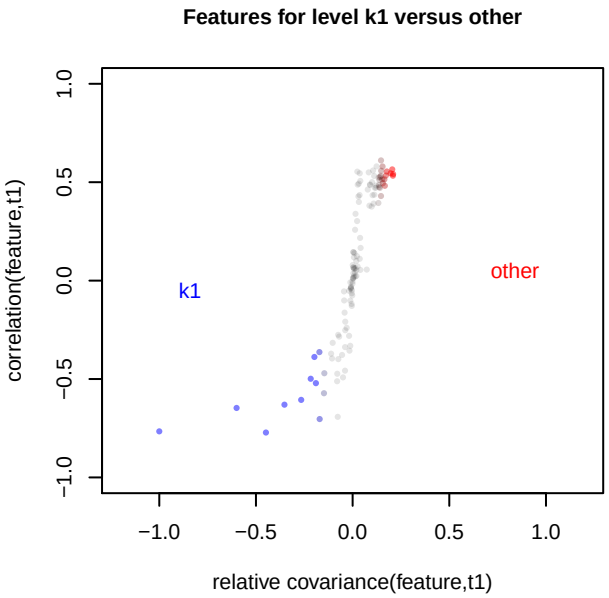
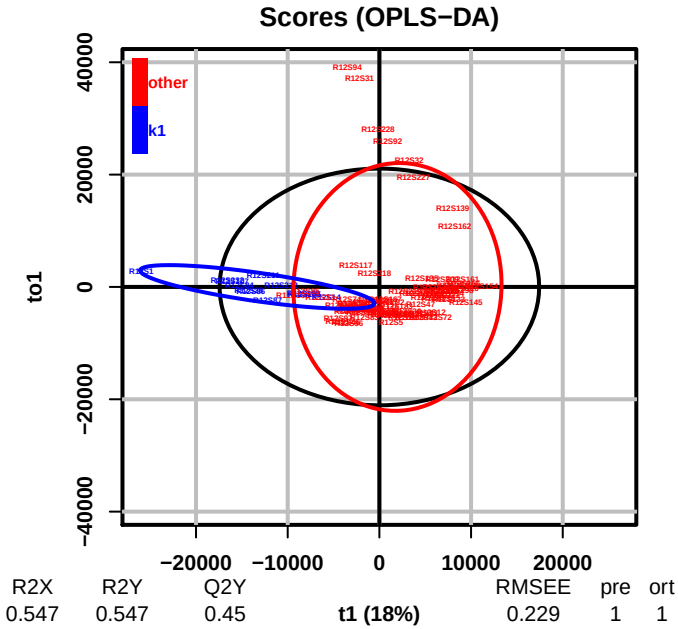
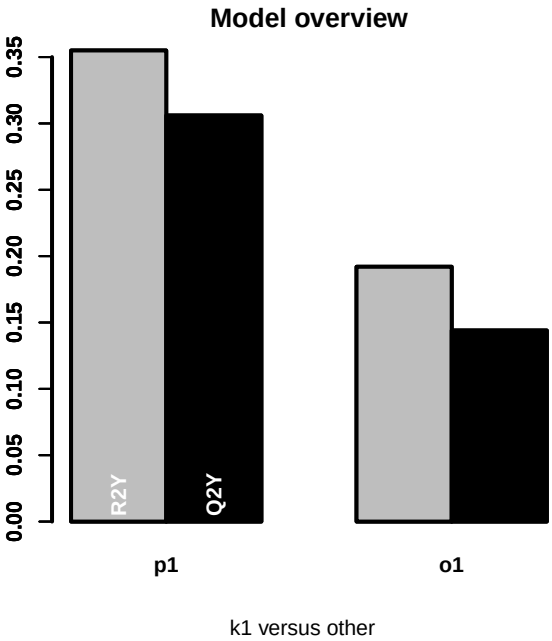
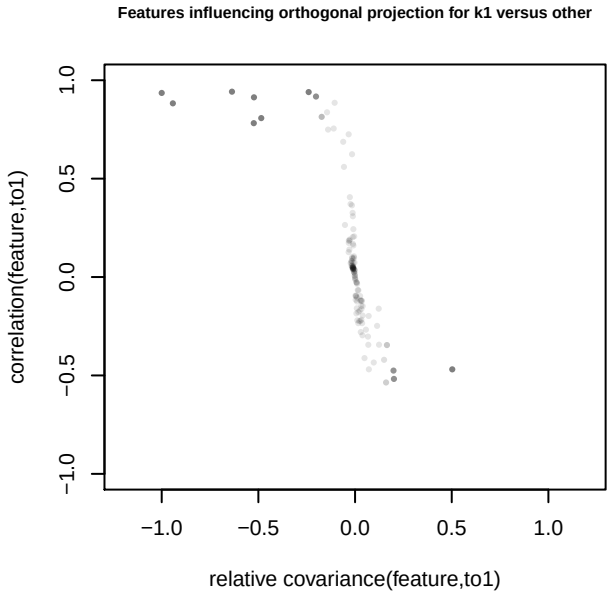
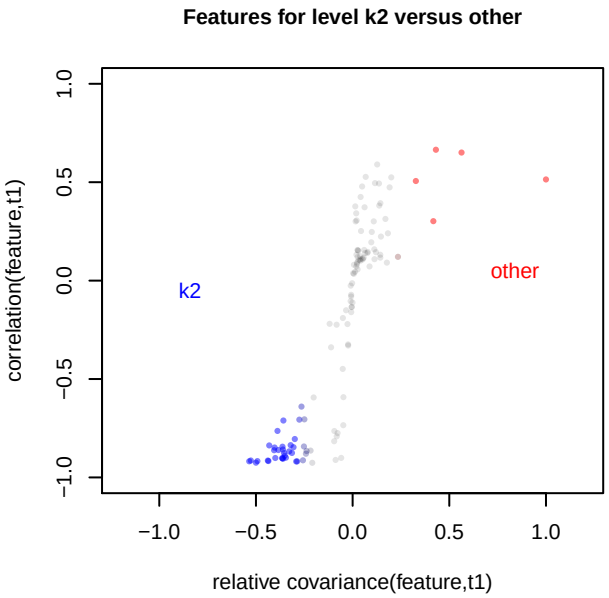
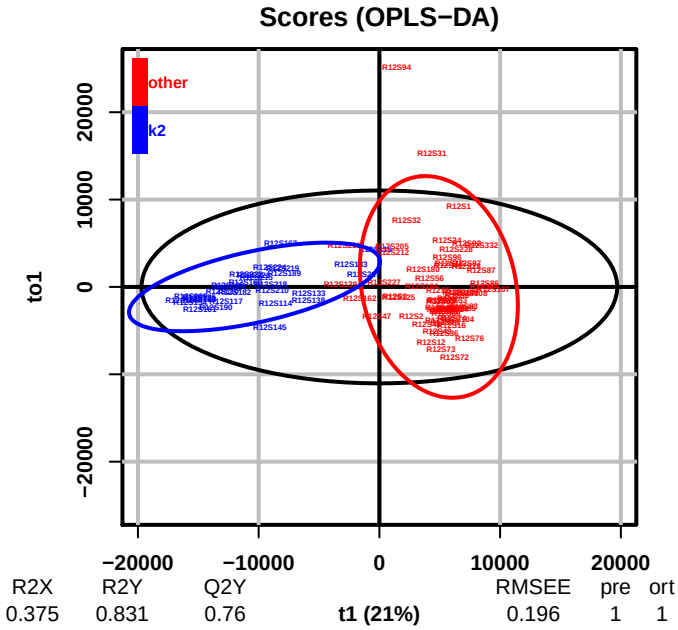

Features for level k1 versus other
correlation(feature,t1)
relative covariance(feature,t1)
k1
other
1.0
0.5
0.0
−0.5
−1.0

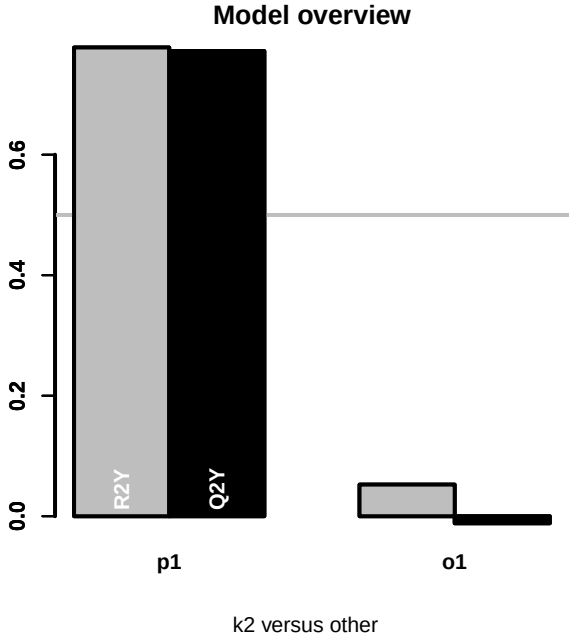

Scores (OPLS−DA)
other
k1
to1
t1 (18%)
40000
20000
0
−20000
−40000
−20000
−10000
0
10000
20000
R2X
0.547
R2Y
0.547
Q2Y
0.45
RMSEE
0.229
pre
1
ort
1

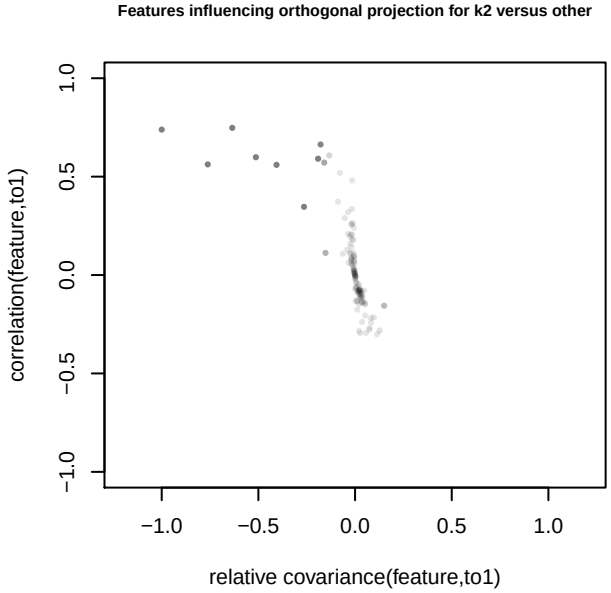

Model overview
R2Y
Q2Y
p1
o1
k1 versus other
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35

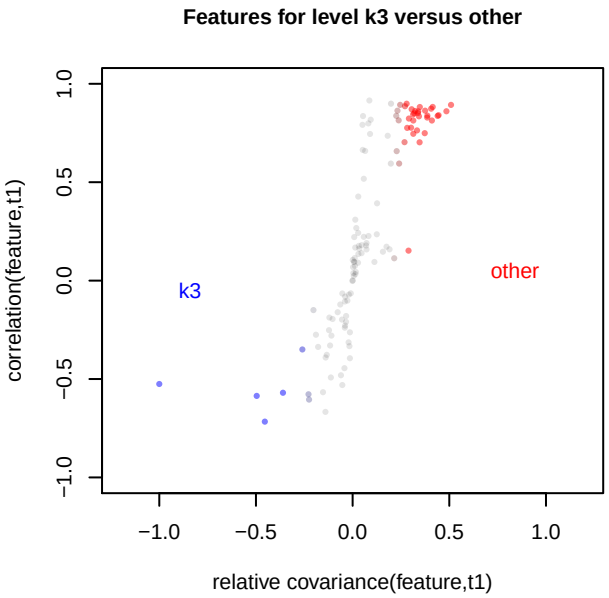

Features influencing orthogonal projection for k1 versus other
correlation(feature,to1)
relative covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0

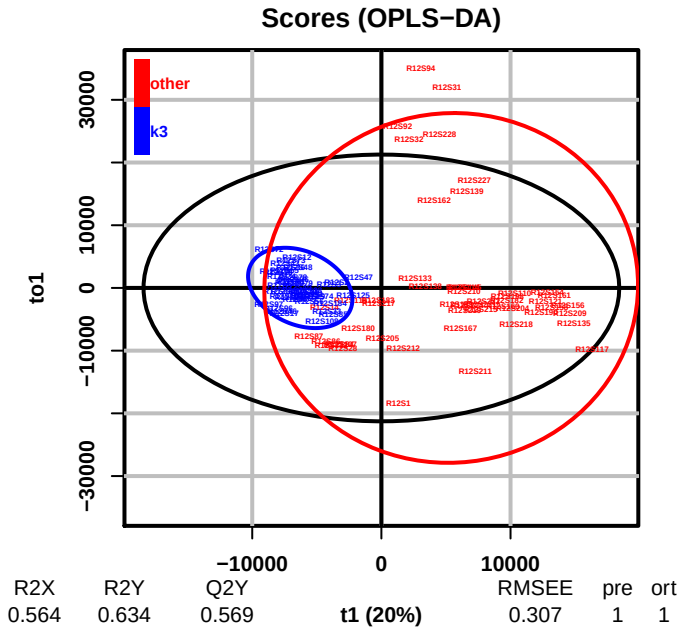

Features for level k2 versus other
correlation(feature,t1)
relative covariance(feature,t1)
k2
other
1.0
0.5
0.0
−0.5
−1.0

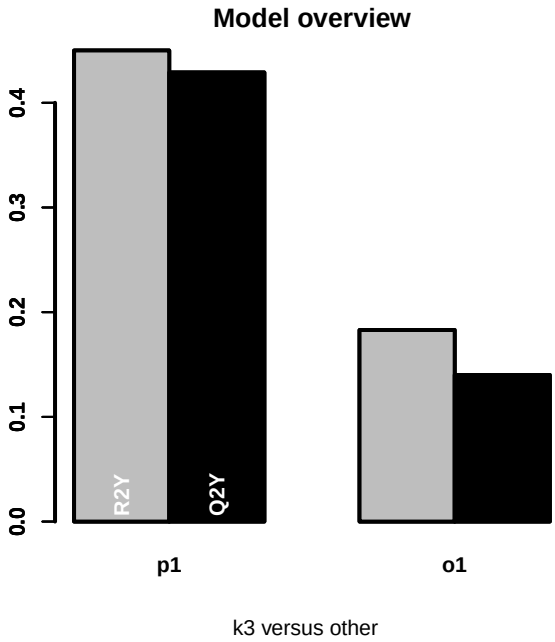

Scores (OPLS−DA)
other
k2
to1
t1 (21%)
20000
10000
0
−10000
−20000
R2X 0.375
R2Y 0.831
Q2Y 0.76
RMSEE 0.196
pre 1
ort 1

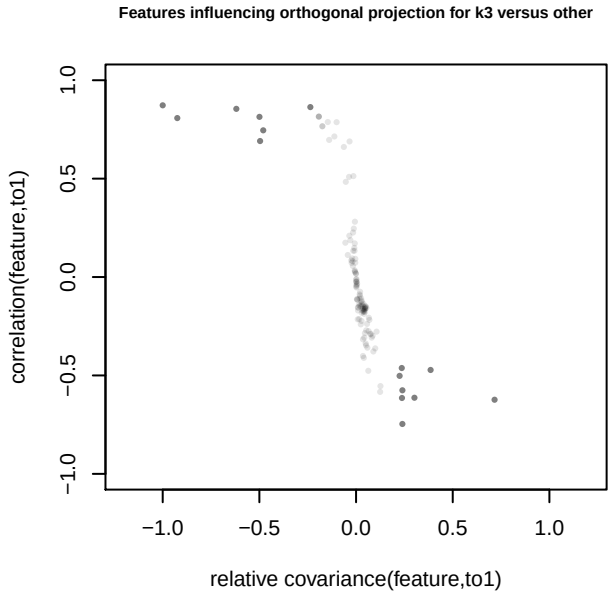

Model overview
R2Y
Q2Y
0.0
0.2
0.4
0.6
p1
o1
k2 versus other

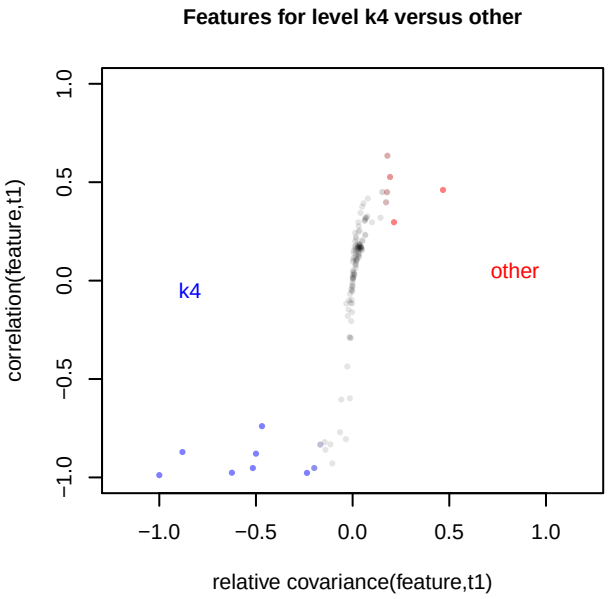

Features influencing orthogonal projection for k2 versus other
correlation(feature,to1)
relative covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0

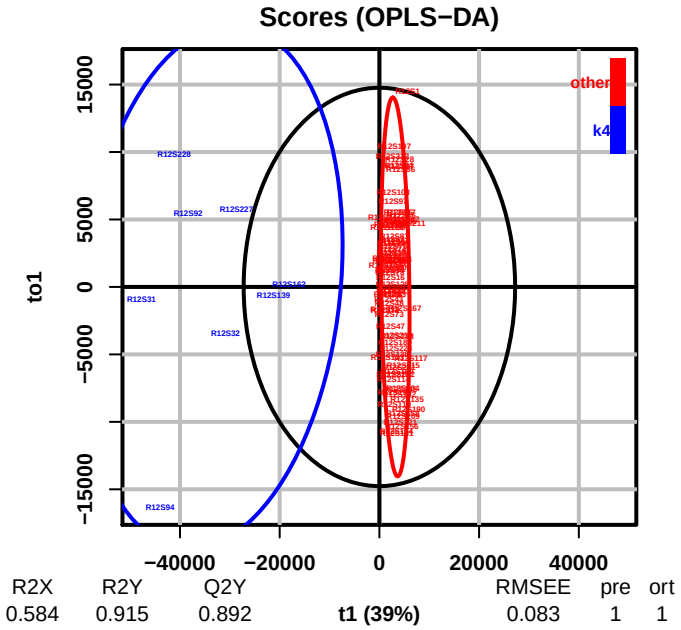

Features for level k3 versus other
correlation(feature,t1)
relative covariance(feature,t1)
k3
other
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0

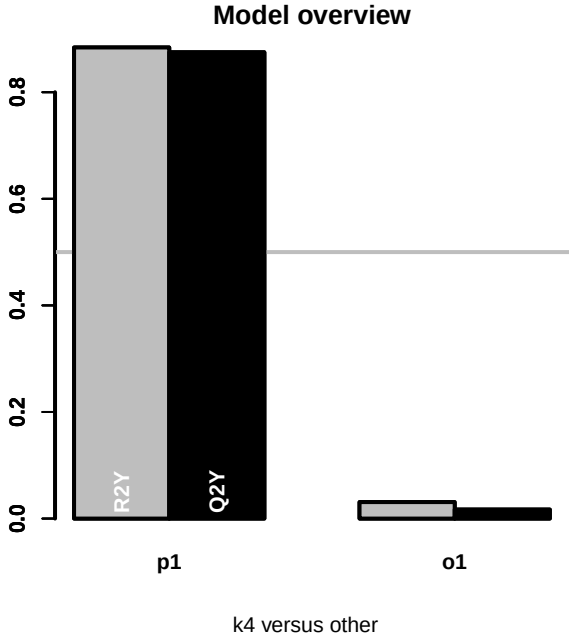

Scores (OPLS−DA)
other
k3
to1
t1 (20%)
30000
10000
0
−10000
−30000
−10000
0
10000
R2X R2Y Q2Y RMSEE pre ort
0.564 0.634 0.569 0.307 1 1

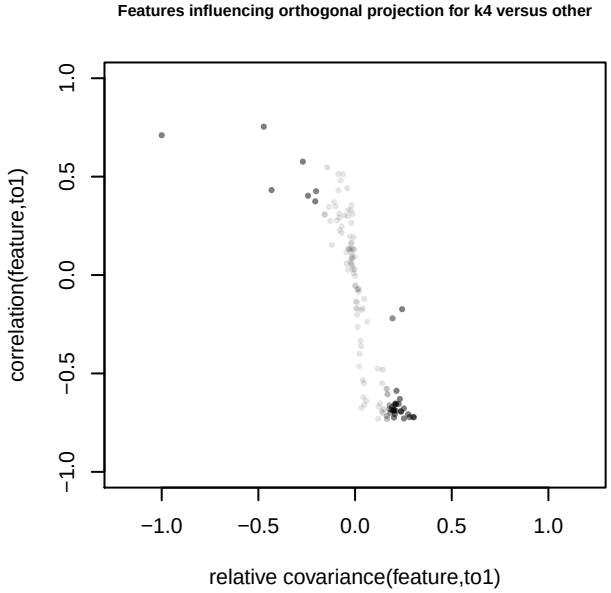

Model overview
R2Y
Q2Y
0.0
0.1
0.2
0.3
0.4
p1
o1
k3 versus other

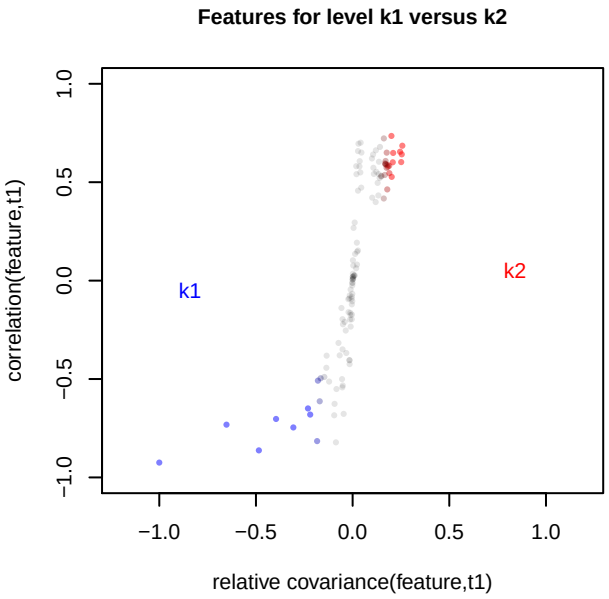

Features influencing orthogonal projection for k3 versus other
correlation(feature,to1)
relative covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0

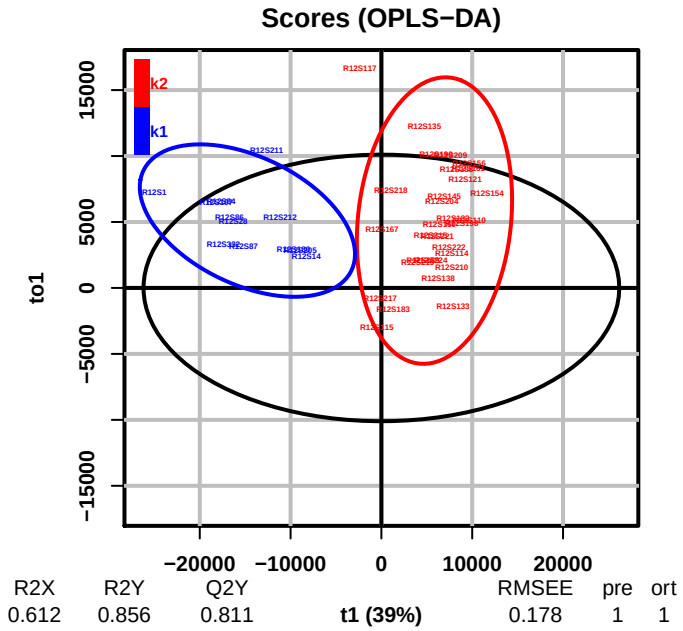

Features for level k4 versus other
correlation(feature,t1)
relative covariance(feature,t1)
k4
other
1.0
0.5
0.0
−0.5
−1.0

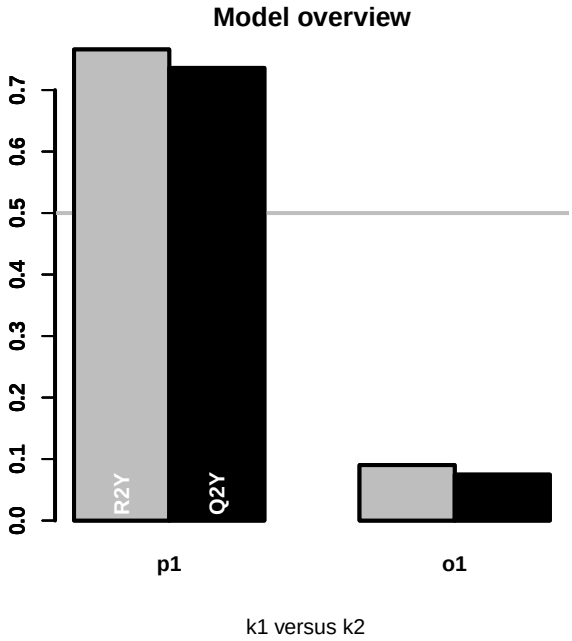

Scores (OPLS−DA)
to1
t1 (39%)
other
k4
15000
5000
0
−5000
−15000
−40000
−20000
0
20000
40000
R2X 0.584
R2Y 0.915
Q2Y 0.892
RMSEE 0.083
pre 1
ort 1

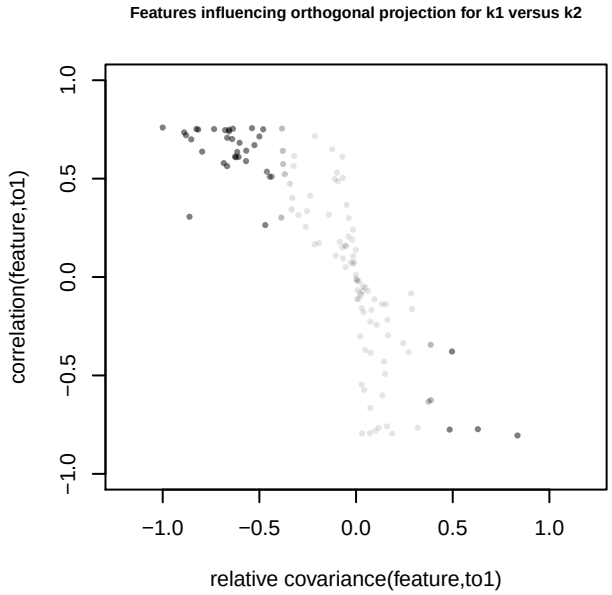

Model overview
R2Y
Q2Y
p1
o1
k4 versus other
0.0
0.2
0.4
0.6
0.8

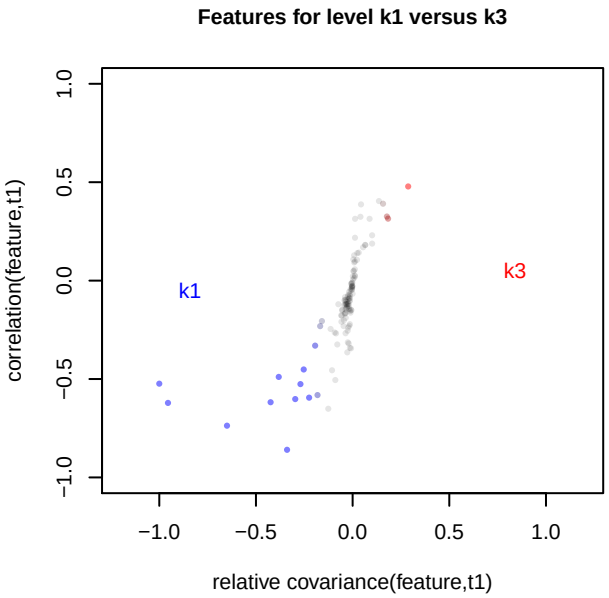

Features influencing orthogonal projection for k4 versus other
correlation(feature,to1)
relative covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0

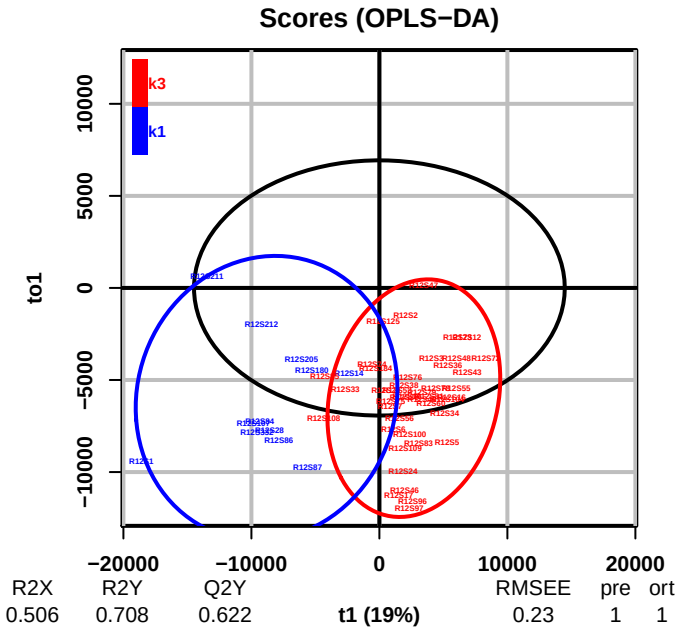

Features for level k1 versus k2
correlation(feature,t1)
relative covariance(feature,t1)
k1
k2
1.0
0.5
0.0
−0.5
−1.0

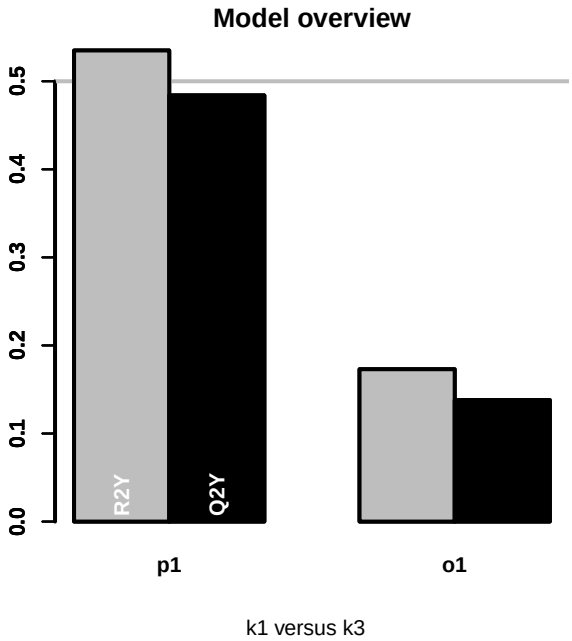

Scores (OPLS−DA)
k2
k1
to1
t1 (39%)
15000
5000
0
−5000
−15000
−20000
−10000
0
10000
20000
R2X R2Y Q2Y RMSEE pre ort
0.612 0.856 0.811 0.178 1 1

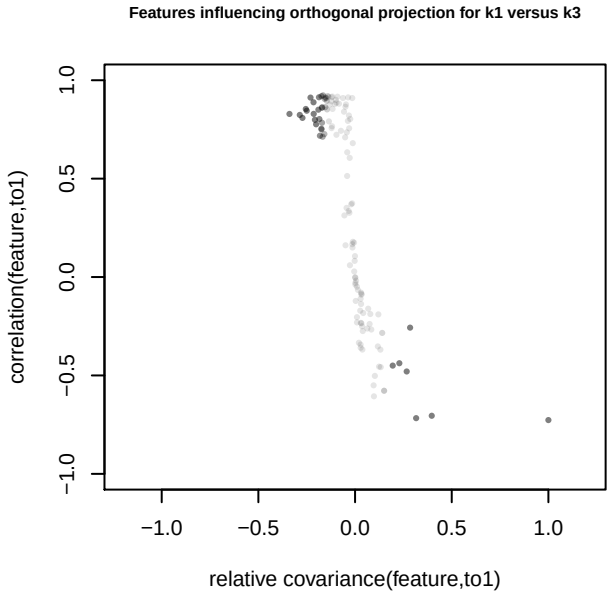

Model overview
R2Y
Q2Y
p1
o1
k1 versus k2
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7

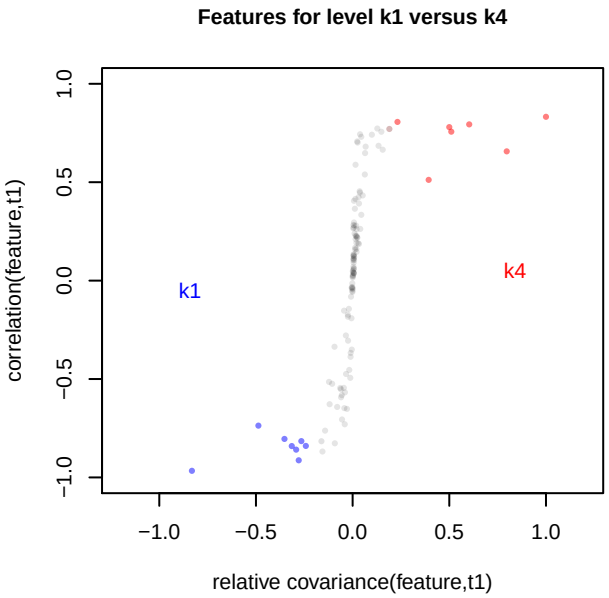

Features influencing orthogonal projection for k1 versus k2
correlation(feature,to1)
relative covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0

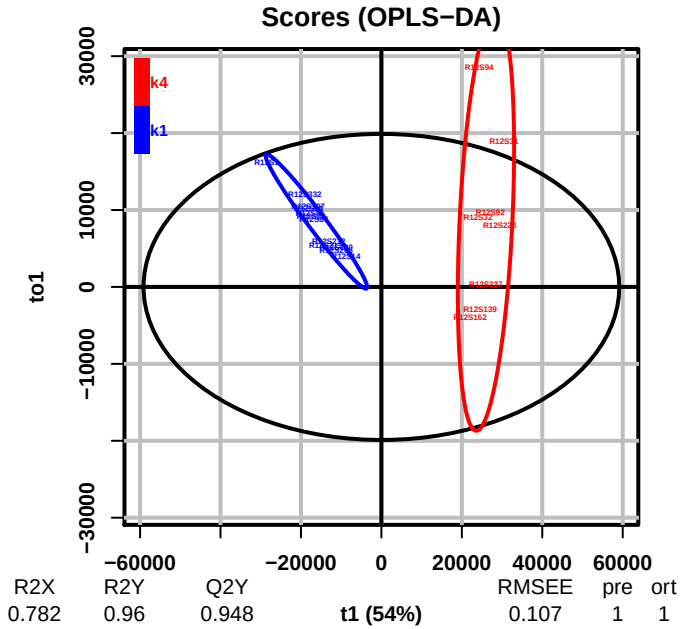

Features for level k1 versus k3
correlation(feature,t1)
relative covariance(feature,t1)
k1
k3
1.0
0.5
0.0
−0.5
−1.0

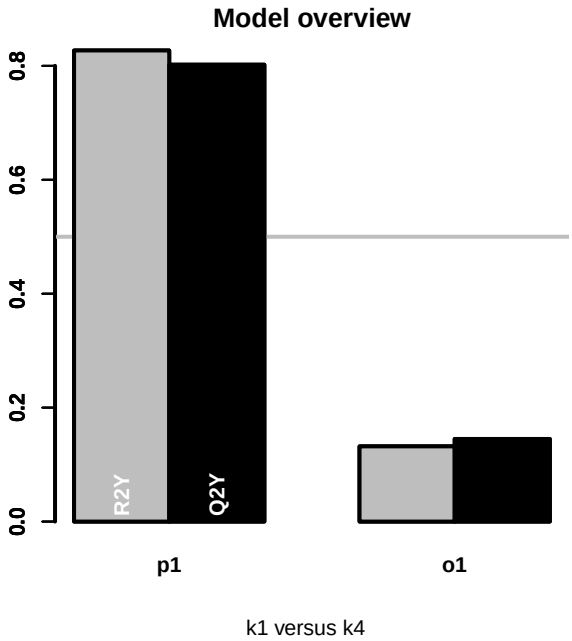

Scores (OPLS−DA)
k3
k1
to1
10000
5000
0
−5000
−10000
−20000
−10000
0
10000
20000
R2X
0.506
R2Y
0.708
Q2Y
0.622
t1 (19%)
RMSEE
0.23
pre
1
ort
1

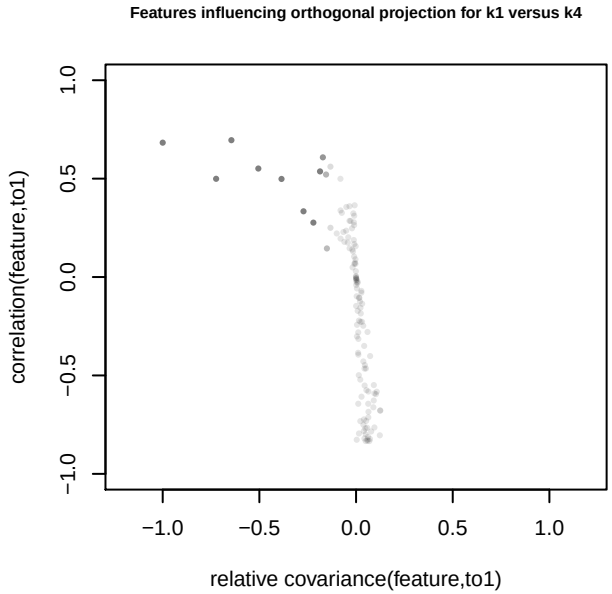

Model overview
0.0
0.1
0.2
0.3
0.4
0.5
R2Y
Q2Y
p1
o1
k1 versus k3

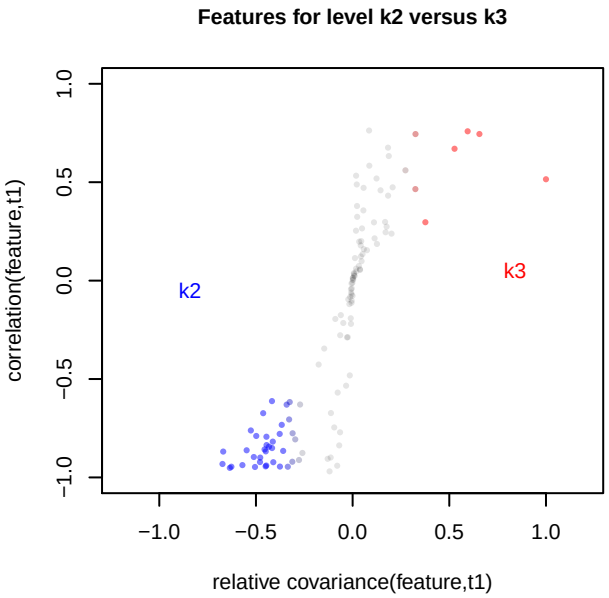

Features influencing orthogonal projection for k1 versus k3
correlation(feature,to1)
relative covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0

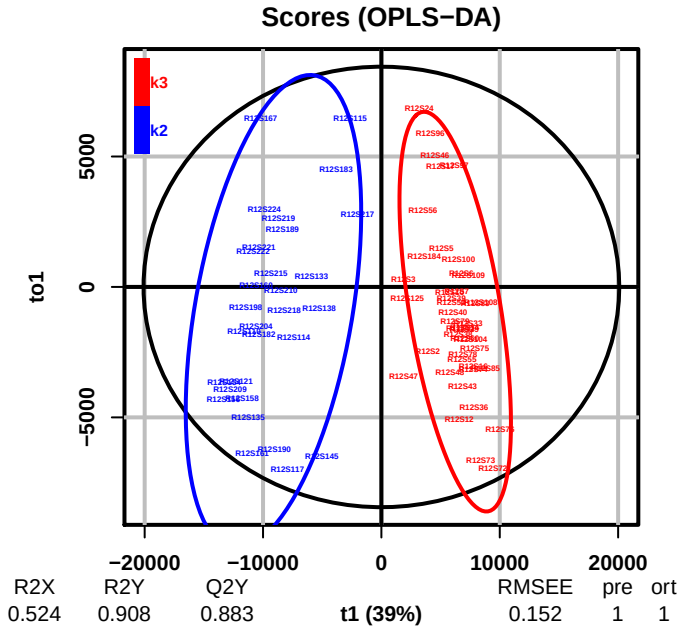

Features for level k1 versus k4
correlation(feature,t1)
relative covariance(feature,t1)
k1
k4
1.0
0.5
0.0
−0.5
−1.0

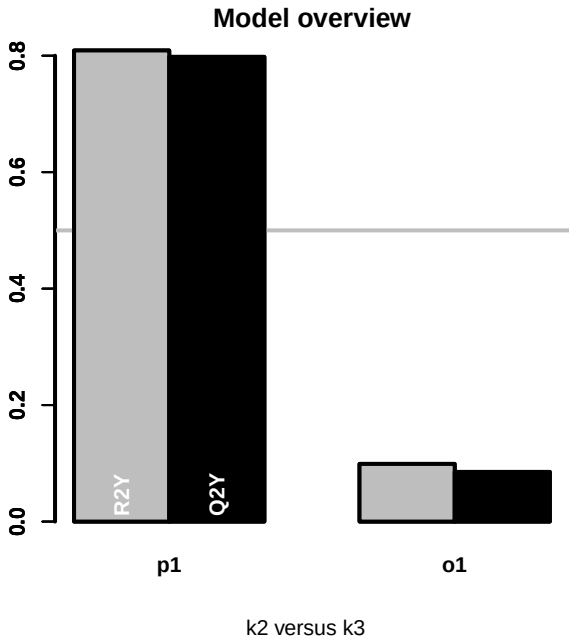

Scores (OPLS−DA)
k4
k1
to1
t1 (54%)
30000
10000
0
−10000
−30000
−60000
−20000
0
20000
40000
60000
R2X
0.782
R2Y
0.96
Q2Y
0.948
RMSEE
0.107
pre
1
ort
1

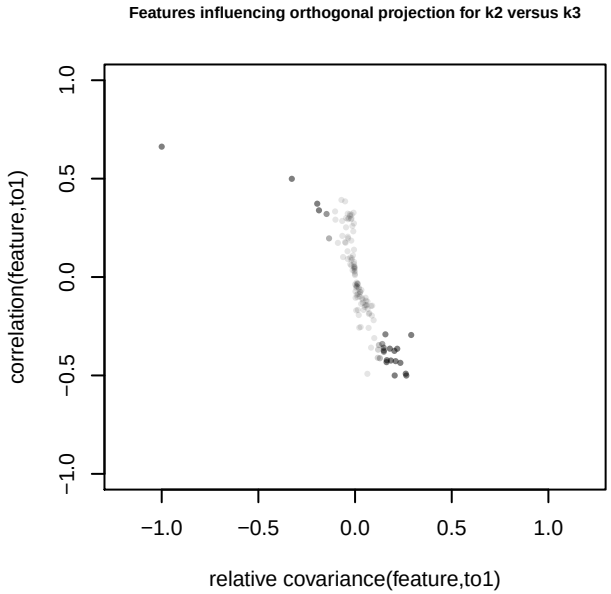

Model overview
R2Y
Q2Y
p1
o1
0.0
0.2
0.4
0.6
0.8
k1 versus k4

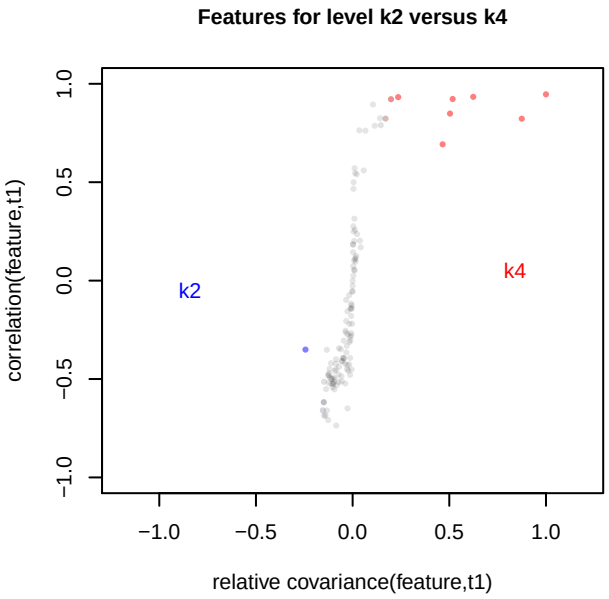

Features influencing orthogonal projection for k1 versus k4
correlation(feature,to1)
relative covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0

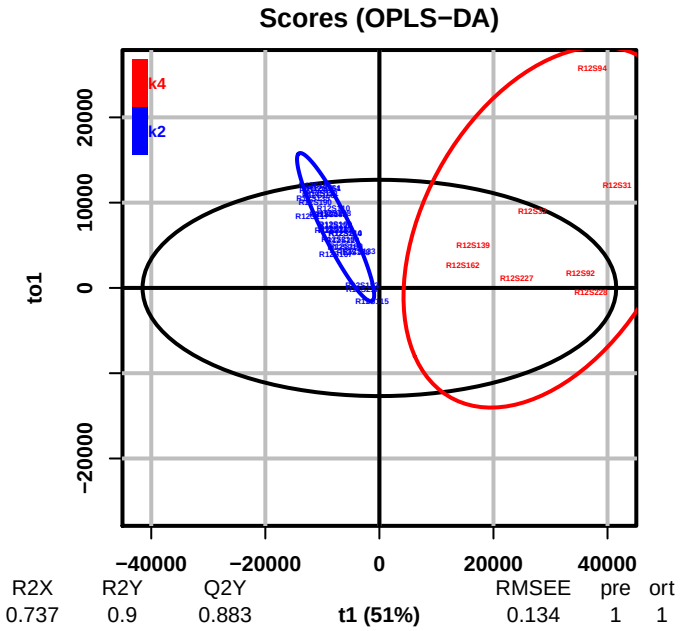

Features for level k2 versus k3
correlation(feature,t1)
relative covariance(feature,t1)
k2
k3
1.0
0.5
0.0
−0.5
−1.0

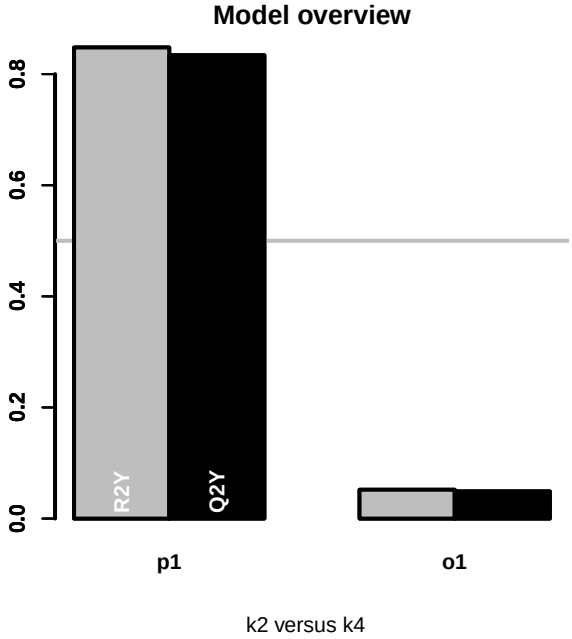

Scores (OPLS−DA)
k3
k2
to1
5000
0
−5000
−20000
−10000
0
10000
20000
R2X
0.524
R2Y
0.908
Q2Y
0.883
t1 (39%)
RMSEE
0.152
pre
1
ort
1

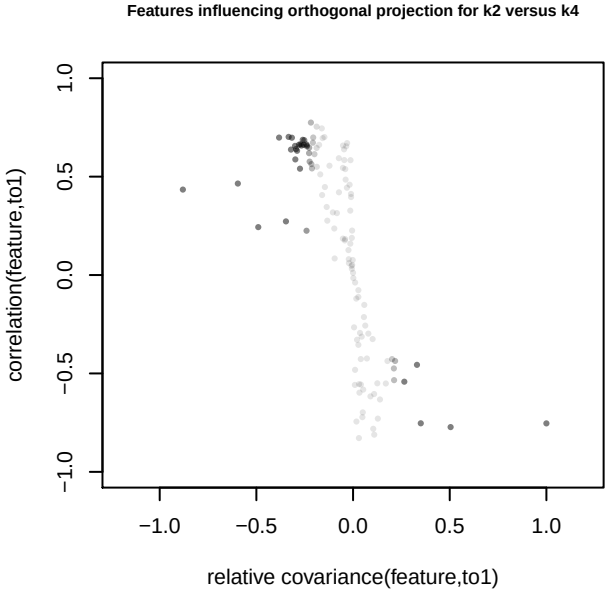

Model overview
0.8
0.6
0.4
0.2
0.0
R2Y
Q2Y
p1
o1
k2 versus k3

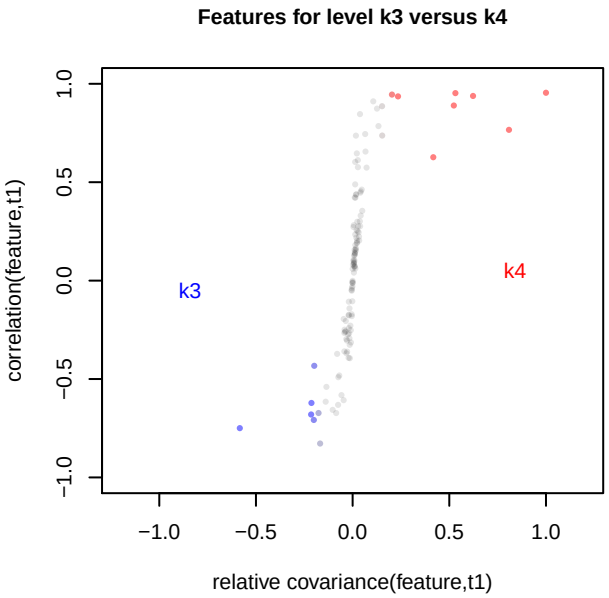

Features influencing orthogonal projection for k2 versus k3
correlation(feature,to1)
relative covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0

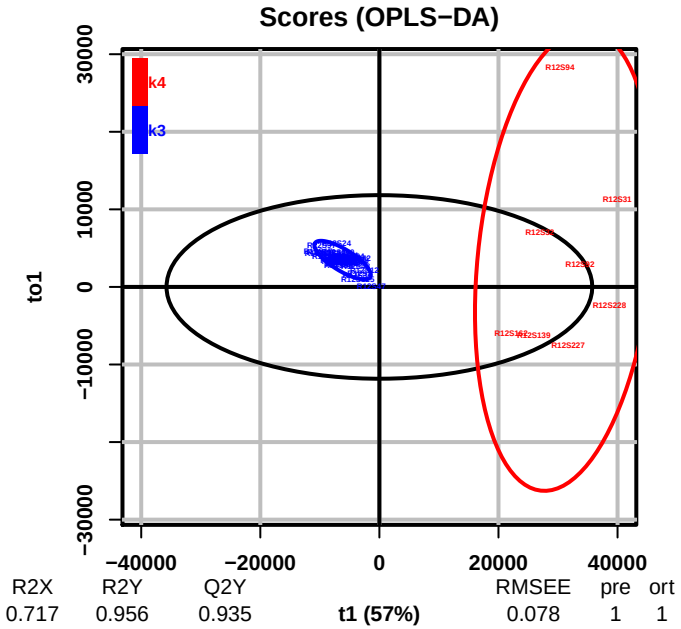

Features for level k2 versus k4
correlation(feature,t1)
relative covariance(feature,t1)
k2
k4
1.0
0.5
0.0
−0.5
−1.0

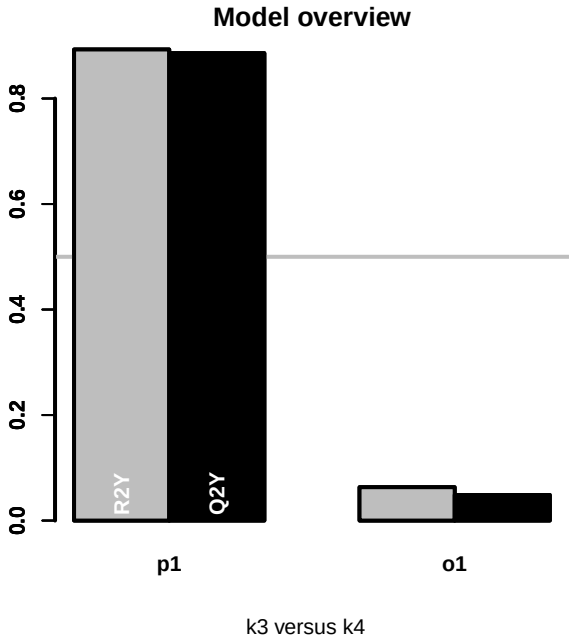

Scores (OPLS−DA)
k4
k2
to1
t1 (51%)
20000
10000
0
−20000
−40000
40000
R12S94
R12S31
R12S139
R12S162
R12S227
R12S92
R12S228
R12S15
R2X
0.737
R2Y
0.9
Q2Y
0.883
RMSEE
0.134
pre
1
ort
1

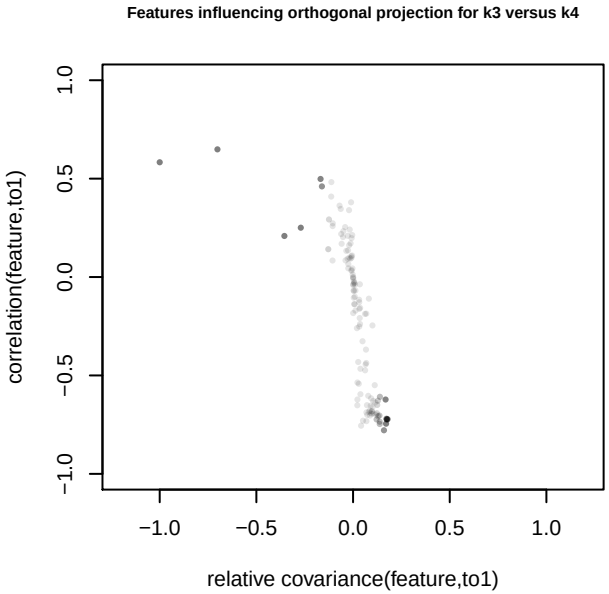

Model overview
R2Y
Q2Y
p1
o1
0.0
0.2
0.4
0.6
0.8
k2 versus k4


Features influencing orthogonal projection for k2 versus k4
correlation(feature,to1)
relative covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0


Features for level k3 versus k4
correlation(feature,t1)
relative covariance(feature,t1)
k3
k4
1.0
0.5
0.0
−0.5
−1.0


Scores (OPLS−DA)
k4
k3
to1
t1 (57%)
30000
10000
0
−10000
−30000
−40000
−20000
0
20000
40000
R2X R2Y Q2Y RMSEE pre ort
0.717 0.956 0.935 0.078 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)
relative covariance(feature,to1)
1.0
0.5
0.0
−0.5
−1.0