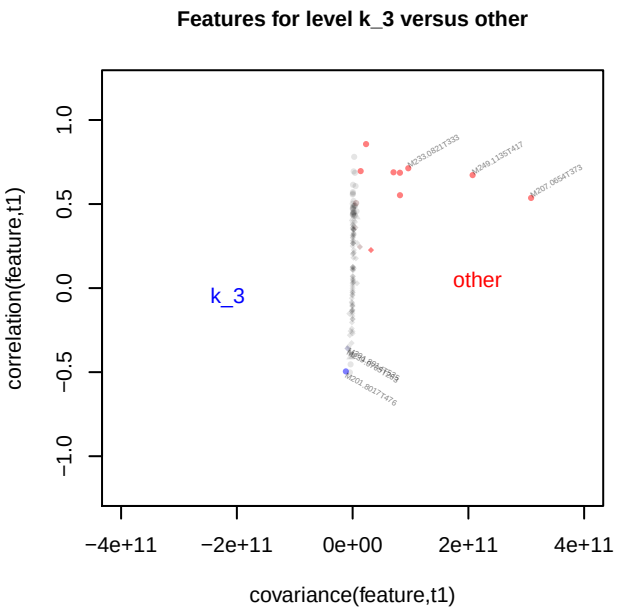
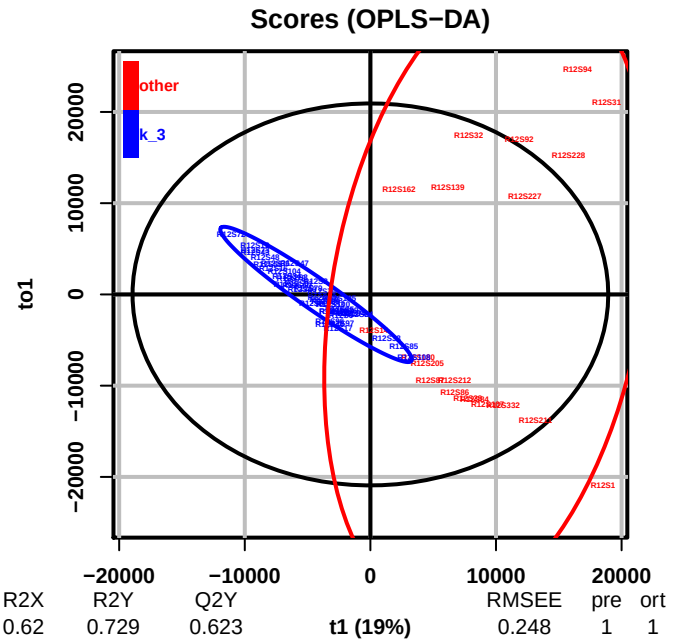
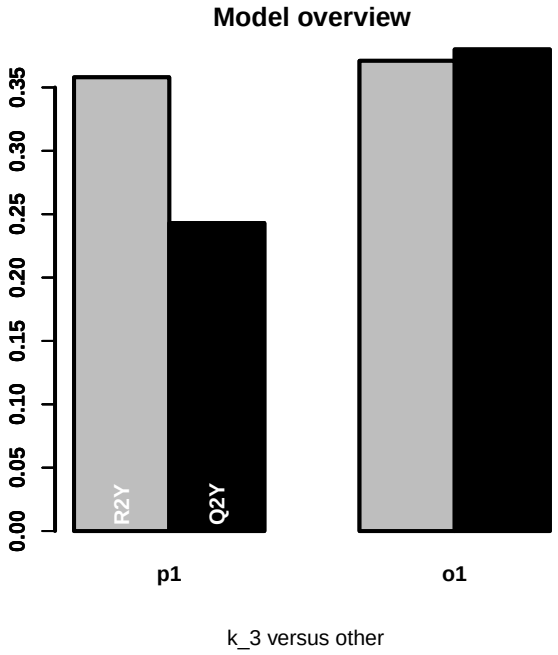
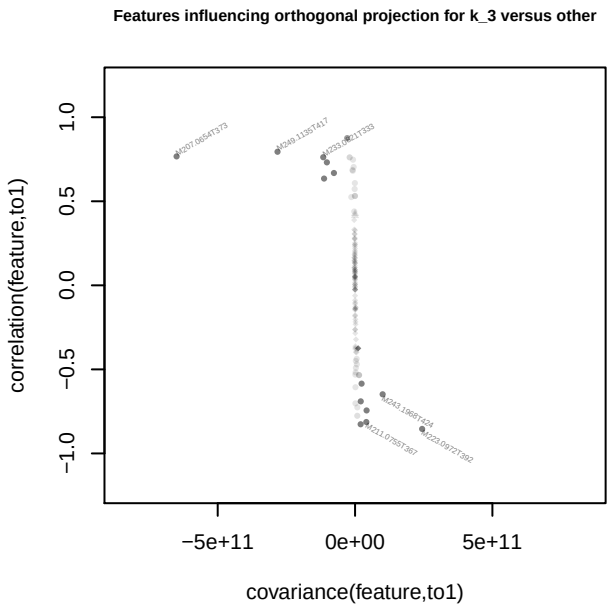
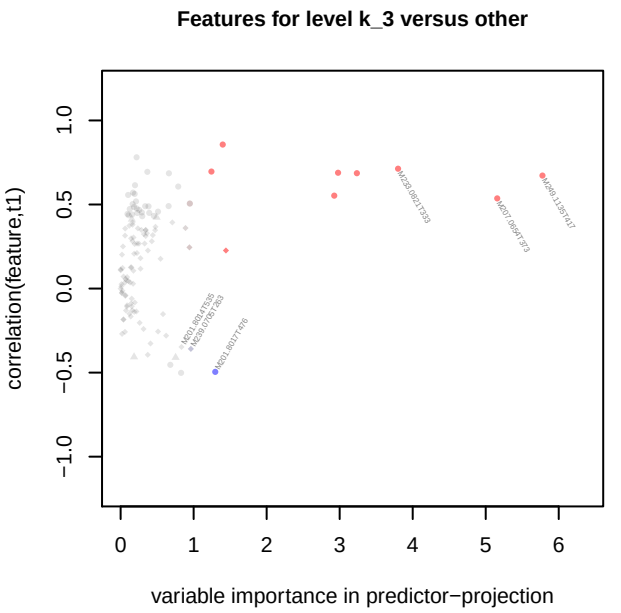
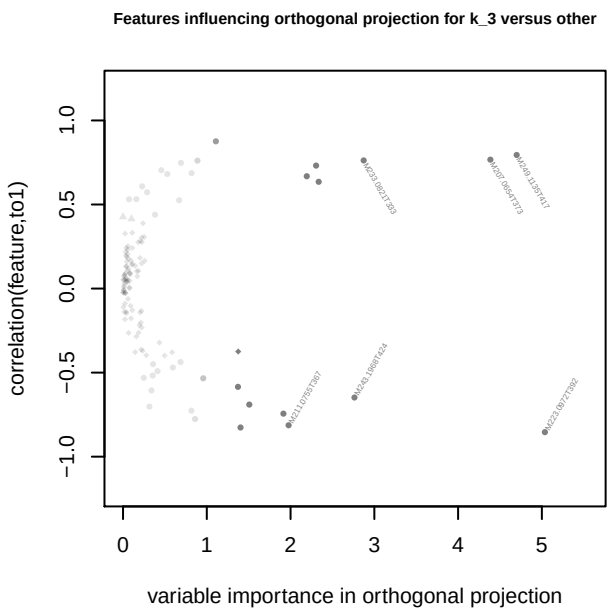

Features for level k_3 versus other
correlation(feature,t1)
covariance(feature,t1)
k_3
other
−4e+11
−2e+11
0e+00
2e+11
4e+11
1.0
0.5
0.0
−0.5
−1.0

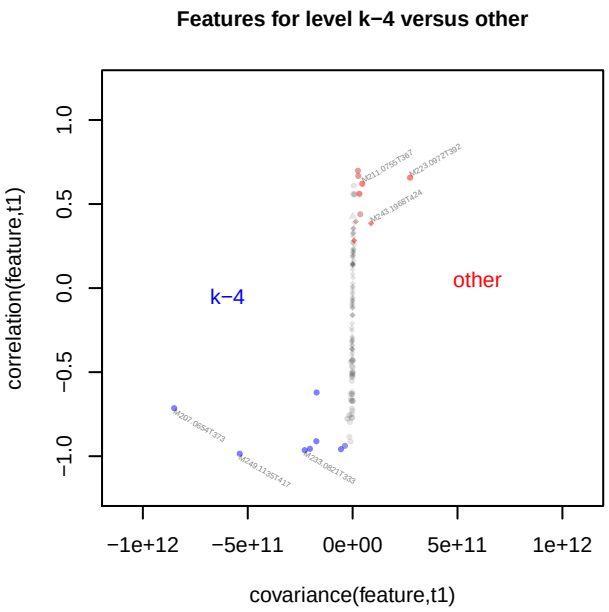

Scores (OPLS−DA)
other
k_3
to1
t1 (19%)
−20000
−10000
0
10000
20000
R2X
R2Y
Q2Y
RMSEE
pre
ort
0.62
0.729
0.623
0.248
1
1

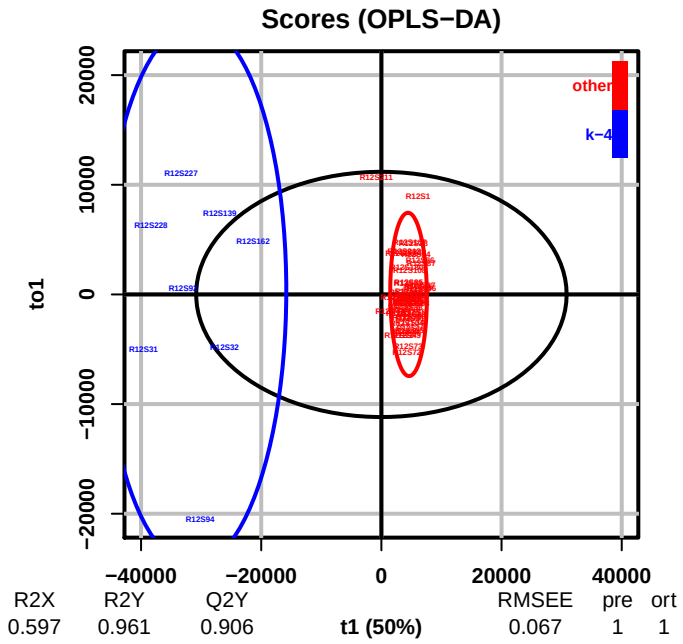

Model overview
R2Y
Q2Y
p1
o1
k_3 versus other
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35

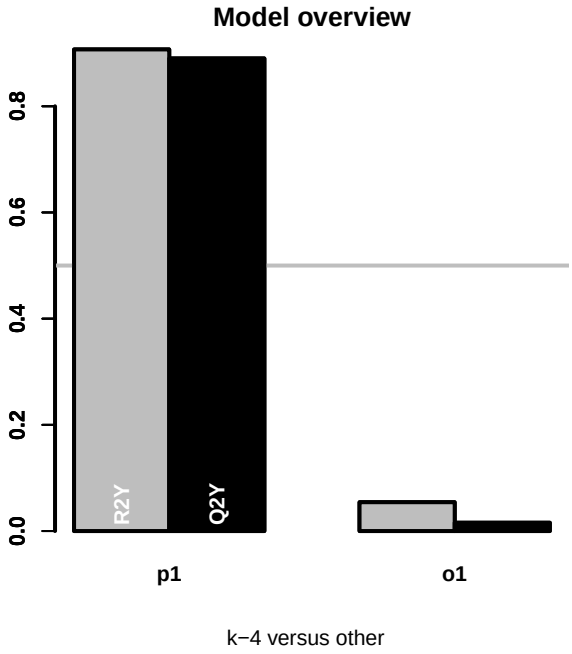

Features influencing orthogonal projection for k_3 versus other
correlation(feature,to1)
covariance(feature,to1)
−5e+11
0e+00
5e+11
1.0
0.5
0.0
−0.5
−1.0

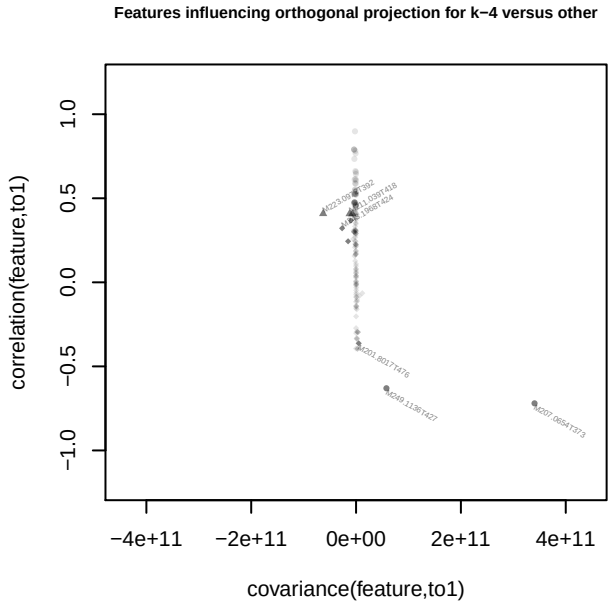

Features for level k_3 versus other
correlation(feature,t1)
variable importance in predictor−projection
0
1
2
3
4
5
6
1.0
0.5
0.0
−0.5
−1.0

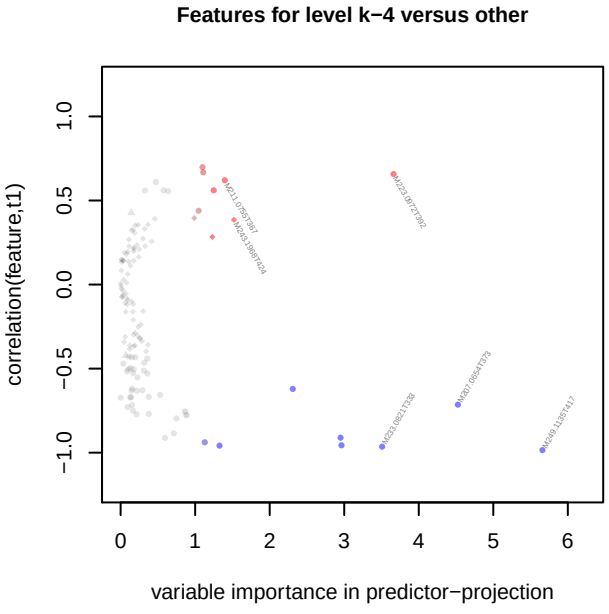

Features influencing orthogonal projection for k_3 versus other
correlation(feature,to1)
variable importance in orthogonal projection
0
1
2
3
4
5
1.0
0.5
0.0
−0.5
−1.0

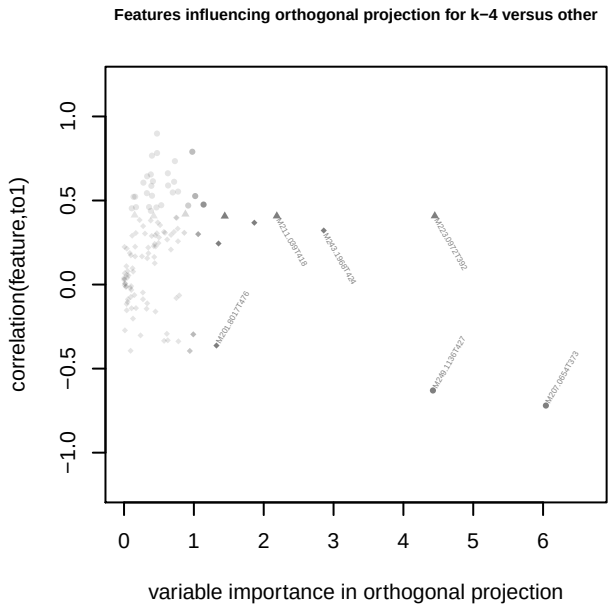

Features for level k−4 versus other
correlation(feature,t1)
covariance(feature,t1)
k−4
other
1.0
0.5
0.0
−0.5
−1.0
−1e+12
−5e+11
0e+00
5e+11
1e+12

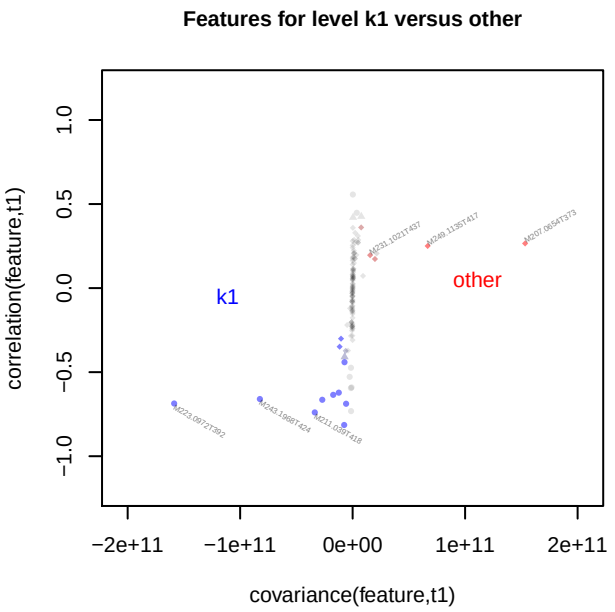

Scores (OPLS−DA)
other
k−4
to1
t1 (50%)
20000
10000
0
−10000
−20000
−40000
−20000
0
20000
40000
R2X
R2Y
Q2Y
RMSEE
pre
ort
0.597
0.961
0.906
0.067
1
1

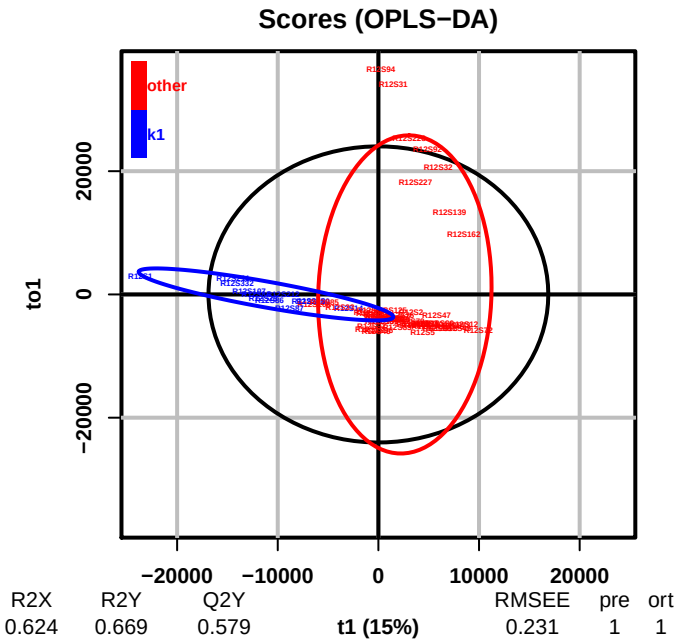

Model overview
R2Y
Q2Y
0.0
0.2
0.4
0.6
0.8
p1
o1
k−4 versus other

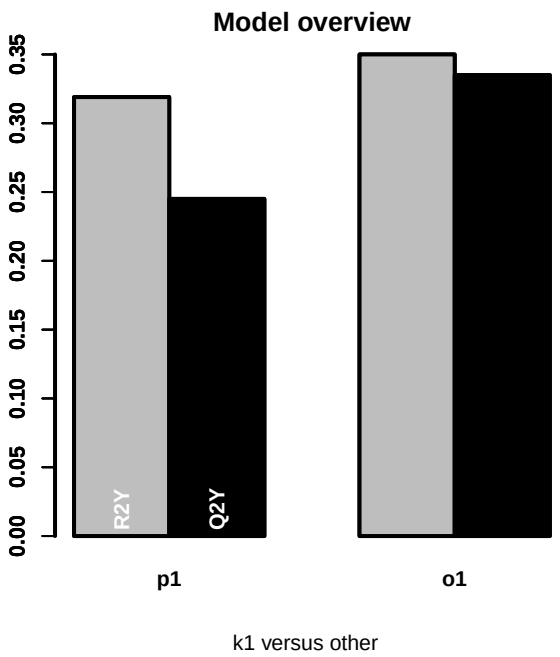

Features influencing orthogonal projection for k−4 versus other
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−4e+11
−2e+11
0e+00
2e+11
4e+11

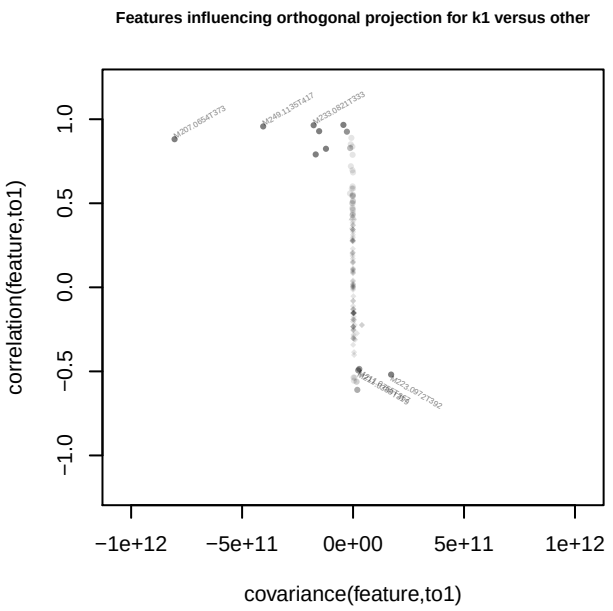

Features for level k−4 versus other
correlation(feature,t1)
variable importance in predictor−projection
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4
5
6

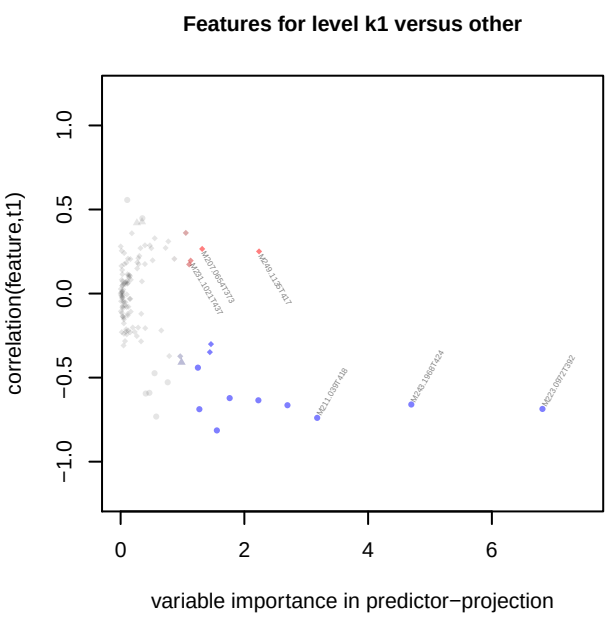

Features influencing orthogonal projection for k−4 versus other
correlation(feature,to1)
variable importance in orthogonal projection
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4
5
6

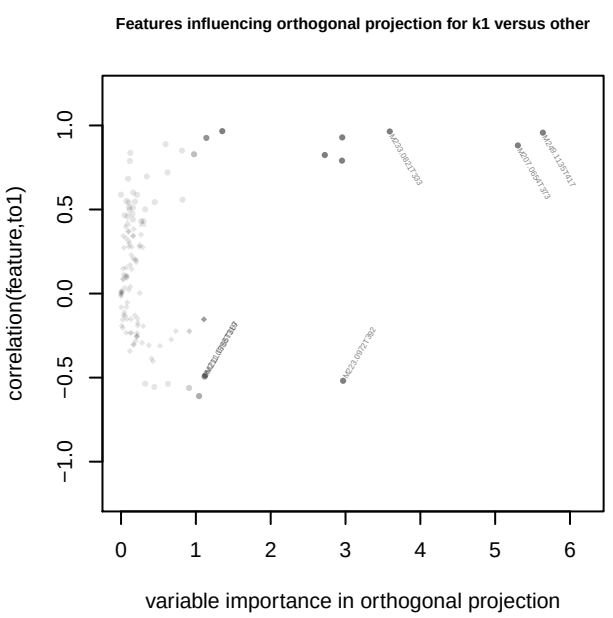

Features for level k1 versus other
correlation(feature,t1)
covariance(feature,t1)
k1
other
−2e+11
−1e+11
0e+00
1e+11
2e+11
−1.0
−0.5
0.0
0.5
1.0

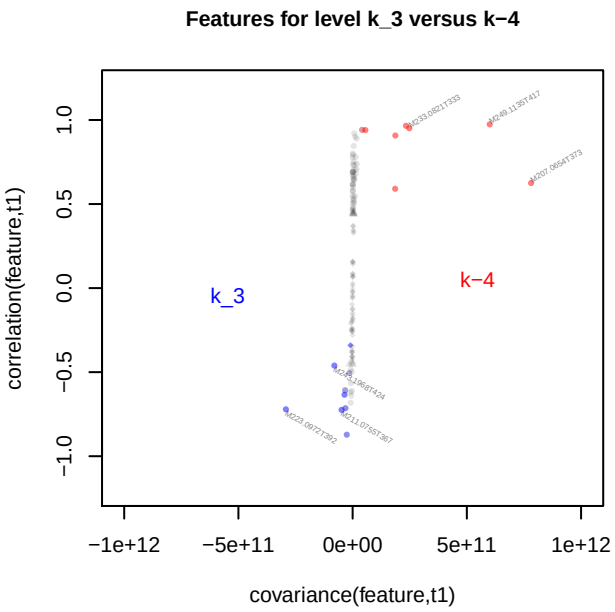

Scores (OPLS−DA)
other
k1
to1
t1 (15%)
−20000
−10000
0
10000
20000
R2X 0.624
R2Y 0.669
Q2Y 0.579
RMSEE 0.231
pre 1
ort 1

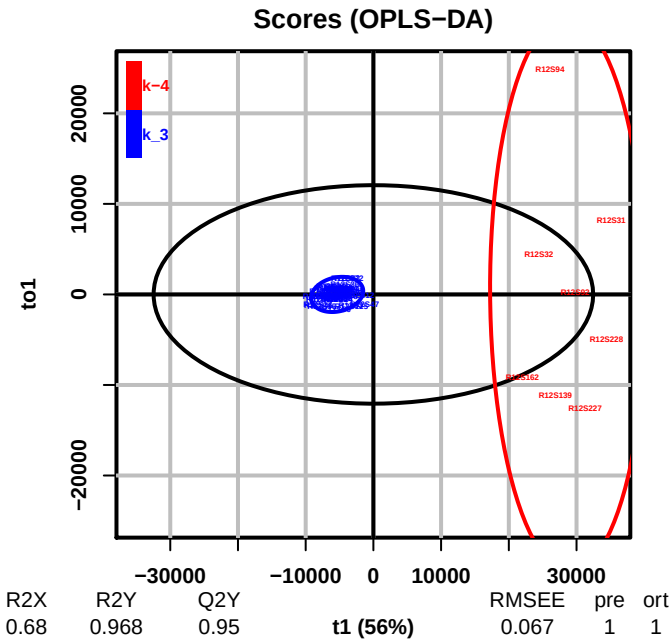

Model overview
R2Y
Q2Y
p1
o1
k1 versus other
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35

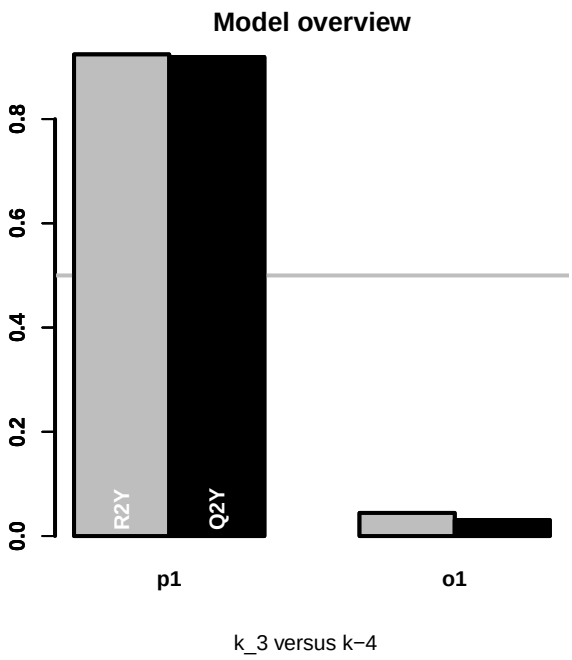

Features influencing orthogonal projection for k1 versus other
correlation(feature,to1)
covariance(feature,to1)
−1e+12
−5e+11
0e+00
5e+11
1e+12
−1.0
−0.5
0.0
0.5
1.0

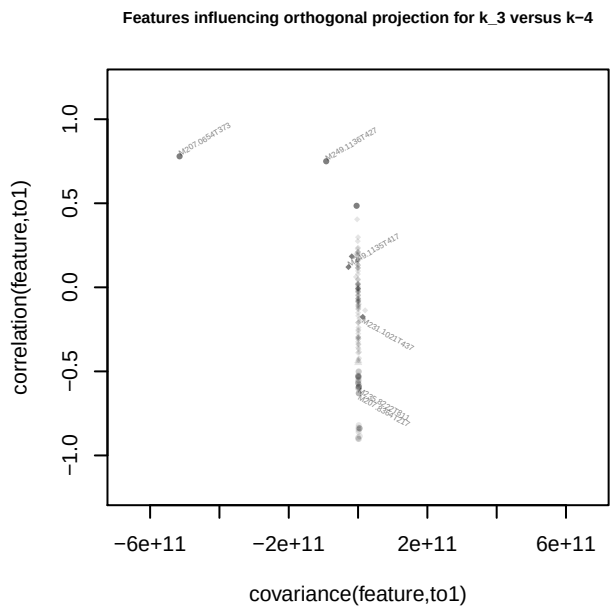

Features for level k1 versus other
correlation(feature,t1)
variable importance in predictor−projection
0
2
4
6
−1.0
−0.5
0.0
0.5
1.0

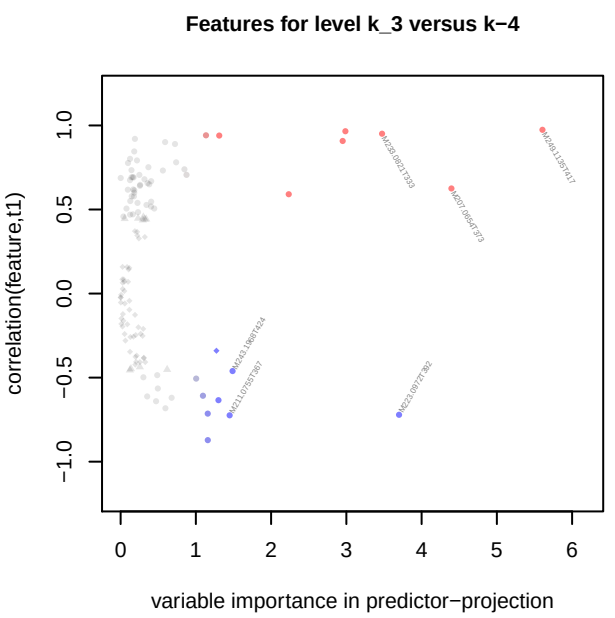

Features influencing orthogonal projection for k1 versus other
correlation(feature,to1)
variable importance in orthogonal projection
0
1
2
3
4
5
6
−1.0
−0.5
0.0
0.5
1.0

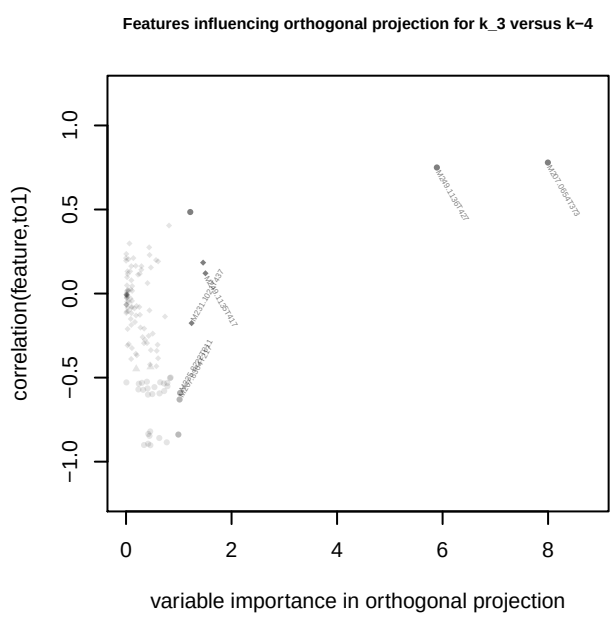

Features for level k_3 versus k−4
correlation(feature,t1)
covariance(feature,t1)
k_3
k−4
1.0
0.5
0.0
−0.5
−1.0
−1e+12
−5e+11
0e+00
5e+11
1e+12

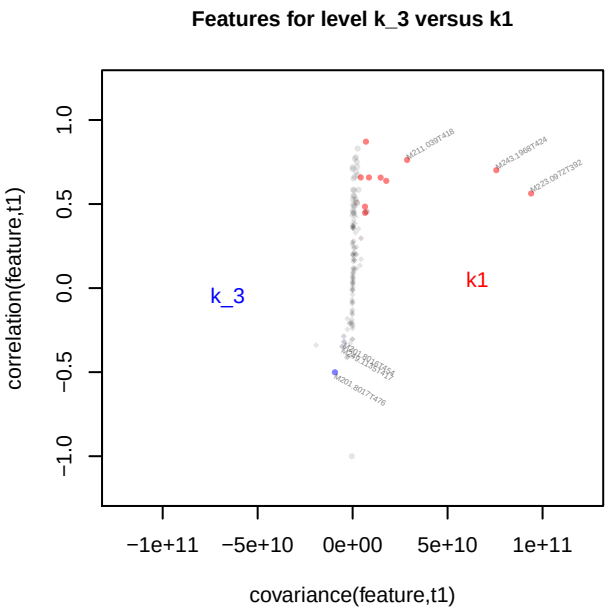

Scores (OPLS−DA)
k−4
k_3
to1
t1 (56%)
20000
10000
0
−20000
−30000
−10000
0
10000
30000
R12S94
R12S31
R12S32
R12S228
R12S162
R12S139
R12S227
R2X R2Y Q2Y RMSEE pre ort
0.68 0.968 0.95 0.067 1 1

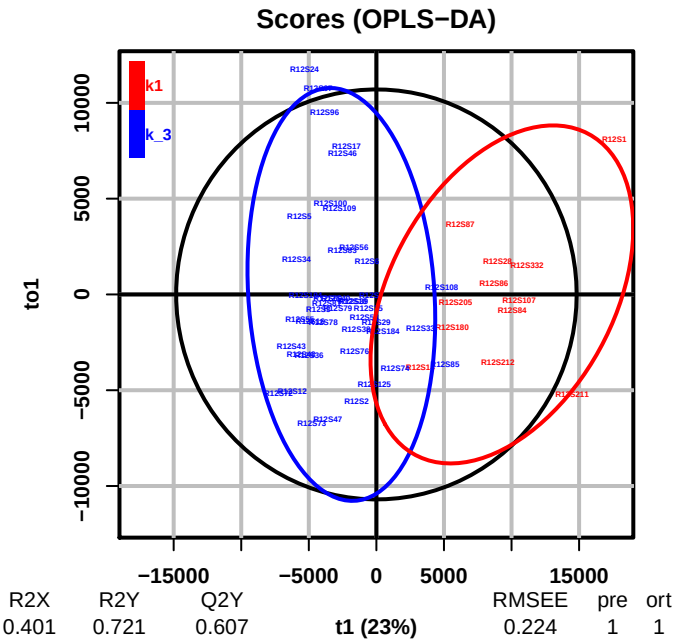

Model overview
R2Y
Q2Y
0.0
0.2
0.4
0.6
0.8
p1
o1
k_3 versus k−4

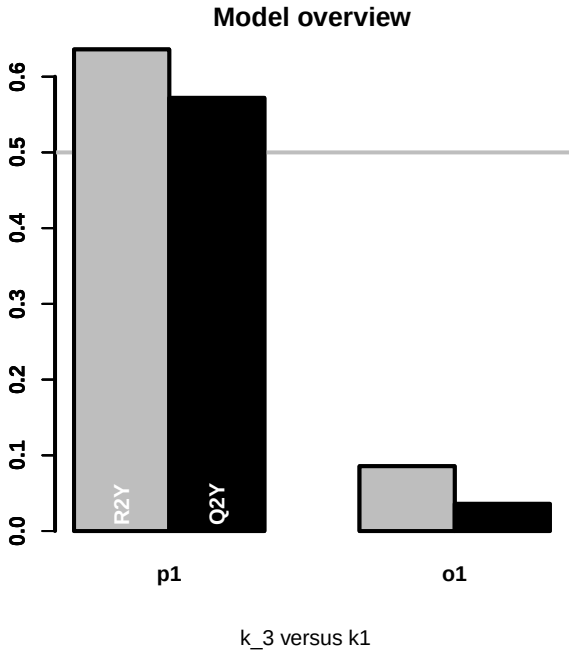

Features influencing orthogonal projection for k_3 versus k−4
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−6e+11
−2e+11
2e+11
6e+11

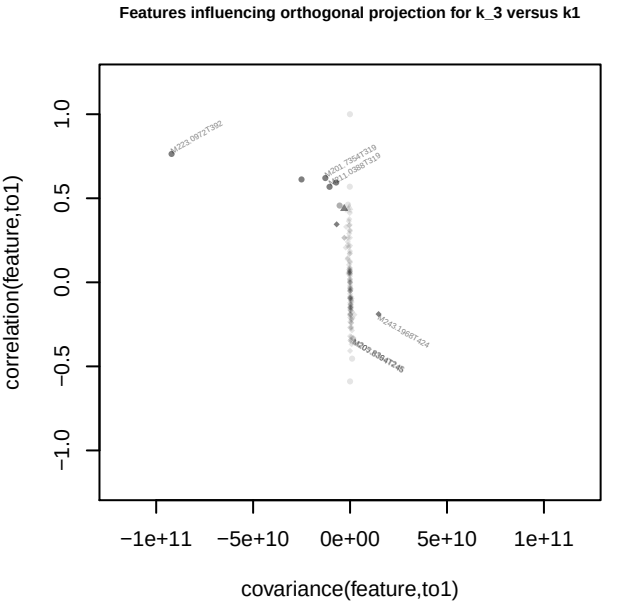

Features for level k_3 versus k−4
correlation(feature,t1)
variable importance in predictor−projection
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4
5
6

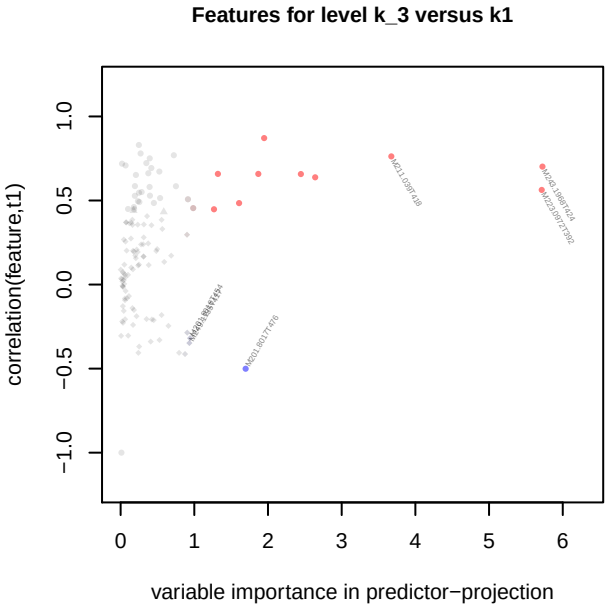

Features influencing orthogonal projection for k_3 versus k−4
correlation(feature,to1)
variable importance in orthogonal projection
1.0
0.5
0.0
−0.5
−1.0
0
2
4
6
8

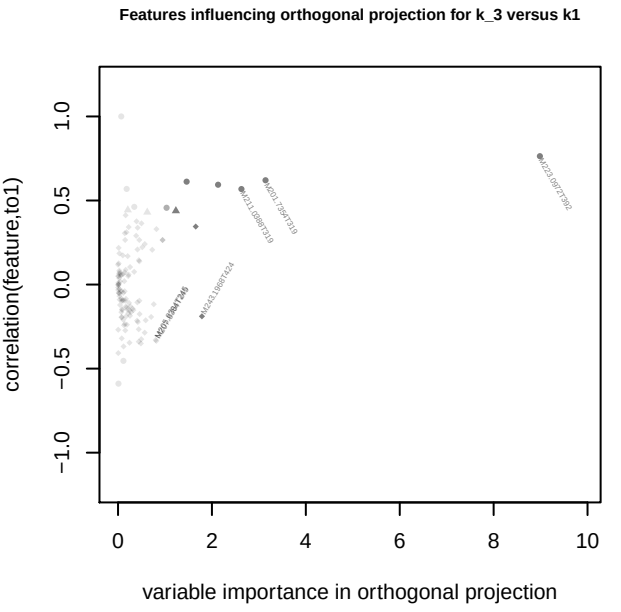

Features for level k_3 versus k1
correlation(feature,t1)
covariance(feature,t1)
k_3
k1
−1e+11
−5e+10
0e+00
5e+10
1e+11
1.0
0.5
0.0
−0.5
−1.0

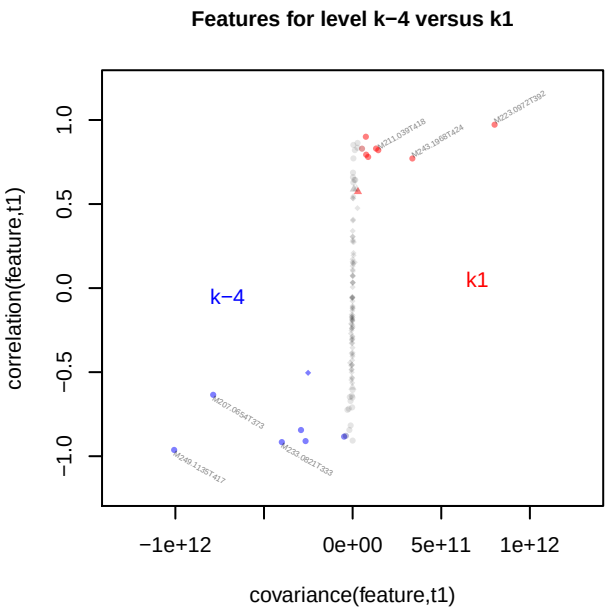

Scores (OPLS−DA)
k1
k_3
to1
t1 (23%)
−15000
−5000
0
5000
15000
10000
−10000
R2X
0.401
R2Y
0.721
Q2Y
0.607
RMSEE
0.224
pre
1
ort
1

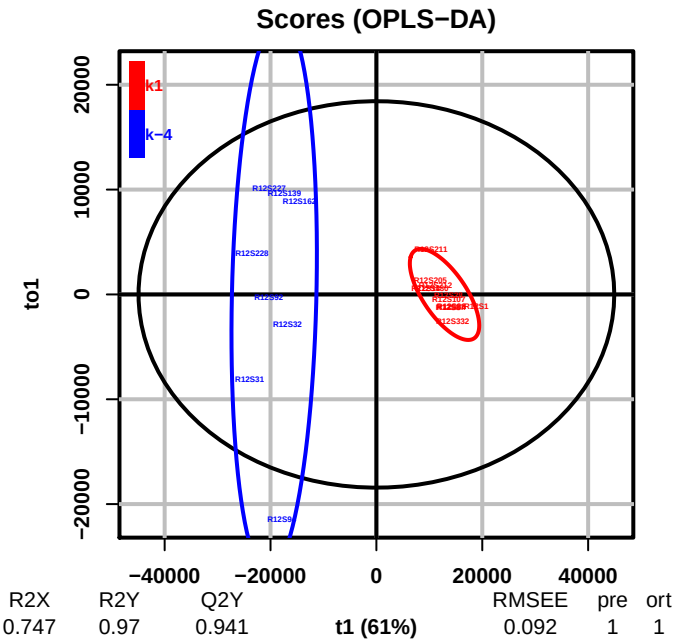

Model overview
R2Y
Q2Y
p1
o1
k_3 versus k1
0.0
0.1
0.2
0.3
0.4
0.5
0.6

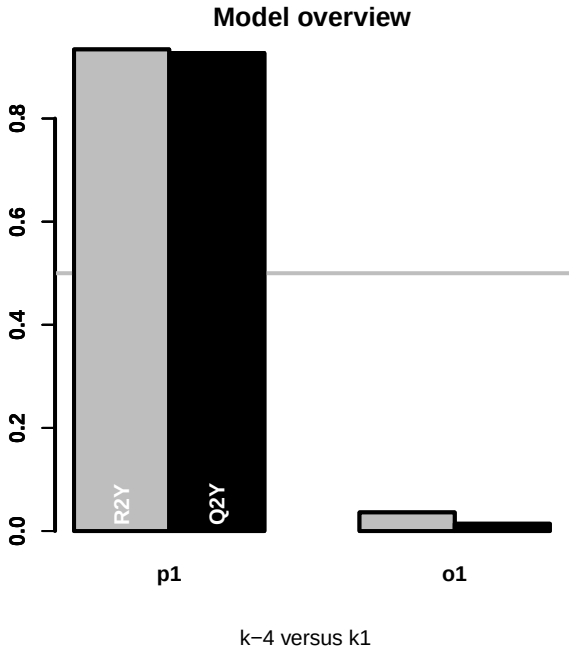

Features influencing orthogonal projection for k_3 versus k1
correlation(feature,to1)
covariance(feature,to1)
−1e+11
−5e+10
0e+00
5e+10
1e+11
1.0
0.5
0.0
−0.5
−1.0

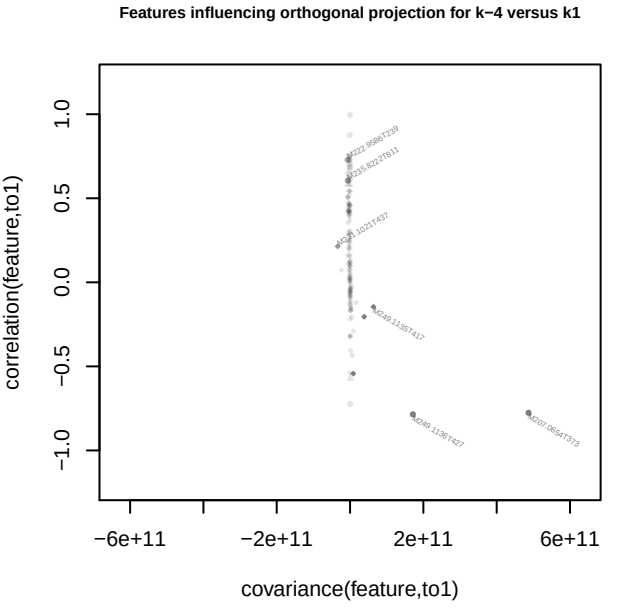

Features for level k_3 versus k1
correlation(feature,t1)
variable importance in predictor−projection
0
1
2
3
4
5
6
1.0
0.5
0.0
−0.5
−1.0

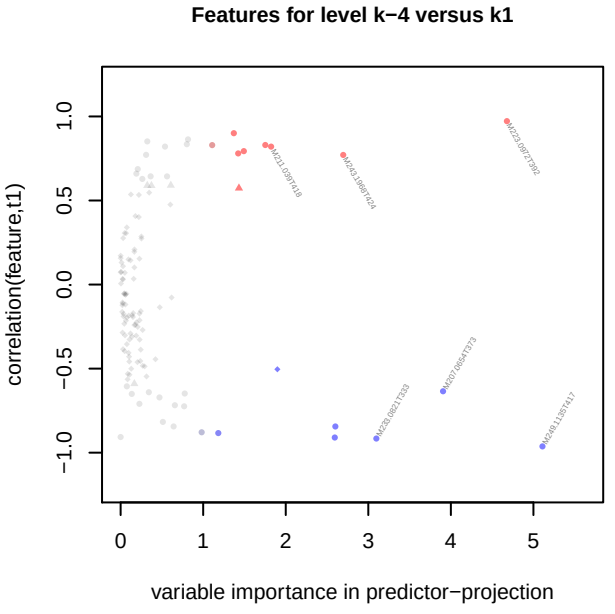

Features influencing orthogonal projection for k_3 versus k1
correlation(feature,to1)
variable importance in orthogonal projection
0
2
4
6
8
10
1.0
0.5
0.0
−0.5
−1.0

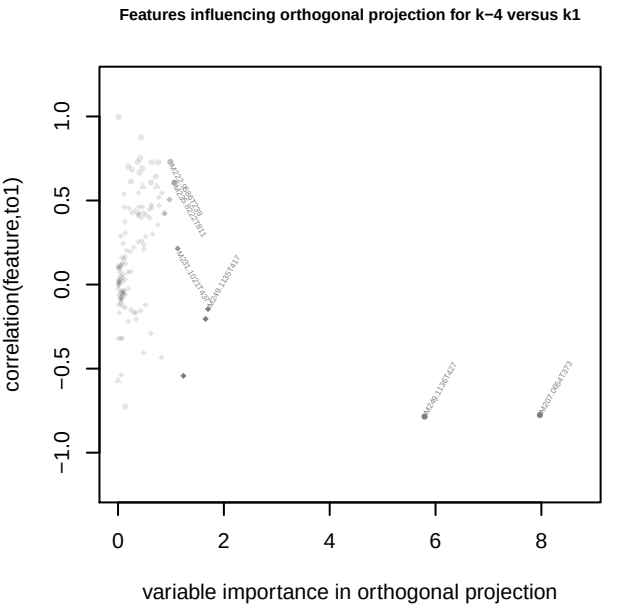

Features for level k−4 versus k1
correlation(feature,t1)
covariance(feature,t1)
k−4
k1
1.0
0.5
0.0
−0.5
−1.0
−1e+12
0e+00
5e+11
1e+12


Scores (OPLS−DA)
k1
k−4
to1
t1 (61%)
20000
10000
0
−10000
−20000
−40000
−20000
0
20000
40000
R2X R2Y Q2Y RMSEE pre ort
0.747 0.97 0.941 0.092 1 1


Model overview
R2Y
Q2Y
p1
o1
k−4 versus k1
0.0
0.2
0.4
0.6
0.8


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


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


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