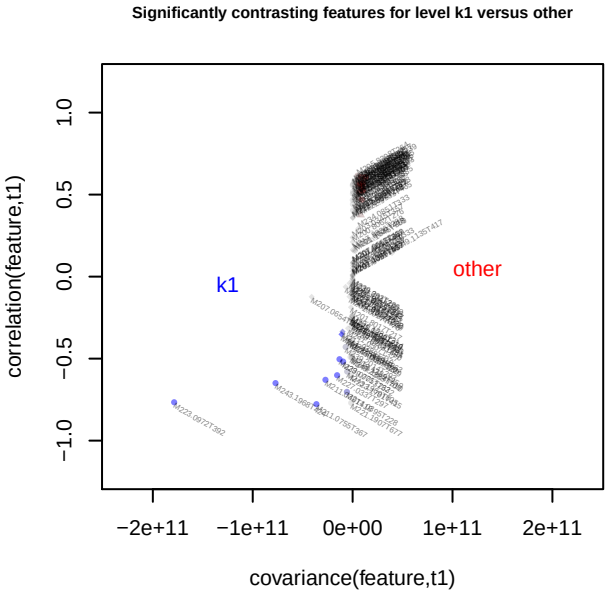
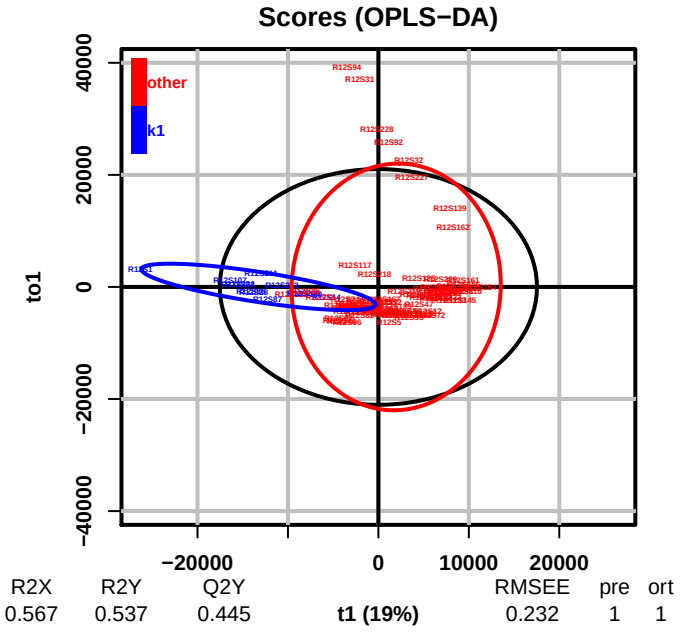
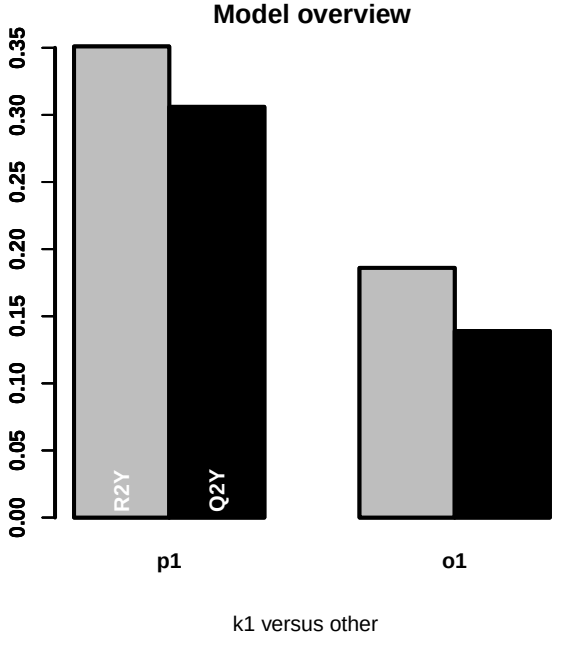
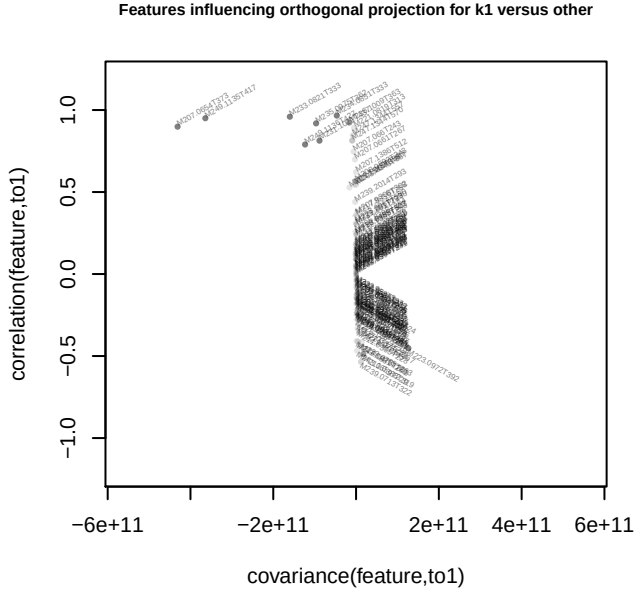
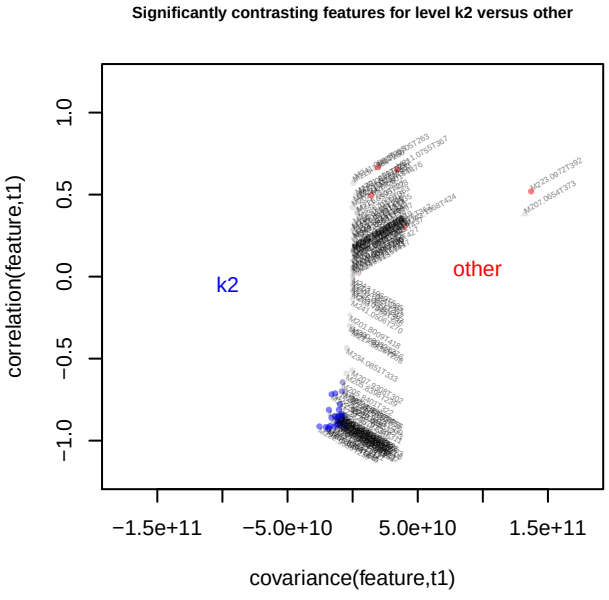
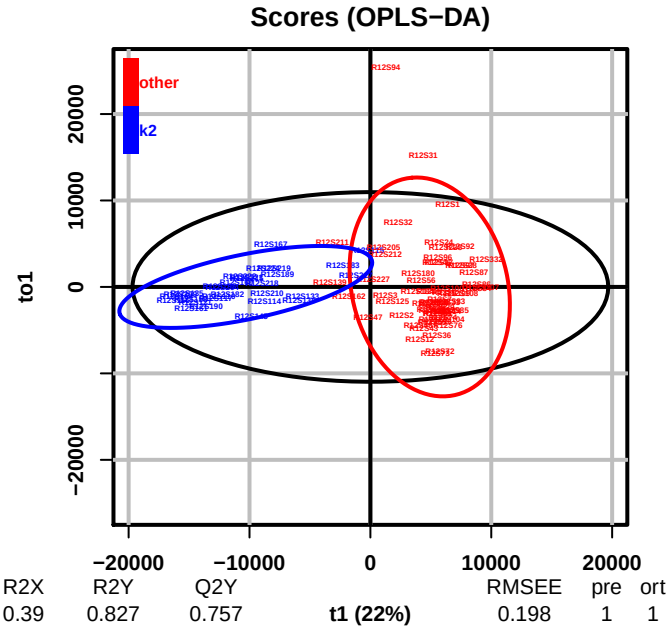

Significantly contrasting features for level k1 versus other
correlation(feature,t1)
covariance(feature,t1)
k1
other
1.0
0.5
0.0
−0.5
−1.0
−2e+11
−1e+11
0e+00
1e+11
2e+11

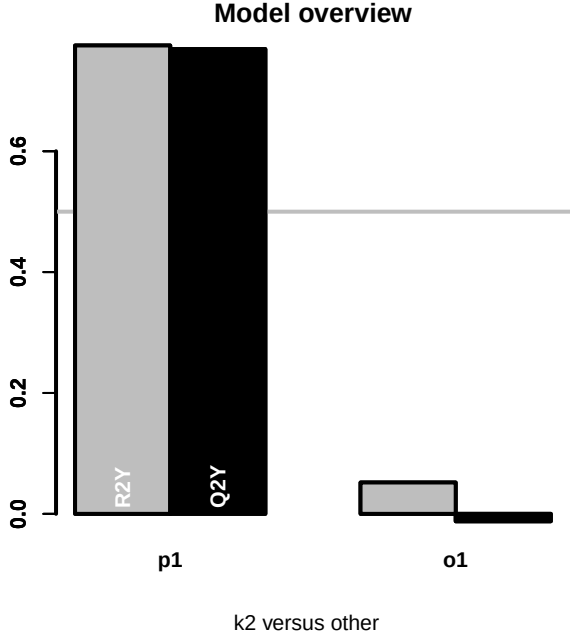

Scores (OPLS−DA)
to1
t1 (19%)
other
k1
40000
20000
0
−20000
−40000
−20000
0
10000
20000
R2X
R2Y
Q2Y
RMSEE
pre
ort
0.567
0.537
0.445
0.232
1
1

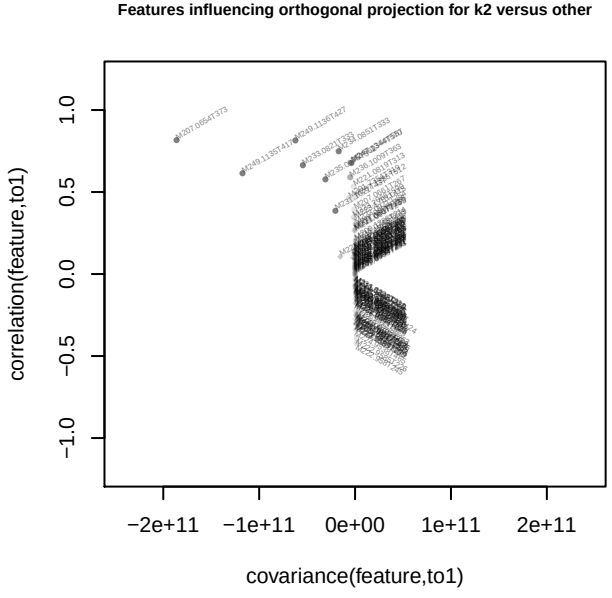

Model overview
R2Y
Q2Y
p1
o1
k1 versus other
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35

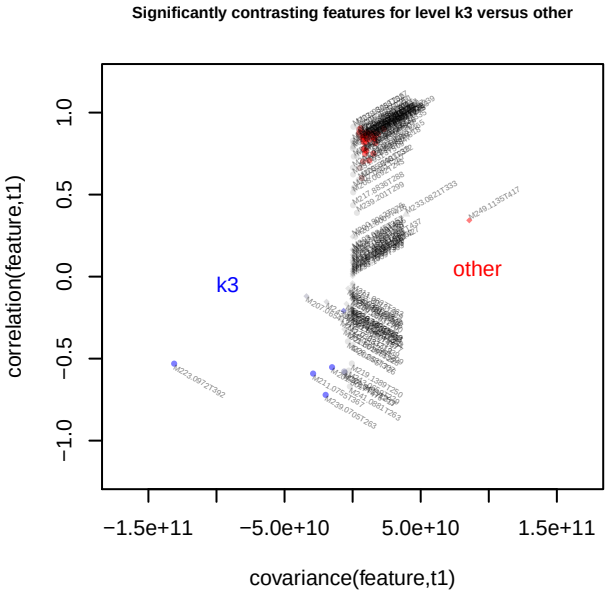

Features influencing orthogonal projection for k1 versus other
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−6e+11
−2e+11
2e+11
4e+11
6e+11

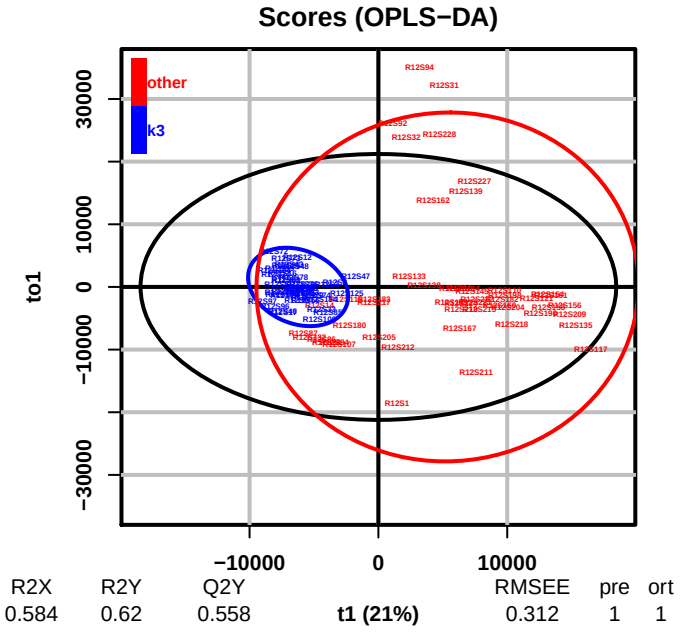

Significantly contrasting features for level k2 versus other
correlation(feature,t1)
covariance(feature,t1)
k2
other
1.0
0.5
0.0
−0.5
−1.0
−1.5e+11
−5.0e+10
5.0e+10
1.5e+11

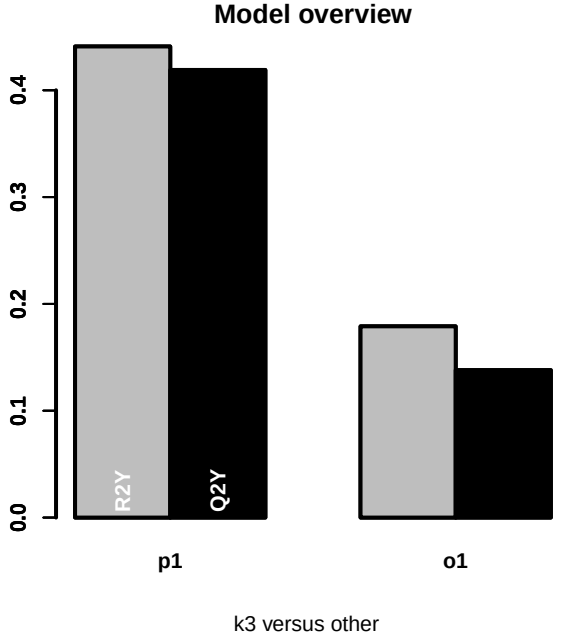

Scores (OPLS−DA)
other
k2
to1
t1 (22%)
20000
10000
0
−20000
−10000
R2X
R2Y
Q2Y
RMSEE
pre
ort
0.39
0.827
0.757
0.198
1
1

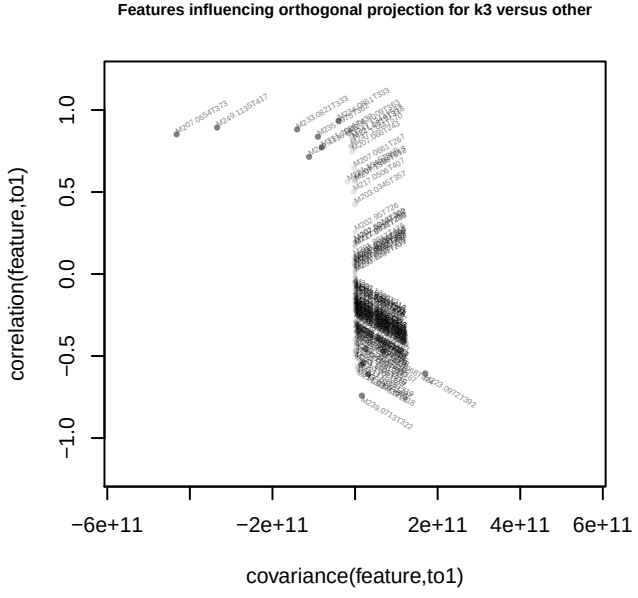

Model overview
R2Y
Q2Y
p1
o1
k2 versus other
0.6
0.4
0.2
0.0

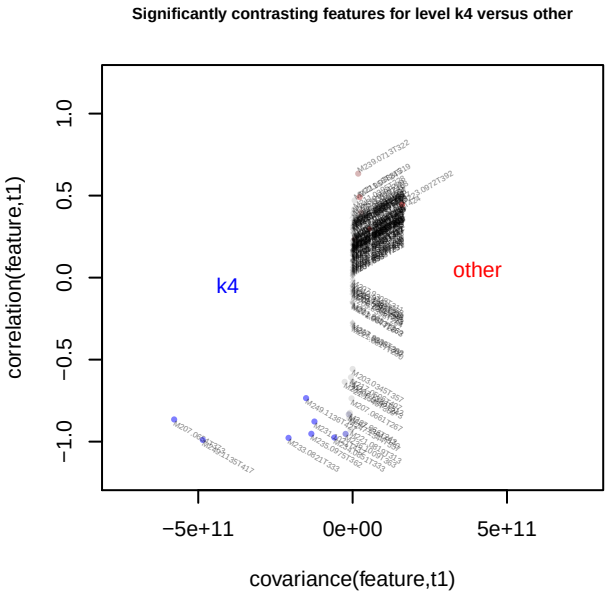

Features influencing orthogonal projection for k2 versus other
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−2e+11
−1e+11
0e+00
1e+11
2e+11

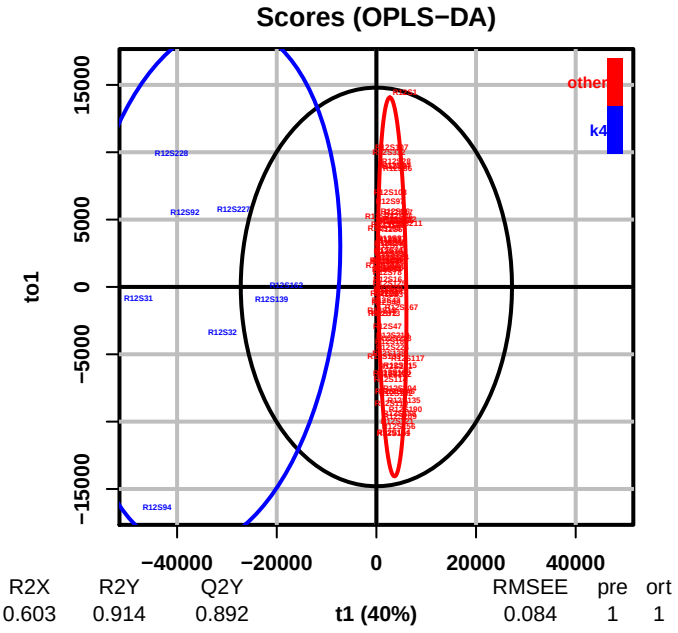

Significantly contrasting features for level k3 versus other
correlation(feature,t1)
covariance(feature,t1)
k3
other
1.0
0.5
0.0
−0.5
−1.0
−1.5e+11
−5.0e+10
5.0e+10
1.5e+11

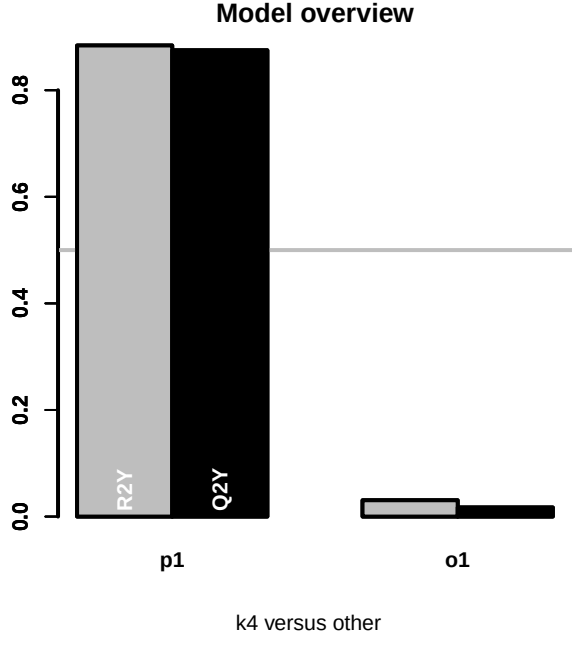

Scores (OPLS−DA)
other
k3
to1
t1 (21%)
30000
10000
0
−10000
−30000
−10000
0
10000
R2X R2Y Q2Y RMSEE pre ort
0.584 0.62 0.558 0.312 1 1

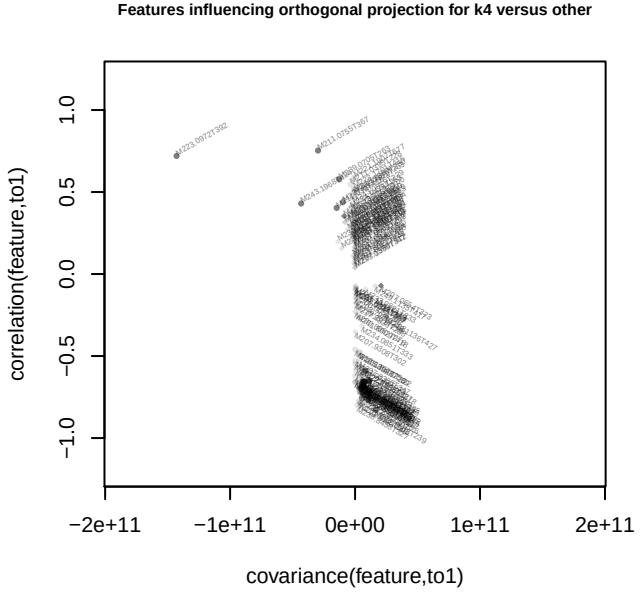

Model overview
R2Y
Q2Y
0.0
0.1
0.2
0.3
0.4
p1
o1
k3 versus other

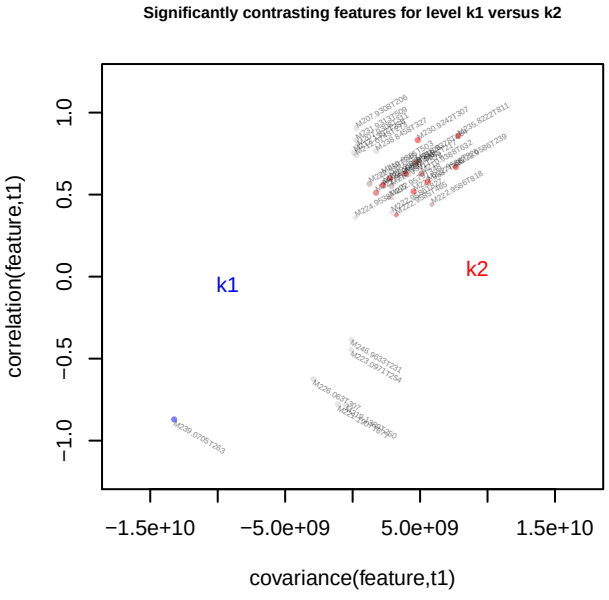

Features influencing orthogonal projection for k3 versus other
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−6e+11
−2e+11
2e+11
4e+11
6e+11

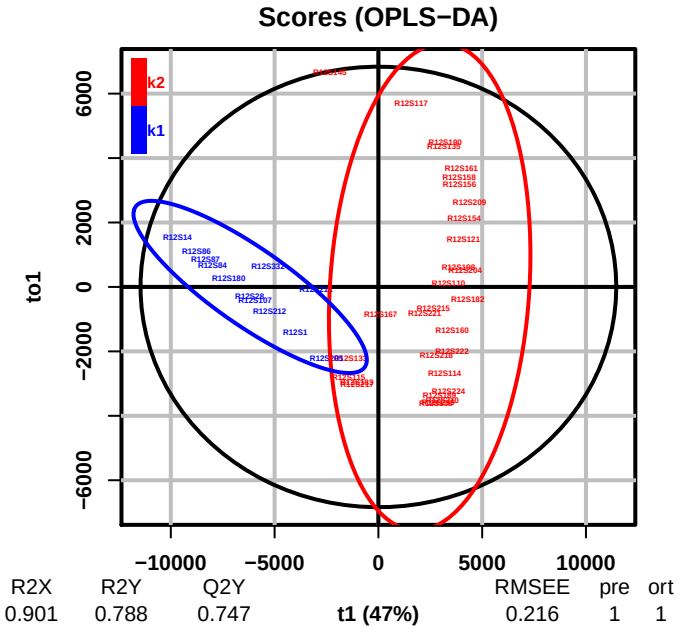

Significantly contrasting features for level k4 versus other
correlation(feature,t1)
covariance(feature,t1)
k4
other
1.0
0.5
0.0
−0.5
−1.0
−5e+11
0e+00
5e+11

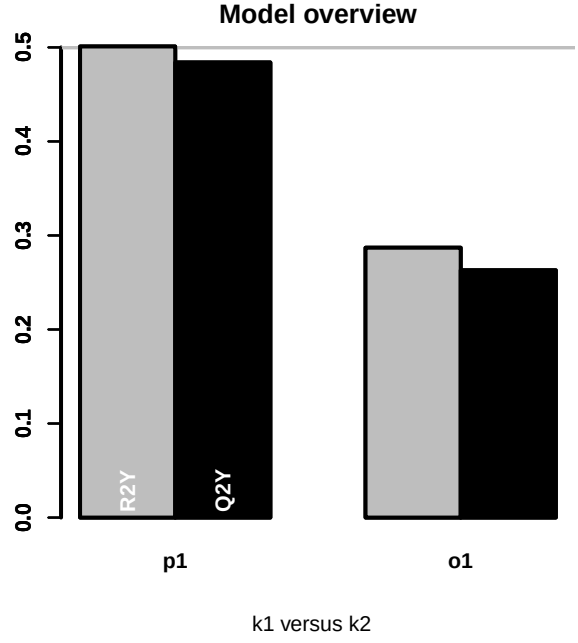

Scores (OPLS−DA)
to1
t1 (40%)
other
k4
15000
5000
0
−5000
−15000
−40000
−20000
0
20000
40000
R2X R2Y Q2Y RMSEE pre ort
0.603 0.914 0.892 0.084 1 1

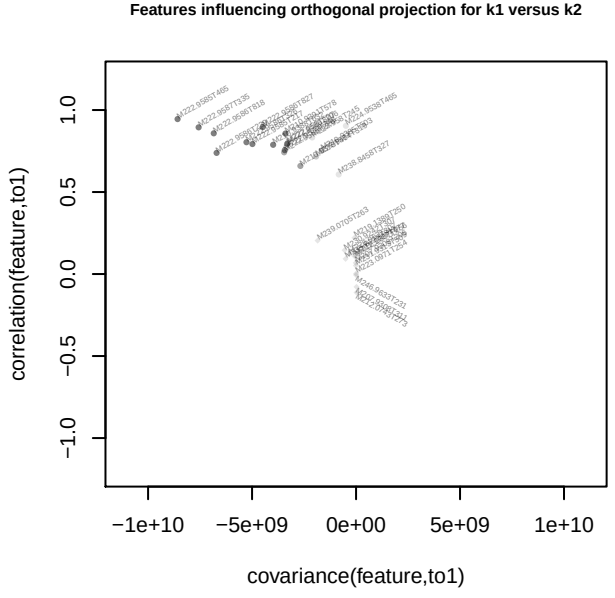

Model overview
R2Y
Q2Y
p1
o1
k4 versus other
0.0
0.2
0.4
0.6
0.8


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


Significantly contrasting features for level k1 versus k2
correlation(feature,t1)
covariance(feature,t1)
k1
k2
1.0
0.5
0.0
−0.5
−1.0
−1.5e+10
−5.0e+09
5.0e+09
1.5e+10

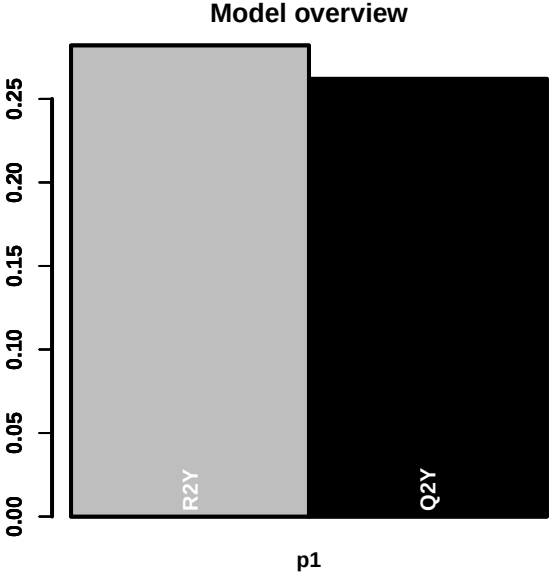

Scores (OPLS−DA)
k2
k1
to1
6000
2000
0
−2000
−6000
−10000
−5000
0
5000
10000
R2X
R2Y
Q2Y
RMSEE
pre
ort
0.901
0.788
0.747
t1 (47%)
0.216
1
1


Model overview
R2Y
Q2Y
0.0
0.1
0.2
0.3
0.4
0.5
p1
o1
k1 versus k2


Features influencing orthogonal projection for k1 versus k2
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−1e+10
−5e+09
0e+00
5e+09
1e+10

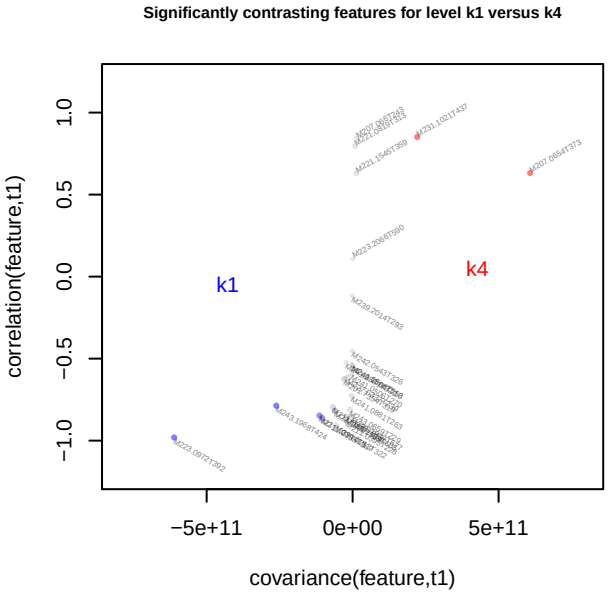
too few covariance data

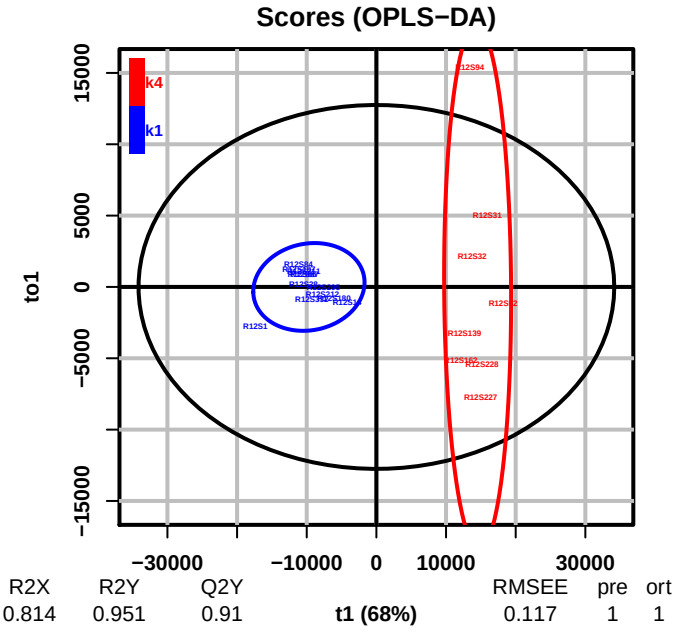
no orthogonal projection is possible

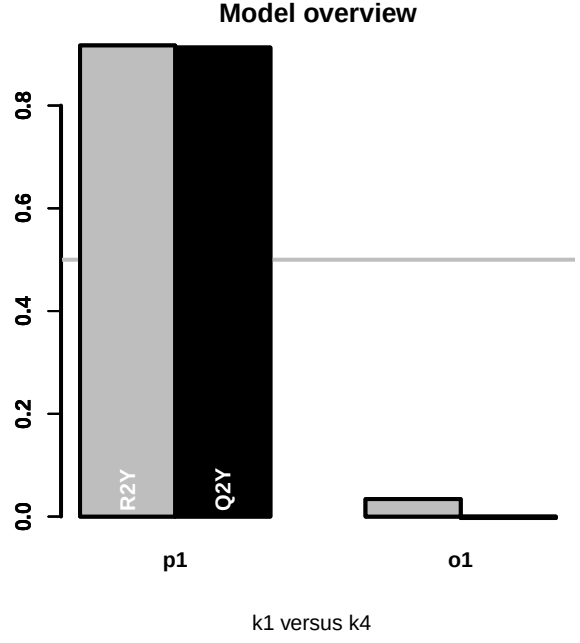


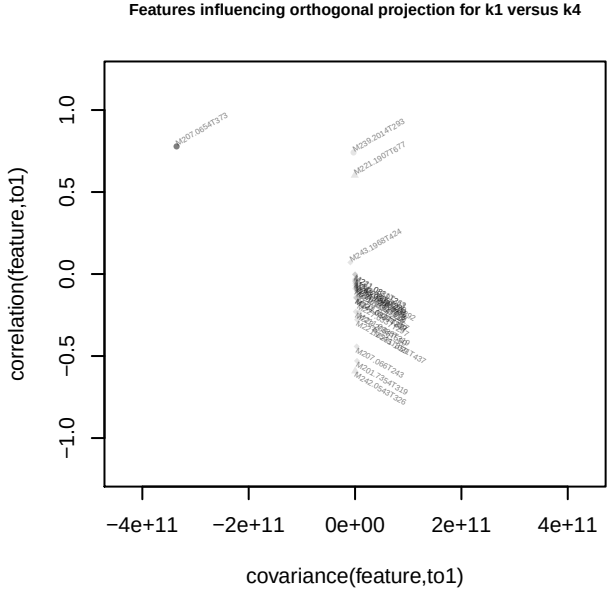
k1 versus k3

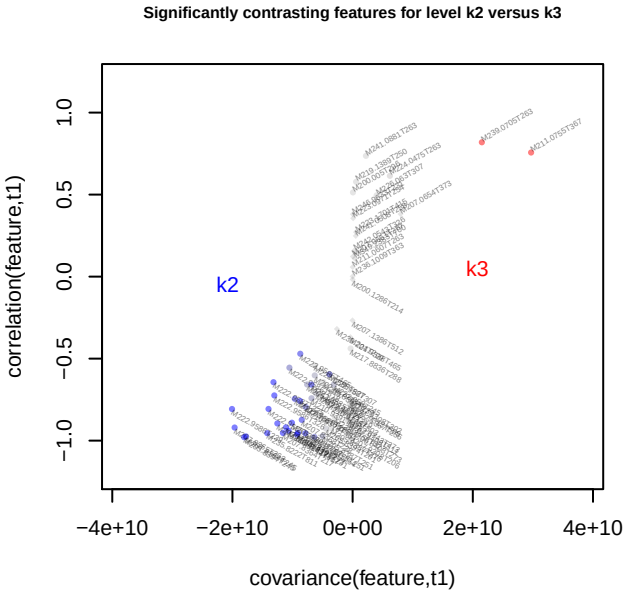
no orthogonal projection is possible

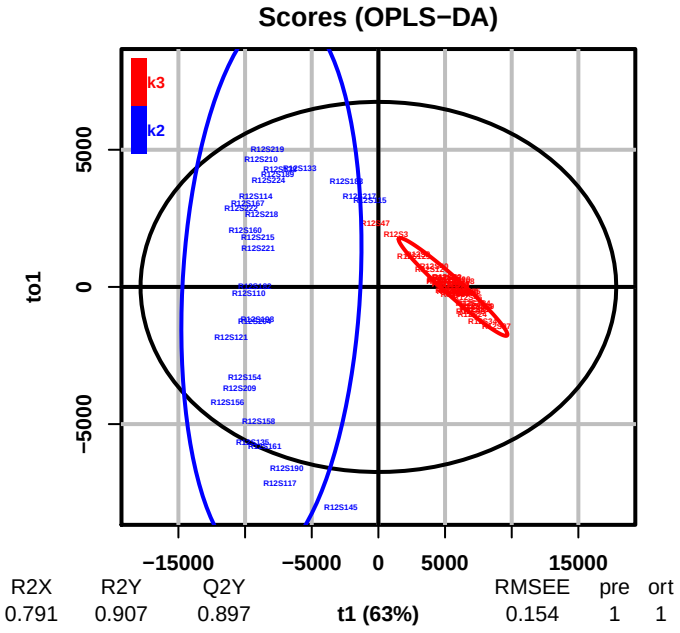

Significantly contrasting features for level k1 versus k4
correlation(feature,t1)
covariance(feature,t1)
k1
k4
1.0
0.5
0.0
−0.5
−1.0
−5e+11
0e+00
5e+11

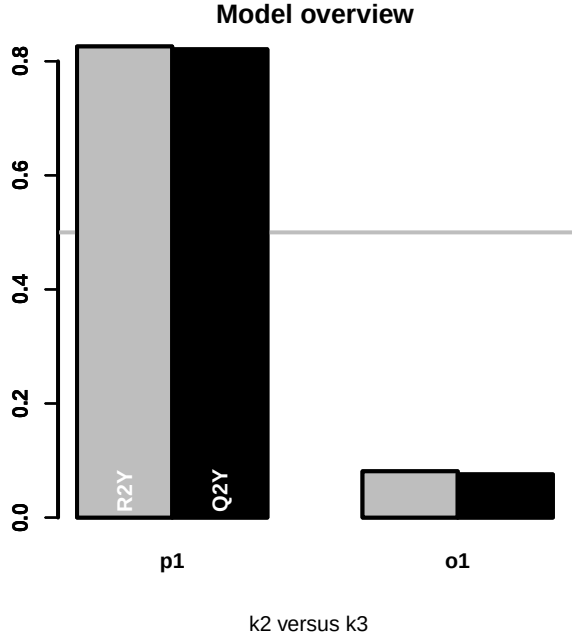

Scores (OPLS−DA)
k4
k1
to1
15000
5000
0
−5000
−15000
−30000
−10000
0
10000
30000
R2X
R2Y
Q2Y
RMSEE
pre
ort
0.814
0.951
0.91
t1 (68%)
0.117
1
1

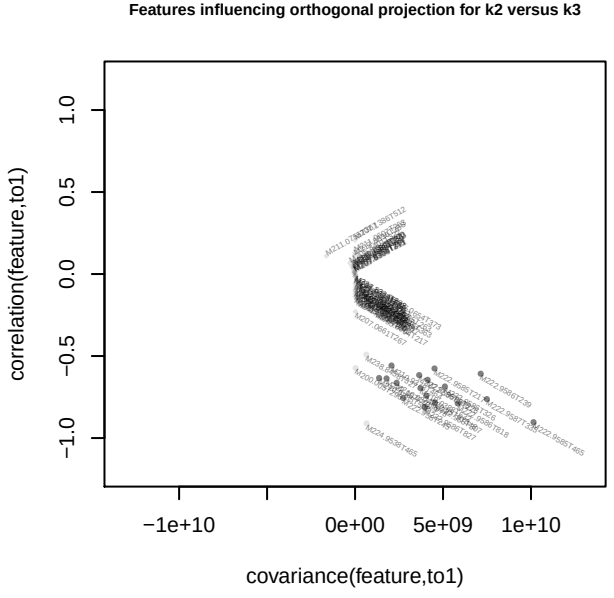

Model overview
R2Y
Q2Y
0.0
0.2
0.4
0.6
0.8
p1
o1
k1 versus k4

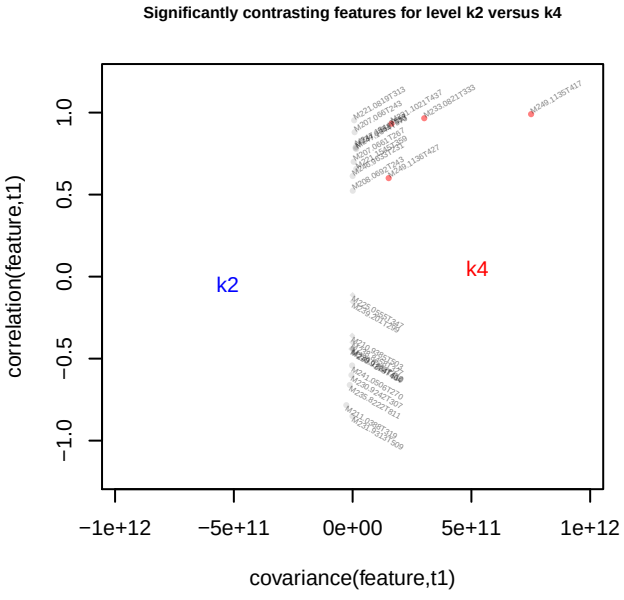

Features influencing orthogonal projection for k1 versus k4
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−4e+11
−2e+11
0e+00
2e+11
4e+11

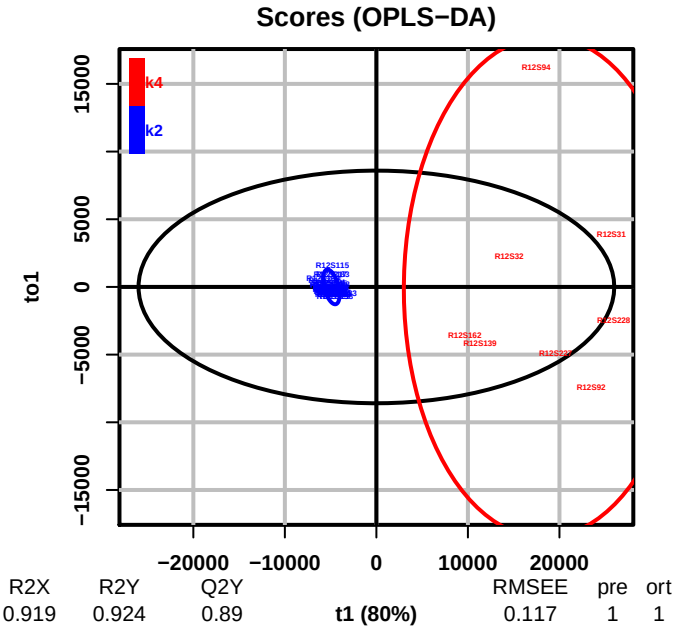

Significantly contrasting features for level k2 versus k3
correlation(feature,t1)
covariance(feature,t1)
k2
k3
1.0
0.5
0.0
−0.5
−1.0
−4e+10
−2e+10
0e+00
2e+10
4e+10

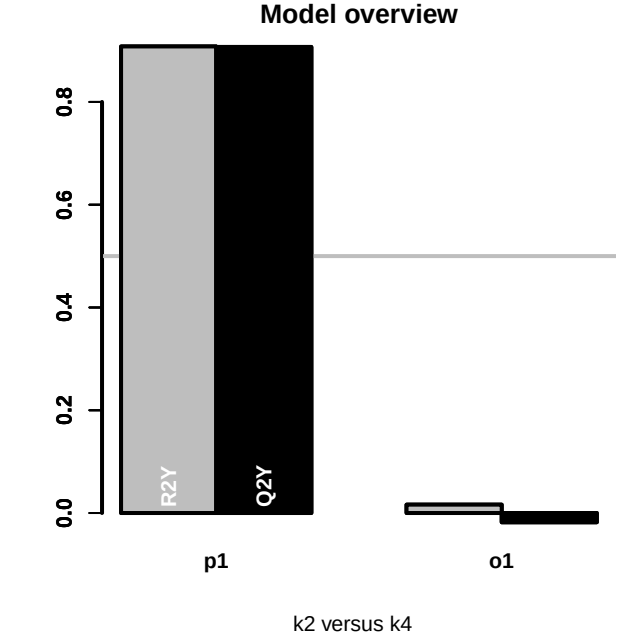

Scores (OPLS−DA)
k3
k2
to1
5000
0
−5000
−15000
−5000
0
5000
15000
R2X
R2Y
Q2Y
RMSEE
pre
ort
0.791
0.907
0.897
t1 (63%)
0.154
1
1

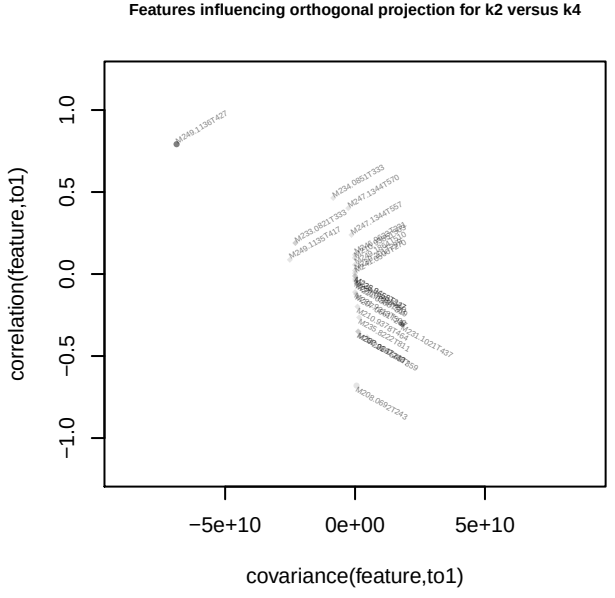

Model overview
R2Y
Q2Y
p1
o1
k2 versus k3
0.0
0.2
0.4
0.6
0.8

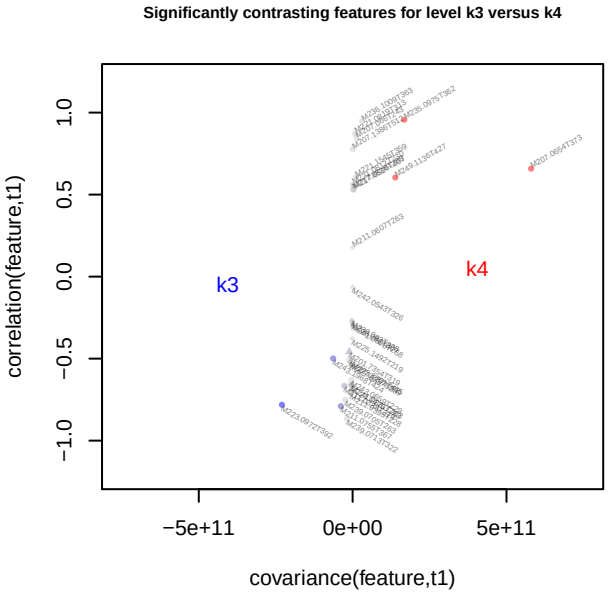

Features influencing orthogonal projection for k2 versus k3
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−1e+10
0e+00
5e+09
1e+10

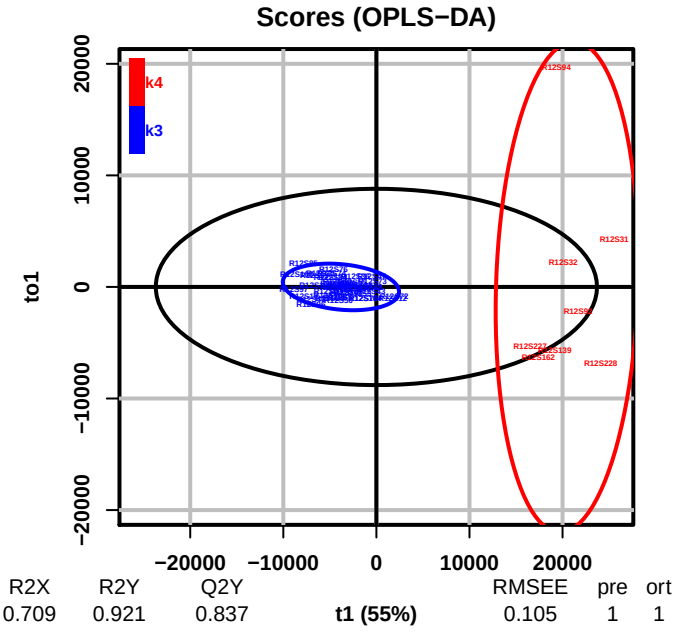

Significantly contrasting features for level k2 versus k4
correlation(feature,t1)
covariance(feature,t1)
k2
k4
1.0
0.5
0.0
−0.5
−1.0
−1e+12
−5e+11
0e+00
5e+11
1e+12

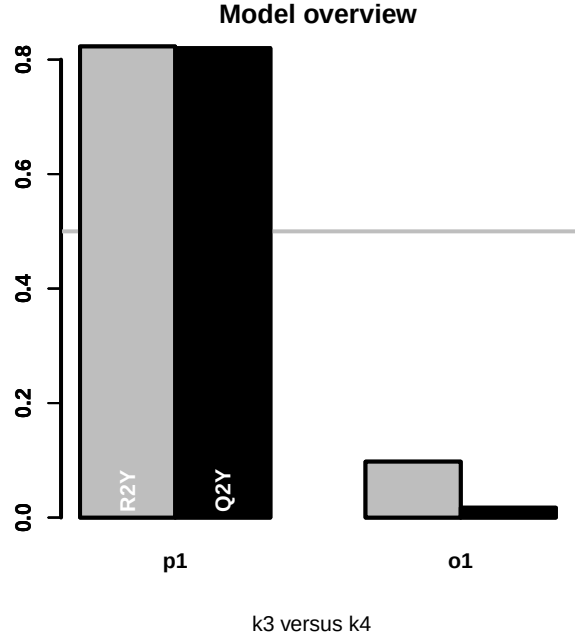

Scores (OPLS−DA)
to1
t1 (80%)
k4
k2
15000
5000
0
−5000
−15000
−20000
−10000
0
10000
20000
R2X
R2Y
Q2Y
RMSEE
pre
ort
0.919
0.924
0.89
0.117
1
1

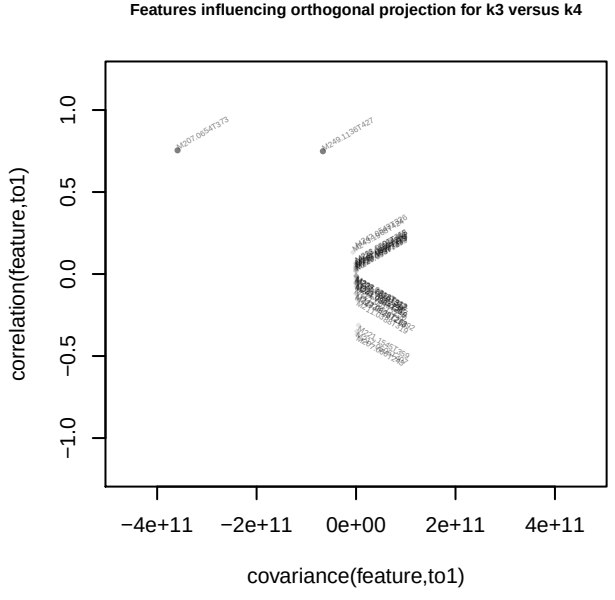

Model overview
R2Y
Q2Y
p1
o1
k2 versus k4
0.0
0.2
0.4
0.6
0.8


Features influencing orthogonal projection for k2 versus k4
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−5e+10
0e+00
5e+10


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


Scores (OPLS−DA)
k4
k3
to1
t1 (55%)
20000
10000
0
−10000
−20000
R2X
R2Y
Q2Y
RMSEE
pre
ort
0.709
0.921
0.837
0.105
1
1


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


Features influencing orthogonal projection for k3 versus k4
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