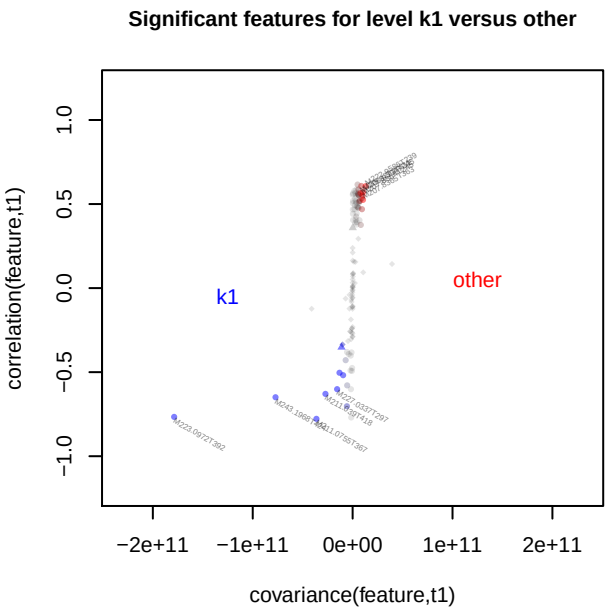
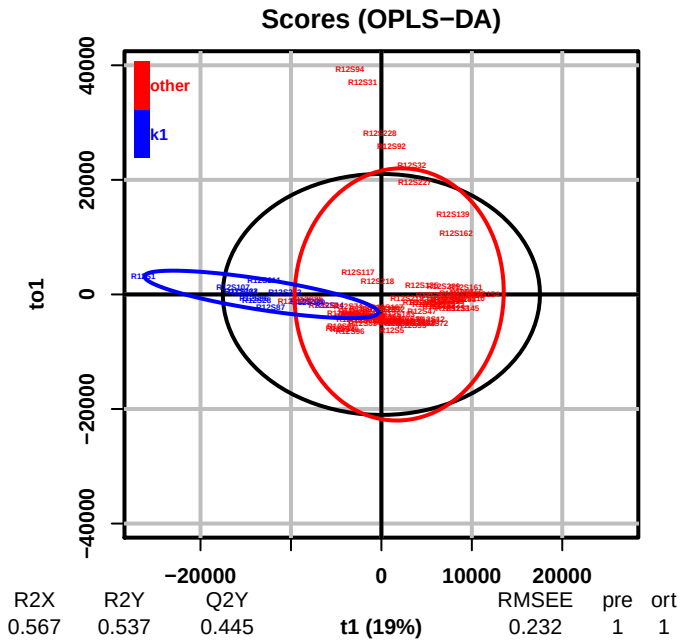
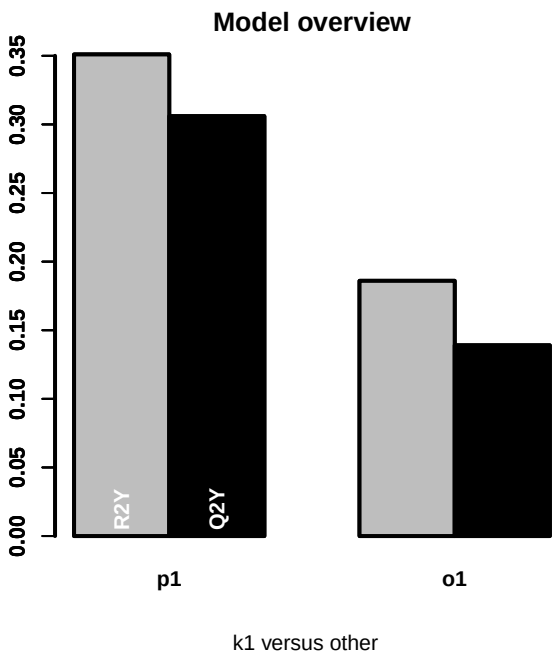
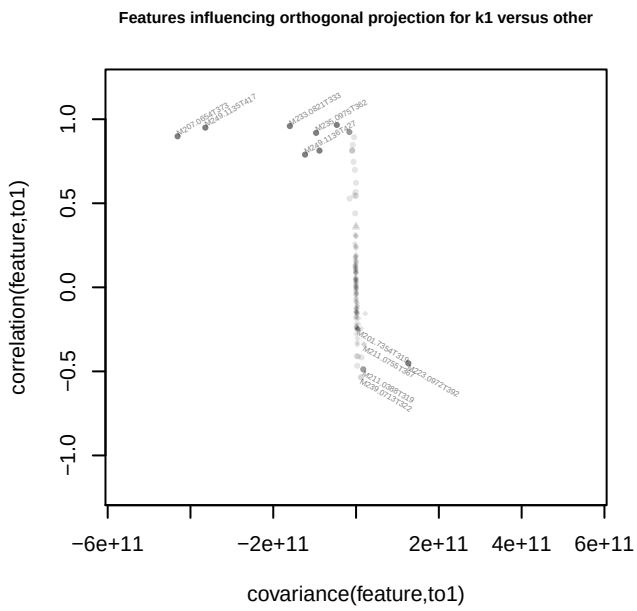
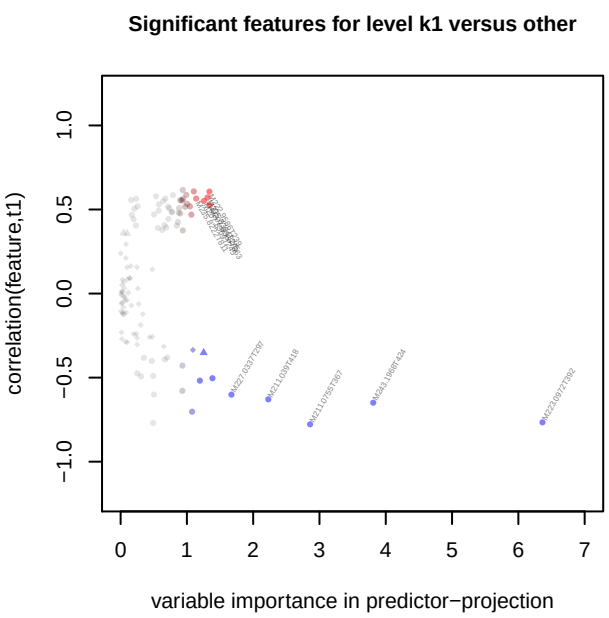
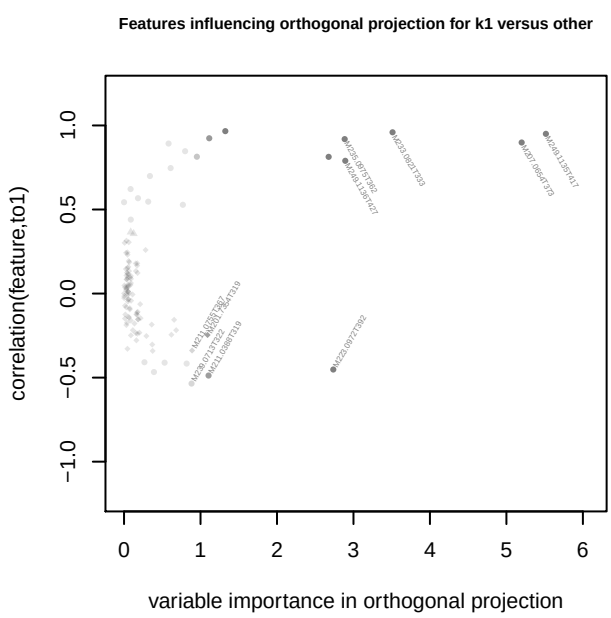

Significant features for level k1 versus other
correlation(feature,t1)
covariance(feature,t1)
k1
other
1.0
0.5
0.0
−0.5
−1.0
−2e+11
−1e+11
0e+00
1e+11
2e+11

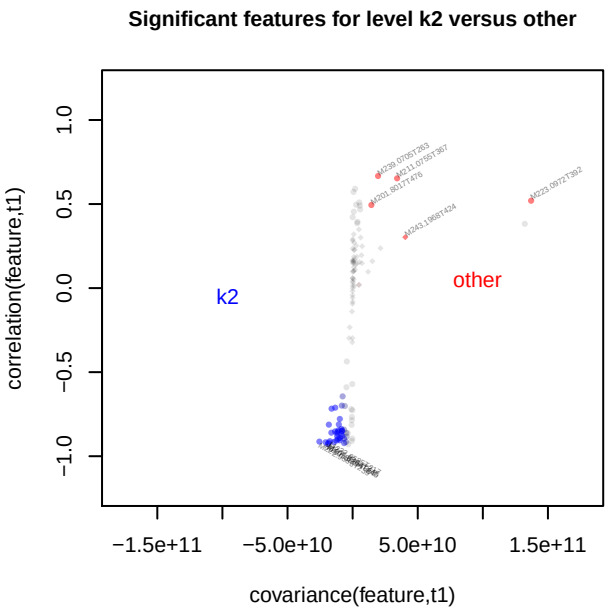

Scores (OPLS−DA)
other
k1
to1
t1 (19%)
40000
20000
0
−20000
−40000
−20000
0
10000
20000
R2X R2Y Q2Y RMSEE pre ort
0.567 0.537 0.445 0.232 1 1

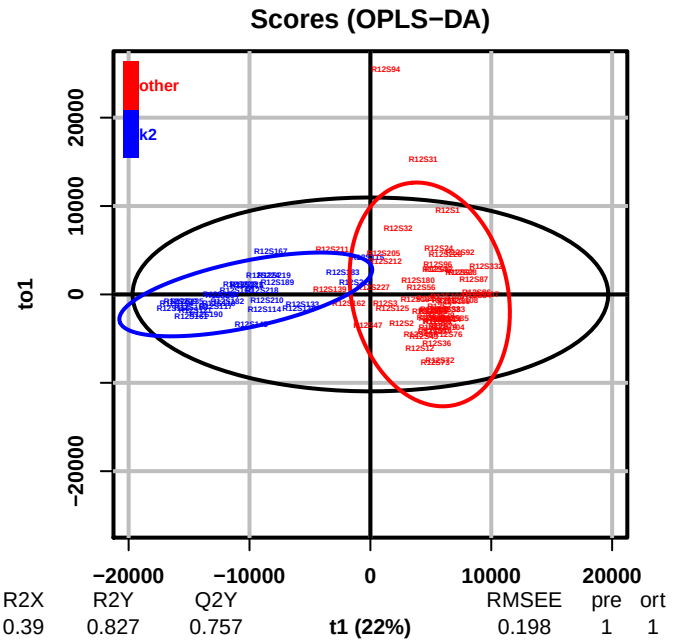

Model overview
R2Y
Q2Y
p1
o1
k1 versus other
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35

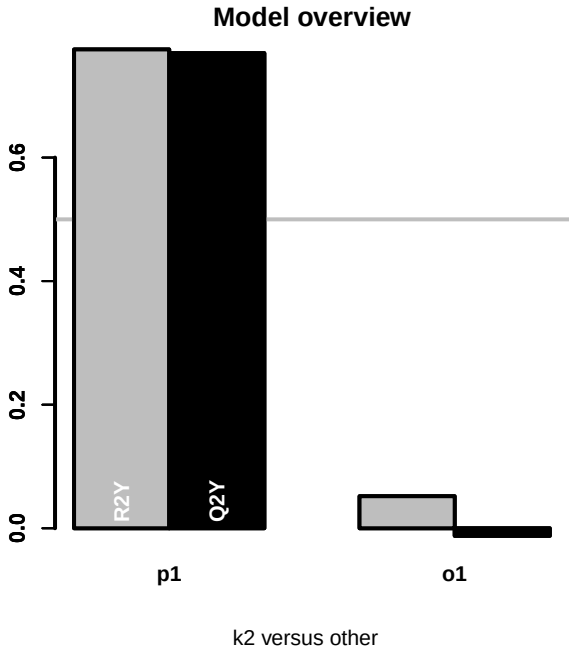

Features influencing orthogonal projection for k1 versus other
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−6e+11
−2e+11
2e+11
4e+11
6e+11

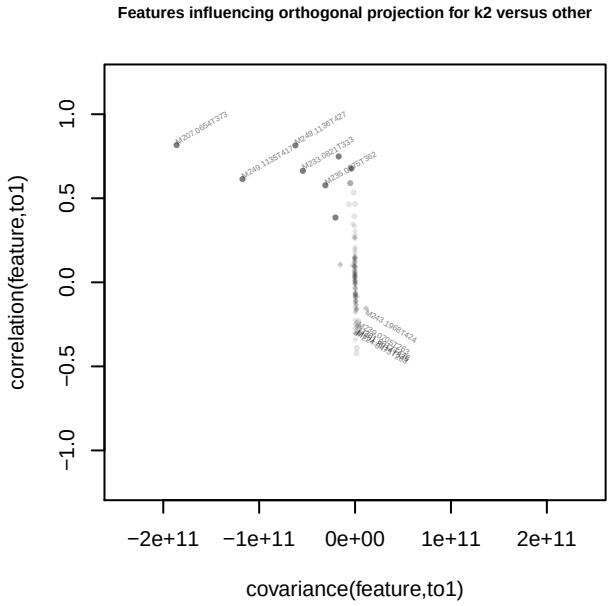

Significant features for level k1 versus other
correlation(feature,t1)
variable importance in predictor−projection
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4
5
6
7

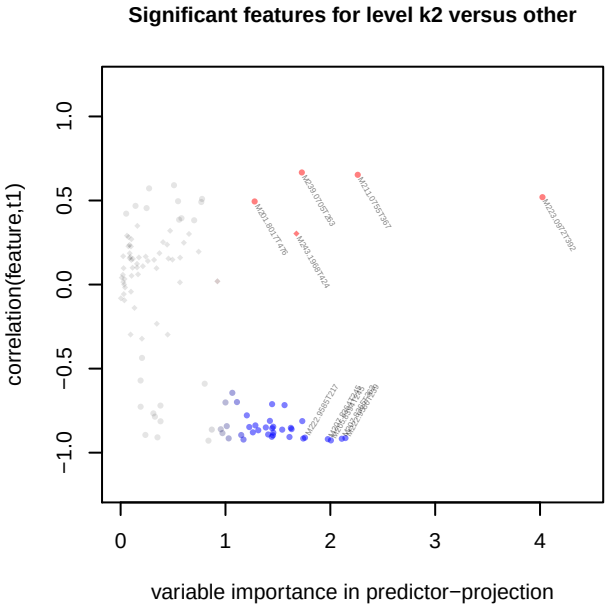

Features influencing orthogonal projection for k1 versus other
correlation(feature,to1)
variable importance in orthogonal projection
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4
5
6

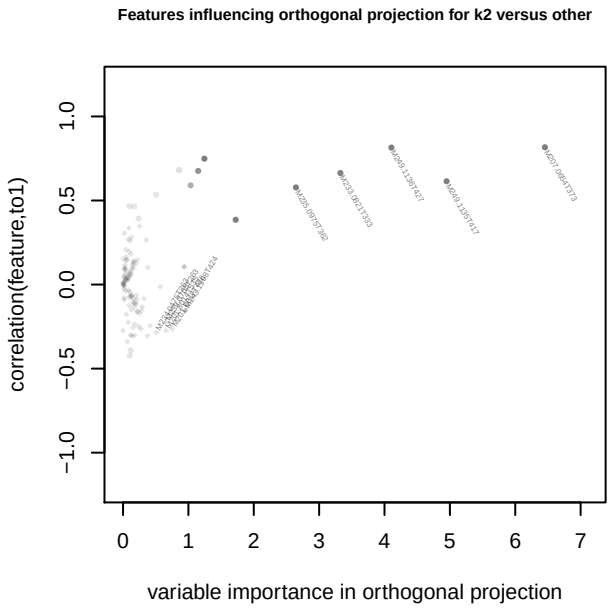

Significant features for level k2 versus other
correlation(feature,t1)
covariance(feature,t1)
k2
other
1.0
0.5
0.0
−0.5
−1.0
−1.5e+11
−5.0e+10
5.0e+10
1.5e+11

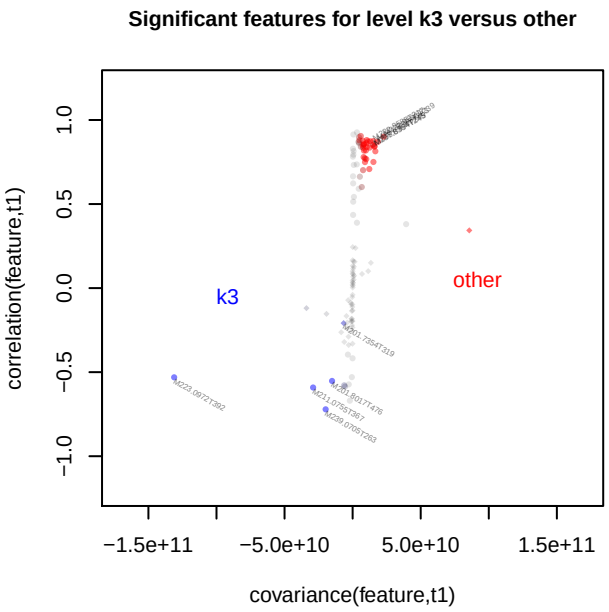

Scores (OPLS−DA)
other
k2
to1
t1 (22%)
20000
10000
0
−10000
−20000
R2X
0.39
R2Y
0.827
Q2Y
0.757
RMSEE
0.198
pre
1
ort
1

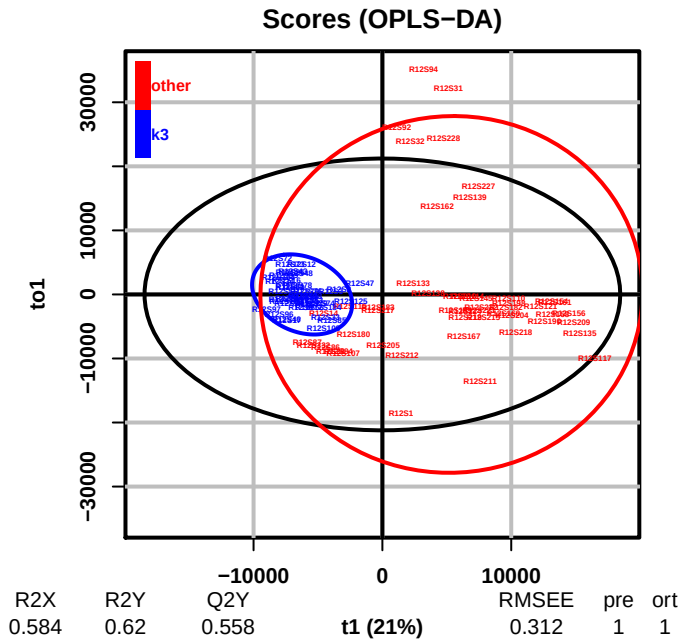

Model overview
R2Y
Q2Y
0.0
0.2
0.4
0.6
p1
o1
k2 versus other

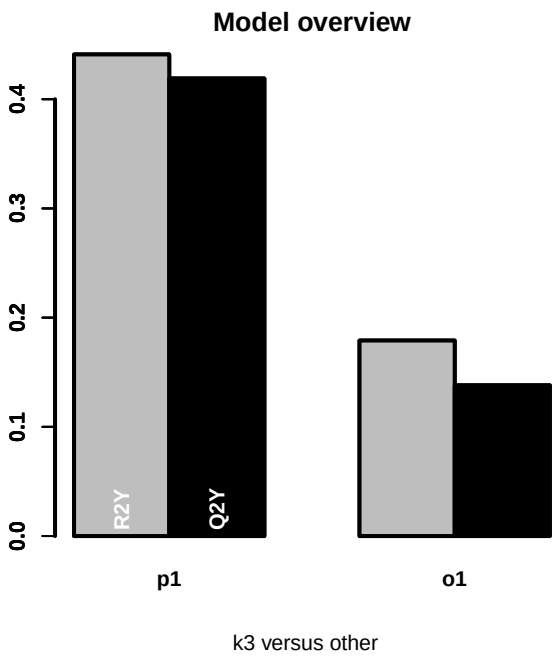

Features influencing orthogonal projection for k2 versus other
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−2e+11
−1e+11
0e+00
1e+11
2e+11

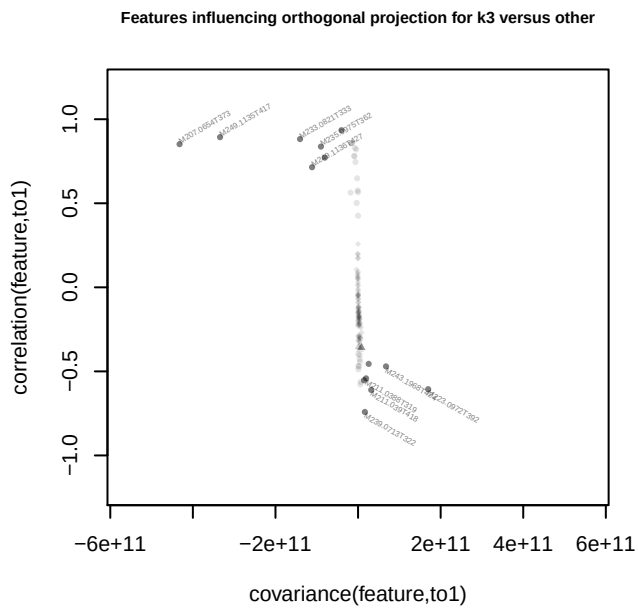

Significant features for level k2 versus other
correlation(feature,t1)
variable importance in predictor−projection
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4

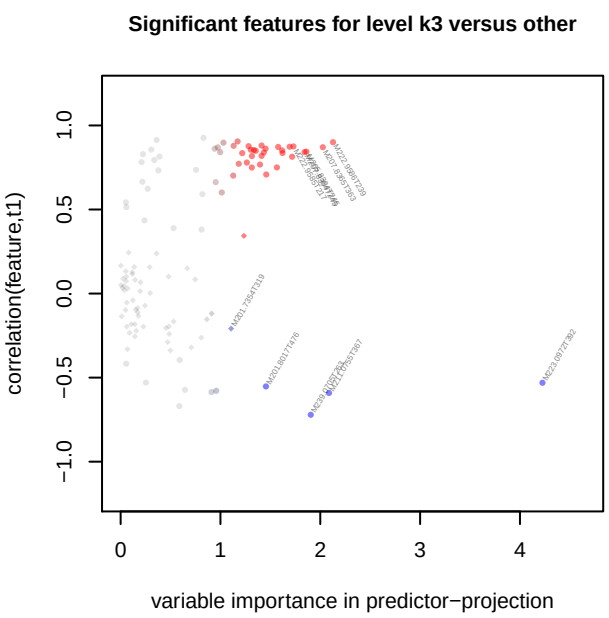

Features influencing orthogonal projection for k2 versus other
correlation(feature,to1)
variable importance in orthogonal projection
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4
5
6
7

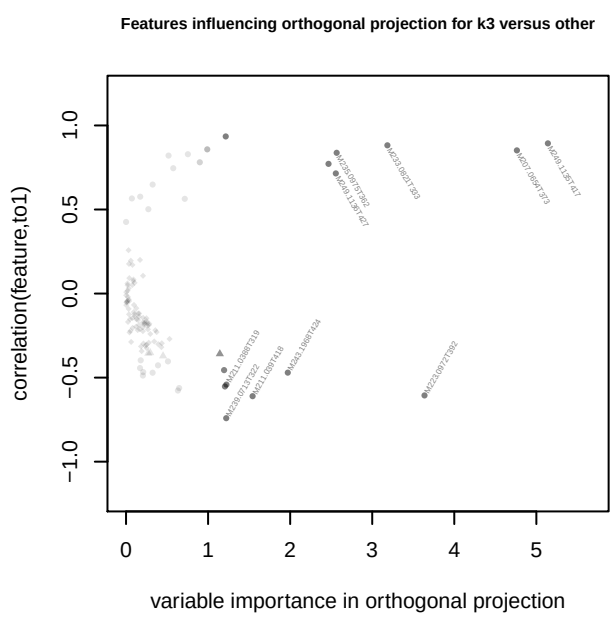

Significant features for level k3 versus other
correlation(feature,t1)
covariance(feature,t1)
k3
other
1.0
0.5
0.0
−0.5
−1.0
−1.5e+11
−5.0e+10
5.0e+10
1.5e+11

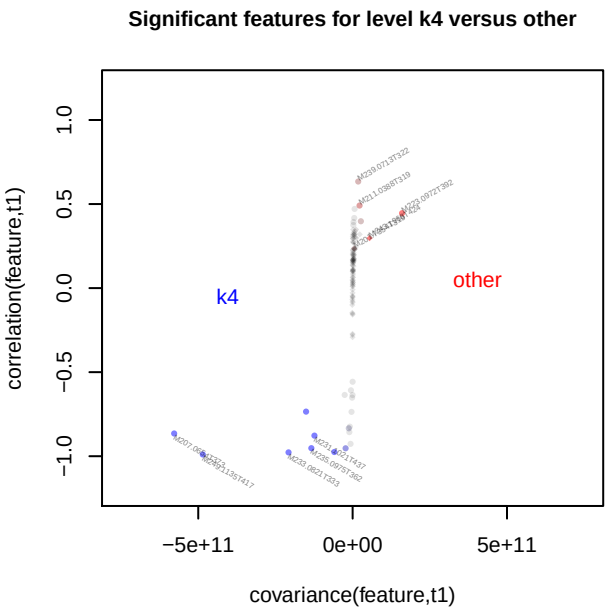

Scores (OPLS−DA)
other
k3
to1
t1 (21%)
30000
10000
0
−10000
−30000
−10000
0
10000
R2X R2Y Q2Y RMSEE pre ort
0.584 0.62 0.558 0.312 1 1

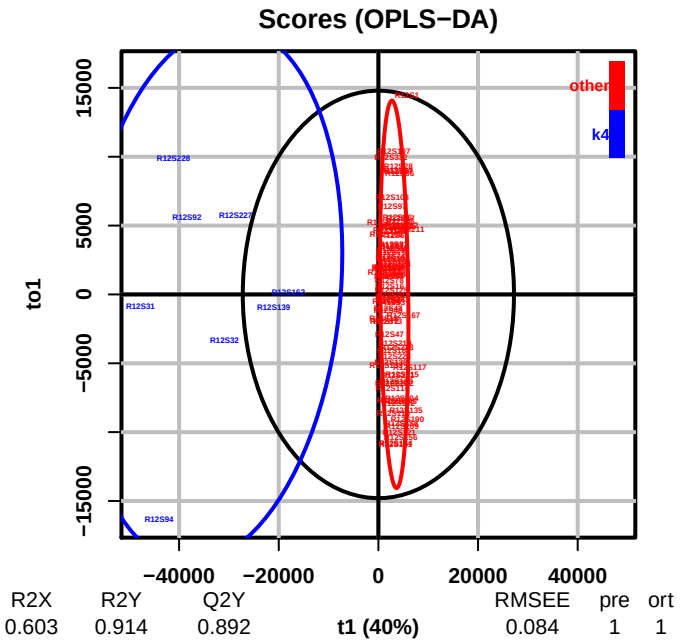

Model overview
R2Y
Q2Y
0.0
0.1
0.2
0.3
0.4
p1
o1
k3 versus other

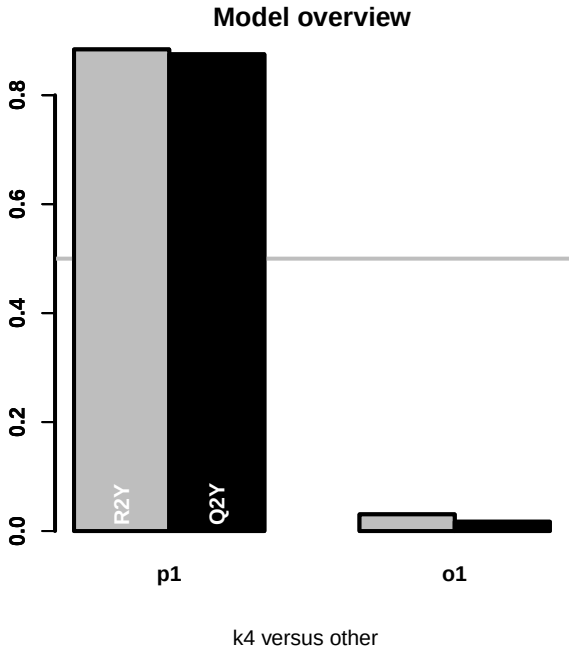

Features influencing orthogonal projection for k3 versus other
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−6e+11
−2e+11
2e+11
4e+11
6e+11

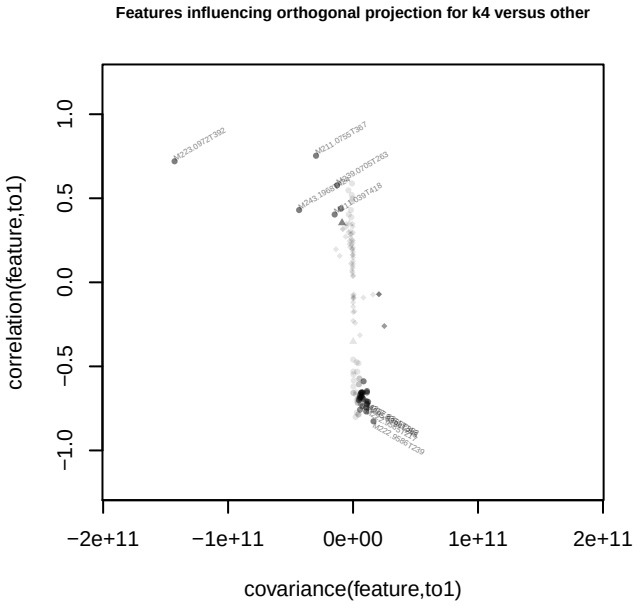

Significant features for level k3 versus other
correlation(feature,t1)
variable importance in predictor−projection
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4

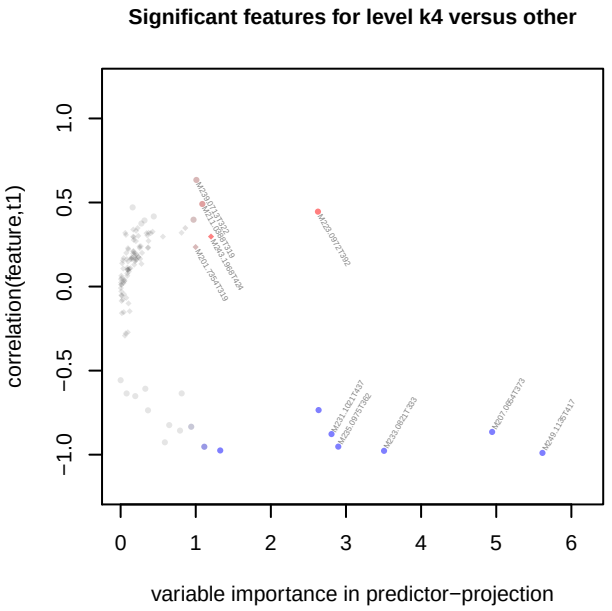

Features influencing orthogonal projection for k3 versus other
correlation(feature,to1)
variable importance in orthogonal projection
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4
5

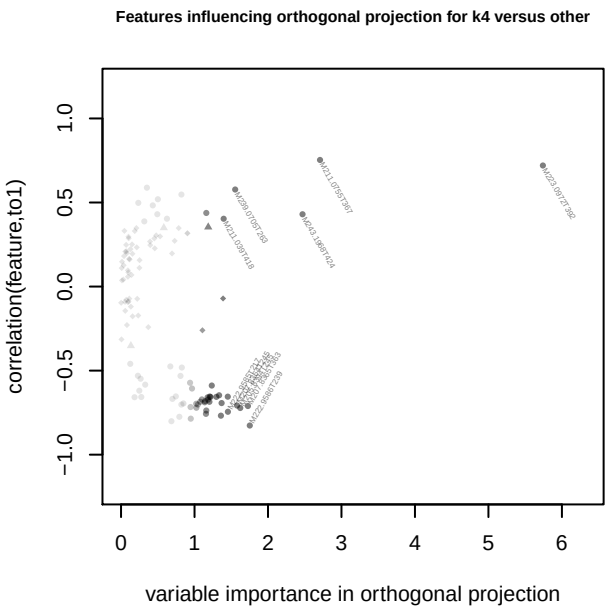

Significant features for level k4 versus other
correlation(feature,t1)
covariance(feature,t1)
k4
other
1.0
0.5
0.0
−0.5
−1.0
−5e+11
0e+00
5e+11

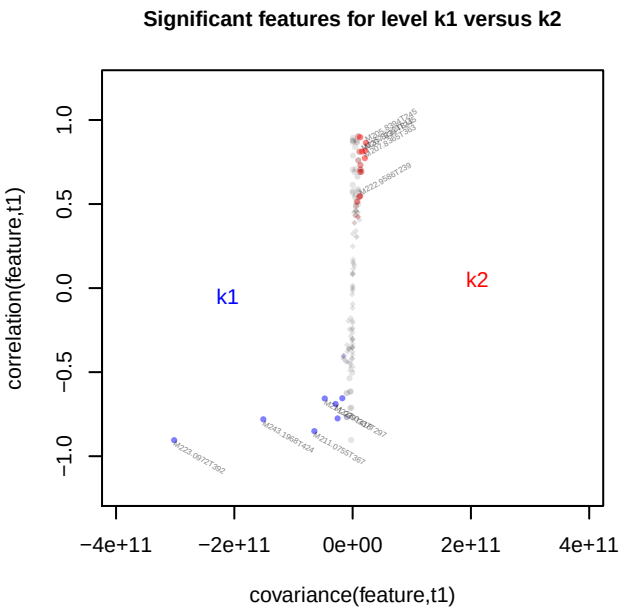

Scores (OPLS−DA)
to1
t1 (40%)
other
k4
15000
5000
0
−5000
−15000
−40000
−20000
0
20000
40000
R2X R2Y Q2Y RMSEE pre ort
0.603 0.914 0.892 0.084 1 1

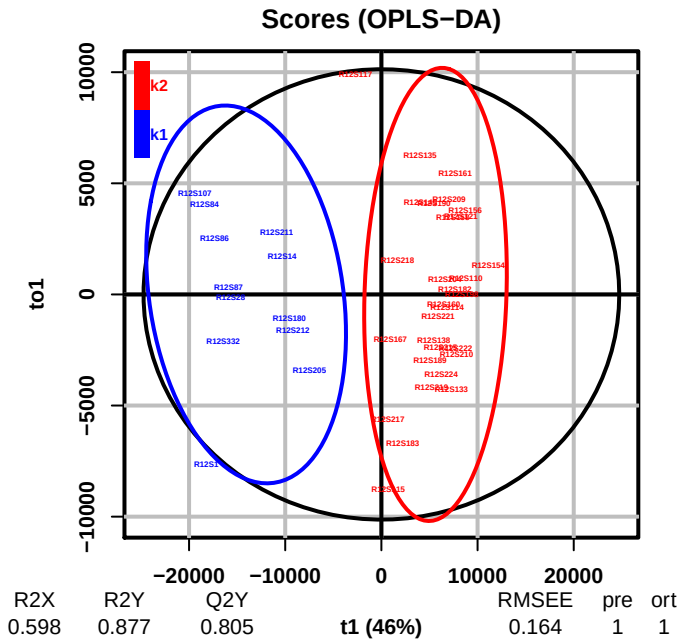

Model overview
R2Y
Q2Y
0.0
0.2
0.4
0.6
0.8
p1
o1
k4 versus other

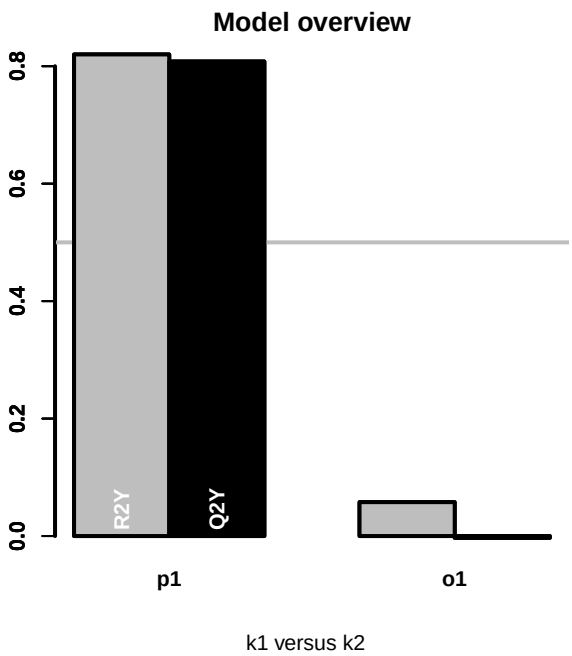

Features influencing orthogonal projection for k4 versus other
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−2e+11
−1e+11
0e+00
1e+11
2e+11

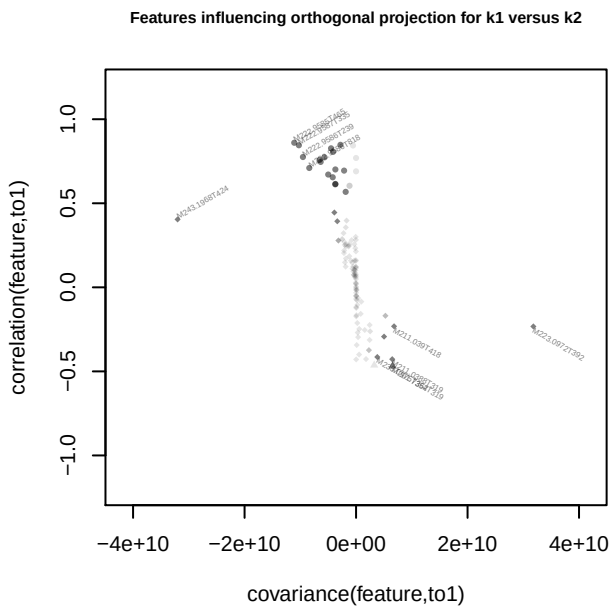

Significant features for level k4 versus other
correlation(feature,t1)
variable importance in predictor−projection
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4
5
6

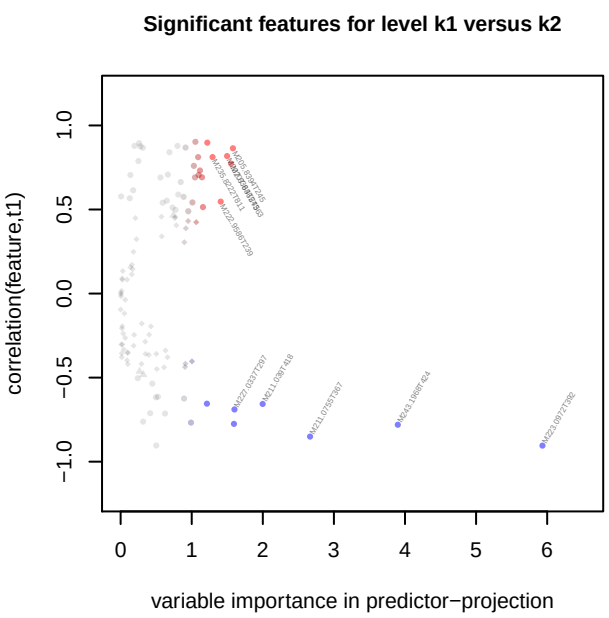

Features influencing orthogonal projection for k4 versus other
correlation(feature,to1)
variable importance in orthogonal projection
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4
5
6

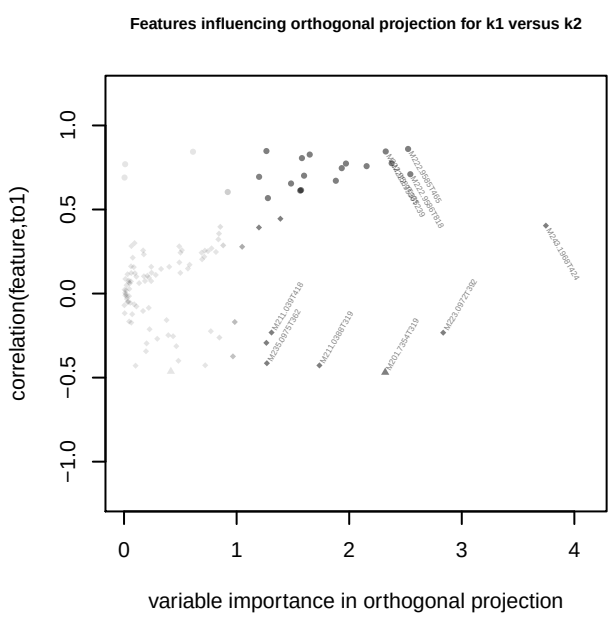

Significant features for level k1 versus k2
correlation(feature,t1)
covariance(feature,t1)
k1
k2
−4e+11
−2e+11
0e+00
2e+11
4e+11
1.0
0.5
0.0
−0.5
−1.0

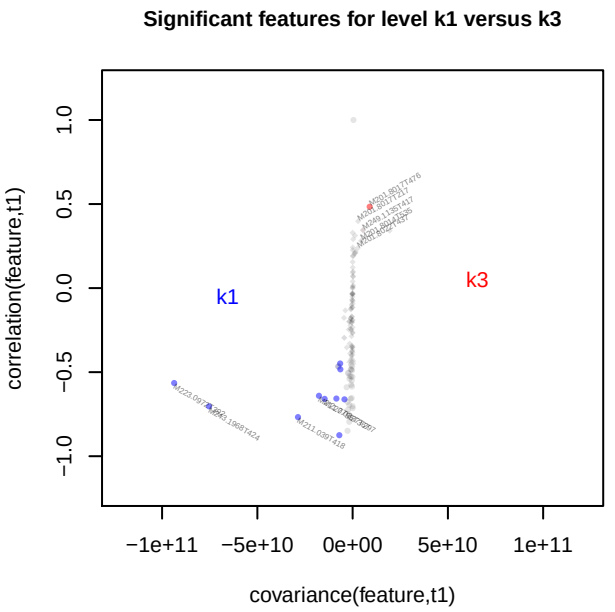

Scores (OPLS−DA)
k2
k1
to1
t1 (46%)
−20000
−10000
0
10000
20000
10000
5000
0
−5000
−10000
R2X R2Y Q2Y RMSEE pre ort
0.598 0.877 0.805 0.164 1 1

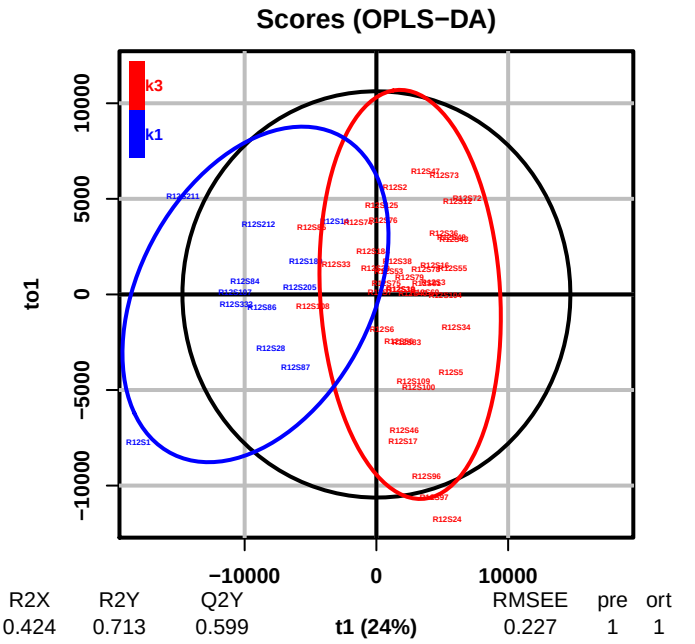

Model overview
R2Y
Q2Y
p1
o1
0.0
0.2
0.4
0.6
0.8
k1 versus k2

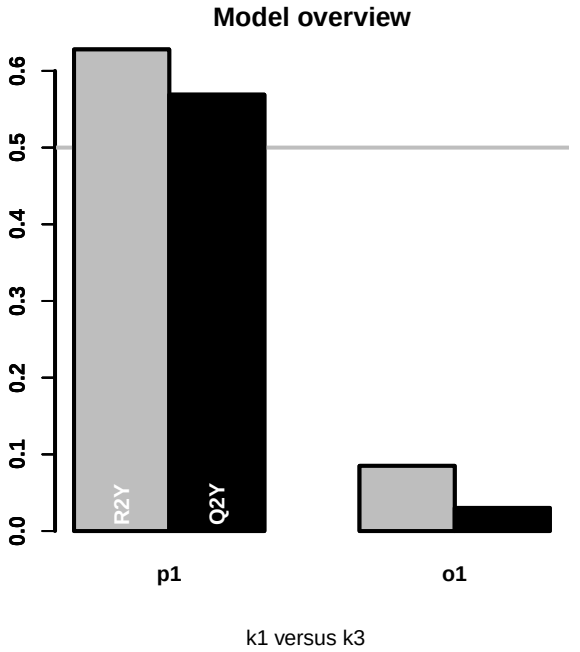

Features influencing orthogonal projection for k1 versus k2
correlation(feature,to1)
covariance(feature,to1)
−4e+10
−2e+10
0e+00
2e+10
4e+10
1.0
0.5
0.0
−0.5
−1.0

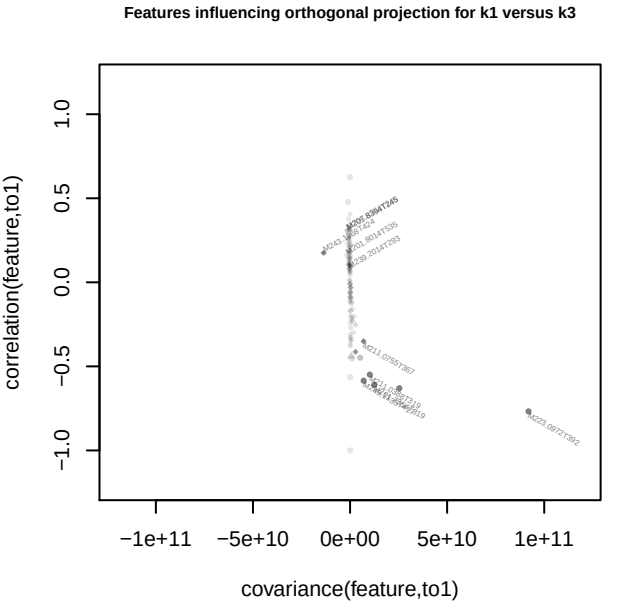

Significant features for level k1 versus k2
correlation(feature,t1)
variable importance in predictor−projection
0
1
2
3
4
5
6
1.0
0.5
0.0
−0.5
−1.0

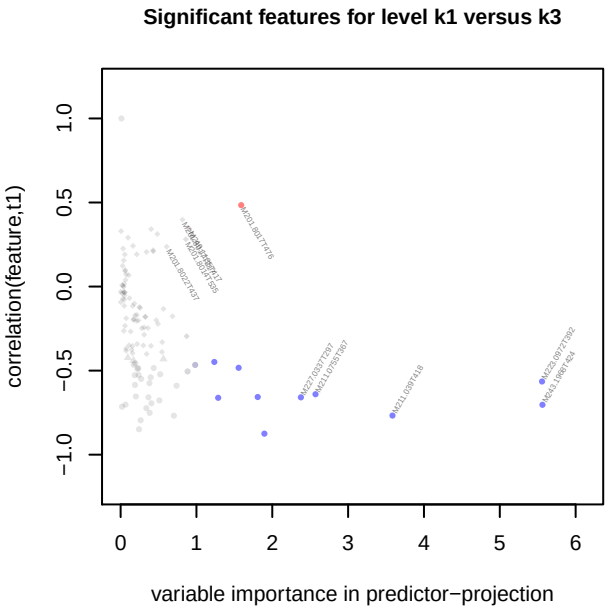

Features influencing orthogonal projection for k1 versus k2
correlation(feature,to1)
variable importance in orthogonal projection
0
1
2
3
4
1.0
0.5
0.0
−0.5
−1.0

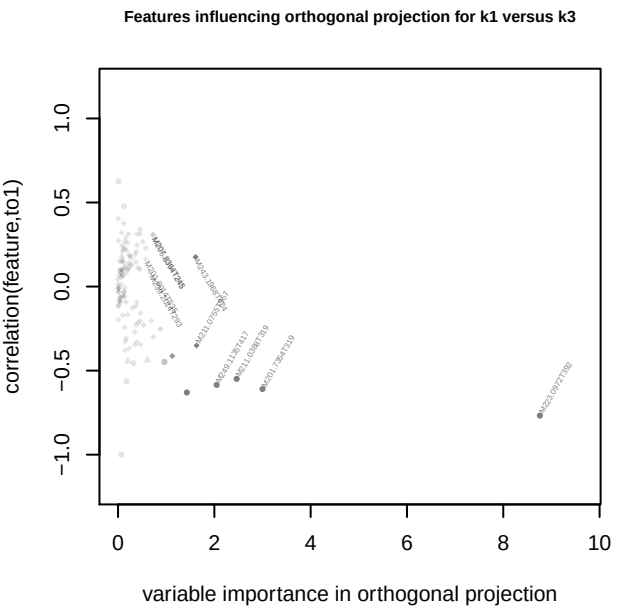

Significant features for level k1 versus k3
correlation(feature,t1)
covariance(feature,t1)
k1
k3
−1e+11
−5e+10
0e+00
5e+10
1e+11
1.0
0.5
0.0
−0.5
−1.0

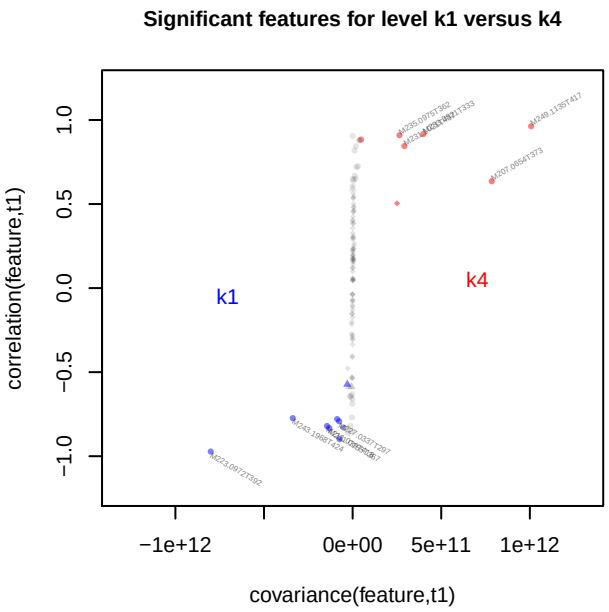

Scores (OPLS−DA)
k3
k1
to1
t1 (24%)
10000
5000
0
−5000
−10000
R2X 0.424
R2Y 0.713
Q2Y 0.599
RMSEE 0.227
pre 1
ort 1

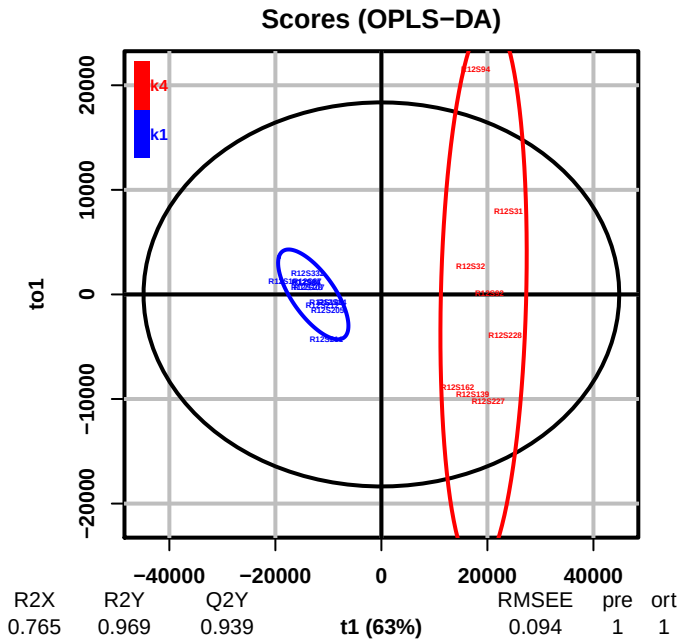

Model overview
R2Y
Q2Y
p1
o1
k1 versus k3
0.0
0.1
0.2
0.3
0.4
0.5
0.6

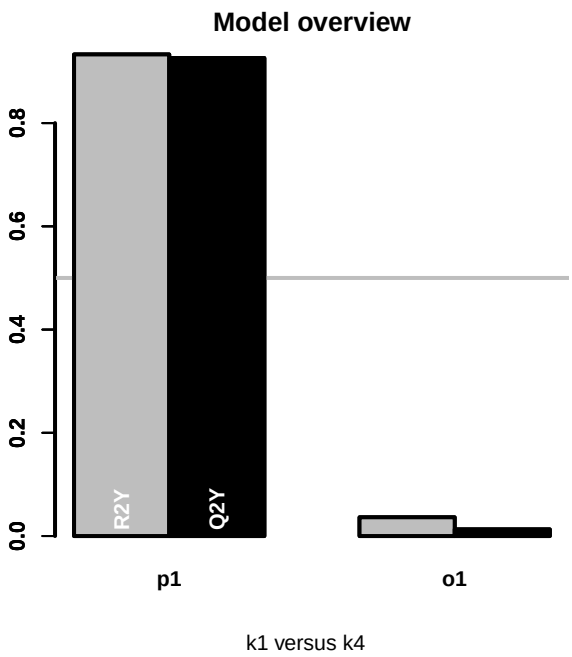

Features influencing orthogonal projection for k1 versus k3
correlation(feature,to1)
covariance(feature,to1)
−1e+11
−5e+10
0e+00
5e+10
1e+11
1.0
0.5
0.0
−0.5
−1.0

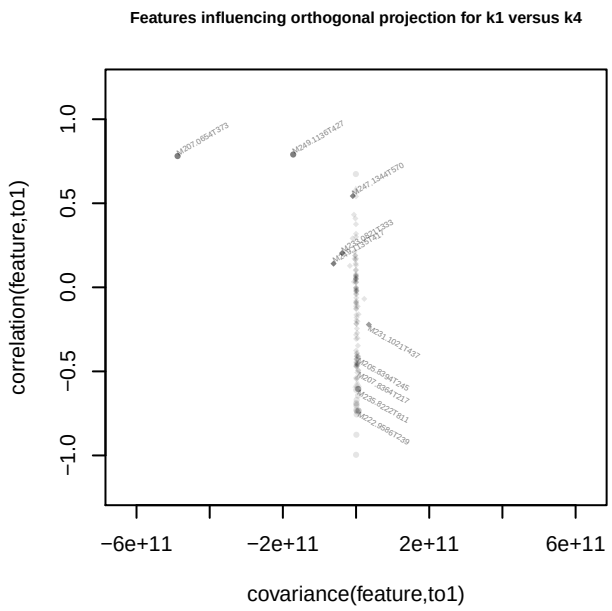

Significant features for level k1 versus k3
correlation(feature,t1)
variable importance in predictor−projection
0
1
2
3
4
5
6
1.0
0.5
0.0
−0.5
−1.0

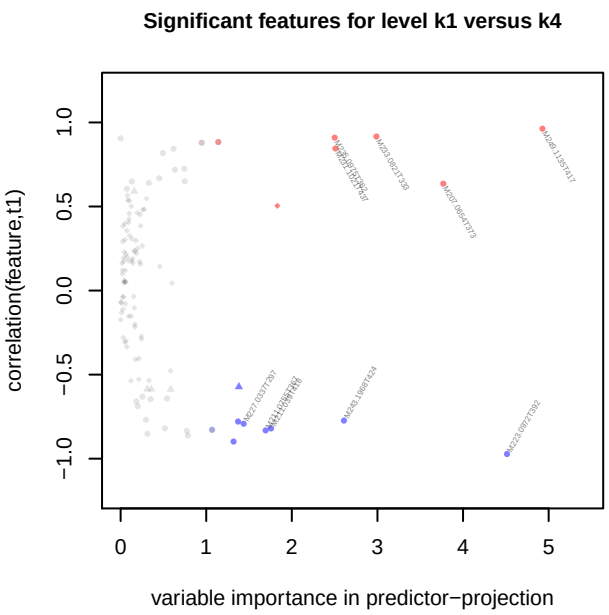

Features influencing orthogonal projection for k1 versus k3
correlation(feature,to1)
variable importance in orthogonal projection
0
2
4
6
8
10
1.0
0.5
0.0
−0.5
−1.0

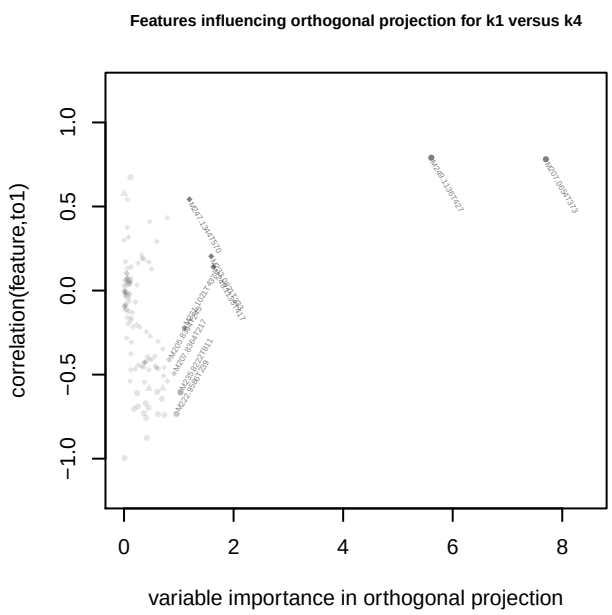

Significant features for level k1 versus k4
correlation(feature,t1)
covariance(feature,t1)
k1
k4
−1e+12
0e+00
5e+11
1e+12
1.0
0.5
0.0
−0.5
−1.0

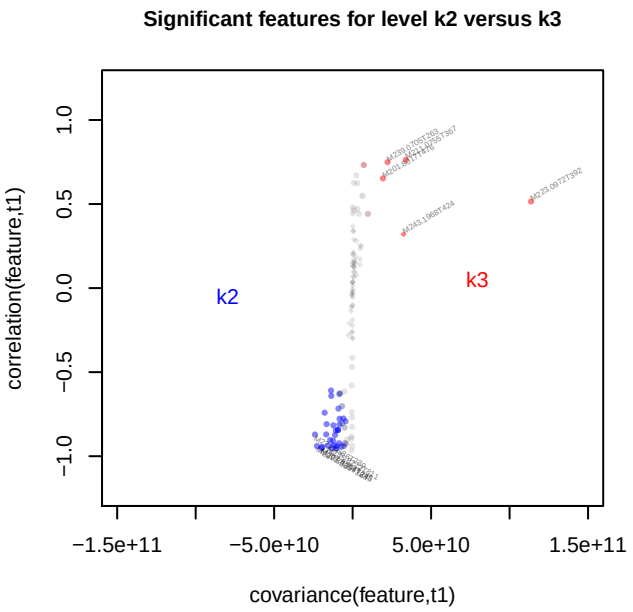

Scores (OPLS−DA)
k4
k1
to1
t1 (63%)
R2X 0.765
R2Y 0.969
Q2Y 0.939
RMSEE 0.094
pre 1
ort 1
−40000
−20000
0
20000
40000
20000
10000
0
−10000
−20000

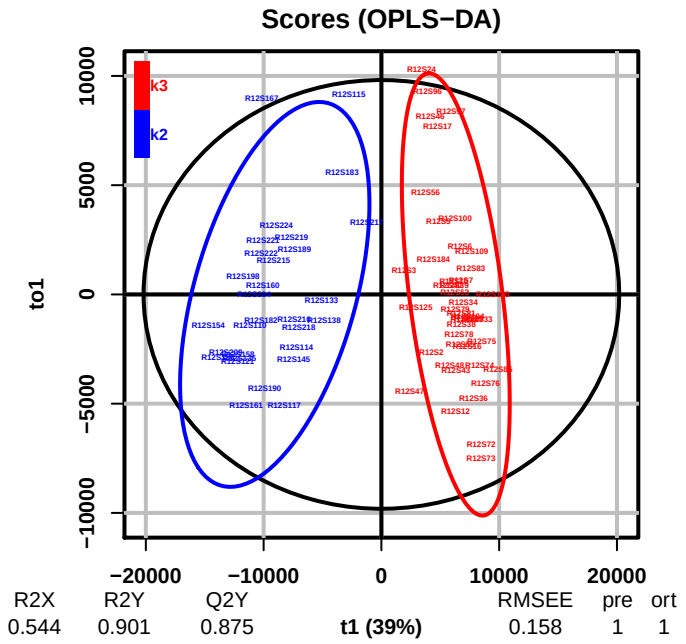

Model overview
R2Y
Q2Y
p1
o1
k1 versus k4
0.0
0.2
0.4
0.6
0.8

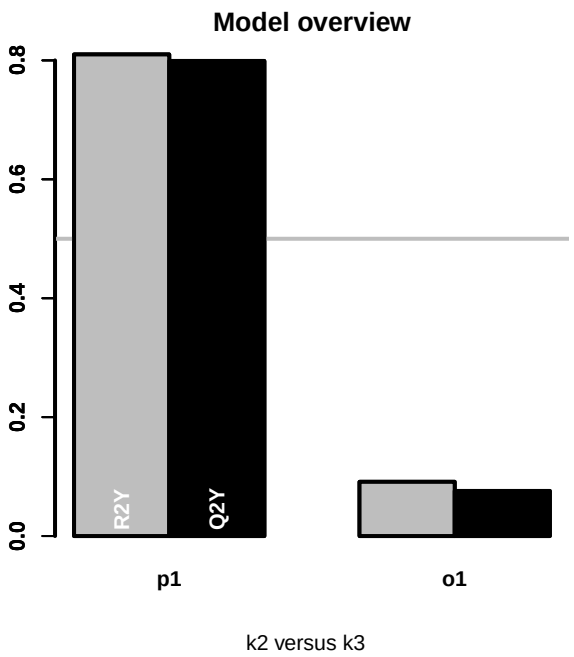

Features influencing orthogonal projection for k1 versus k4
correlation(feature,to1)
covariance(feature,to1)
−6e+11
−2e+11
2e+11
6e+11
1.0
0.5
0.0
−0.5
−1.0

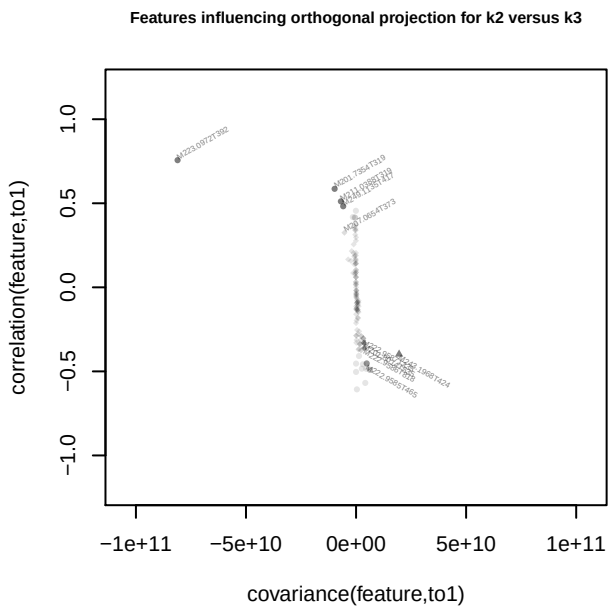

Significant features for level k1 versus k4
correlation(feature,t1)
variable importance in predictor−projection
0
1
2
3
4
5
1.0
0.5
0.0
−0.5
−1.0

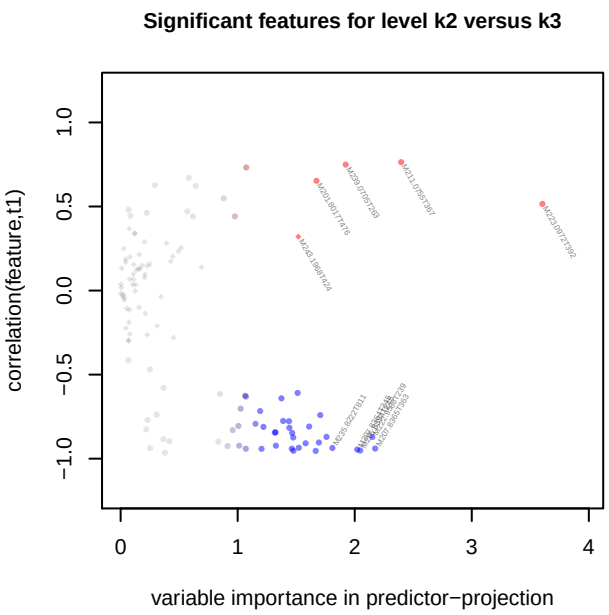

Features influencing orthogonal projection for k1 versus k4
correlation(feature,to1)
variable importance in orthogonal projection
0
2
4
6
8
1.0
0.5
0.0
−0.5
−1.0

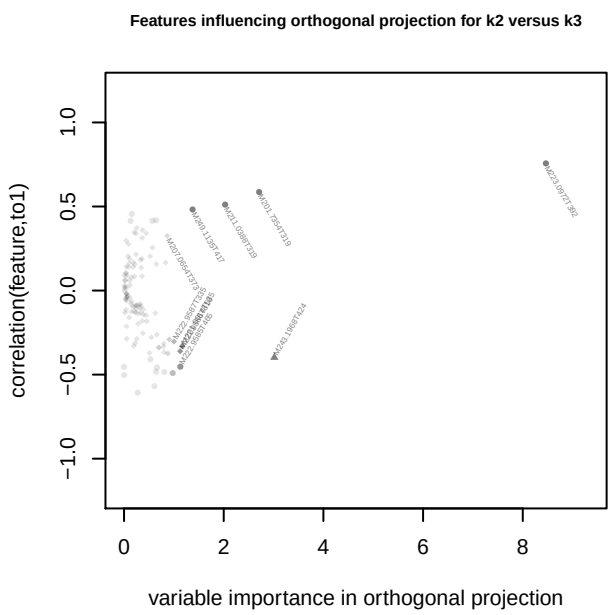

Significant features for level k2 versus k3
correlation(feature,t1)
covariance(feature,t1)
k2
k3
1.0
0.5
0.0
−0.5
−1.0
−1.5e+11
−5.0e+10
5.0e+10
1.5e+11

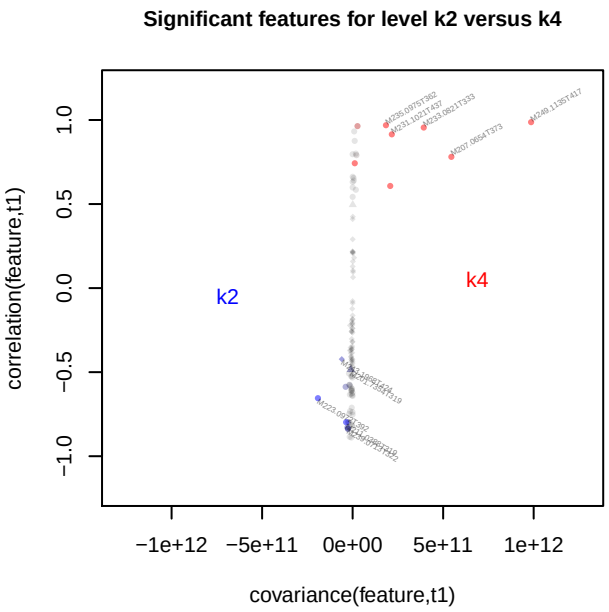

Scores (OPLS−DA)
k3
k2
to1
t1 (39%)
10000
5000
0
−5000
−10000
−20000
−10000
0
10000
20000
R2X R2Y Q2Y RMSEE pre ort
0.544 0.901 0.875 0.158 1 1

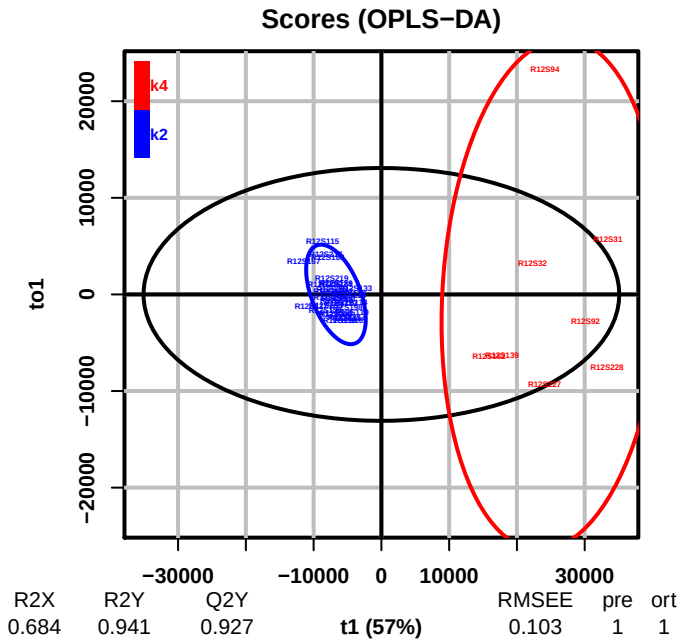

Model overview
R2Y
Q2Y
p1
o1
0.0
0.2
0.4
0.6
0.8
k2 versus k3

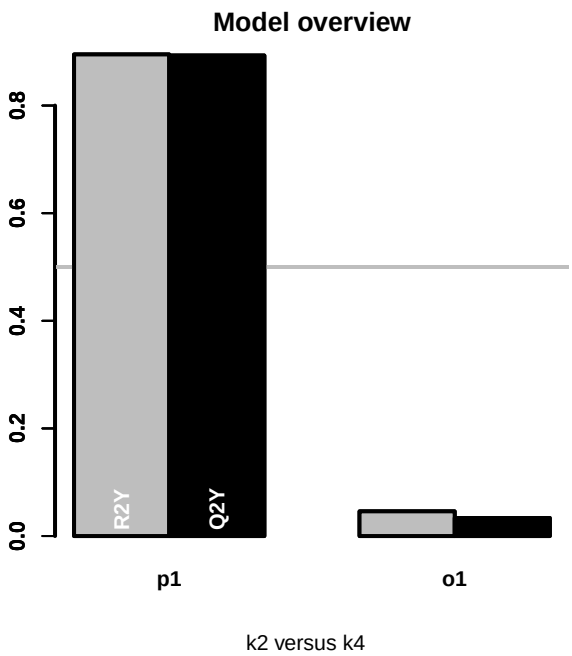

Features influencing orthogonal projection for k2 versus k3
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−1e+11
−5e+10
0e+00
5e+10
1e+11

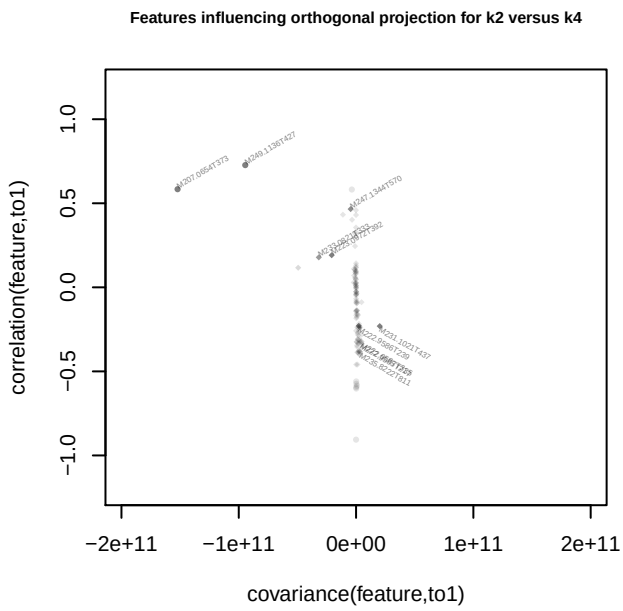

Significant features for level k2 versus k3
correlation(feature,t1)
variable importance in predictor−projection
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4

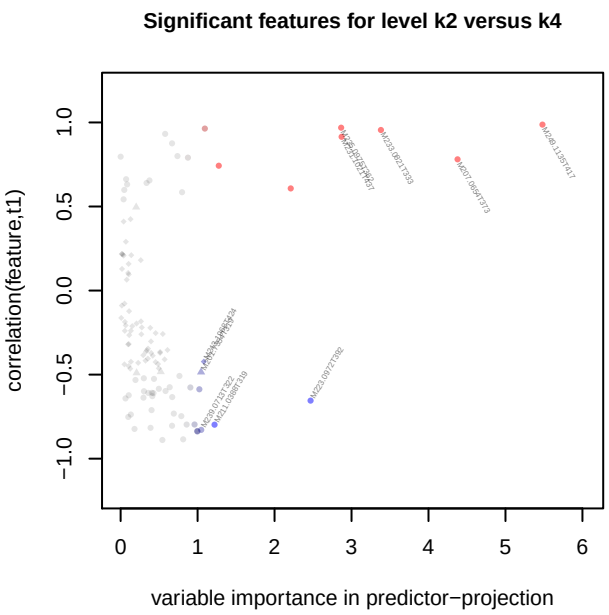

Features influencing orthogonal projection for k2 versus k3
correlation(feature,to1)
variable importance in orthogonal projection
1.0
0.5
0.0
−0.5
−1.0
0
2
4
6
8

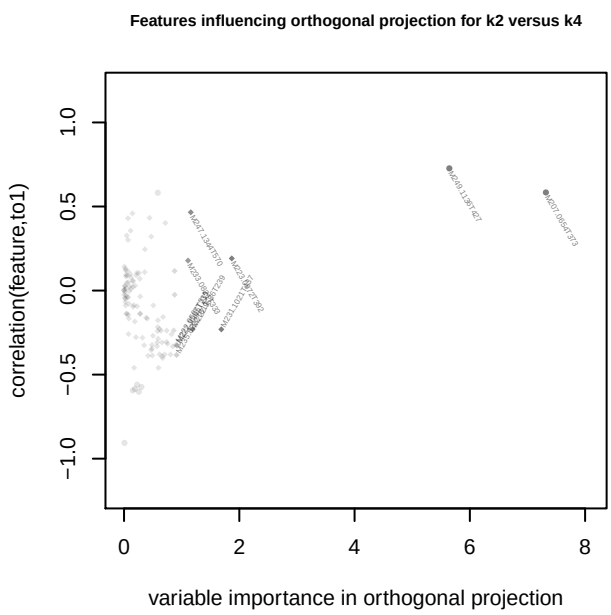

Significant features for level k2 versus k4
correlation(feature,t1)
covariance(feature,t1)
k2
k4
1.0
0.5
0.0
−0.5
−1.0
−1e+12
−5e+11
0e+00
5e+11
1e+12

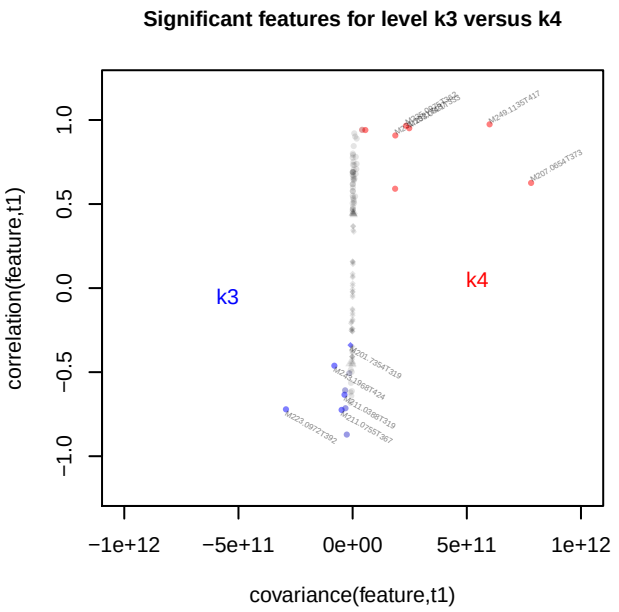

Scores (OPLS−DA)
k4
k2
to1
t1 (57%)
20000
10000
0
−10000
−20000
−30000
−10000
0
10000
30000
R2X
R2Y
Q2Y
RMSEE
pre
ort
0.684
0.941
0.927
0.103
1
1

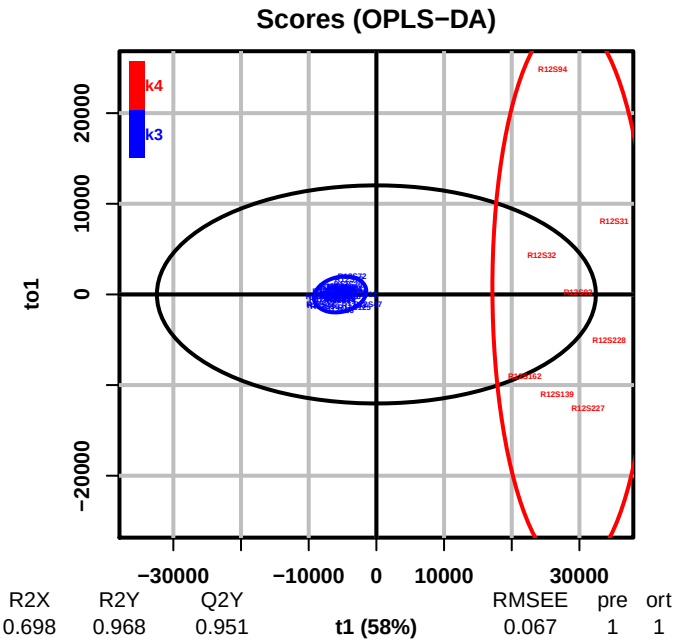

Model overview
R2Y
Q2Y
0.0
0.2
0.4
0.6
0.8
p1
o1
k2 versus k4

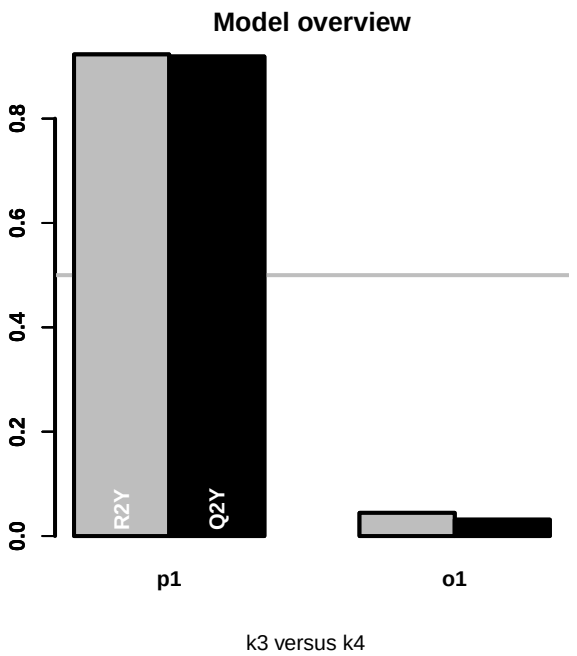

Features influencing orthogonal projection for k2 versus k4
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−2e+11
−1e+11
0e+00
1e+11
2e+11

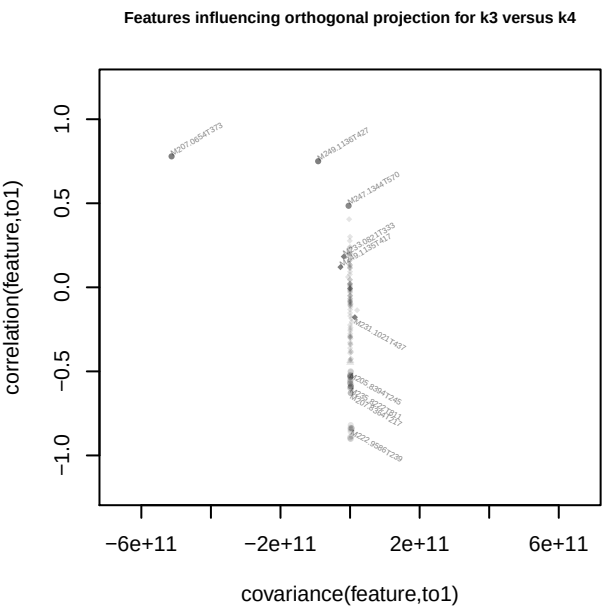

Significant features for level k2 versus k4
correlation(feature,t1)
variable importance in predictor−projection
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4
5
6

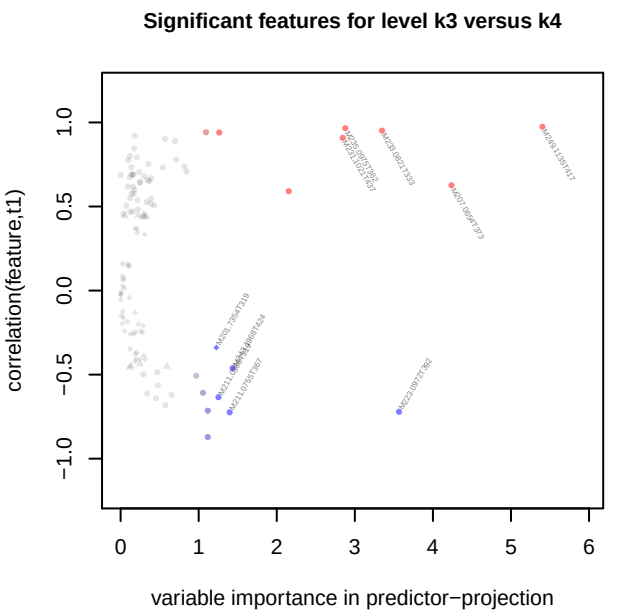

Features influencing orthogonal projection for k2 versus k4
correlation(feature,to1)
variable importance in orthogonal projection
1.0
0.5
0.0
−0.5
−1.0
0
2
4
6
8

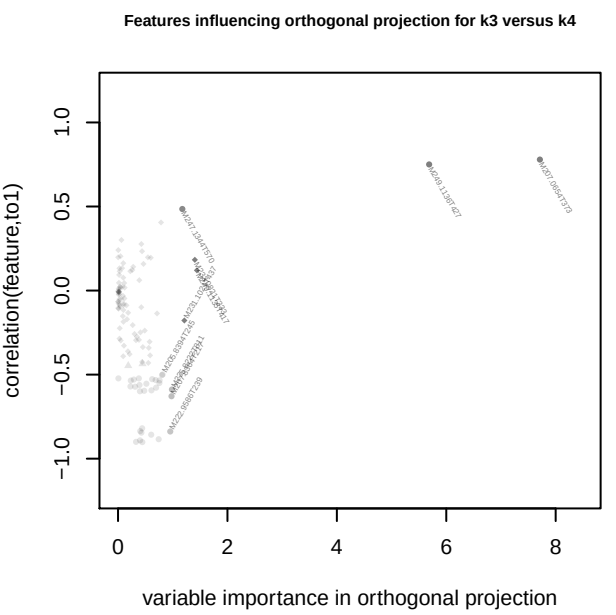

Significant features for level k3 versus k4
correlation(feature,t1)
covariance(feature,t1)
k3
k4
1.0
0.5
0.0
−0.5
−1.0
−1e+12
−5e+11
0e+00
5e+11
1e+12


Scores (OPLS−DA)
k4
k3
to1
t1 (58%)
20000
10000
0
−20000
−30000
−10000
0
10000
30000
R2X R2Y Q2Y RMSEE pre ort
0.698 0.968 0.951 0.067 1 1


Model overview
R2Y
Q2Y
p1
o1
0.0
0.2
0.4
0.6
0.8
k3 versus k4


Features influencing orthogonal projection for k3 versus k4
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−6e+11
−2e+11
2e+11
6e+11


Significant features for level k3 versus k4
correlation(feature,t1)
variable importance in predictor−projection
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4
5
6


Features influencing orthogonal projection for k3 versus k4
correlation(feature,to1)
variable importance in orthogonal projection
1.0
0.5
0.0
−0.5
−1.0
0
2
4
6
8