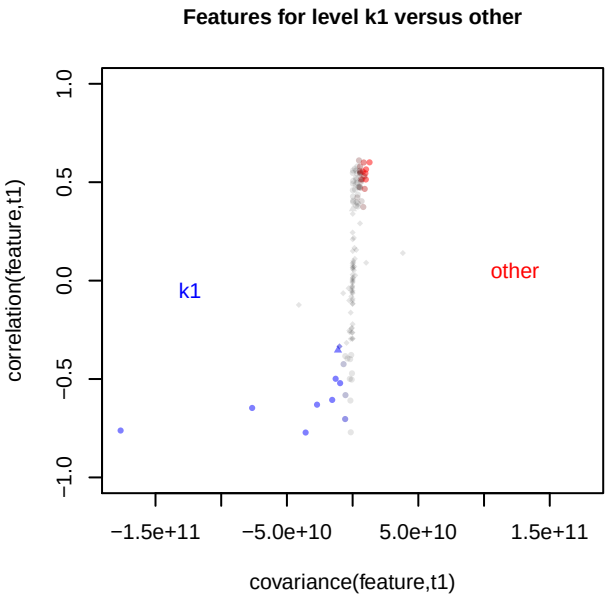
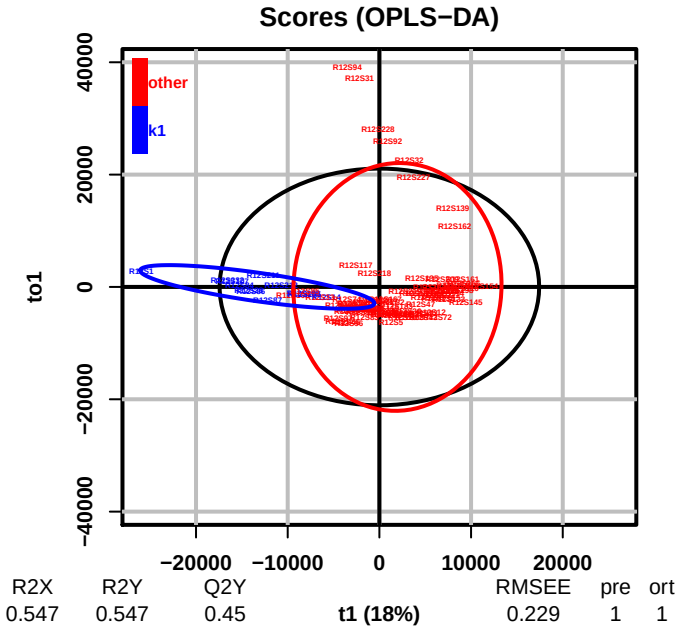
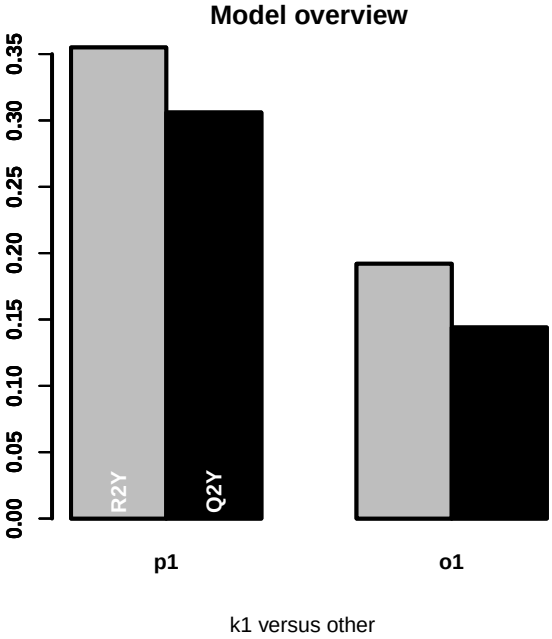
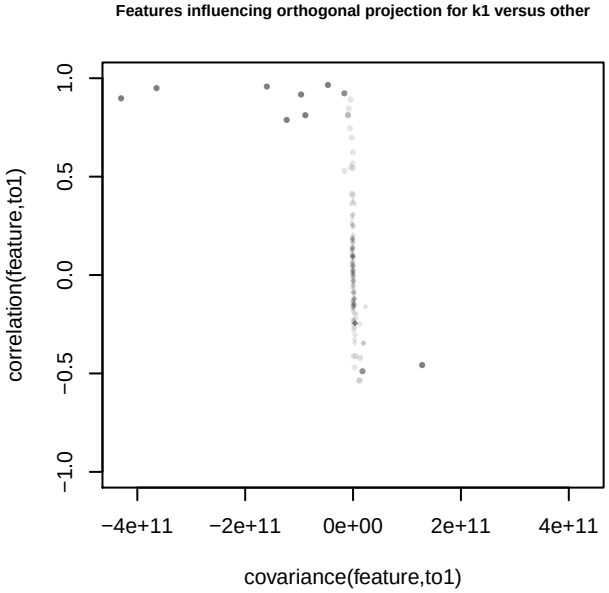
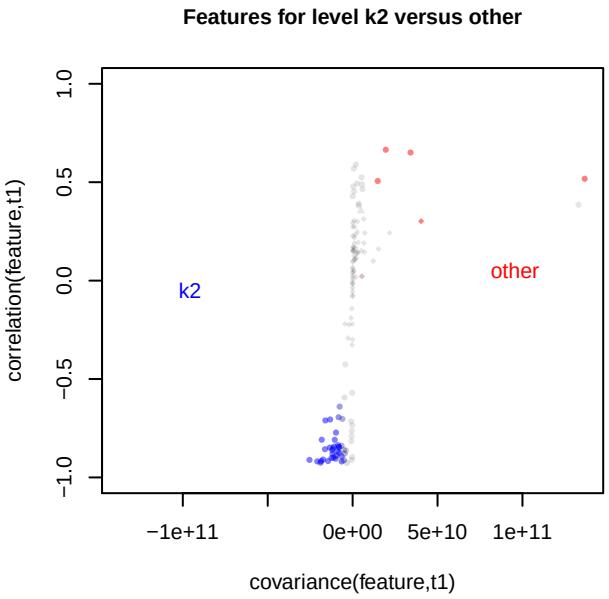
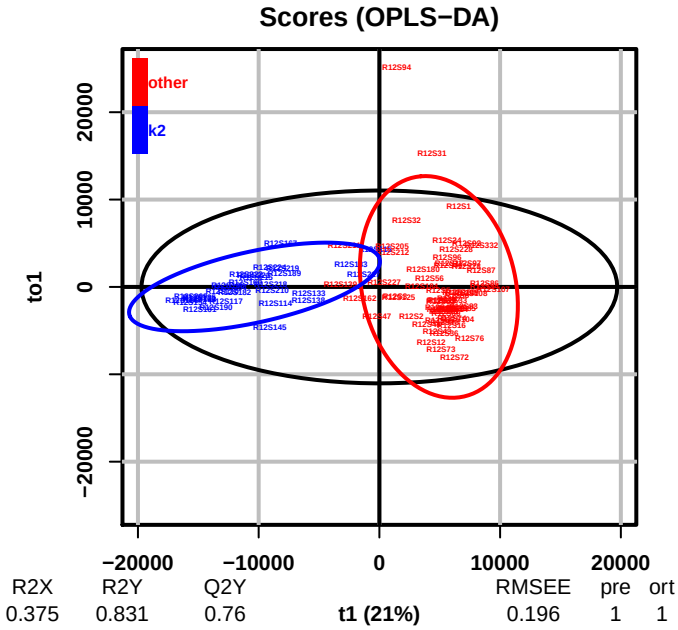

Features for level k1 versus other
correlation(feature,t1)
covariance(feature,t1)
k1
other
1.0
0.5
0.0
−0.5
−1.0
−1.5e+11
−5.0e+10
5.0e+10
1.5e+11

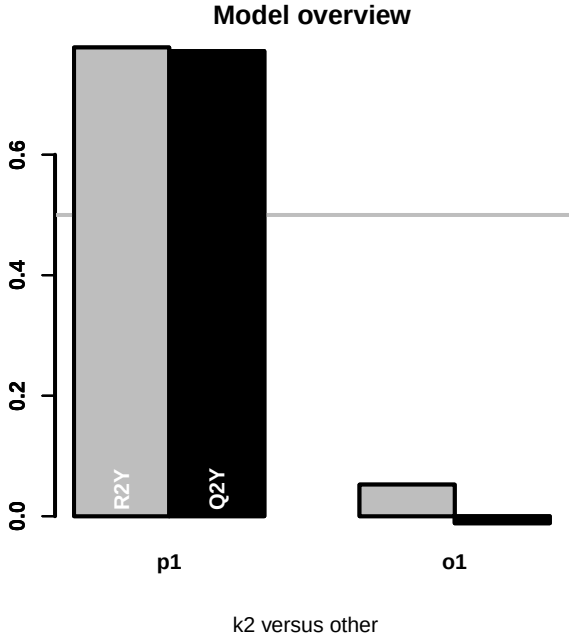

Scores (OPLS−DA)
other
k1
to1
t1 (18%)
40000
20000
0
−20000
−40000
−20000
−10000
0
10000
20000
R2X R2Y Q2Y RMSEE pre ort
0.547 0.547 0.45 0.229 1 1

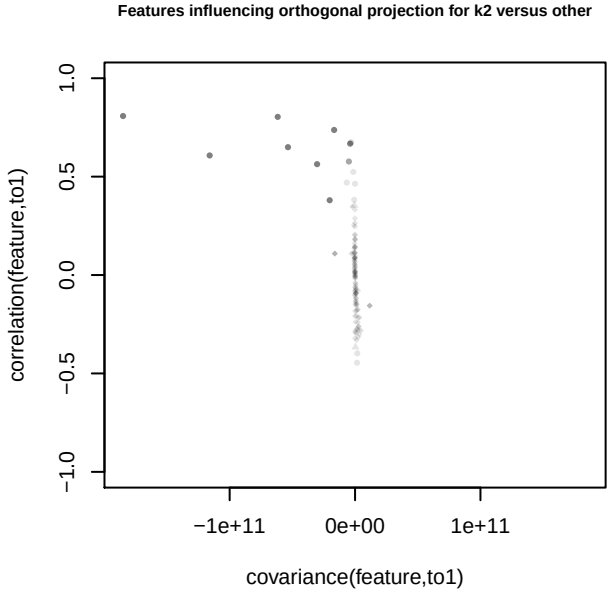

Model overview
R2Y
Q2Y
p1
o1
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
k1 versus other

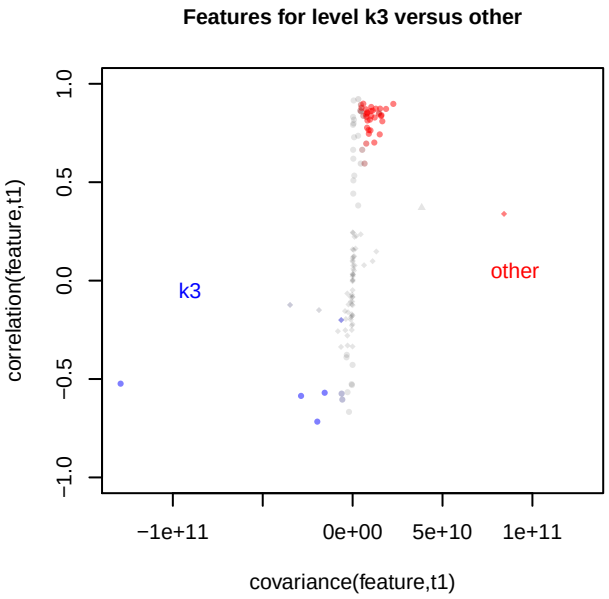

Features influencing orthogonal projection for k1 versus other
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−4e+11
−2e+11
0e+00
2e+11
4e+11

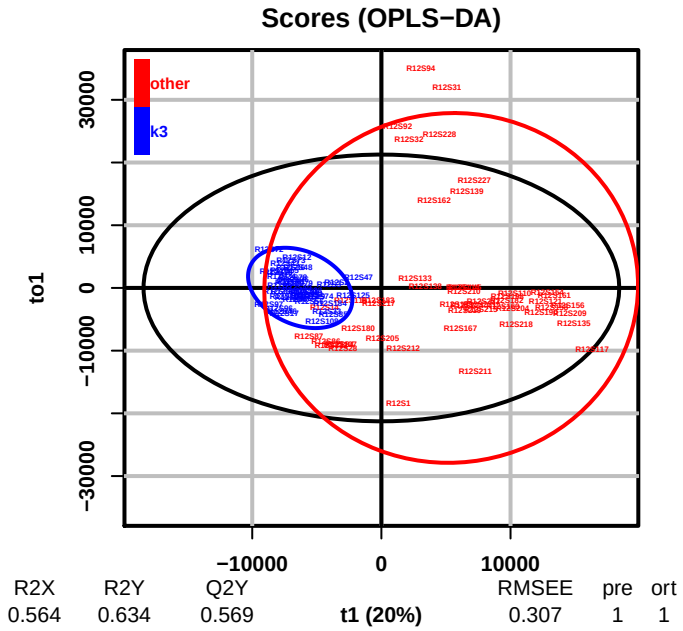

Features for level k2 versus other
correlation(feature,t1)
covariance(feature,t1)
k2
other
1.0
0.5
0.0
−0.5
−1.0
−1e+11
0e+00
5e+10
1e+11

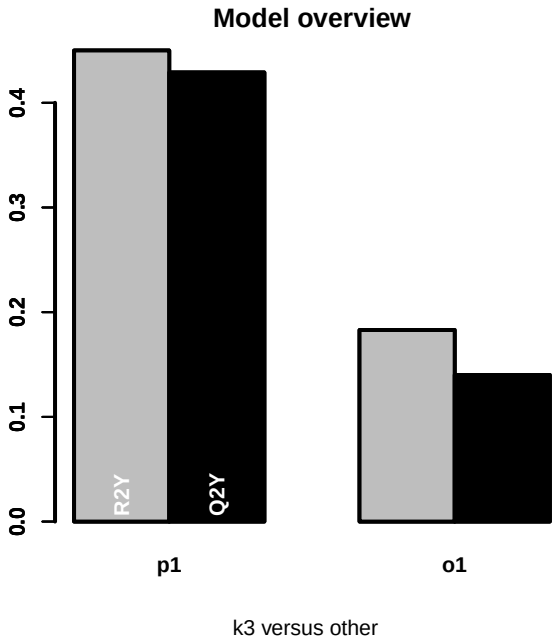

Scores (OPLS−DA)
other
k2
to1
t1 (21%)
20000
10000
0
−20000
−20000
−10000
0
10000
20000
R2X R2Y Q2Y RMSEE pre ort
0.375 0.831 0.76 0.196 1 1

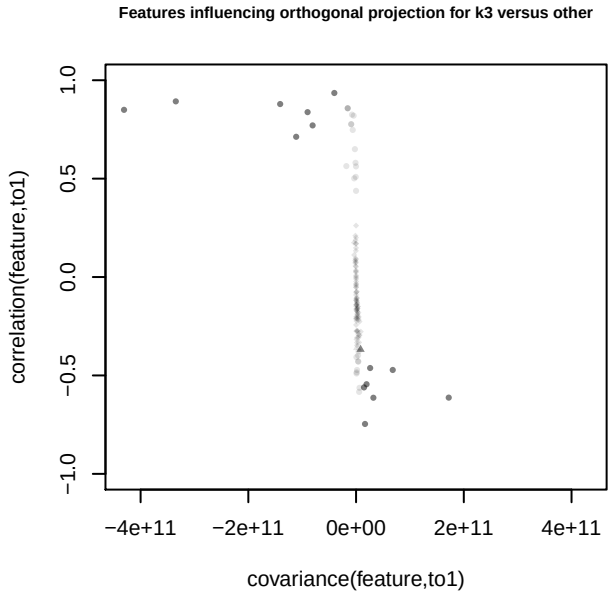

Model overview
R2Y
Q2Y
0.0
0.2
0.4
0.6
p1
o1
k2 versus other

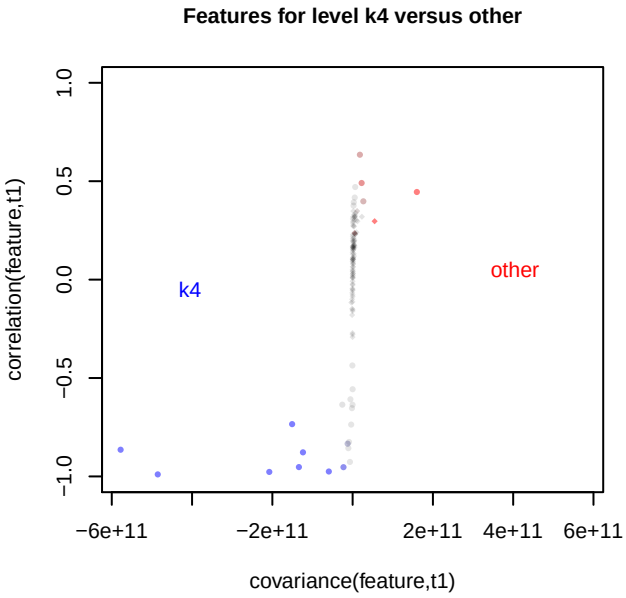

Features influencing orthogonal projection for k2 versus other
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−1e+11
0e+00
1e+11

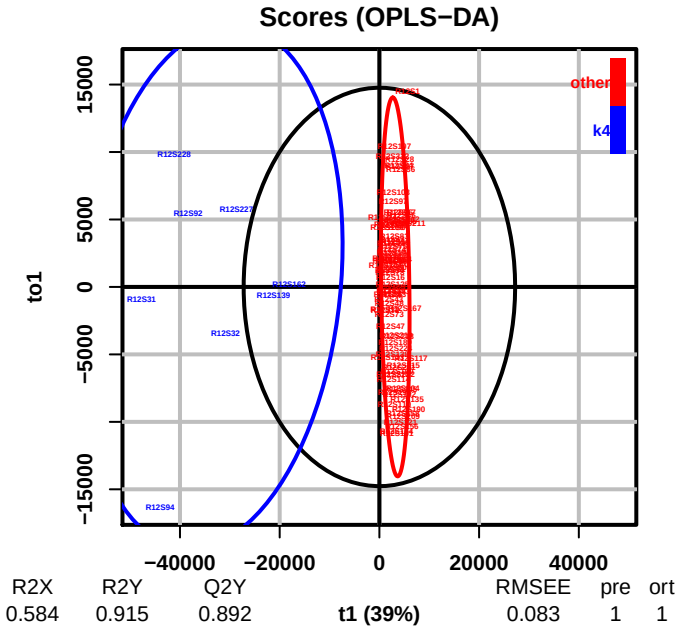

Features for level k3 versus other
correlation(feature,t1)
covariance(feature,t1)
k3
other
1.0
0.5
0.0
−0.5
−1.0
−1e+11
0e+00
5e+10
1e+11

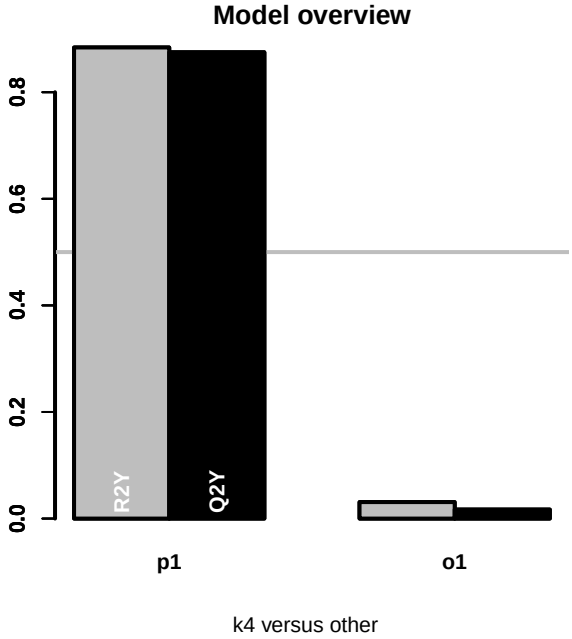

Scores (OPLS−DA)
other
k3
to1
t1 (20%)
30000
10000
0
−10000
−30000
−10000
0
10000
R2X R2Y Q2Y RMSEE pre ort
0.564 0.634 0.569 0.307 1 1

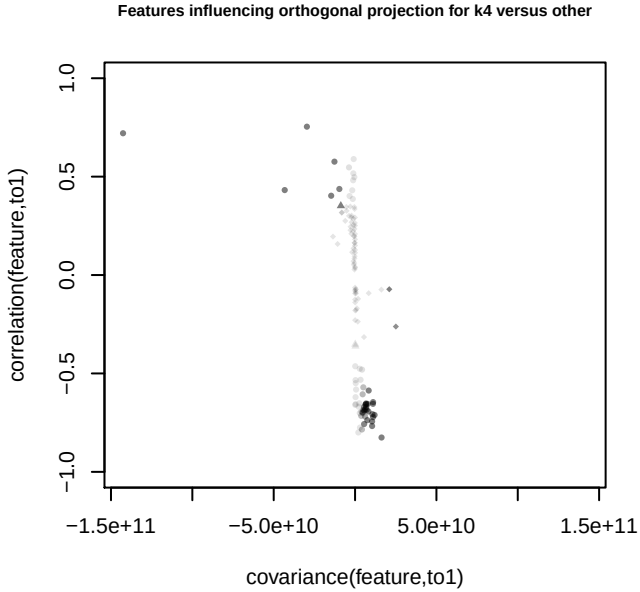

Model overview
R2Y
Q2Y
0.0
0.1
0.2
0.3
0.4
p1
o1
k3 versus other

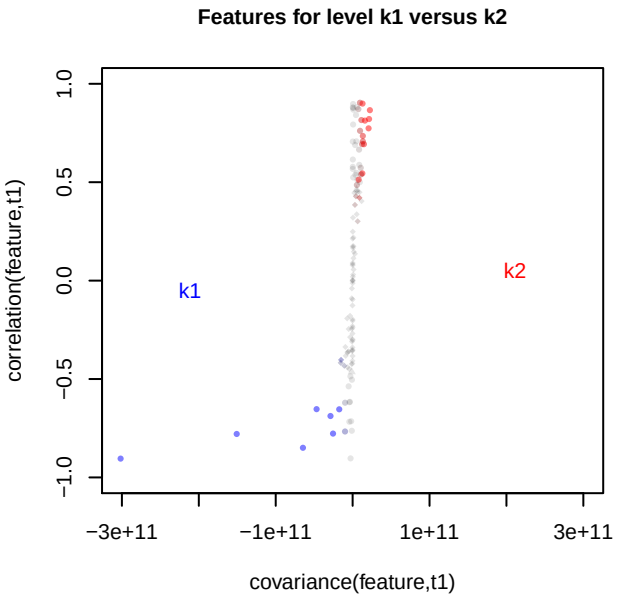

Features influencing orthogonal projection for k3 versus other
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−4e+11
−2e+11
0e+00
2e+11
4e+11

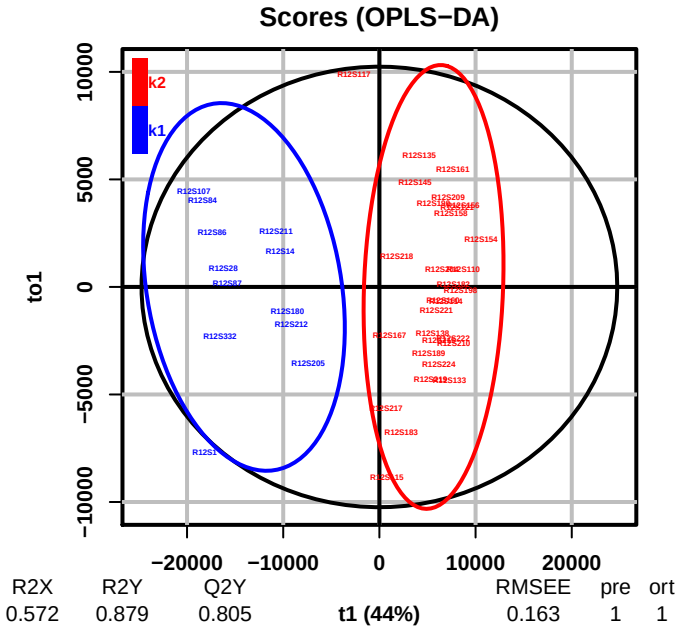

Features for level k4 versus other
correlation(feature,t1)
covariance(feature,t1)
k4
other
1.0
0.5
0.0
−0.5
−1.0
−6e+11
−2e+11
2e+11
4e+11
6e+11

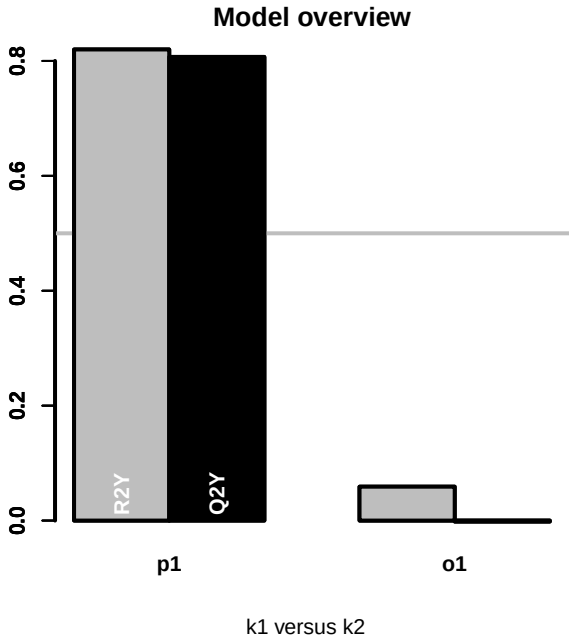

Scores (OPLS−DA)
other
k4
to1
t1 (39%)
15000
5000
0
−5000
−15000
−40000
−20000
0
20000
40000
R2X
0.584
R2Y
0.915
Q2Y
0.892
RMSEE
0.083
pre
1
ort
1

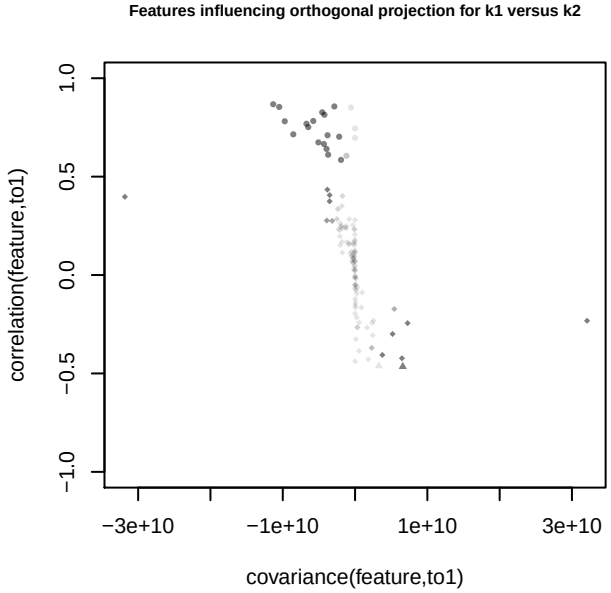

Model overview
R2Y
Q2Y
p1
o1
0.0
0.2
0.4
0.6
0.8
k4 versus other

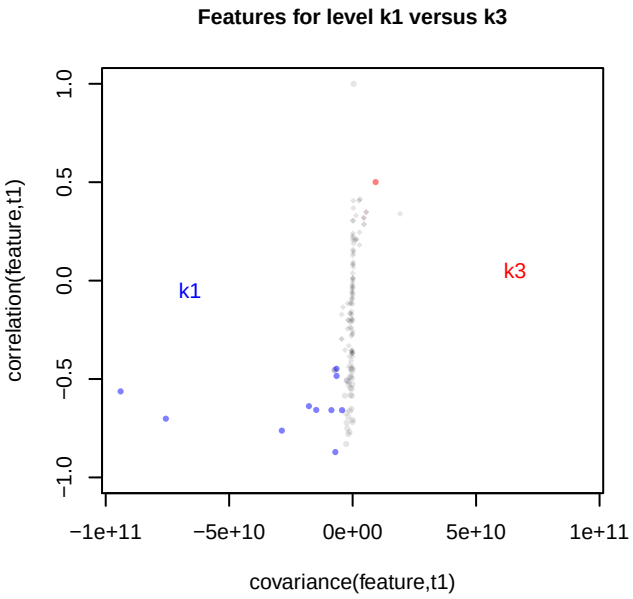

Features influencing orthogonal projection for k4 versus other
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−1.5e+11
−5.0e+10
5.0e+10
1.5e+11

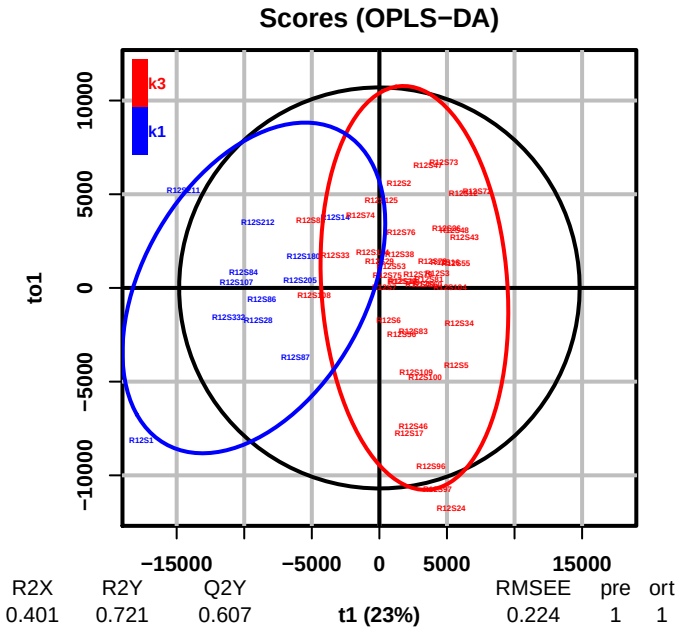

Features for level k1 versus k2
correlation(feature,t1)
covariance(feature,t1)
k1
k2
1.0
0.5
0.0
−0.5
−1.0
−3e+11
−1e+11
1e+11
3e+11

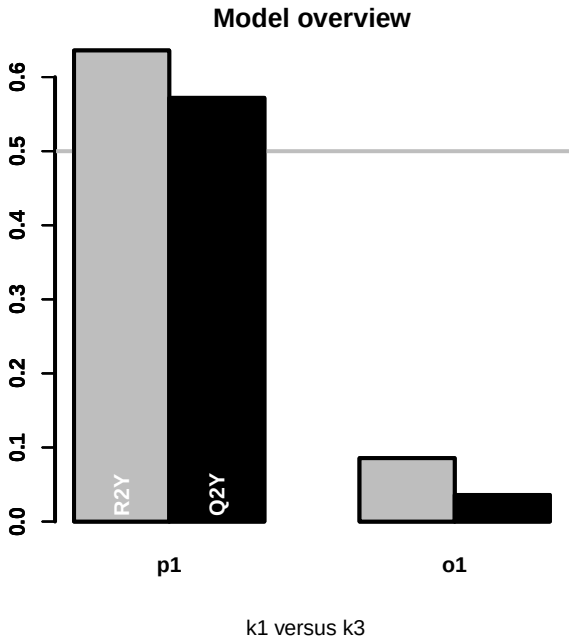

Scores (OPLS−DA)
k2
k1
to1
t1 (44%)
10000
5000
0
−5000
−10000
−20000
−10000
0
10000
20000
R2X R2Y Q2Y RMSEE pre ort
0.572 0.879 0.805 0.163 1 1

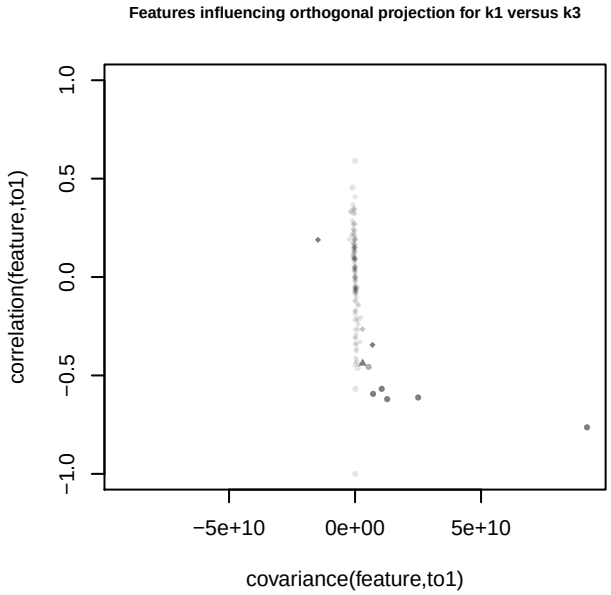

Model overview
R2Y
Q2Y
p1
o1
0.0
0.2
0.4
0.6
0.8
k1 versus k2

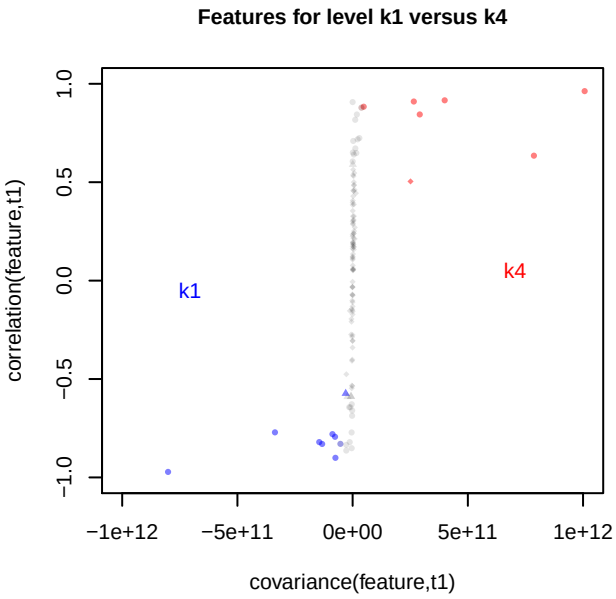

Features influencing orthogonal projection for k1 versus k2
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−3e+10
−1e+10
1e+10
3e+10

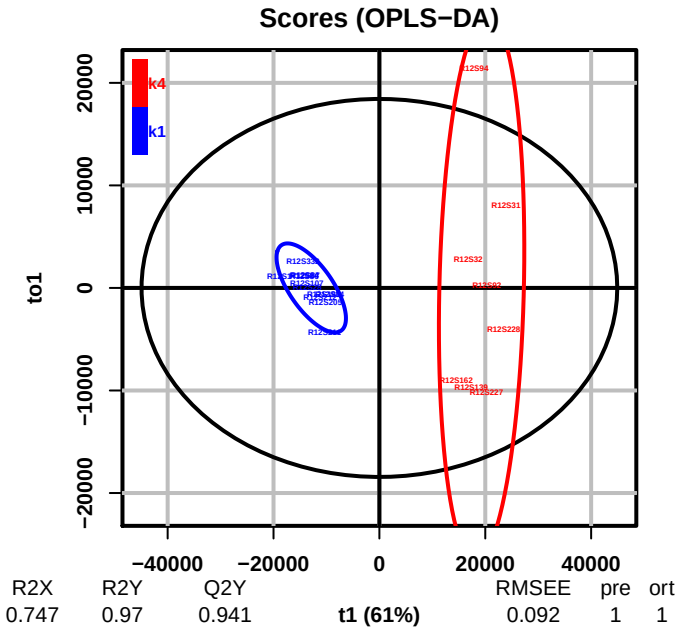

Features for level k1 versus k3
correlation(feature,t1)
covariance(feature,t1)
k1
k3
1.0
0.5
0.0
−0.5
−1.0
−1e+11
−5e+10
0e+00
5e+10
1e+11

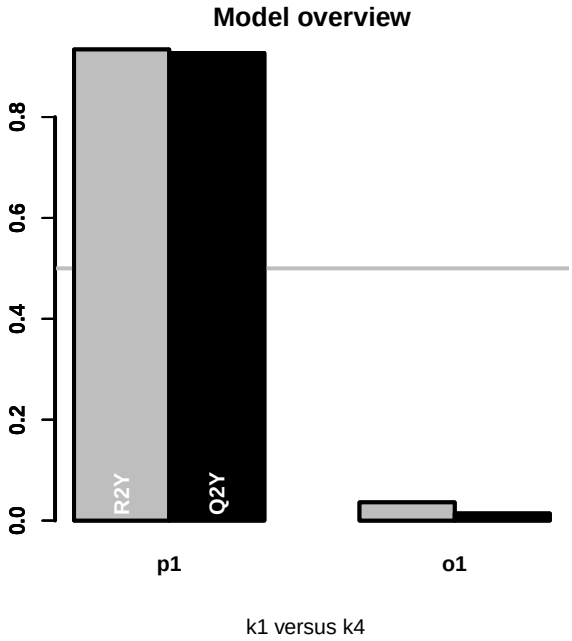

Scores (OPLS−DA)
k3
k1
to1
t1 (23%)
10000
5000
0
−5000
−10000
−15000
−5000
0
5000
15000
R2X
0.401
R2Y
0.721
Q2Y
0.607
RMSEE
0.224
pre
1
ort
1

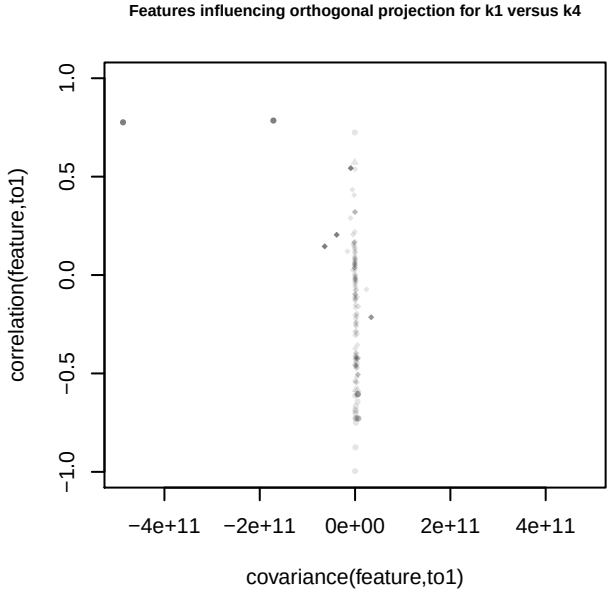

Model overview
R2Y
Q2Y
p1
o1
0.0
0.1
0.2
0.3
0.4
0.5
0.6
k1 versus k3

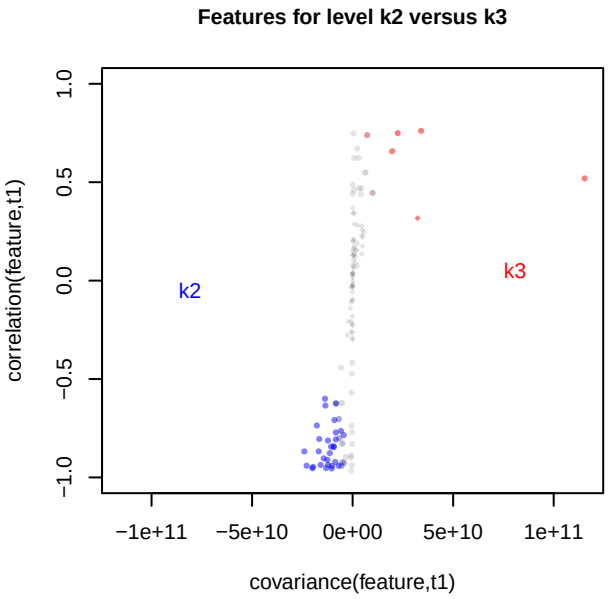

Features influencing orthogonal projection for k1 versus k3
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−5e+10
0e+00
5e+10

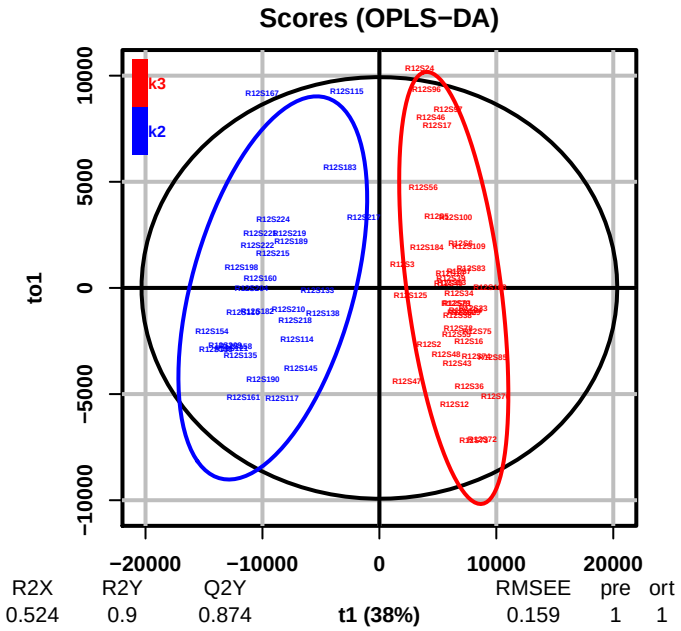

Features for level k1 versus k4
correlation(feature,t1)
covariance(feature,t1)
k1
k4
1.0
0.5
0.0
−0.5
−1.0
−1e+12
−5e+11
0e+00
5e+11
1e+12

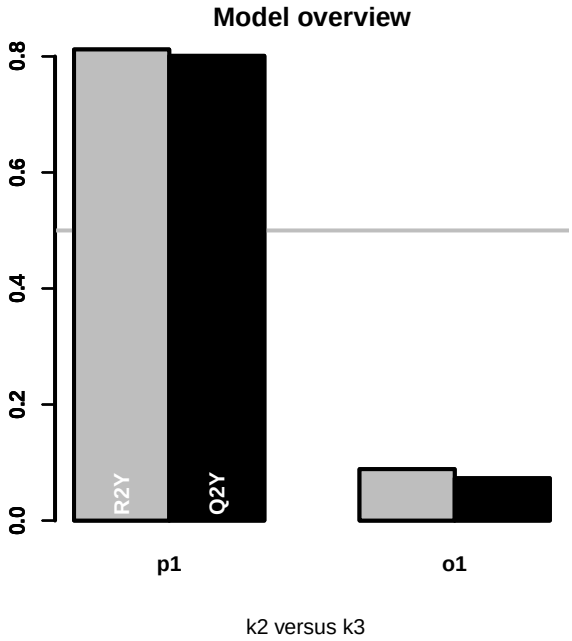

Scores (OPLS−DA)
k4
k1
to1
t1 (61%)
20000
10000
0
−10000
−20000
−40000
−20000
0
20000
40000
R2X R2Y Q2Y RMSEE pre ort
0.747 0.97 0.941 0.092 1 1

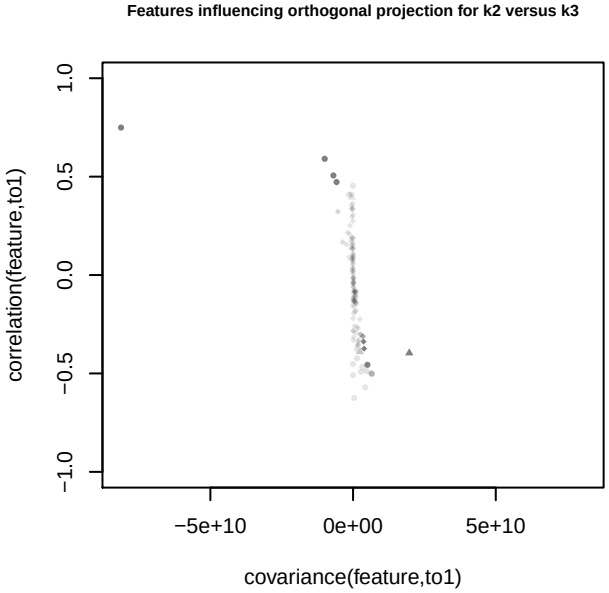

Model overview
R2Y
Q2Y
0.0
0.2
0.4
0.6
0.8
p1
o1
k1 versus k4

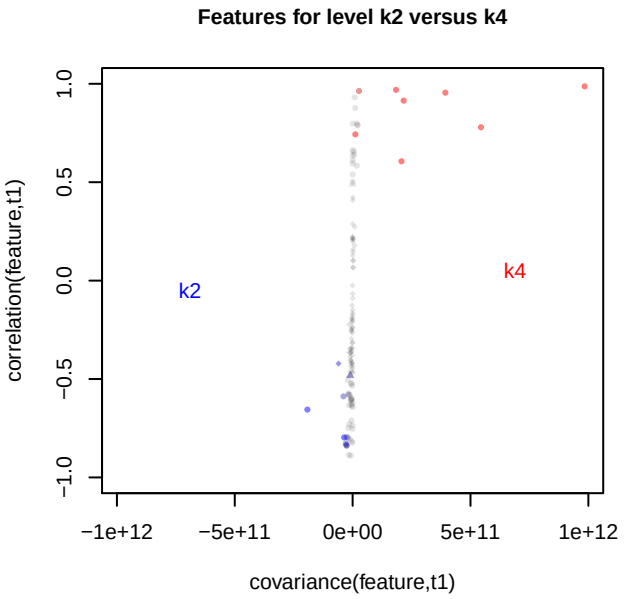

Features influencing orthogonal projection for k1 versus k4
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−4e+11
−2e+11
0e+00
2e+11
4e+11

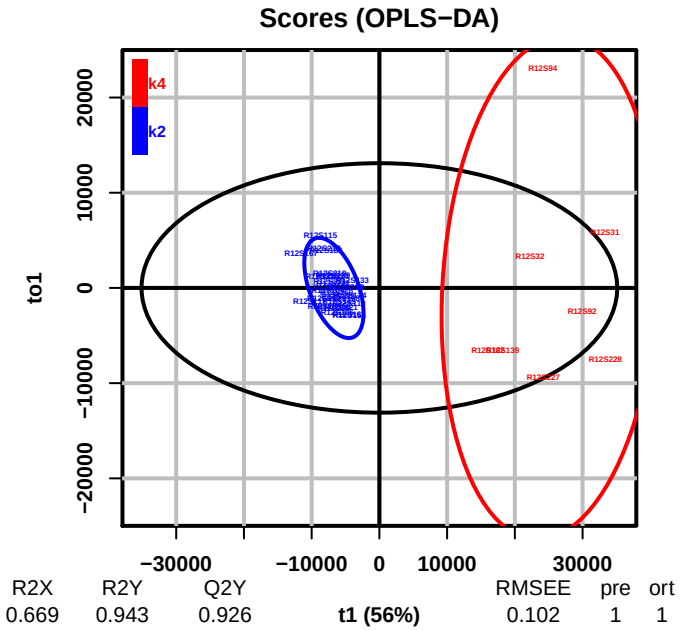

Features for level k2 versus k3
correlation(feature,t1)
covariance(feature,t1)
k2
k3
1.0
0.5
0.0
−0.5
−1.0
−1e+11
−5e+10
0e+00
5e+10
1e+11

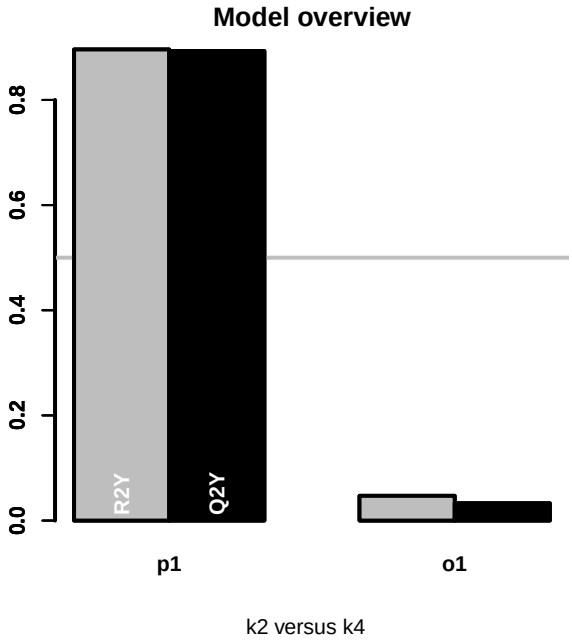

Scores (OPLS−DA)
k3
k2
to1
t1 (38%)
10000
5000
0
−5000
−10000
−20000
−10000
0
10000
20000
R2X R2Y Q2Y RMSEE pre ort
0.524 0.9 0.874 0.159 1 1

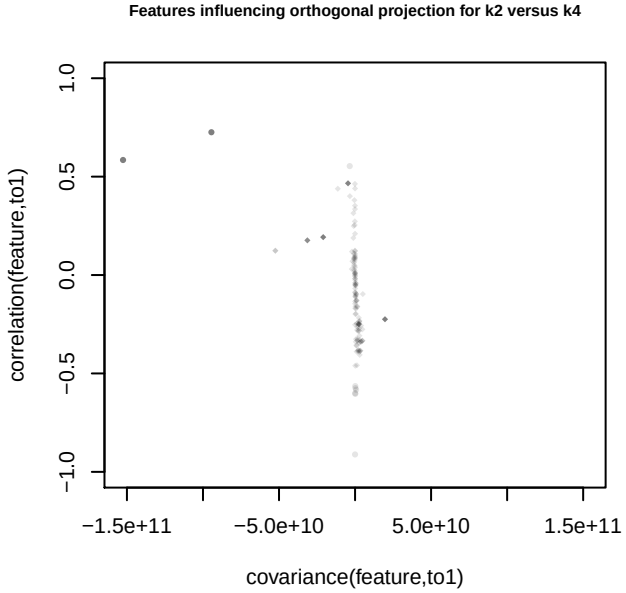

Model overview
R2Y
Q2Y
0.0
0.2
0.4
0.6
0.8
p1
o1
k2 versus k3

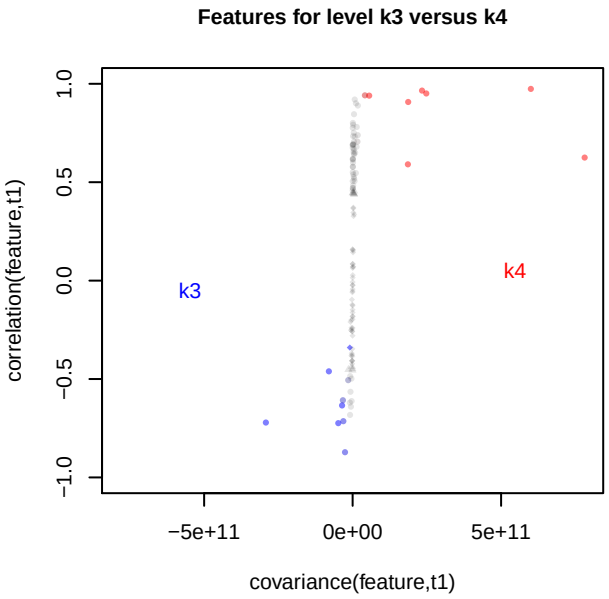

Features influencing orthogonal projection for k2 versus k3
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−5e+10
0e+00
5e+10

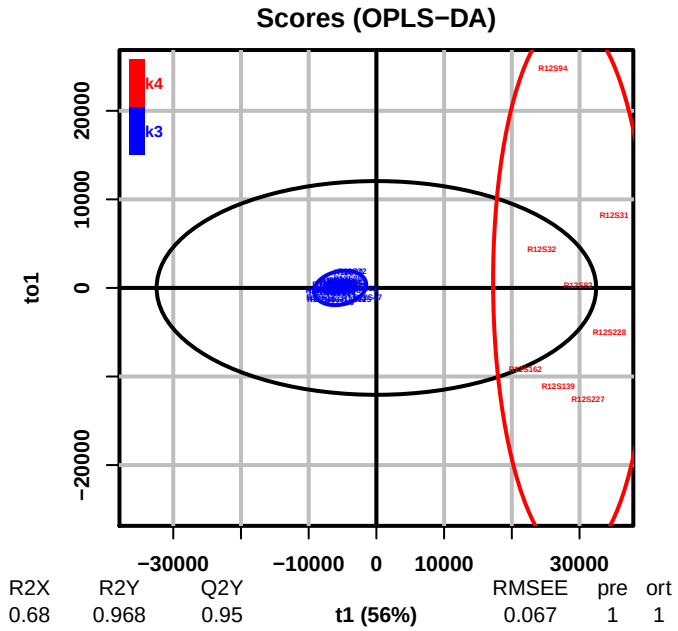

Features for level k2 versus k4
correlation(feature,t1)
covariance(feature,t1)
k2
k4
1.0
0.5
0.0
−0.5
−1.0
−1e+12
−5e+11
0e+00
5e+11
1e+12

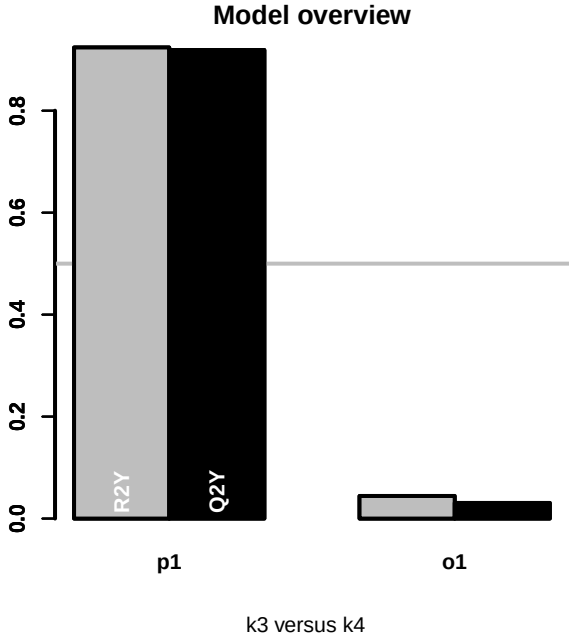

Scores (OPLS−DA)
k4
k2
to1
t1 (56%)
20000
10000
0
−10000
−20000
−30000
−10000
0
10000
30000
R2X
0.669
R2Y
0.943
Q2Y
0.926
RMSEE
0.102
pre
1
ort
1

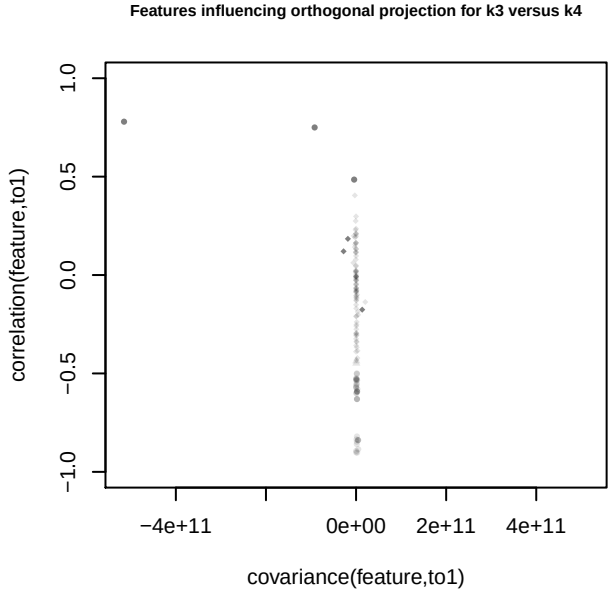

Model overview
R2Y
Q2Y
0.0
0.2
0.4
0.6
0.8
p1
o1
k2 versus k4


Features influencing orthogonal projection for k2 versus k4
correlation(feature,to1)
covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−1.5e+11
−5.0e+10
5.0e+10
1.5e+11


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 (56%)
20000
10000
0
−20000
−30000
−10000
0
10000
30000
R2X
0.68
R2Y
0.968
Q2Y
0.95
RMSEE
0.067
pre
1
ort
1


Model overview
R2Y
Q2Y
0.0
0.2
0.4
0.6
0.8
p1
o1
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
−4e+11
0e+00
2e+11
4e+11