Features for level k1 versus other

Scores (OPLS-DA)

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.547	0.547	0.45	**t1 (18%)**	0.229	1	1

Model overview

k1 versus other

Features influencing orthogonal projection for k1 versus other

Features for level k2 versus other

correlation(feature,t1)

1.0

0.5

0.0

−0.5

−1.0

k2

other

−1.0   −0.5   0.0   0.5   1.0

relative covariance(feature,t1)

Scores (OPLS−DA)

other

k2

to1

20000

10000

0

−20000

R12S94

R12S31

R12S32   R12S1

R12S145

−20000   −10000   0   10000   20000

t1 (21%)

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.375	0.831	0.76		0.196	1	1

Model overview

0.6

0.4

0.2

0.0

R2Y   Q2Y

p1   o1

k2 versus other

Features influencing orthogonal projection for k2 versus other

correlation(feature,to1)

1.0

0.5

0.0

−0.5

−1.0

−1.0   −0.5   0.0   0.5   1.0

relative covariance(feature,to1)

Features for level k3 versus other

correlation(feature,t1) vs relative covariance(feature,t1)

k3   other

Scores (OPLS−DA)

other
k3

to1 vs t1 (20%)

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.564	0.634	0.569		0.307	1	1

Model overview

R2Y   Q2Y

p1   o1

k3 versus other

Features influencing orthogonal projection for k3 versus other

correlation(feature,to1) vs relative covariance(feature,to1)

Features for level k4 versus other

Scores (OPLS−DA)

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.584	0.915	0.892	**t1 (39%)**	0.083	1	1

Model overview

k4 versus other

Features influencing orthogonal projection for k4 versus other

Features for level k1 versus k2

correlation(feature,t1)

relative covariance(feature,t1)

k1

k2

Scores (OPLS−DA)

k2
k1

to1

R12S117

R12S135
R12S161
R12S145
R12S209
R12S107
R12S84
R12S156
R12S154
R12S86
R12S211
R12S14
R12S218
R12S110
R12S28
R12S87
R12S196
R12S180
R12S212
R12S332
R12S167
R12S189
R12S224
R12S205
R12S133
R12S217
R12S183
R12S1
R12S15

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.572	0.879	0.805	**t1 (44%)**	0.163	1	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)

Features for level k1 versus k3

correlation(feature,t1)

1.0

0.5

k1

k3

0.0

−0.5

−1.0

−1.0 −0.5 0.0 0.5 1.0

relative covariance(feature,t1)

Scores (OPLS−DA)

k3
k1

to1

10000

5000

0

−5000

−10000

−15000 −5000 0 5000 15000

R2X	R2Y	Q2Y	**t1 (23%)**	RMSEE	pre	ort
0.401	0.721	0.607		0.224	1	1

Model overview

0.6

0.5

0.4

0.3

0.2

0.1

0.0

R2Y Q2Y

p1   o1

k1 versus k3

Features influencing orthogonal projection for k1 versus k3

correlation(feature,to1)

1.0

0.5

0.0

−0.5

−1.0

−1.0 −0.5 0.0 0.5 1.0

relative covariance(feature,to1)

Features for level k1 versus k4

correlation(feature,t1)

relative covariance(feature,t1)

k1

k4

Scores (OPLS−DA)

k4

k1

to1

R12S94

R12S31

R12S32

R12S92

R12S228

R12S162
R12S13
R12S227

R12S33
R12S107
R12S28

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.747	0.97	0.941	**t1 (61%)**	0.092	1	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)

Features for level k2 versus k3

correlation(feature,t1)

relative covariance(feature,t1)

k2

k3

Scores (OPLS−DA)

k3

k2

to1

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.524	0.9	0.874	**t1 (38%)**	0.159	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)

Features for level k2 versus k4

correlation(feature,t1)

relative covariance(feature,t1)

k2

k4

Scores (OPLS−DA)

k4

k2

to1

R12S94

R12S115

R12S31

R12S32

R12S92

R12S228

R2X R2Y Q2Y RMSEE pre ort
0.669 0.943 0.926 **t1 (56%)** 0.102 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)

Features for level k3 versus k4

correlation(feature,t1)

k3

k4

relative covariance(feature,t1)

Scores (OPLS–DA)

k4

k3

to1

R12S94

R12S31

R12S32

R12S99

R12S228

R12S162

R12S139

R12S227

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.68	0.968	0.95	**t1 (56%)**	0.067	1	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)