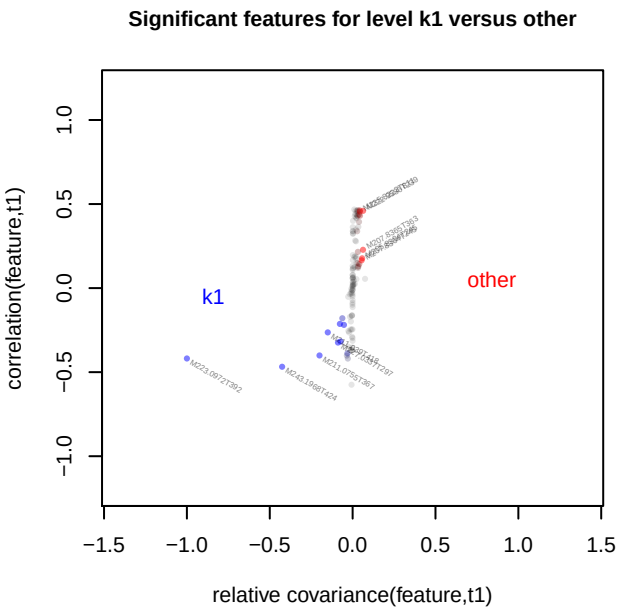
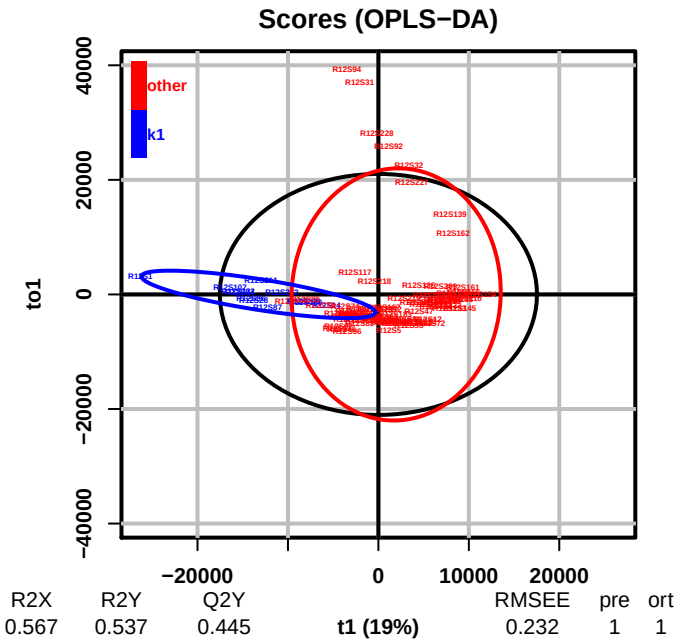
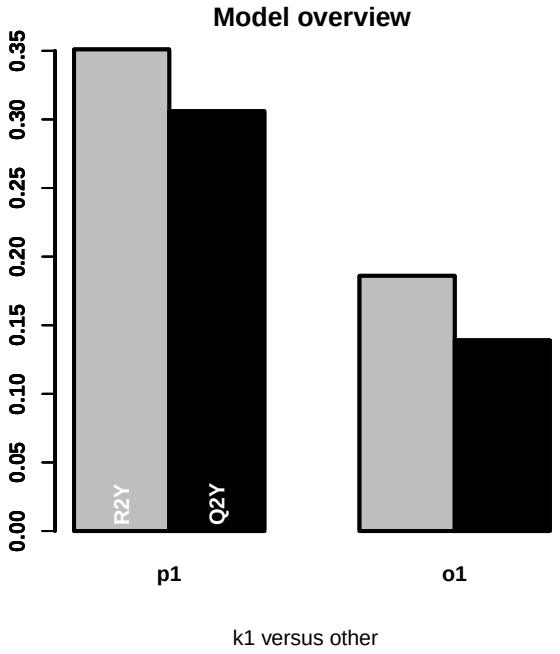
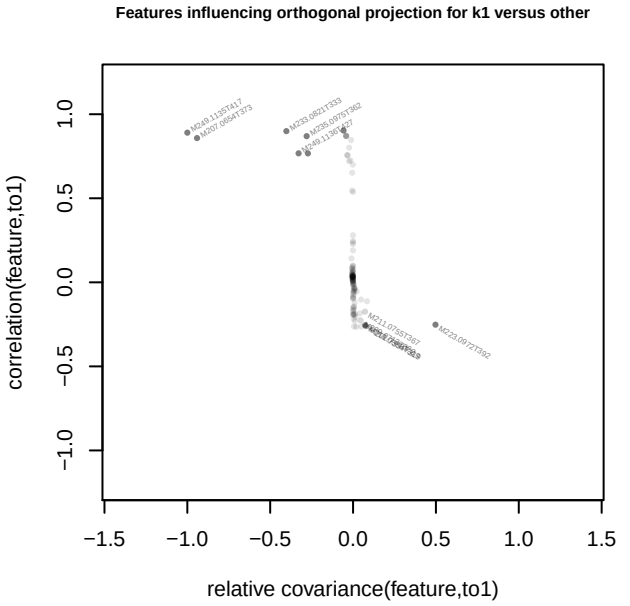
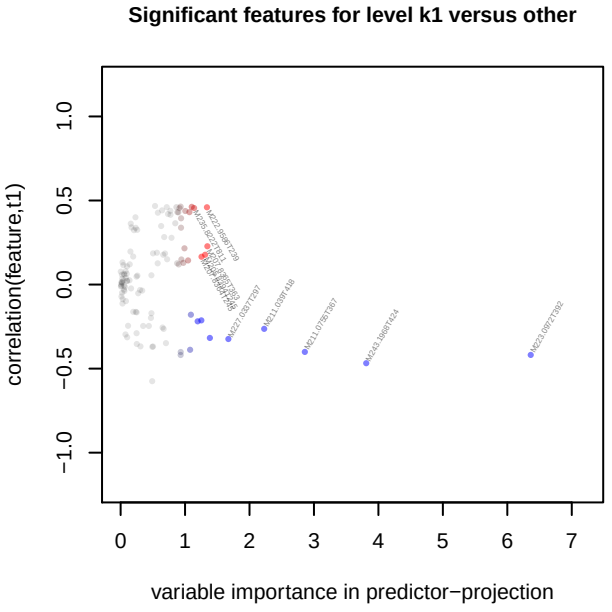
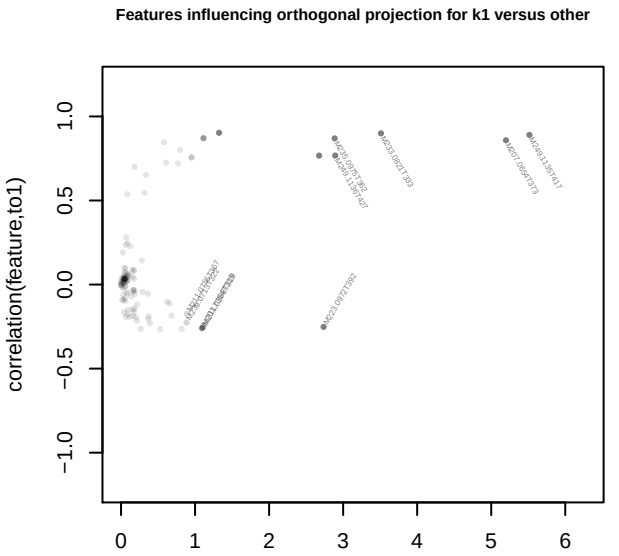

Significant features for level k1 versus other
k1
other
correlation(feature,t1)
relative covariance(feature,t1)

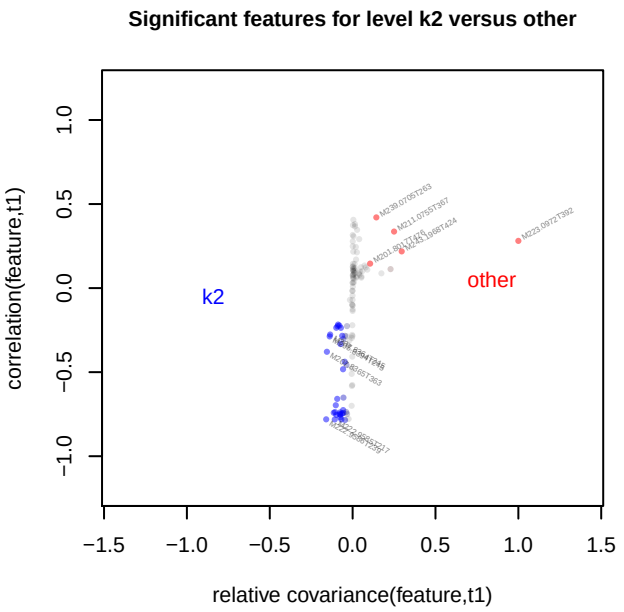

Scores (OPLS−DA)
other
k1
to1
t1 (19%)
R2X R2Y Q2Y RMSEE pre ort
0.567 0.537 0.445 0.232 1 1

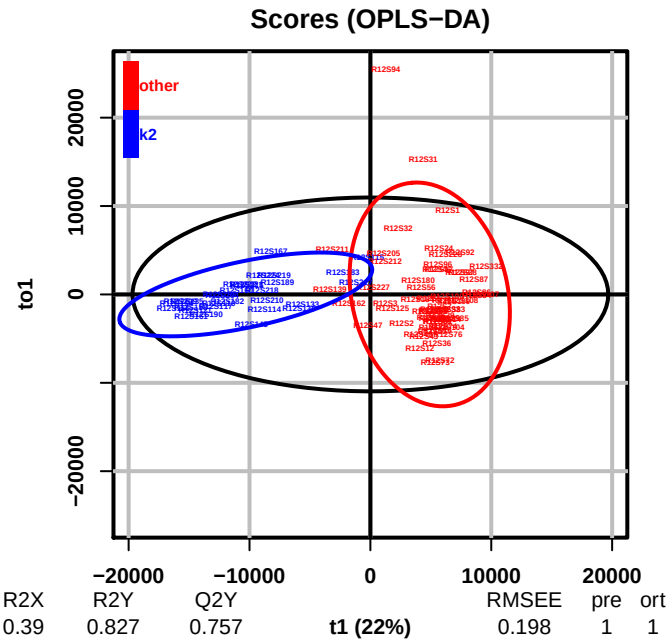

Model overview
R2Y
Q2Y
p1
o1
k1 versus other

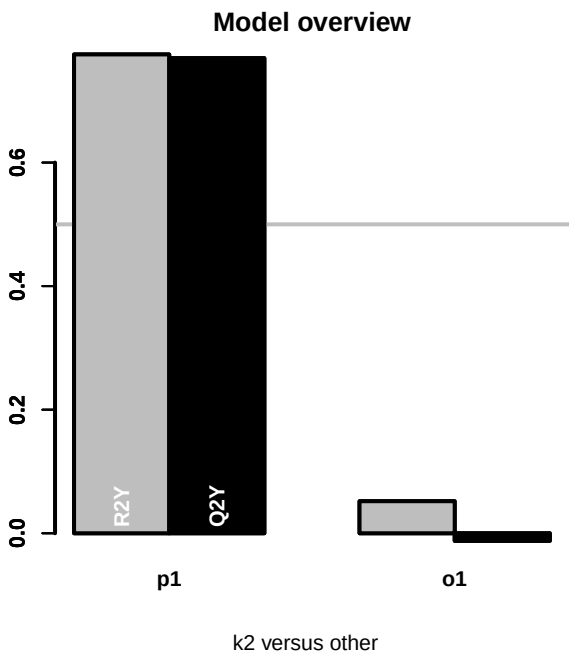

Features influencing orthogonal projection for k1 versus other
correlation(feature,to1)
relative covariance(feature,to1)

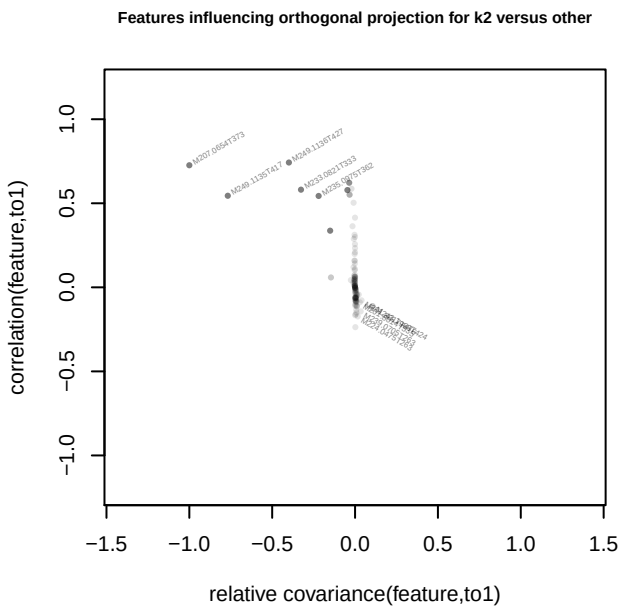

Significant features for level k1 versus other
correlation(feature,t1)
variable importance in predictor−projection

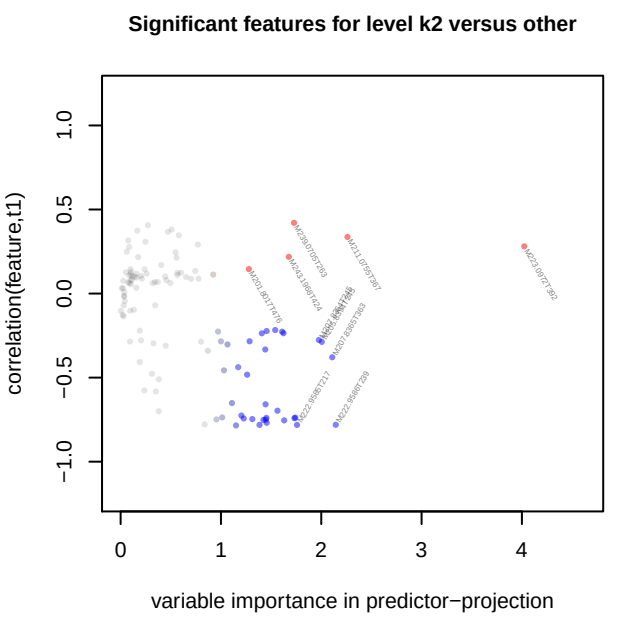

Features influencing orthogonal projection for k1 versus other
correlation(feature,to1)
variable importance in orthogonal projection

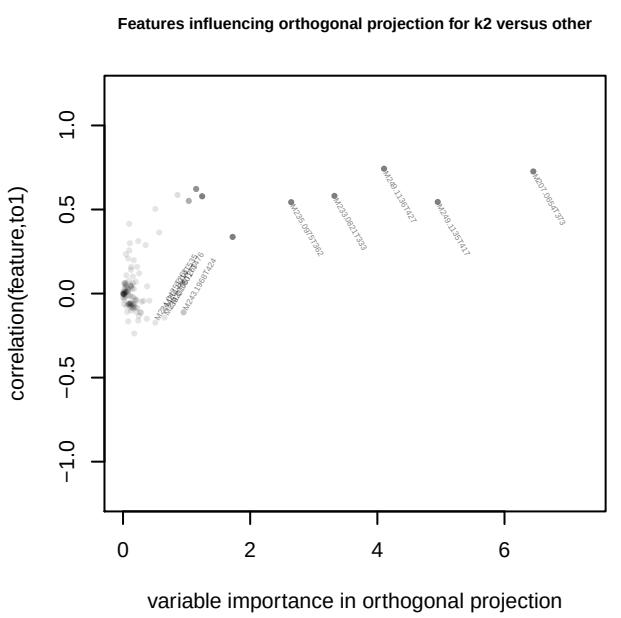

Significant features for level k2 versus other
correlation(feature,t1)
relative covariance(feature,t1)
k2
other

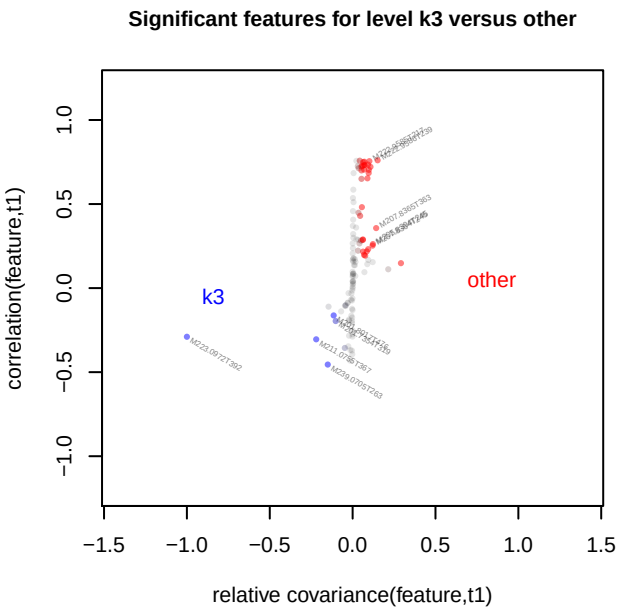

Scores (OPLS−DA)
other
k2
to1
t1 (22%)
R2X 0.39
R2Y 0.827
Q2Y 0.757
RMSEE 0.198
pre 1
ort 1

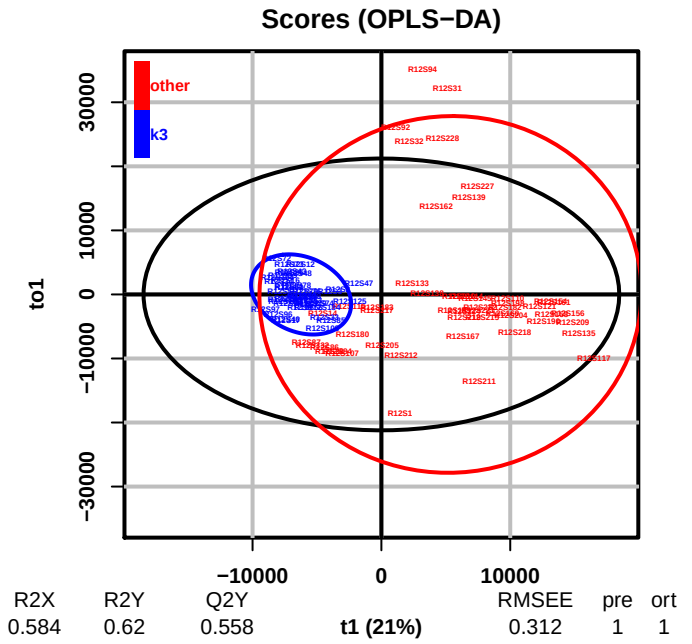

Model overview
R2Y
Q2Y
p1
o1
k2 versus other

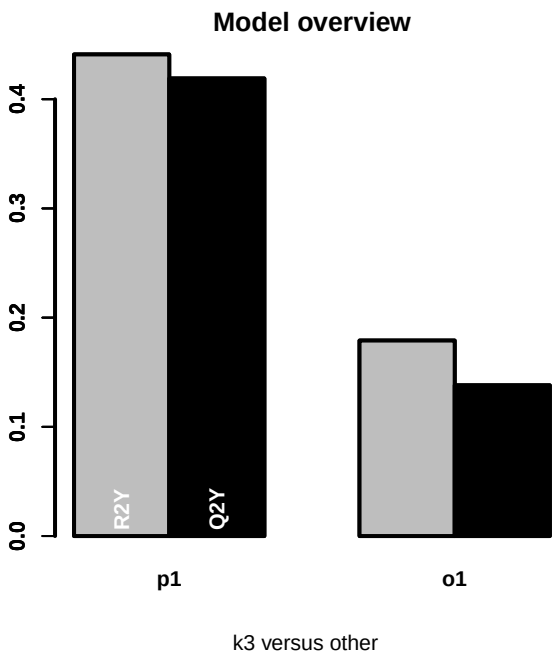

Features influencing orthogonal projection for k2 versus other
correlation(feature,to1)
relative covariance(feature,to1)

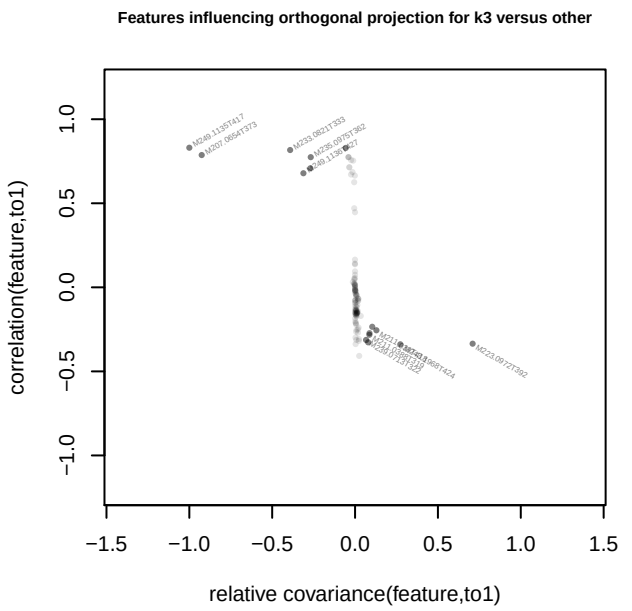

Significant features for level k2 versus other
correlation(feature,t1)
variable importance in predictor−projection

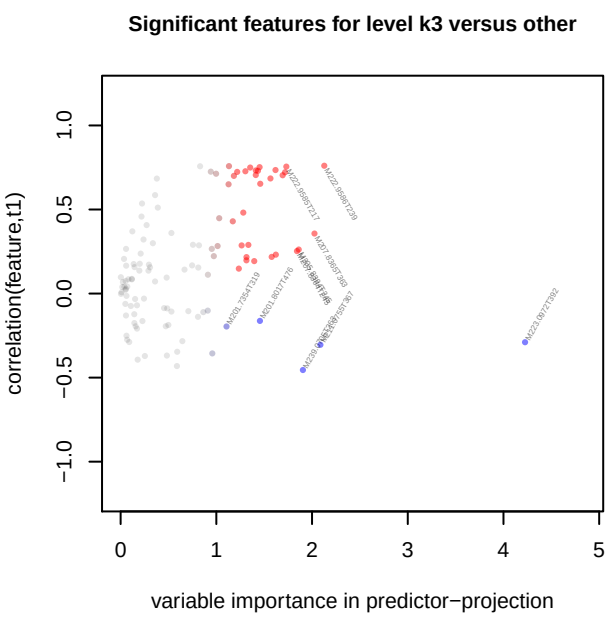

Features influencing orthogonal projection for k2 versus other
correlation(feature,to1)
variable importance in orthogonal projection

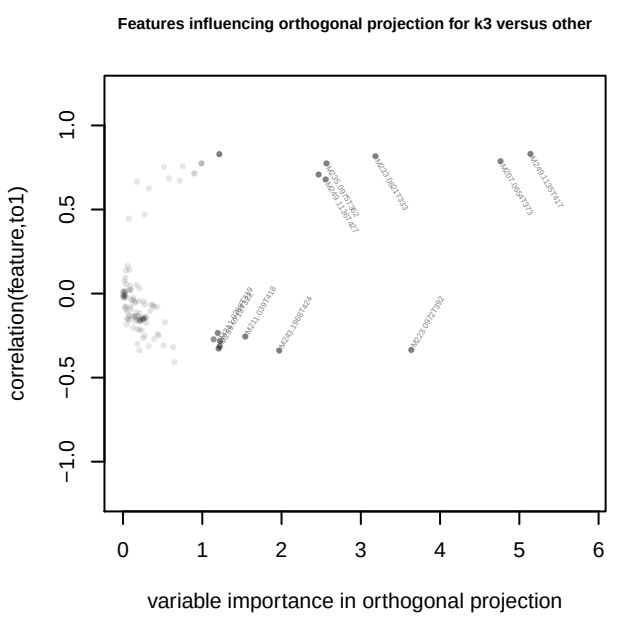

Significant features for level k3 versus other
k3
other
correlation(feature,t1)
relative covariance(feature,t1)

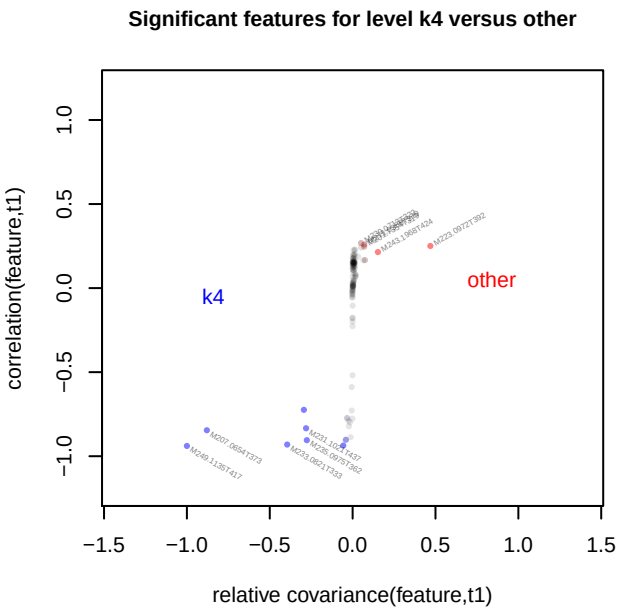

Scores (OPLS−DA)
other
k3
to1
t1 (21%)
R2X 0.584
R2Y 0.62
Q2Y 0.558
RMSEE 0.312
pre 1
ort 1

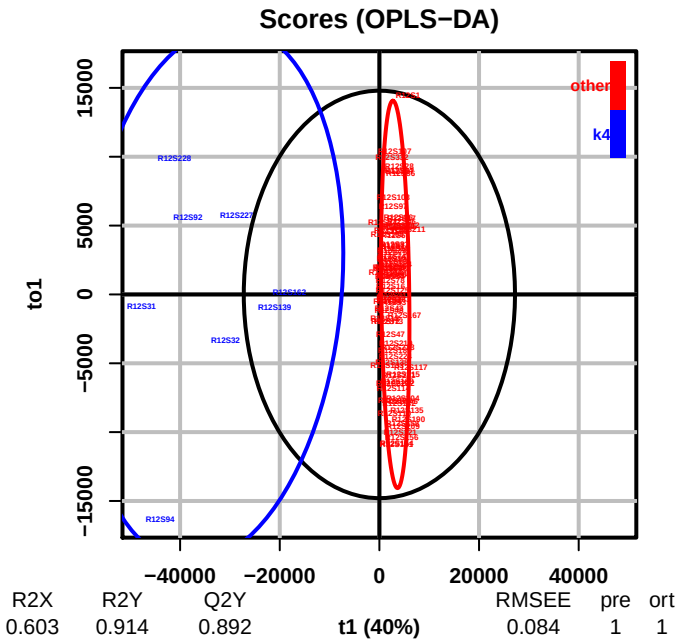

Model overview
R2Y
Q2Y
p1
o1
k3 versus other

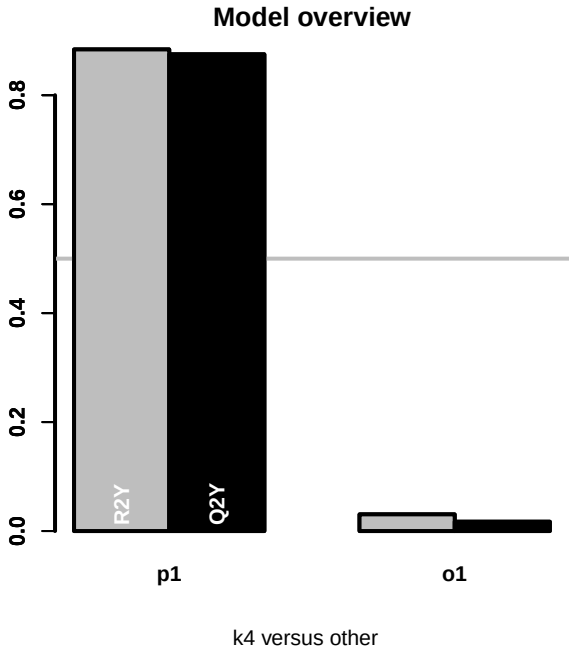

Features influencing orthogonal projection for k3 versus other
correlation(feature,to1)
relative covariance(feature,to1)

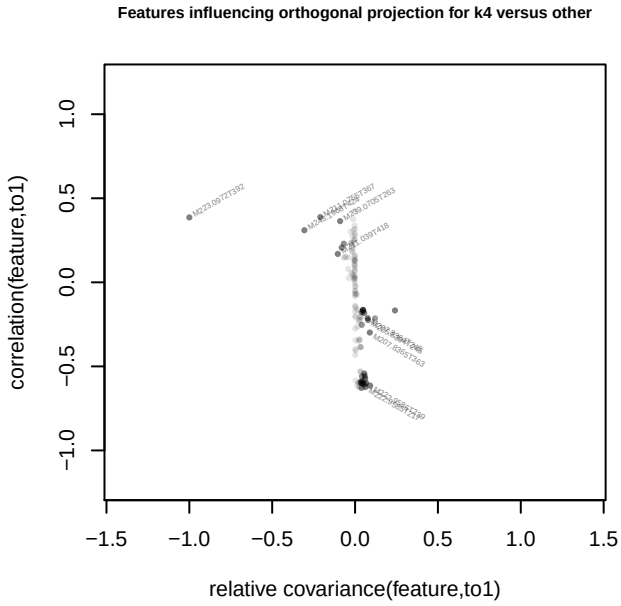

Significant features for level k3 versus other
correlation(feature,t1)
variable importance in predictor−projection

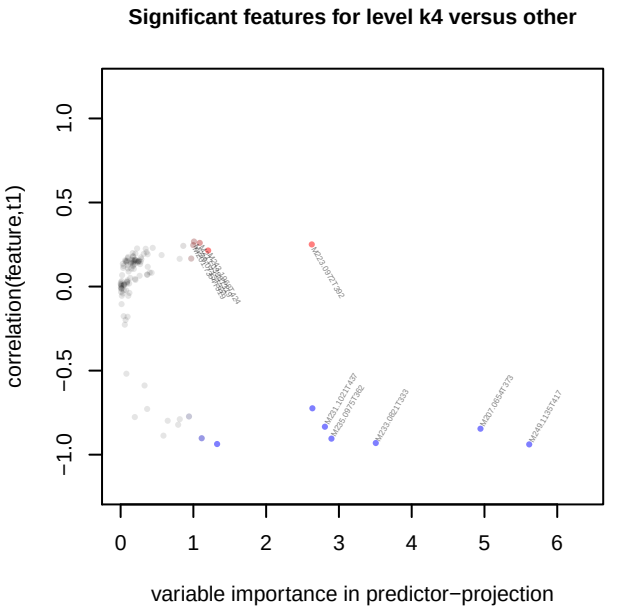

Features influencing orthogonal projection for k3 versus other
correlation(feature,to1)
variable importance in orthogonal projection

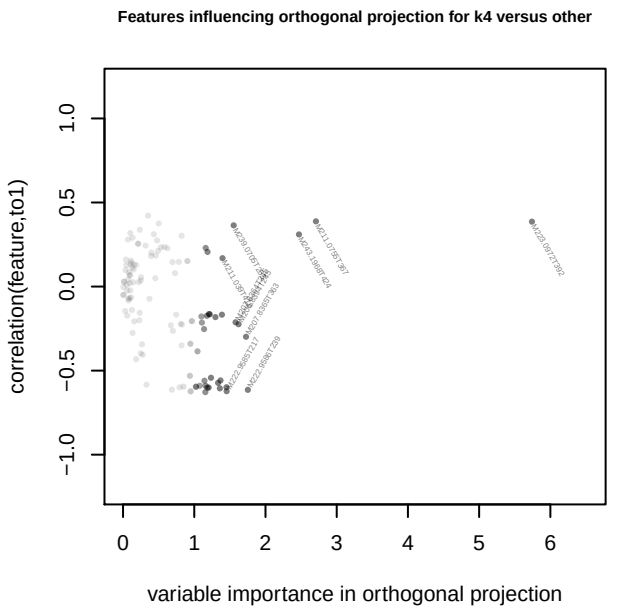

Significant features for level k4 versus other
correlation(feature,t1)
relative covariance(feature,t1)
k4
other

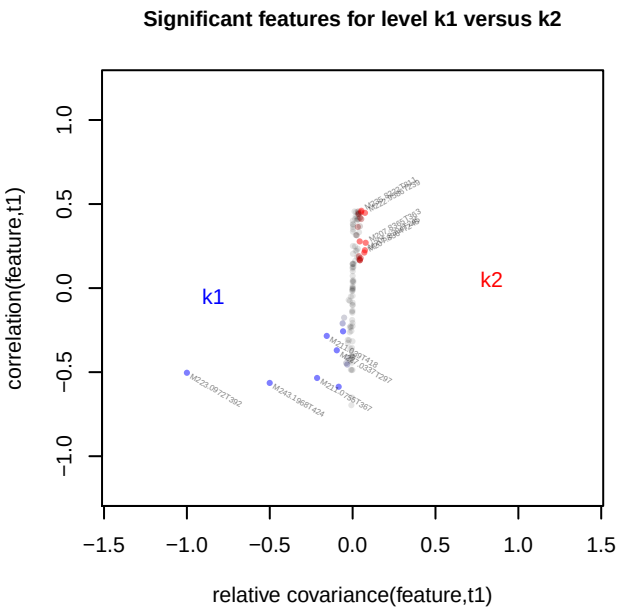

Scores (OPLS−DA)
other
k4
to1
t1 (40%)
R2X 0.603
R2Y 0.914
Q2Y 0.892
RMSEE 0.084
pre 1
ort 1

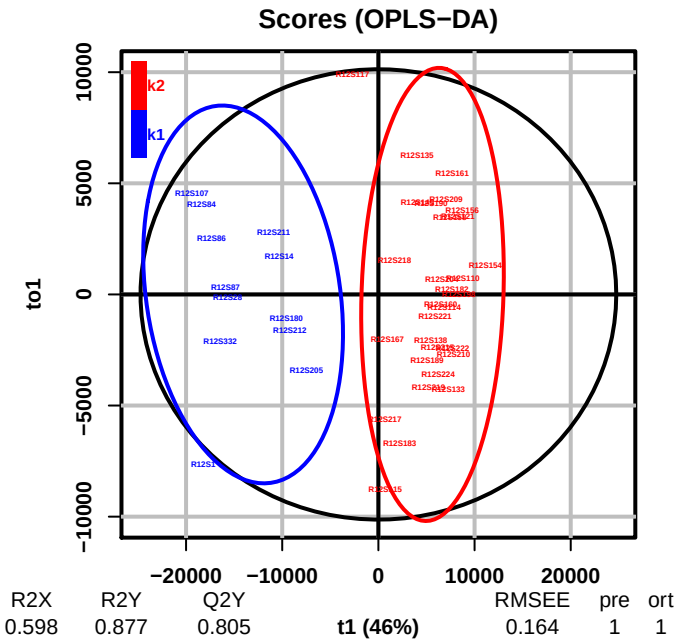

Model overview
R2Y
Q2Y
p1
o1
k4 versus other

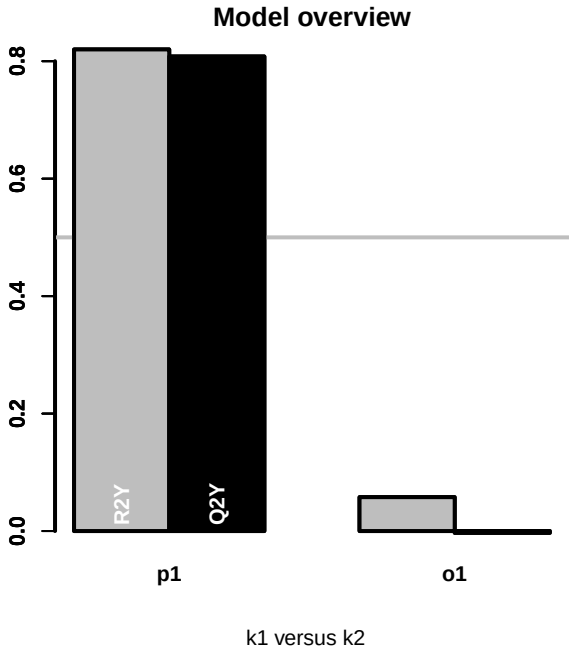

Features influencing orthogonal projection for k4 versus other
correlation(feature,to1)
relative covariance(feature,to1)

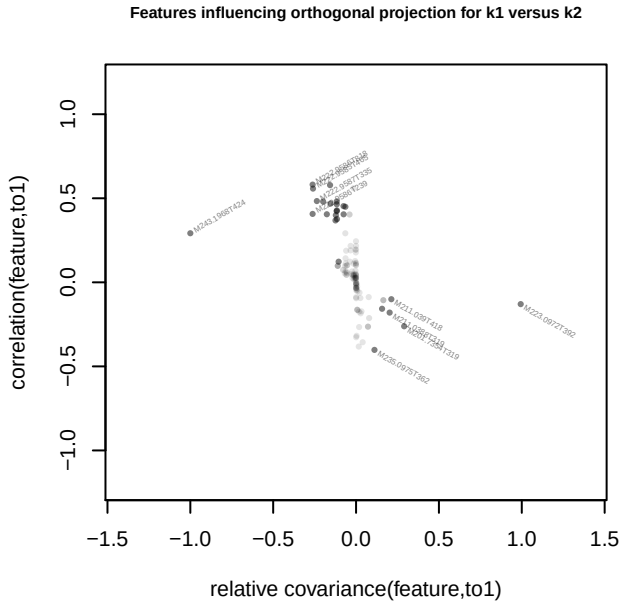

Significant features for level k4 versus other
correlation(feature,t1)
variable importance in predictor−projection

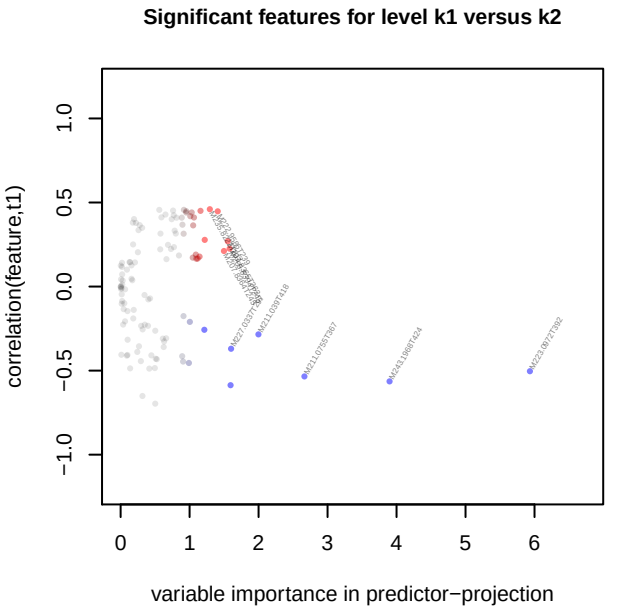

Features influencing orthogonal projection for k4 versus other
correlation(feature,to1)
variable importance in orthogonal projection

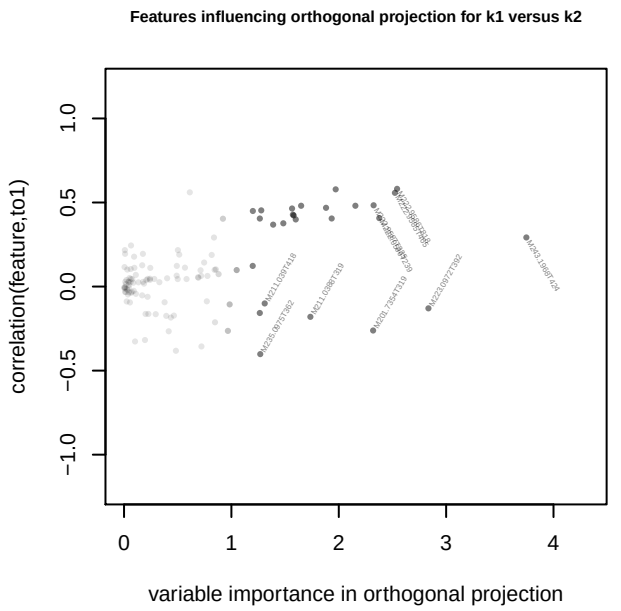

Significant features for level k1 versus k2
correlation(feature,t1)
relative covariance(feature,t1)
k1
k2

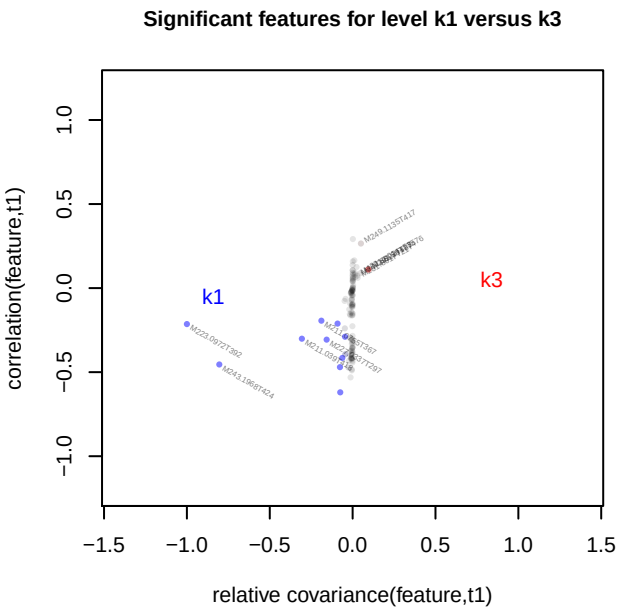

Scores (OPLS−DA)
k2
k1
to1
t1 (46%)
R2X 0.598
R2Y 0.877
Q2Y 0.805
RMSEE 0.164
pre 1
ort 1

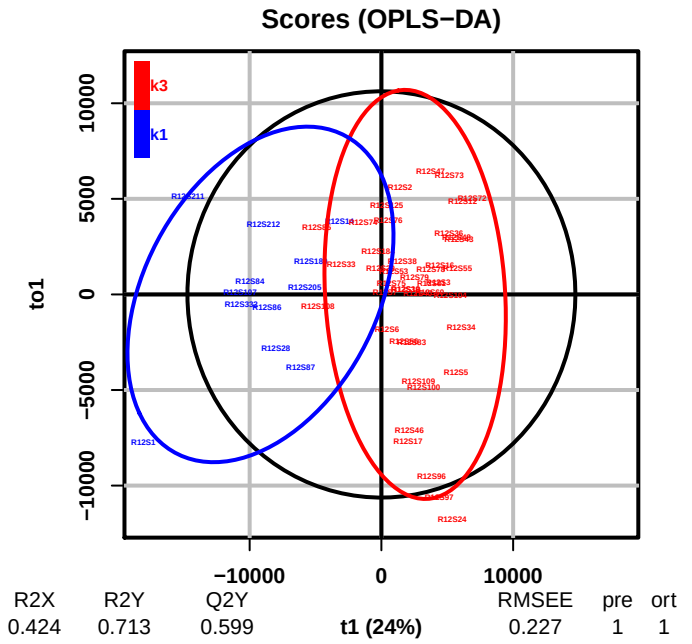

Model overview
R2Y
Q2Y
p1
o1
k1 versus k2

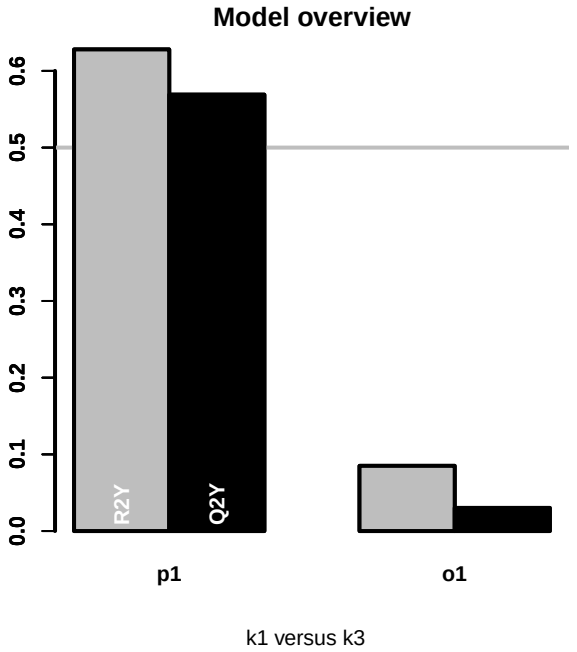

Features influencing orthogonal projection for k1 versus k2
correlation(feature,to1)
relative covariance(feature,to1)

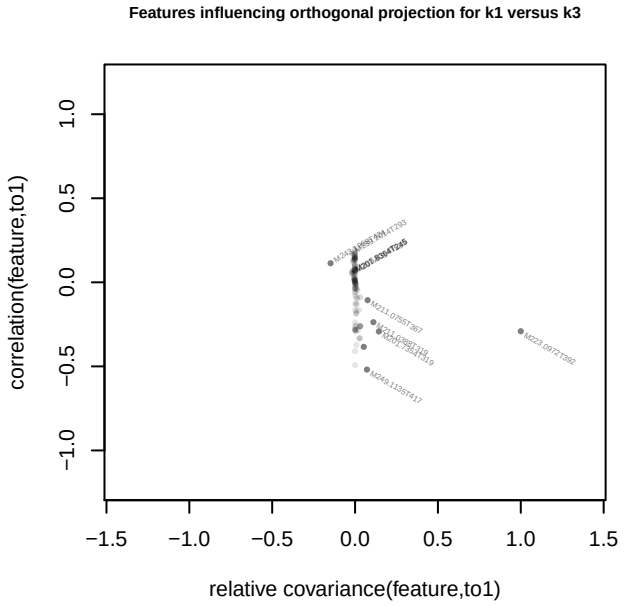

Significant features for level k1 versus k2
correlation(feature,t1)
variable importance in predictor−projection

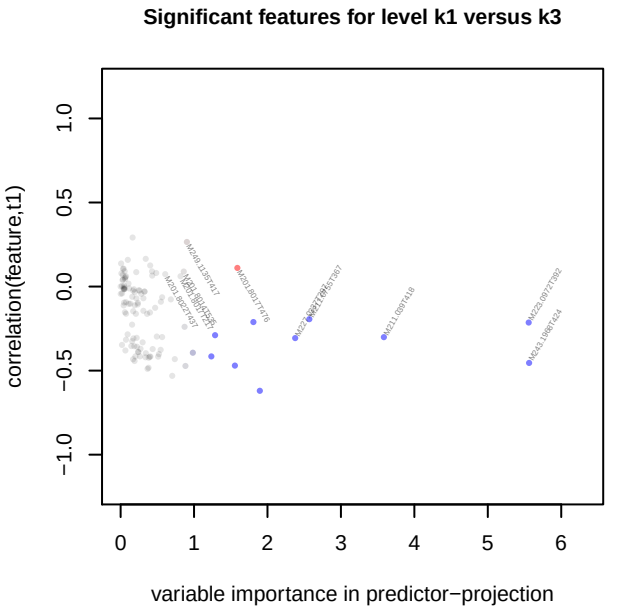

Features influencing orthogonal projection for k1 versus k2
correlation(feature,to1)
variable importance in orthogonal projection

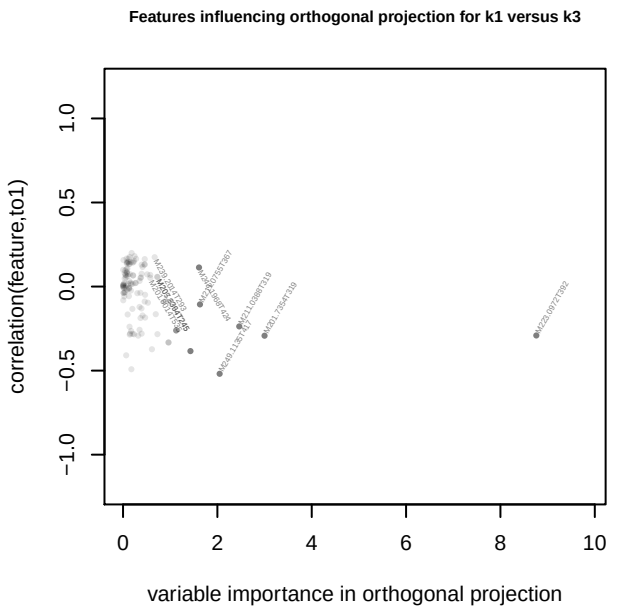

Significant features for level k1 versus k3
correlation(feature,t1)
relative covariance(feature,t1)
k1
k3

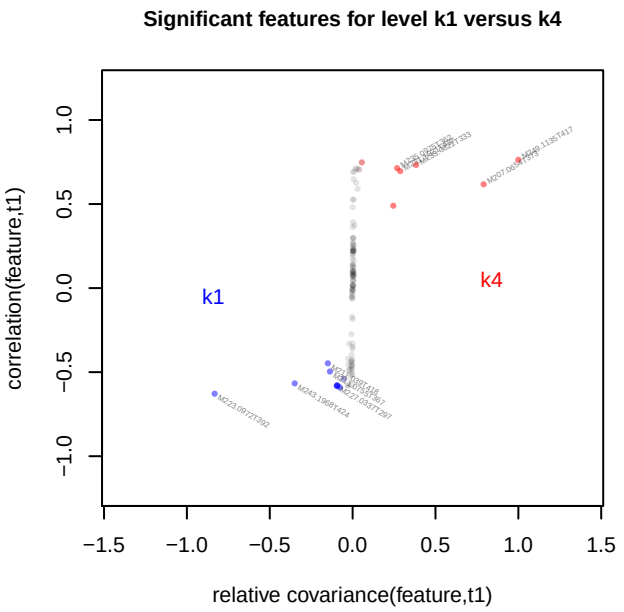

Scores (OPLS−DA)
k3
k1
to1
t1 (24%)
R2X 0.424
R2Y 0.713
Q2Y 0.599
RMSEE 0.227
pre 1
ort 1

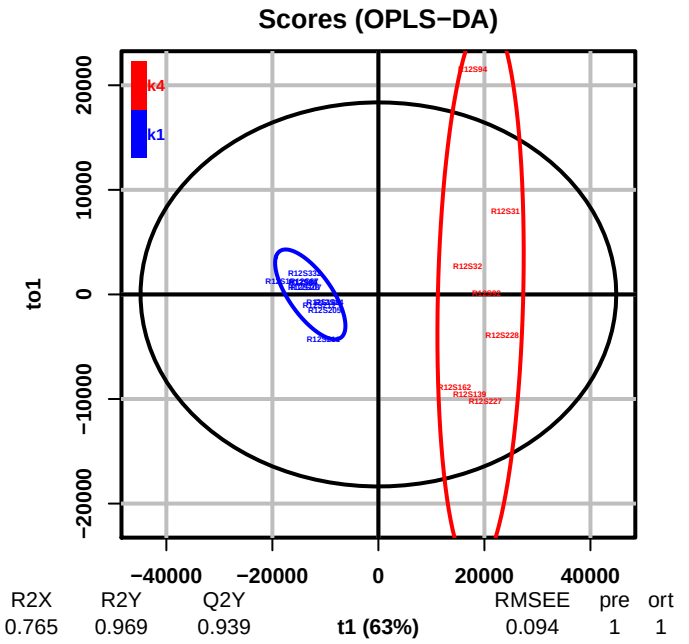

Model overview
R2Y
Q2Y
p1
o1
k1 versus k3

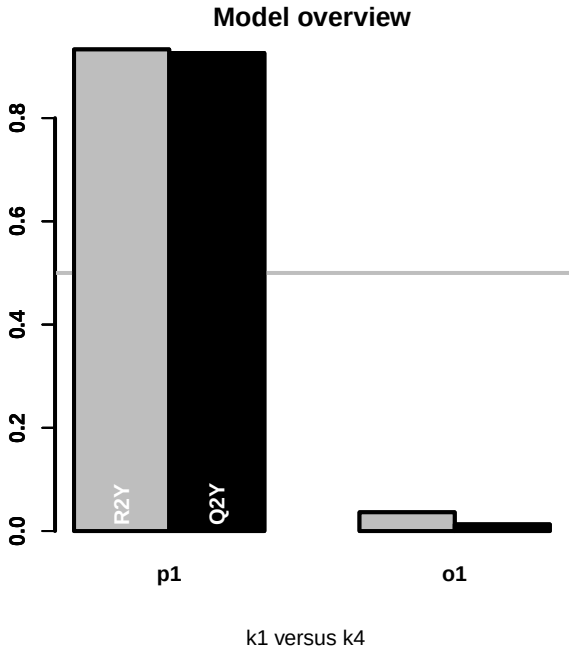

Features influencing orthogonal projection for k1 versus k3
correlation(feature,to1)
relative covariance(feature,to1)

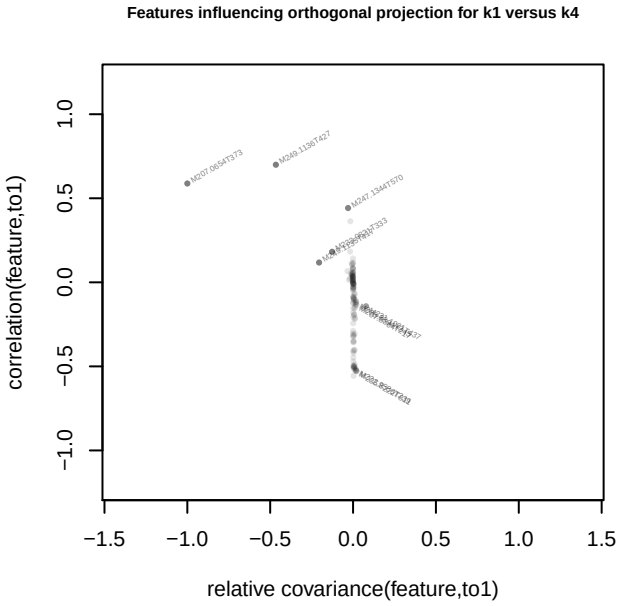

Significant features for level k1 versus k3
correlation(feature,t1)
variable importance in predictor−projection

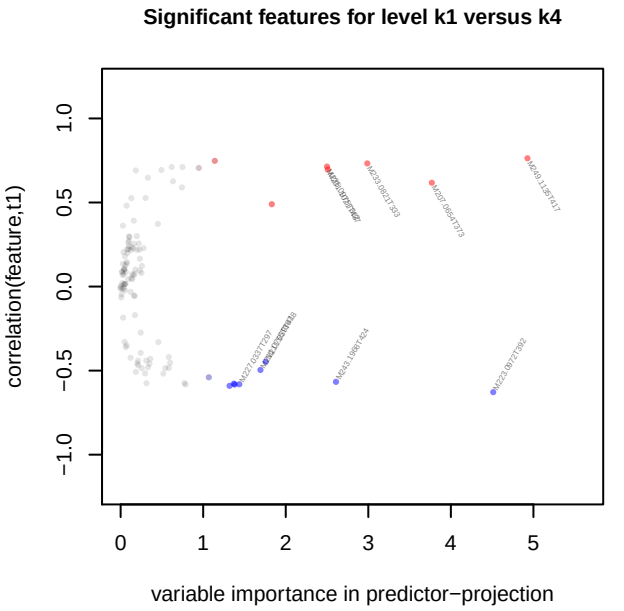

Features influencing orthogonal projection for k1 versus k3
correlation(feature,to1)
variable importance in orthogonal projection

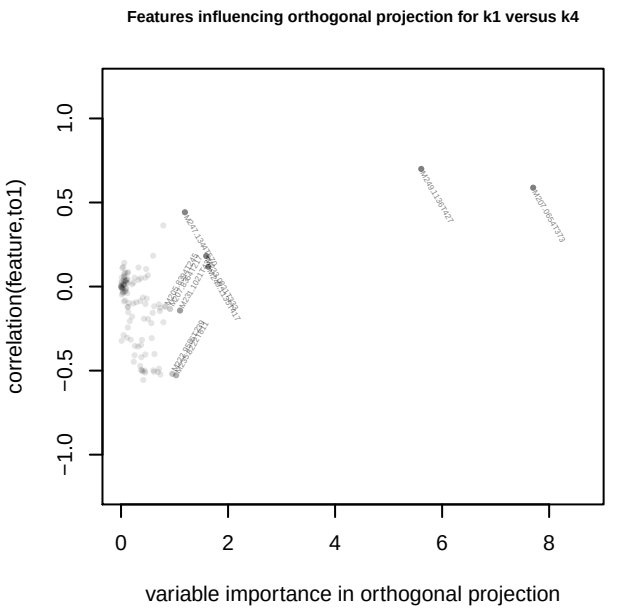

Significant features for level k1 versus k4
correlation(feature,t1)
relative covariance(feature,t1)
k1
k4

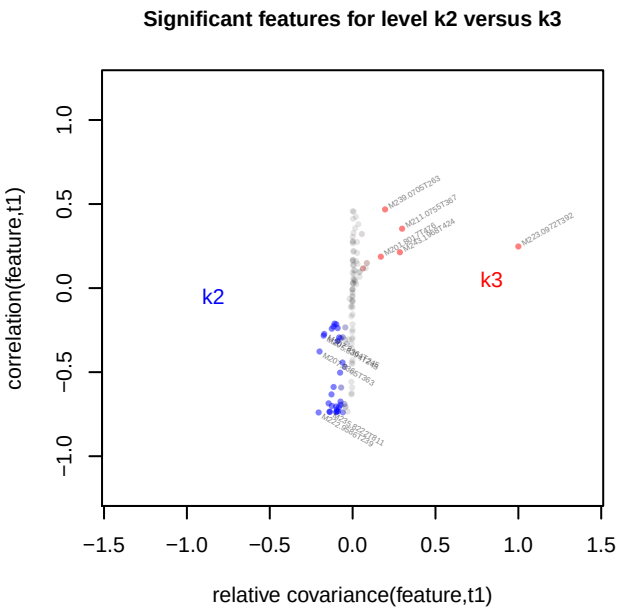

Scores (OPLS−DA)
k4
k1
to1
t1 (63%)
R2X 0.765
R2Y 0.969
Q2Y 0.939
RMSEE 0.094
pre 1
ort 1

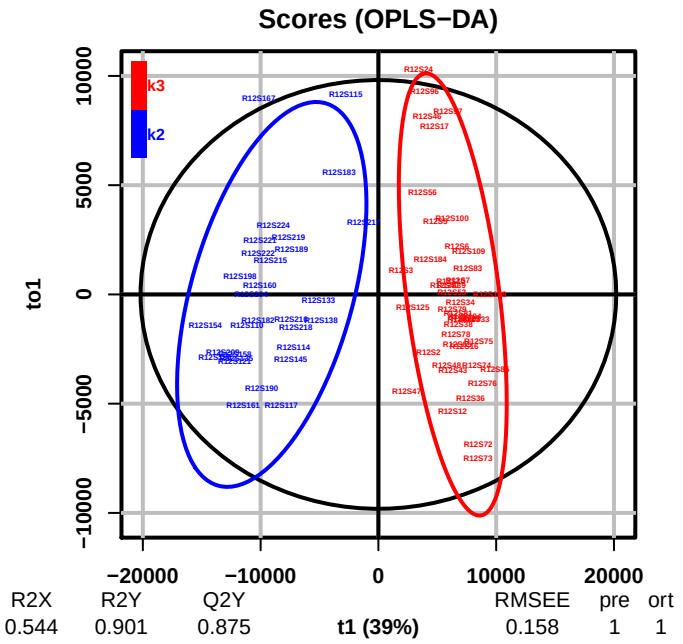

Model overview
R2Y
Q2Y
p1
o1
k1 versus k4

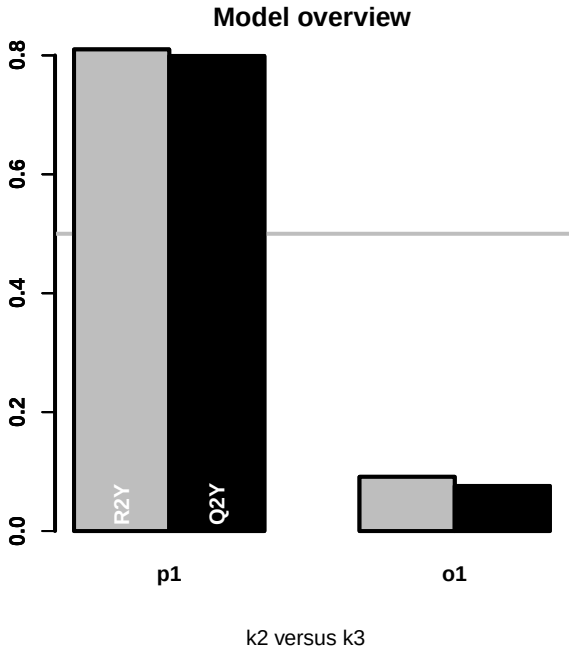

Features influencing orthogonal projection for k1 versus k4
correlation(feature,to1)
relative covariance(feature,to1)

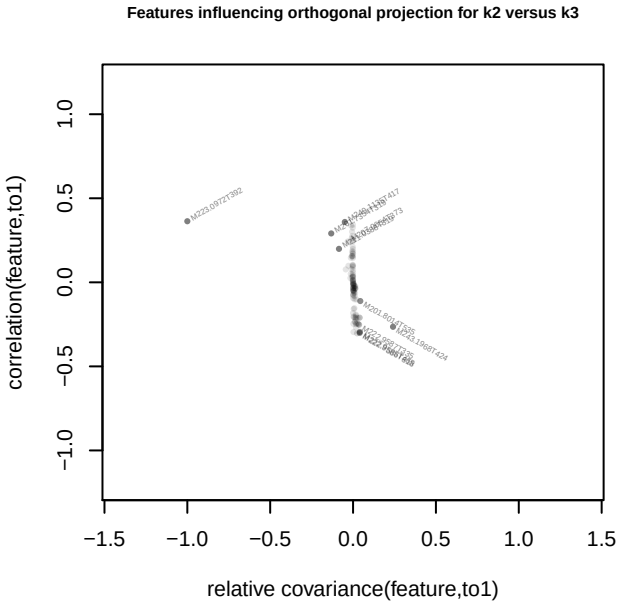

Significant features for level k1 versus k4
correlation(feature,t1)
variable importance in predictor−projection

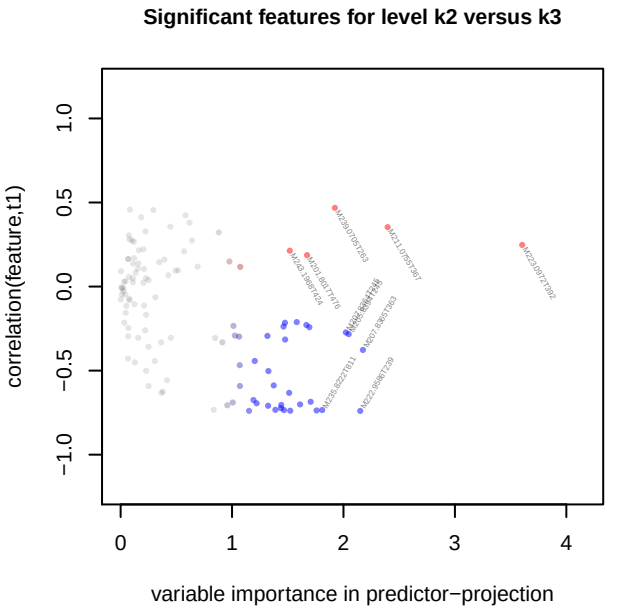

Features influencing orthogonal projection for k1 versus k4
correlation(feature,to1)
variable importance in orthogonal projection

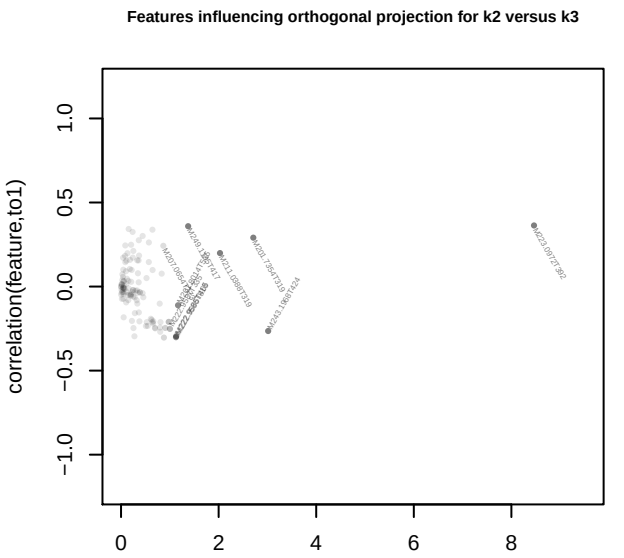

Significant features for level k2 versus k3
correlation(feature,t1)
relative covariance(feature,t1)
k2
k3

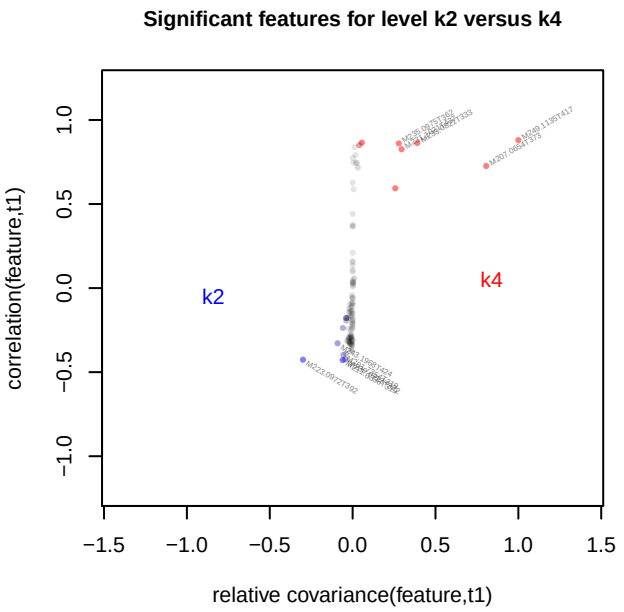

Scores (OPLS−DA)
k3
k2
to1
t1 (39%)
R2X R2Y Q2Y RMSEE pre ort
0.544 0.901 0.875 0.158 1 1

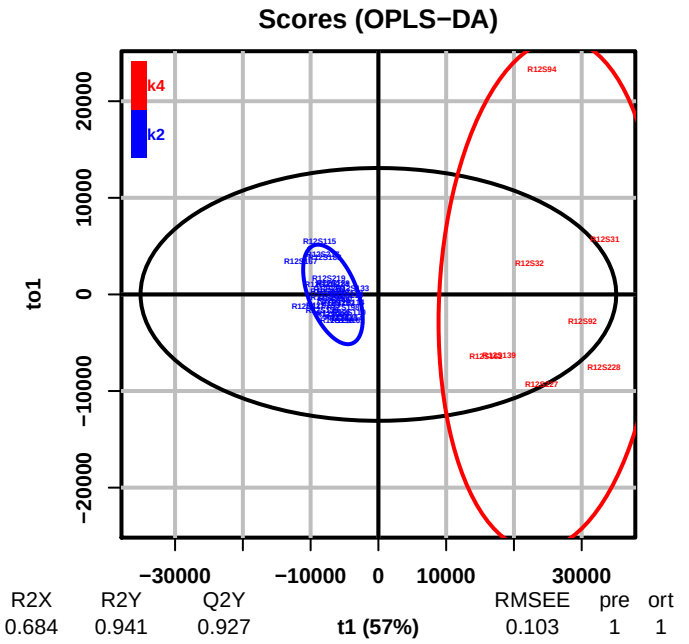

Model overview
R2Y
Q2Y
p1
o1
k2 versus k3

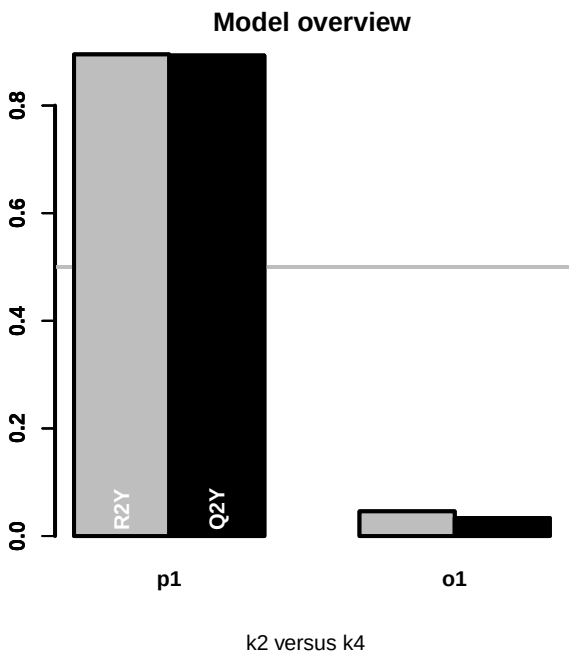

Features influencing orthogonal projection for k2 versus k3
correlation(feature,to1)
relative covariance(feature,to1)

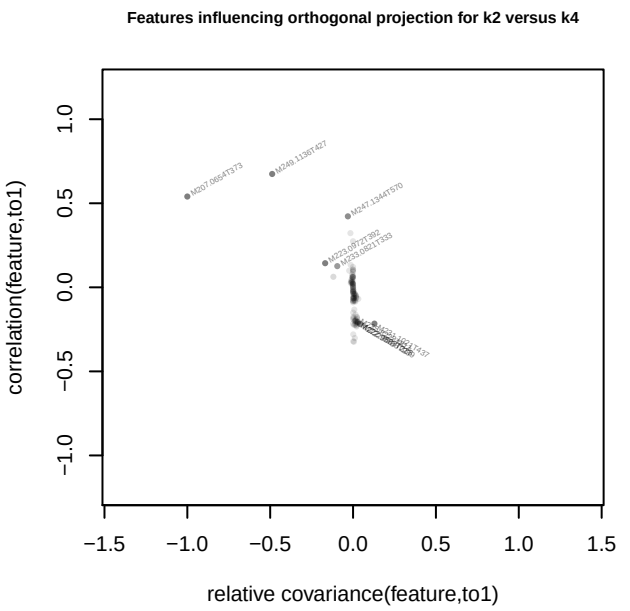

Significant features for level k2 versus k3
correlation(feature,t1)
variable importance in predictor−projection

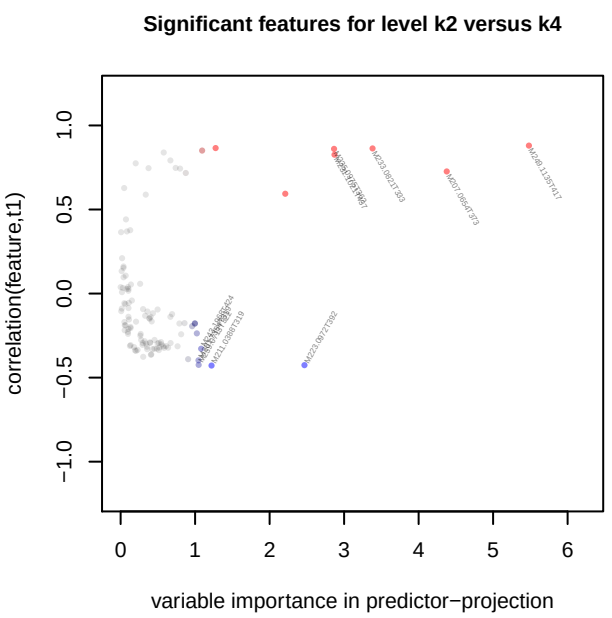

Features influencing orthogonal projection for k2 versus k3
correlation(feature,to1)
variable importance in orthogonal projection

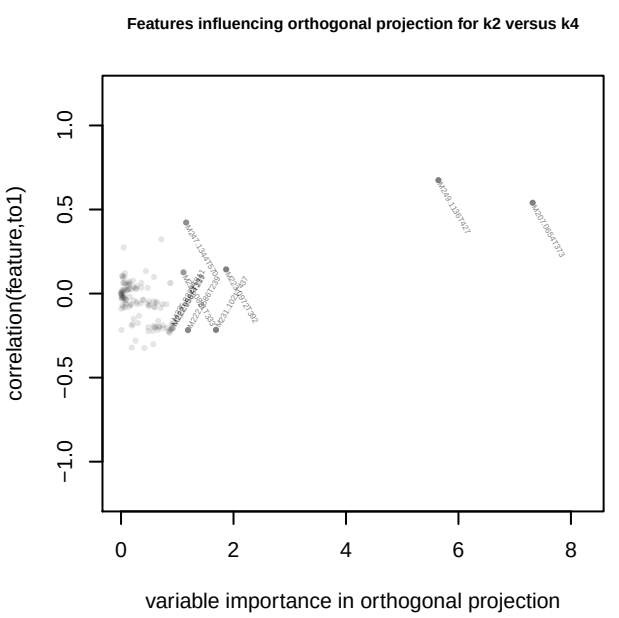

Significant features for level k2 versus k4
correlation(feature,t1)
relative covariance(feature,t1)
k2
k4

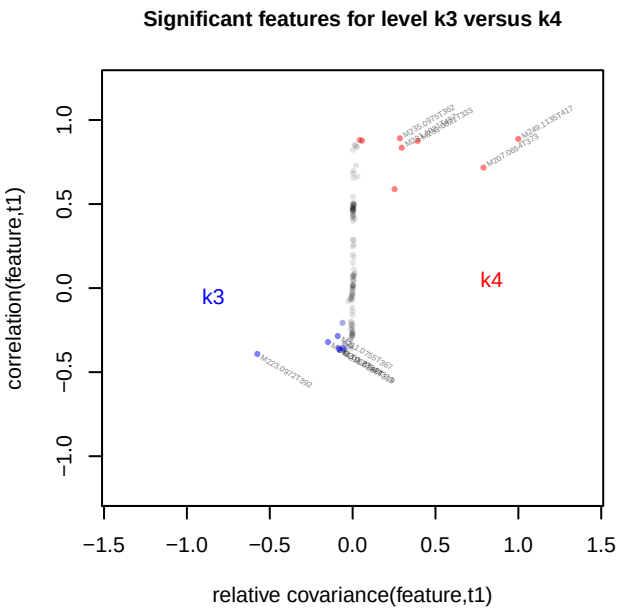

Scores (OPLS−DA)
k4
k2
to1
t1 (57%)
R2X R2Y Q2Y RMSEE pre ort
0.684 0.941 0.927 0.103 1 1

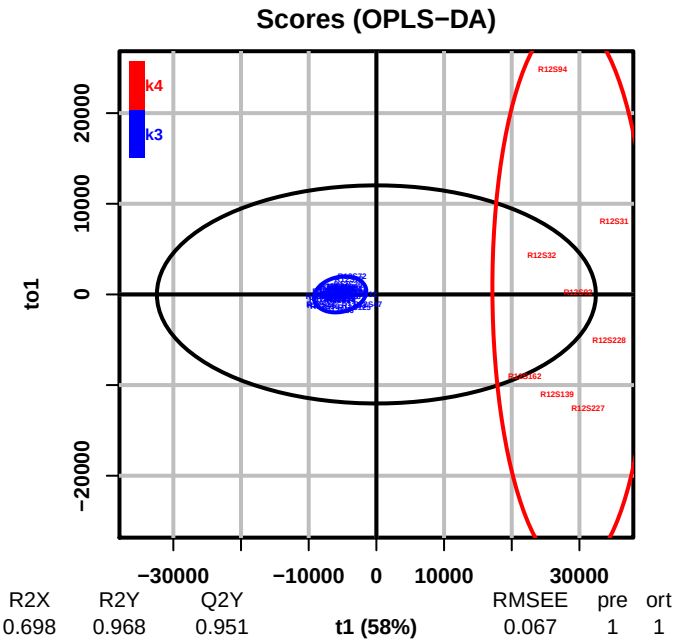

Model overview
R2Y
Q2Y
p1
o1
k2 versus k4

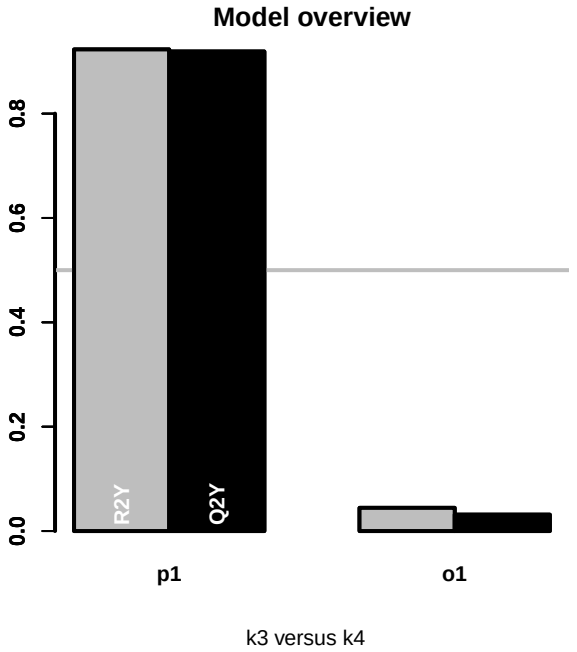

Features influencing orthogonal projection for k2 versus k4
correlation(feature,to1)
relative covariance(feature,to1)

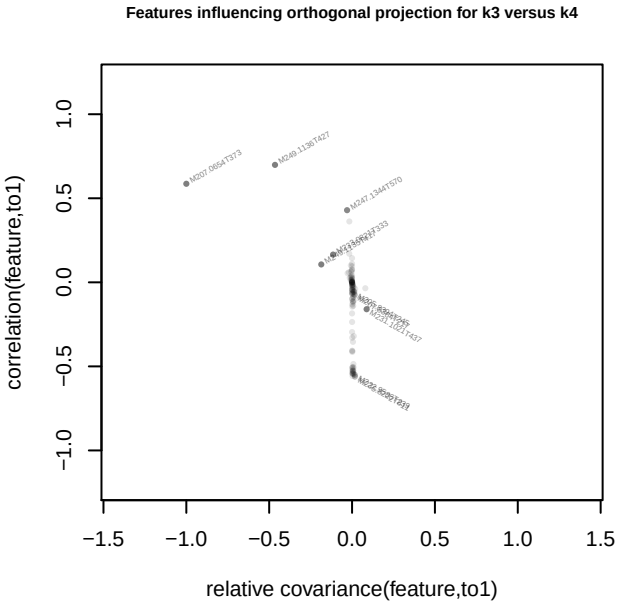

Significant features for level k2 versus k4
correlation(feature,t1)
variable importance in predictor−projection

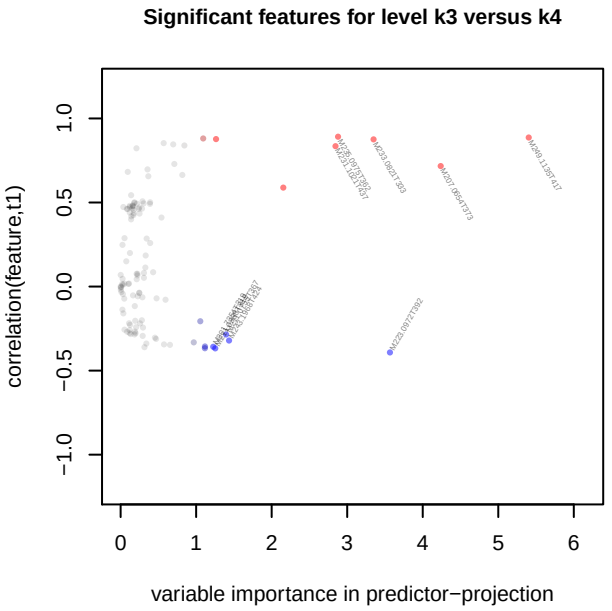

Features influencing orthogonal projection for k2 versus k4
correlation(feature,to1)
variable importance in orthogonal projection

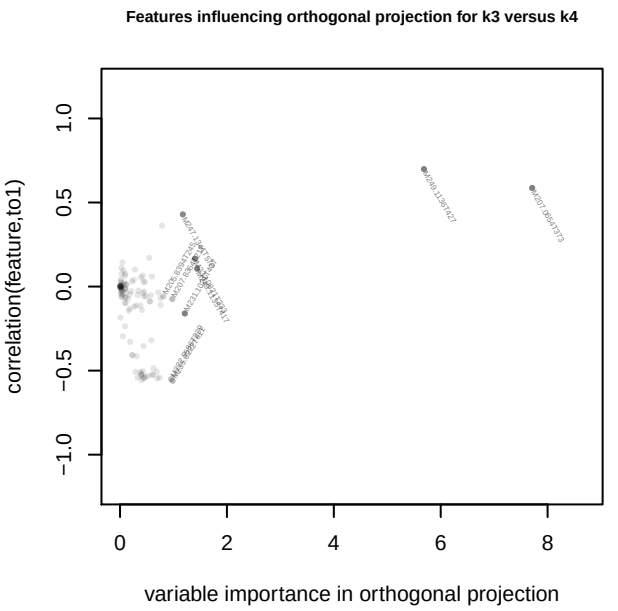

Significant features for level k3 versus k4
correlation(feature,t1)
relative covariance(feature,t1)
k3
k4


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


Model overview
R2Y
Q2Y
p1
o1
k3 versus k4


Features influencing orthogonal projection for k3 versus k4
correlation(feature,to1)
relative covariance(feature,to1)


Significant features for level k3 versus k4
correlation(feature,t1)
variable importance in predictor−projection


Features influencing orthogonal projection for k3 versus k4
correlation(feature,to1)
variable importance in orthogonal projection