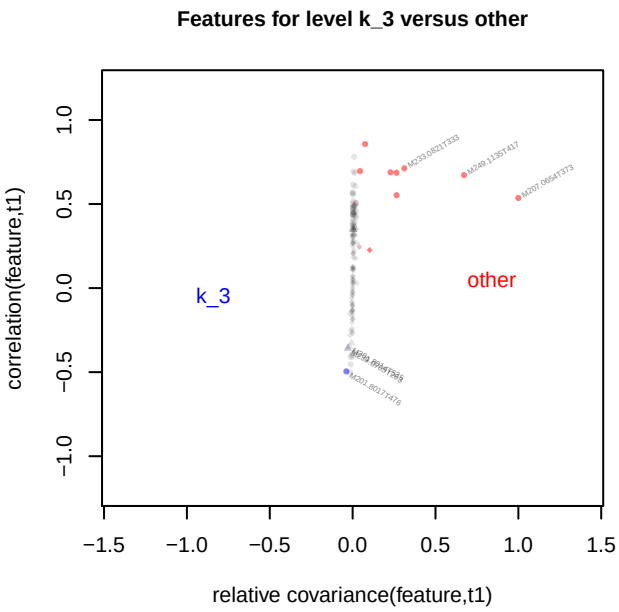
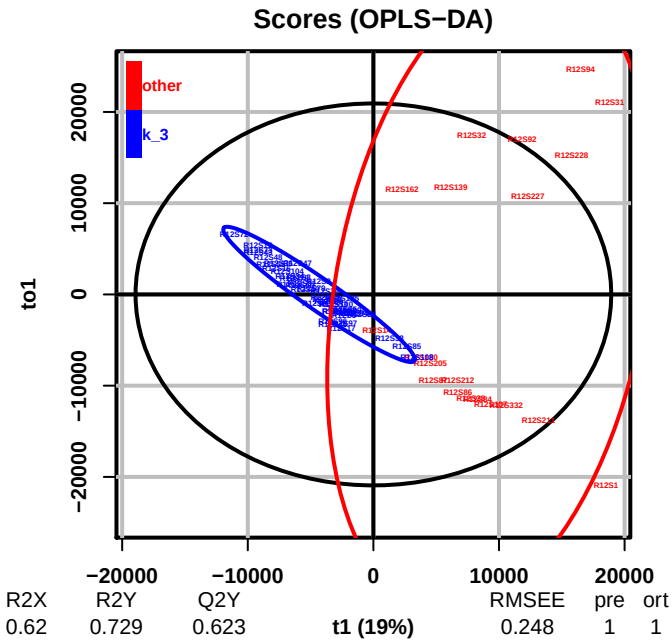
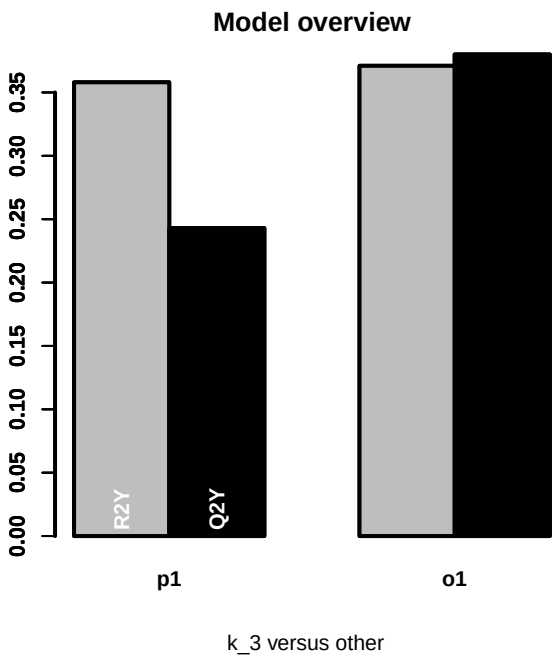
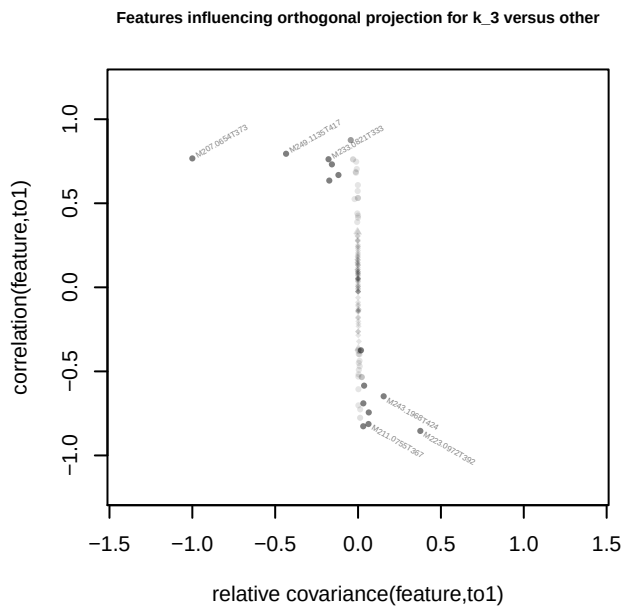
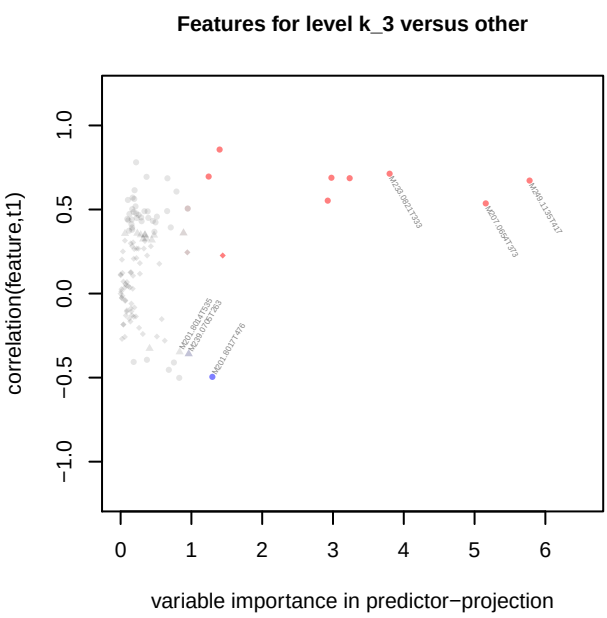
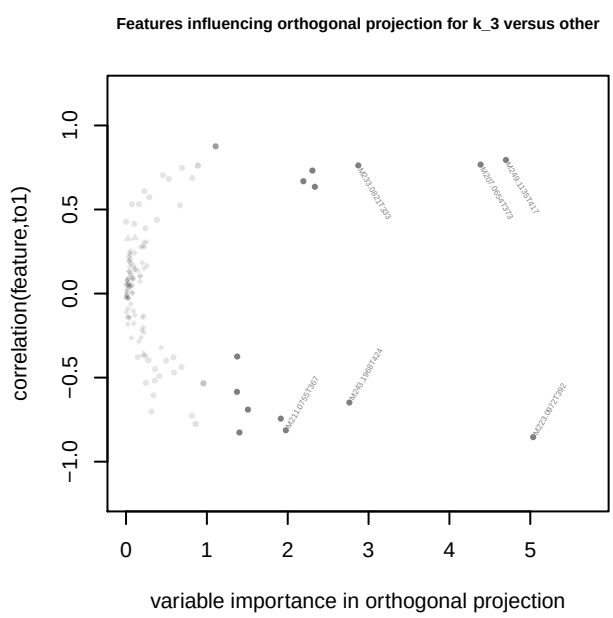

Features for level k_3 versus other
correlation(feature,t1)
relative covariance(feature,t1)
k_3
other

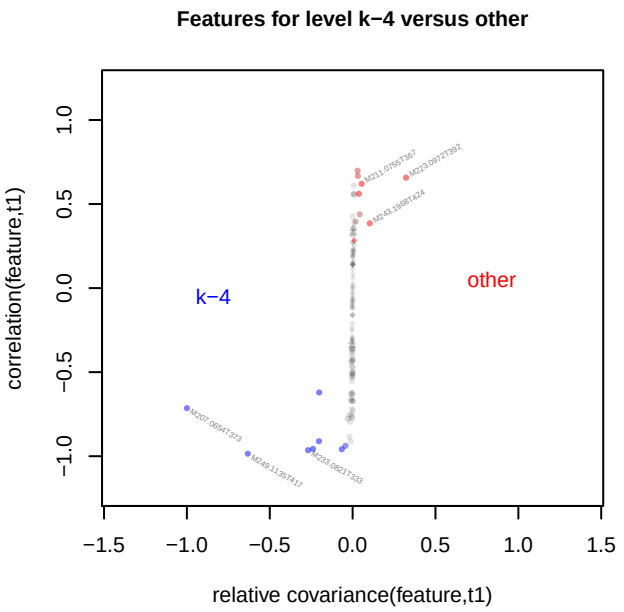

Scores (OPLS−DA)
other
k_3
to1
t1 (19%)
R2X 0.62
R2Y 0.729
Q2Y 0.623
RMSEE 0.248
pre 1
ort 1

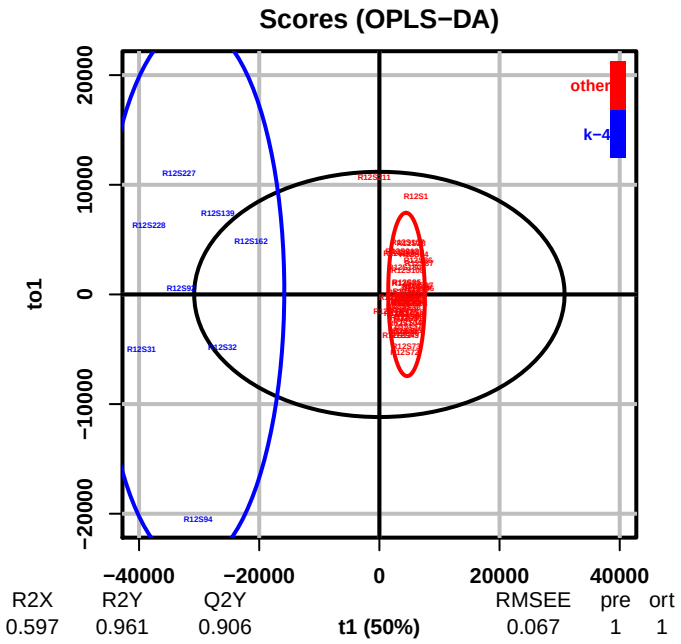

Model overview
R2Y
Q2Y
p1
o1
k_3 versus other

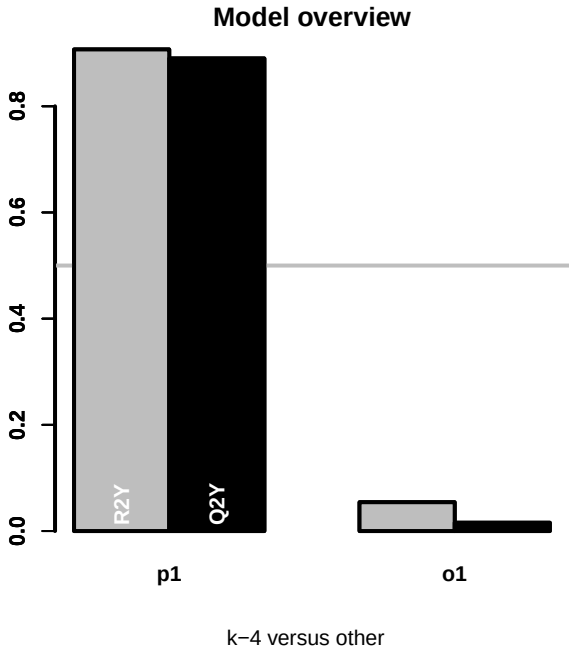

Features influencing orthogonal projection for k_3 versus other
correlation(feature,to1)
relative covariance(feature,to1)

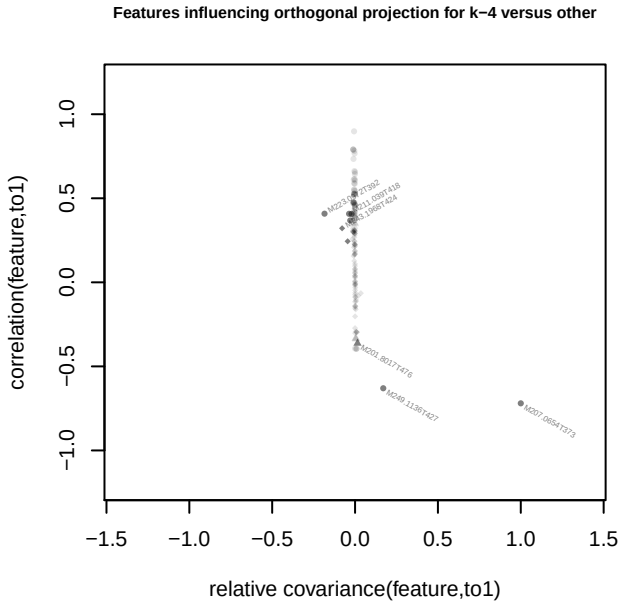

Features for level k_3 versus other
correlation(feature,t1)
variable importance in predictor−projection

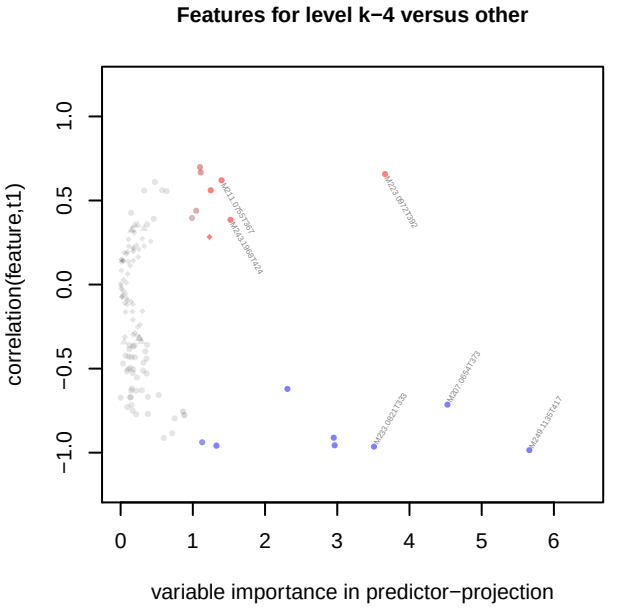

Features influencing orthogonal projection for k_3 versus other
correlation(feature,to1)
variable importance in orthogonal projection

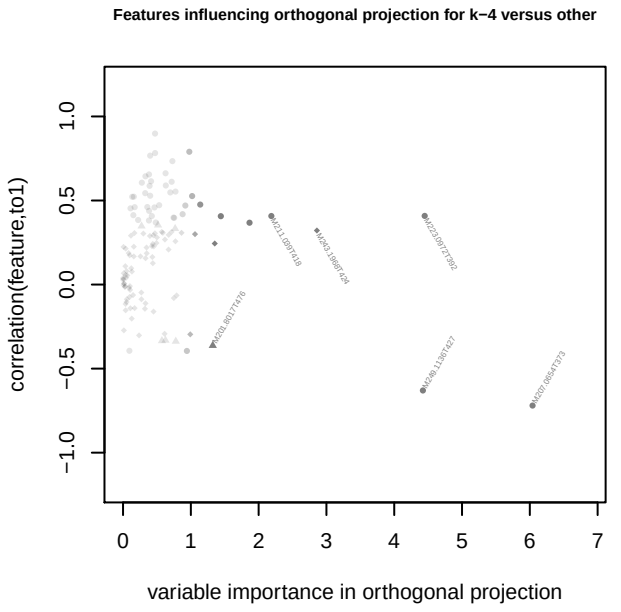

Features for level k−4 versus other
correlation(feature,t1)
relative covariance(feature,t1)
k−4
other

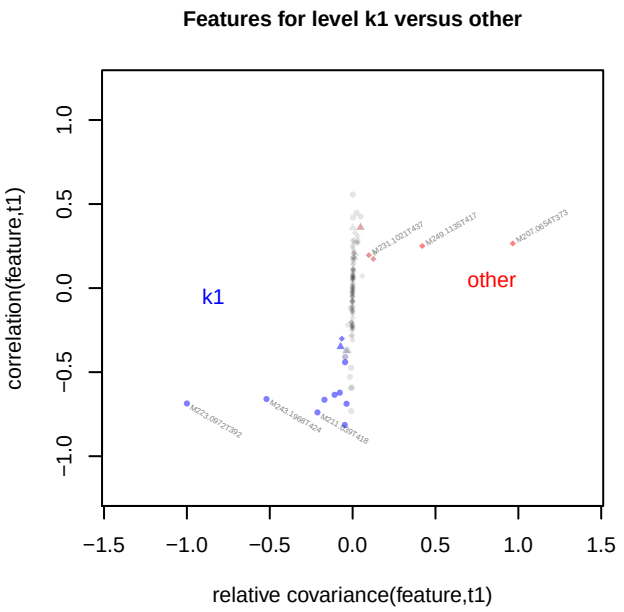

Scores (OPLS−DA)
other
k−4
to1
t1 (50%)
R2X R2Y Q2Y RMSEE pre ort
0.597 0.961 0.906 0.067 1 1

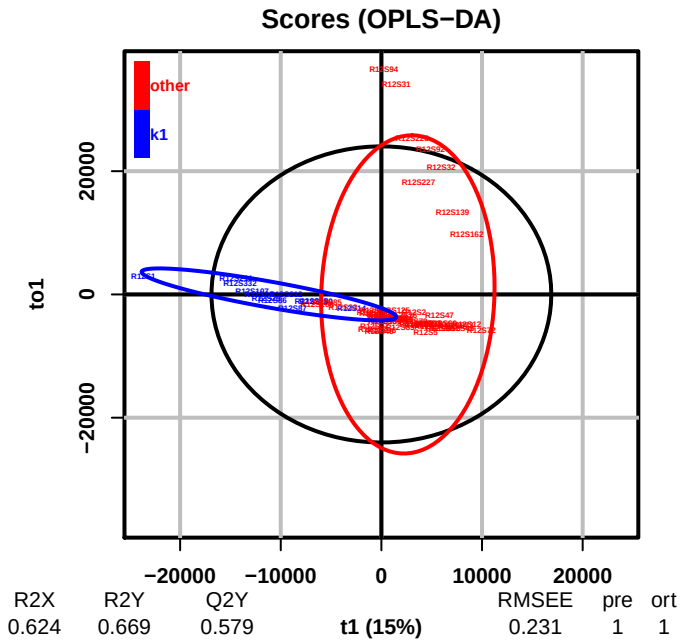

Model overview
R2Y
Q2Y
p1
o1
k−4 versus other

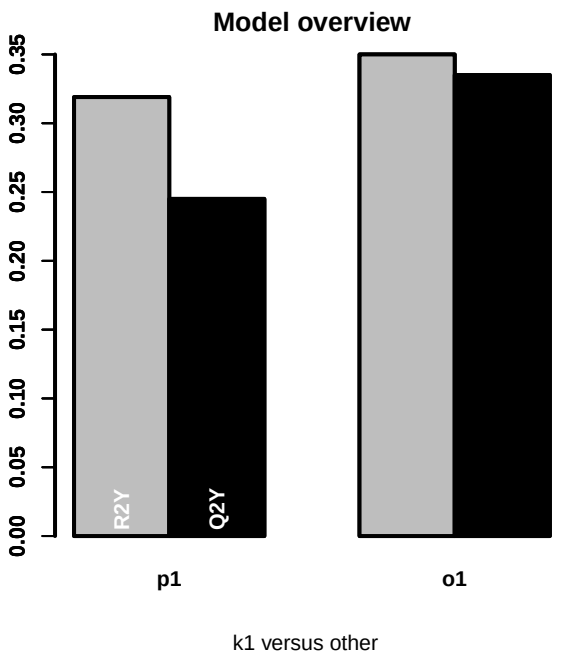

Features influencing orthogonal projection for k−4 versus other
correlation(feature,to1)
relative covariance(feature,to1)

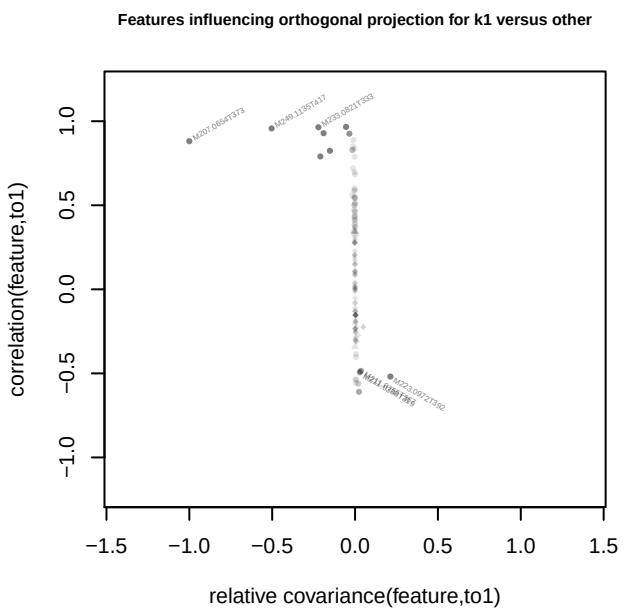

Features for level k−4 versus other
correlation(feature,t1)
variable importance in predictor−projection

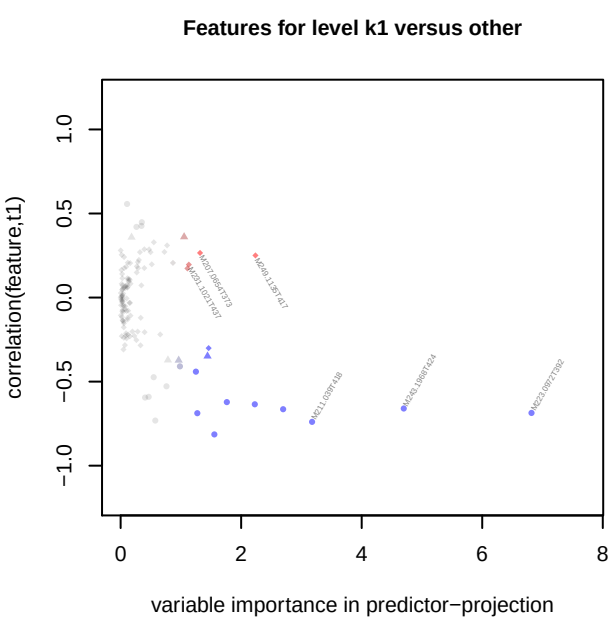

Features influencing orthogonal projection for k−4 versus other
correlation(feature,to1)
variable importance in orthogonal projection

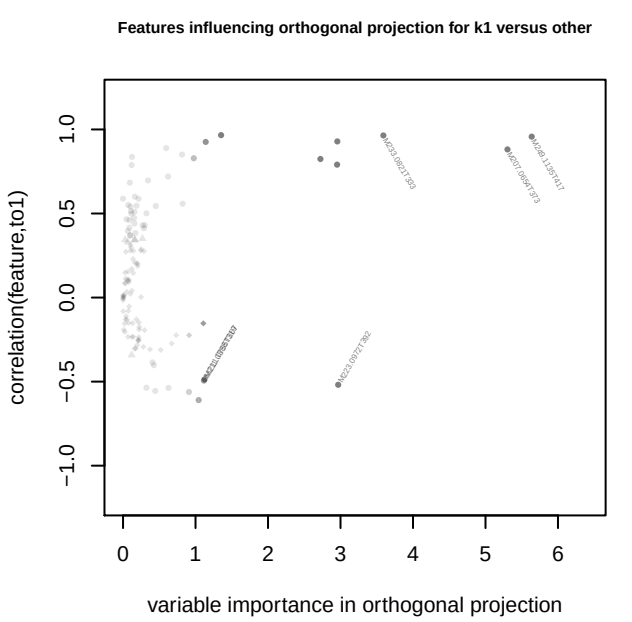

Features for level k1 versus other
correlation(feature,t1)
relative covariance(feature,t1)
k1
other

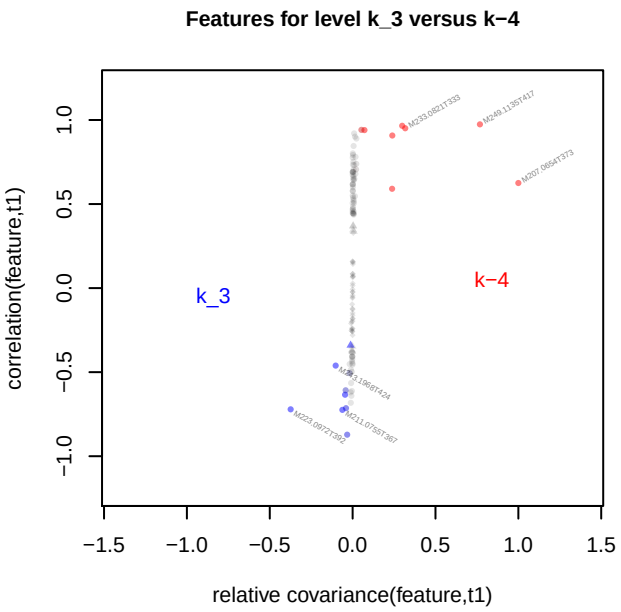

Scores (OPLS−DA)
other
k1
to1
t1 (15%)
R2X 0.624
R2Y 0.669
Q2Y 0.579
RMSEE 0.231
pre 1
ort 1

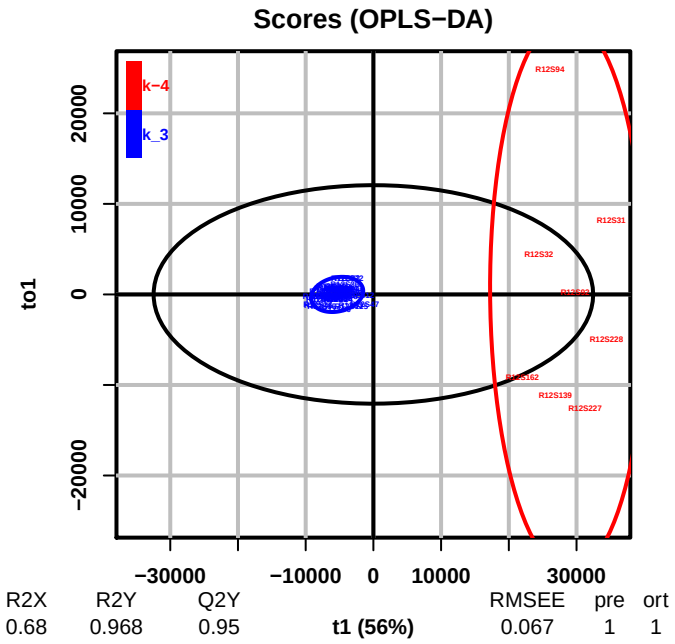

Model overview
R2Y
Q2Y
p1
o1
k1 versus other

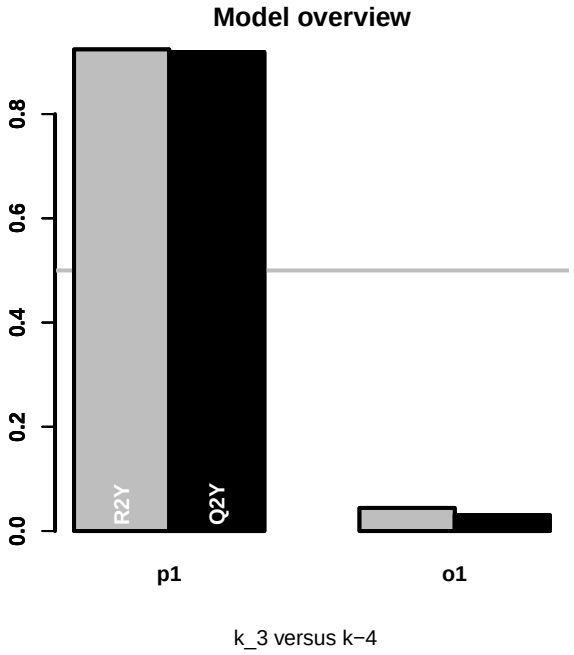

Features influencing orthogonal projection for k1 versus other
correlation(feature,to1)
relative covariance(feature,to1)

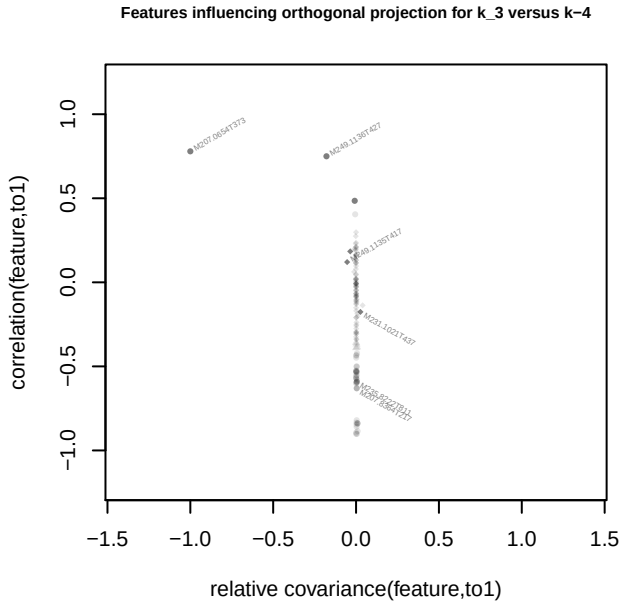

Features for level k1 versus other
correlation(feature,t1)
variable importance in predictor−projection

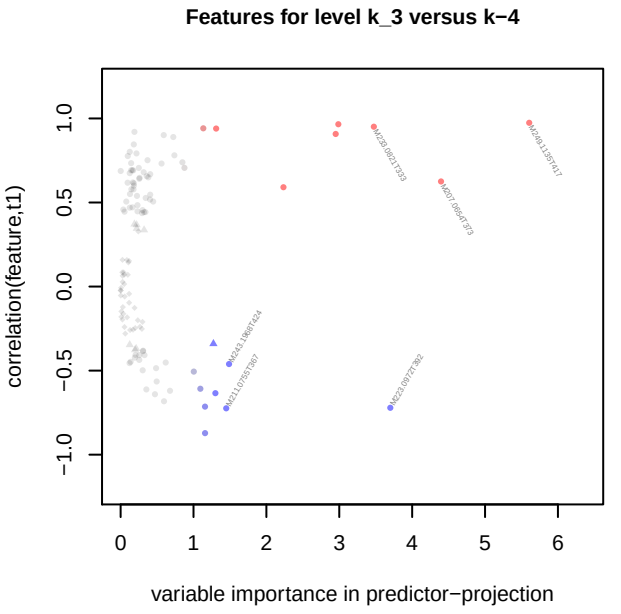

Features influencing orthogonal projection for k1 versus other
correlation(feature,to1)
variable importance in orthogonal projection

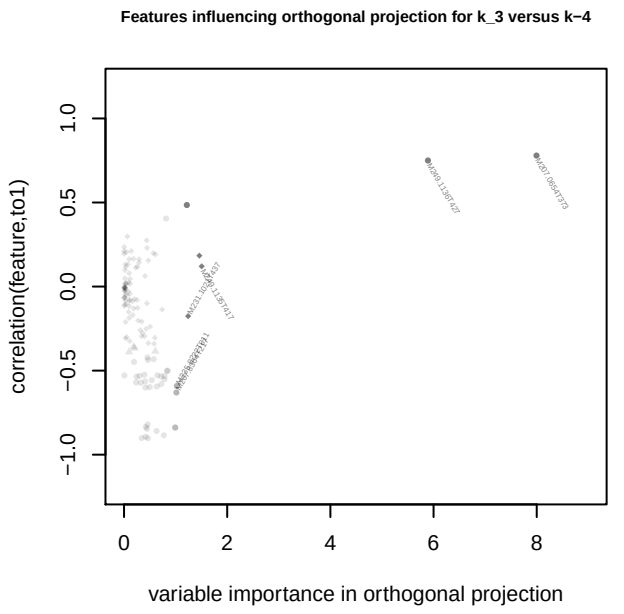

Features for level k_3 versus k−4
correlation(feature,t1)
relative covariance(feature,t1)
k_3
k−4

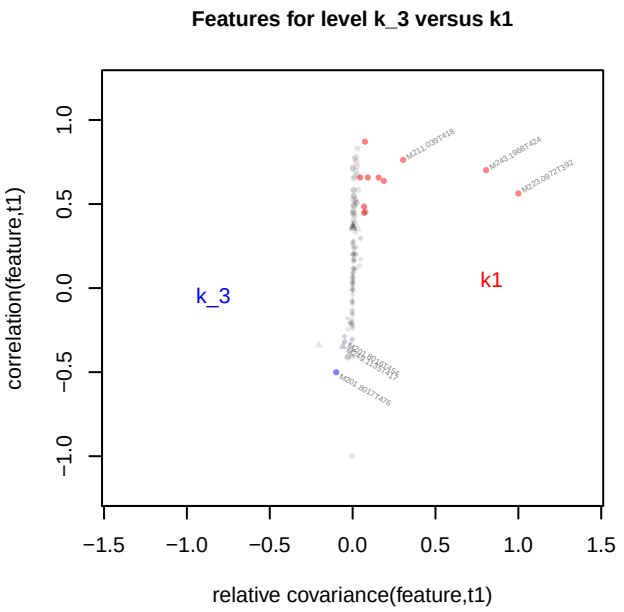

Scores (OPLS−DA)
k−4
k_3
to1
t1 (56%)
R2X 0.68
R2Y 0.968
Q2Y 0.95
RMSEE 0.067
pre 1
ort 1

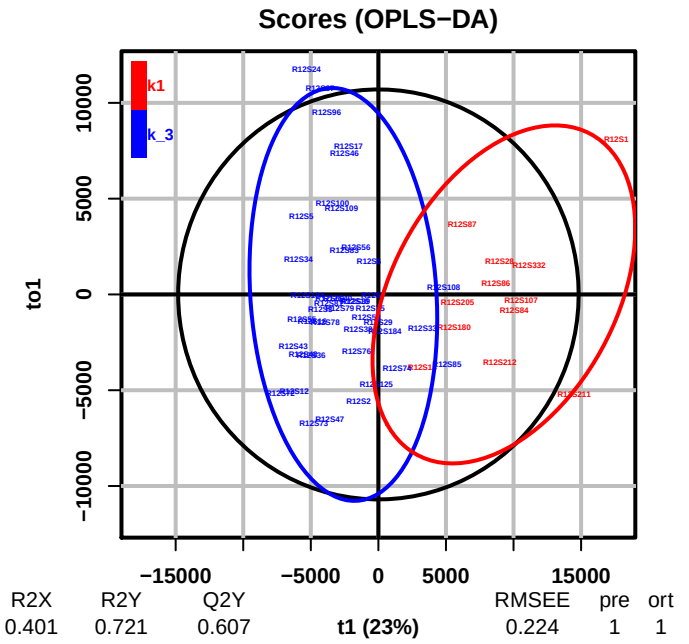

Model overview
R2Y
Q2Y
p1
o1
k_3 versus k−4

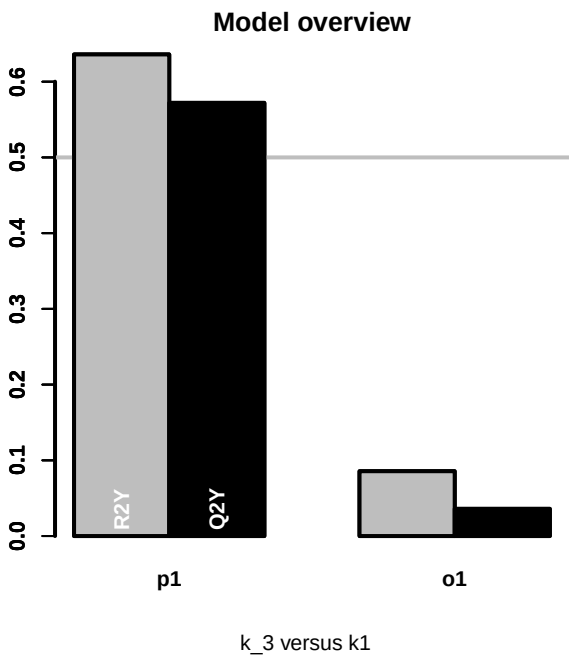

Features influencing orthogonal projection for k_3 versus k−4
correlation(feature,to1)
relative covariance(feature,to1)

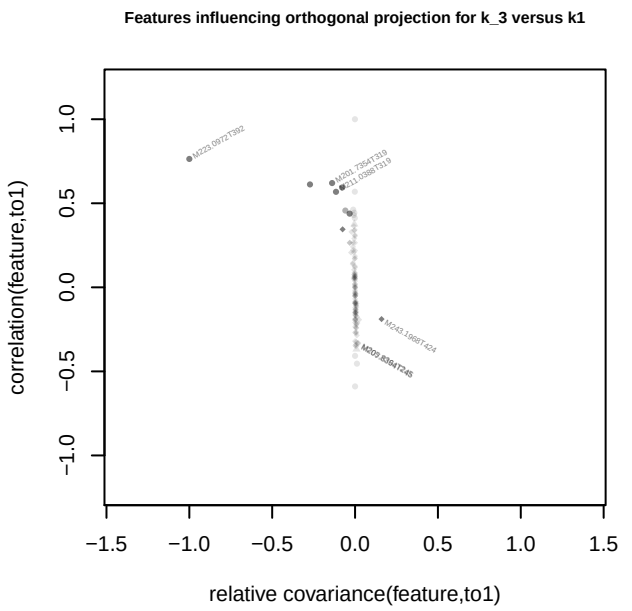

Features for level k_3 versus k−4
correlation(feature,t1)
variable importance in predictor−projection

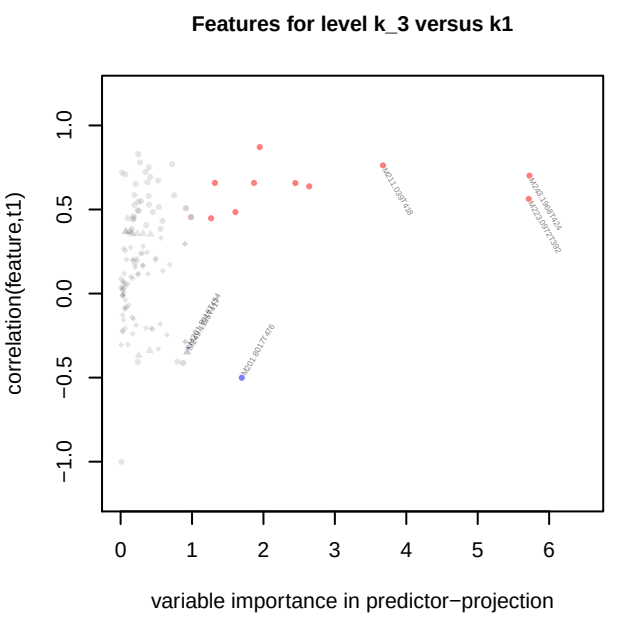

Features influencing orthogonal projection for k_3 versus k−4
correlation(feature,to1)
variable importance in orthogonal projection

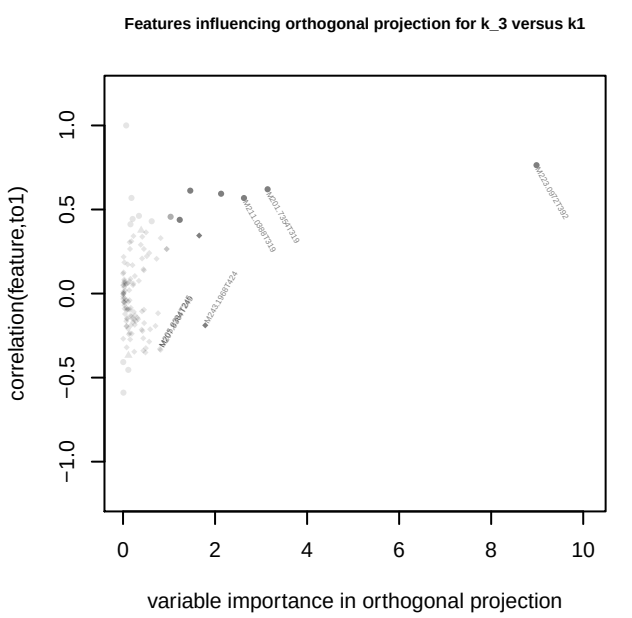

Features for level k_3 versus k1
correlation(feature,t1)
relative covariance(feature,t1)
k_3
k1

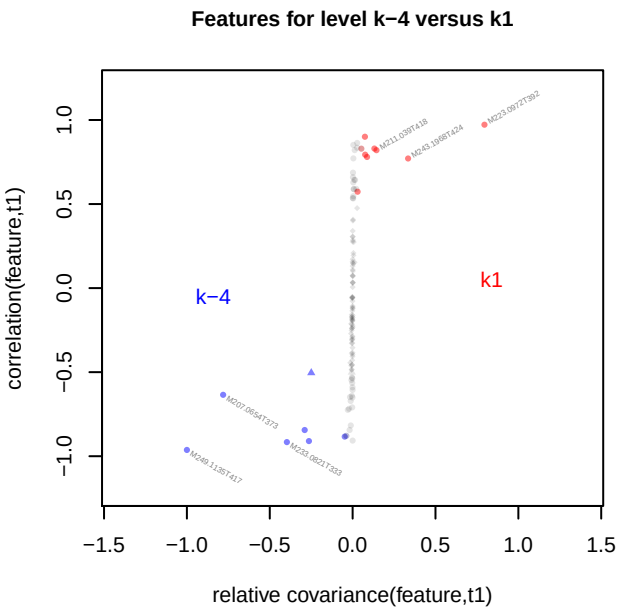

Scores (OPLS−DA)
k1
k_3
to1
t1 (23%)
R2X 0.401
R2Y 0.721
Q2Y 0.607
RMSEE 0.224
pre 1
ort 1

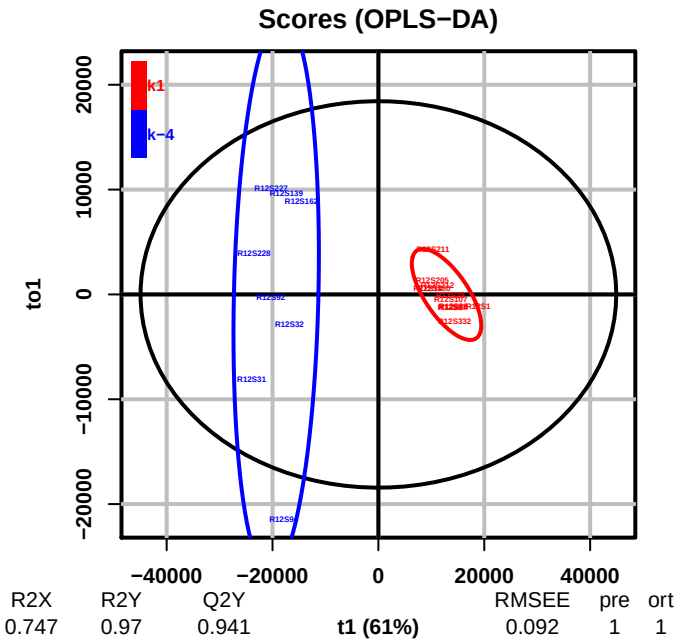

Model overview
R2Y
Q2Y
p1
o1
k_3 versus k1

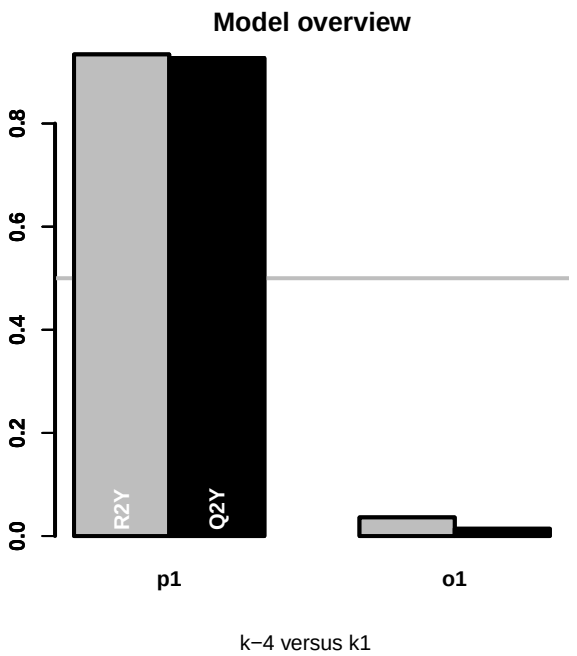

Features influencing orthogonal projection for k_3 versus k1
correlation(feature,to1)
relative covariance(feature,to1)

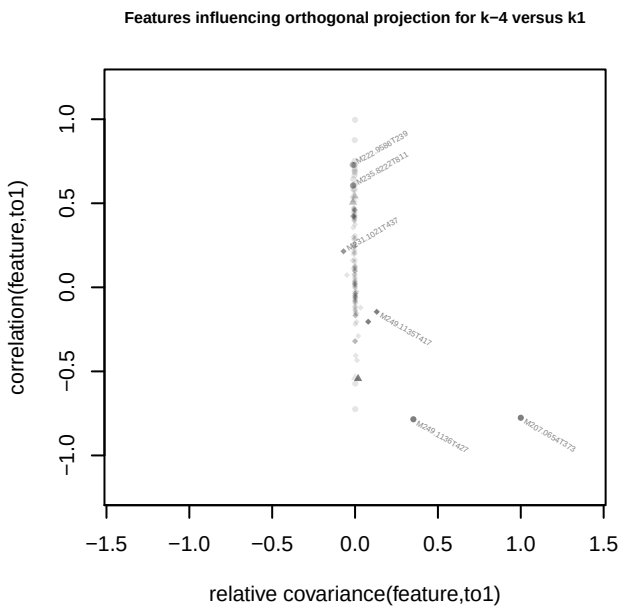

Features for level k_3 versus k1
correlation(feature,t1)
variable importance in predictor−projection

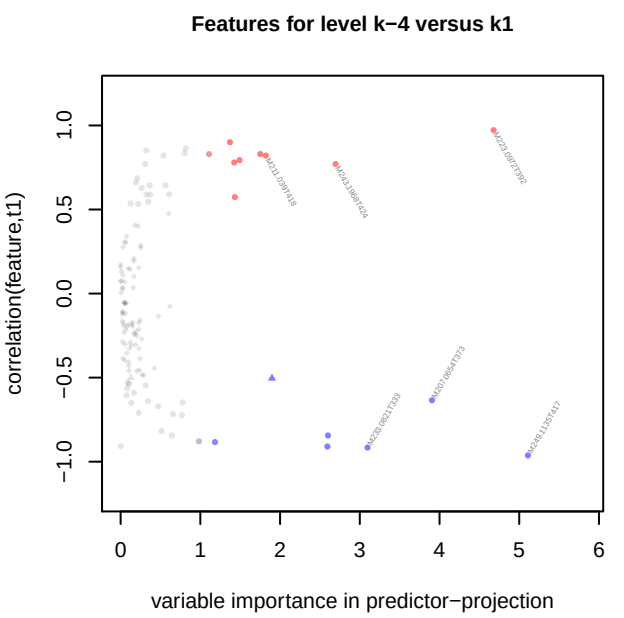

Features influencing orthogonal projection for k_3 versus k1
correlation(feature,to1)
variable importance in orthogonal projection

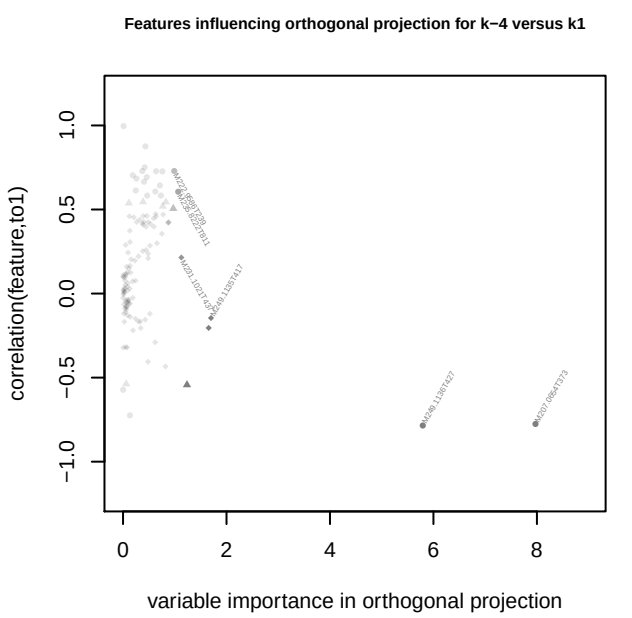

Features for level k−4 versus k1
correlation(feature,t1)
relative covariance(feature,t1)
k−4
k1
M211.0397T418
M243.1868T424
M223.0972T392
M207.0654T373
M233.0621T333
M249.1135T417


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


Model overview
R2Y
Q2Y
p1
o1
k−4 versus k1


Features influencing orthogonal projection for k−4 versus k1
correlation(feature,to1)
relative covariance(feature,to1)


Features for level k−4 versus k1
correlation(feature,t1)
variable importance in predictor−projection


Features influencing orthogonal projection for k−4 versus k1
correlation(feature,to1)
variable importance in orthogonal projection