example of output from dynOmics time delay detection
##
##  Feature1  Feature2     delay     pBefore   pAfter    corBefore     corAfter
## ---------  ----------  ------  ----------  -------  -----------  -----------
##         1  M271T1466        -3   0.0002208    6e-07   -0.7966729   -0.9509863
##         1  M179T1018         2   0.0000000    0e+00    0.9837388    0.9960687
##         1  M207T1196        -2   0.0000047    2e-07   -0.8867378   -0.9513271
##         1  M106T894         -2   0.0000000    0e+00   -0.9565143   -0.9707634
##         1  M308T1437        -2   0.0000000    0e+00    0.9565143    0.9707634
##         1  M310T1500         1   0.0000000    0e+00   -0.9889401   -0.9964419
##         1  M290T1524         1   0.0000000    0e+00    0.9893887    0.9950648
##         1  M285T1569         1   0.0000000    0e+00   -0.9896766   -0.9904458
##         1  M379T1799         1   0.0000000    0e+00    0.9890879    0.9950224
##         1  M357T2099        -2   0.0000000    0e+00    0.9565143    0.9707634
##         1  M415T2220        -2   0.0000000    0e+00   -0.9565143   -0.9707634
##         1  M229T1227         2   0.0000000    0e+00   -0.9737807   -0.9935894
##         1  M205T1473         1   0.0000000    0e+00   -0.9968339   -0.9969254
##         1  M292T1383         1   0.0000000    0e+00    0.9971562    0.9985083
##         1  M291T1584        -2   0.0000000    0e+00    0.9565143    0.9707634
```

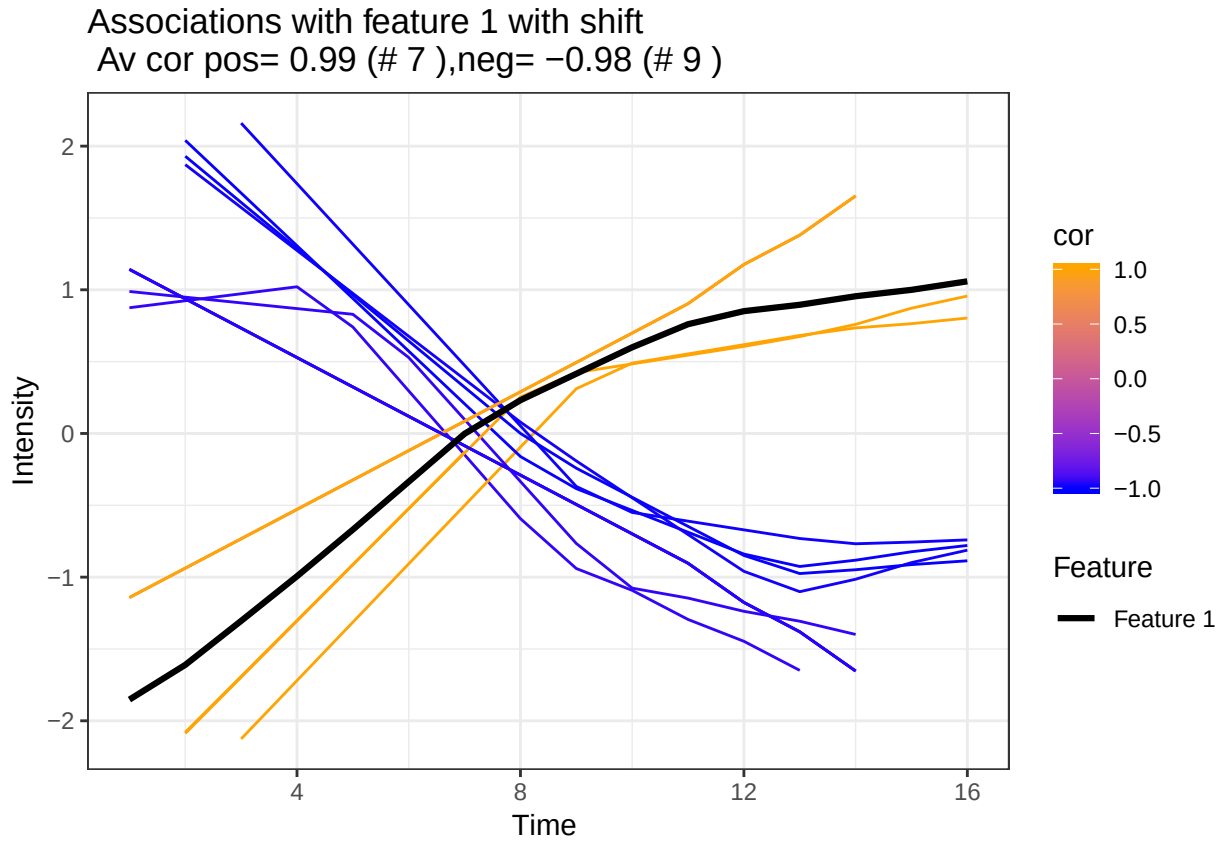
```
##         1  M398T1643       -2   0.0000000    0e+00   -0.9565143   -0.9707634
```

```
## Identifying associations between time profiles using fast Fourier transform.
##
##  Significant associations <0.05 found with shift and without shift:
##                      object$pBefore < 0.05
## object$pAfter < 0.05 TRUE
##                 TRUE   16
##
##  Predicted delays:
##
## -3 -2  1  2
##  1  7  6  2
```

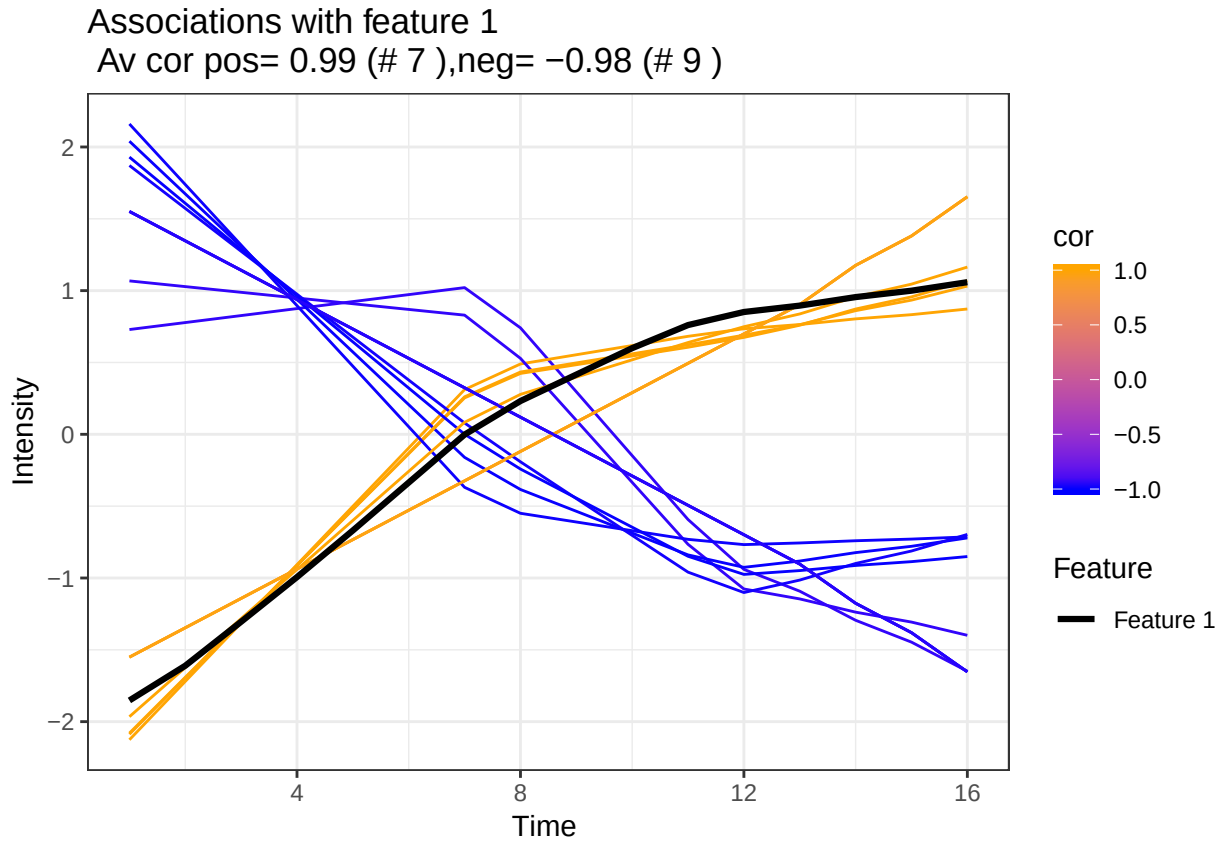
```
## number of delays with a correlation > 0.9 once reshifted
```

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

```
## Warning: Removed 23 rows containing missing values (geom_path).
```




```
## without shift
```



7.4 metabolites versus propionate

```
## reference is propionate concentration.
```

```
##
##
## Table: Example of output from dynOmics time delay detection
##
##  Feature1  Feature2     delay     pBefore     pAfter    corBefore     corAfter
## ---------  ----------  ------  ----------  ---------  -----------  -----------
##         1  M271T1466         0   0.0000000   0.00e+00    0.9988893    0.9988893
##         1  M179T1018         3   0.0035267   3.24e-05   -0.6832561   -0.8969935
##         1  M207T1196         1   0.0000000   0.00e+00    0.9861893    0.9902715
##         1  M106T894          2   0.0000008   4.00e-07    0.9133549    0.9442819
##         1  M308T1437         2   0.0000008   4.00e-07   -0.9133549   -0.9442819
##         1  M310T1500         3   0.0017767   4.30e-06    0.7168884    0.9293746
##         1  M290T1524         3   0.0016247   2.74e-05   -0.7209614   -0.9001832
##         1  M285T1569         3   0.0003286   3.00e-07    0.7836333    0.9571313
##         1  M379T1799         3   0.0018368   2.71e-05   -0.7153550   -0.9004353
##         1  M357T2099         2   0.0000008   4.00e-07   -0.9133549   -0.9442819
##         1  M415T2220         2   0.0000008   4.00e-07    0.9133549    0.9442819
##         1  M229T1227         3   0.0068597   4.25e-05    0.6460264    0.8915720
##         1  M205T1473         3   0.0003685   9.00e-07    0.7797139    0.9477251
##         1  M292T1383         3   0.0003331   4.70e-06   -0.7831688   -0.9283542
##         1  M291T1584         2   0.0000008   4.00e-07   -0.9133549   -0.9442819
```

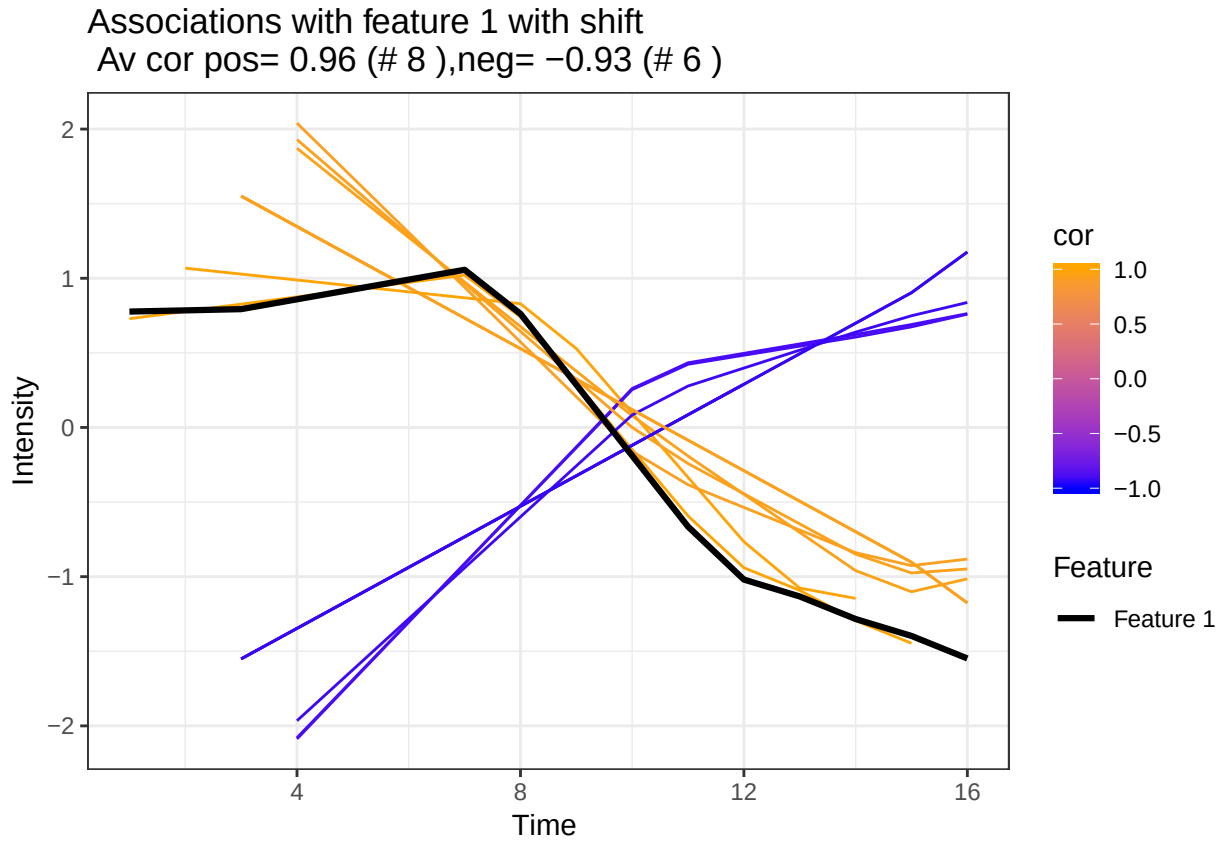
```
##         1  M398T1643        2   0.0000008   4.00e-07    0.9133549    0.9442819
```

```
## Identifying associations between time profiles using fast Fourier transform.
##
##  Significant associations <0.05 found with shift and without shift:
##                      object$pBefore < 0.05
## object$pAfter < 0.05 TRUE
##                TRUE   16
##
##  Predicted delays:
##
## 0 1 2 3
## 1 1 6 8
```

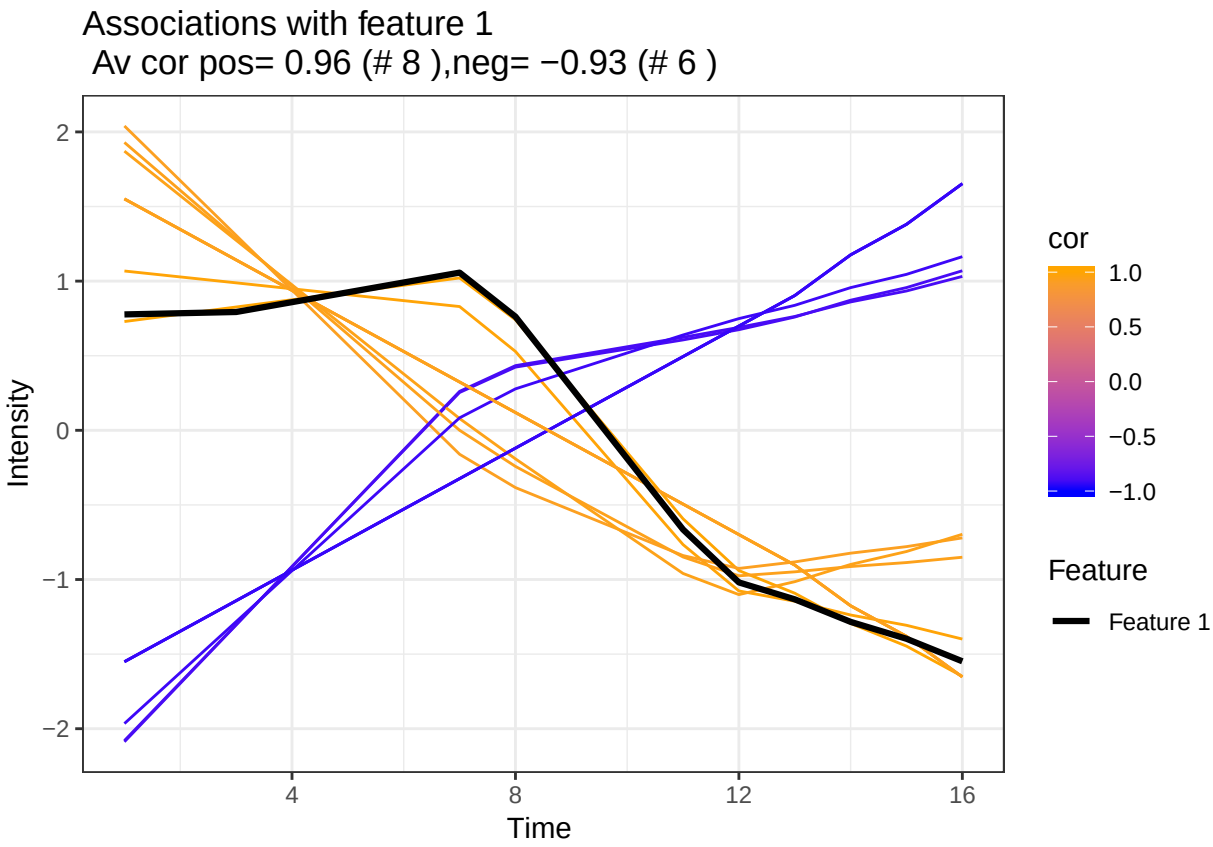
```
## number of delays with a correlation > 0.9 once reshifted
```

```
## [1] 14
```

```
## Warning: Removed 20 rows containing missing values (geom_path).
```




```
## without shift
```


Associations with feature 1
Av cor pos= 0.96 (# 8),neg= −0.93 (# 6)
Intensity
2
1
0
−1
−2
4
8
12
16
Time
cor
1.0
0.5
0.0
−0.5
−1.0
Feature
Feature 1