

PLS

PLSはpartial least squares : 部分最小二乗法

Partial least squares (PLS)

- 部分最小二乗法は連立方程式を解く方法の一つ. (PLS1)
 - $y = XB$

$$\bullet y: \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} \quad X: \begin{pmatrix} x_{11} & x_{12} & \cdot & \cdot & x_{1m} \\ x_{21} & x_{22} & \cdot & \cdot & x_{2m} \\ & & \cdot & & \\ & & \cdot & & \\ x_{n1} & x_{n2} & \cdot & \cdot & x_{nm} \end{pmatrix}$$

$$\bullet B: \begin{pmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ b_m \end{pmatrix}$$

$$\bullet y_1 = b_1 x_{11} + b_2 x_{12} + \cdot \cdot + b_m x_{1m}$$

- PLS1はXとyを線形分解します
 - $X = TP^t + E$ と $y = Tq + f$, ここで
 - T: スコア
 - P: X 負荷量 q: y 負荷量
 - E: X 残差 f: y 残差
- Tとyの共分散が最大になるように分解されます。

$$w = \frac{\mathbf{x}^T \mathbf{y}}{\|\mathbf{x}^T \mathbf{y}\|} \quad \mathbf{b} = \mathbf{W}(\mathbf{P}^T \mathbf{W})^{-1} \mathbf{q}$$

PLSの目的

• PLS で次の方程式を解きます

• $Y = XB$

• この例だと

- Y: ユーザー入力
- X: 各m/zの信号強度
- B: regression coefficient

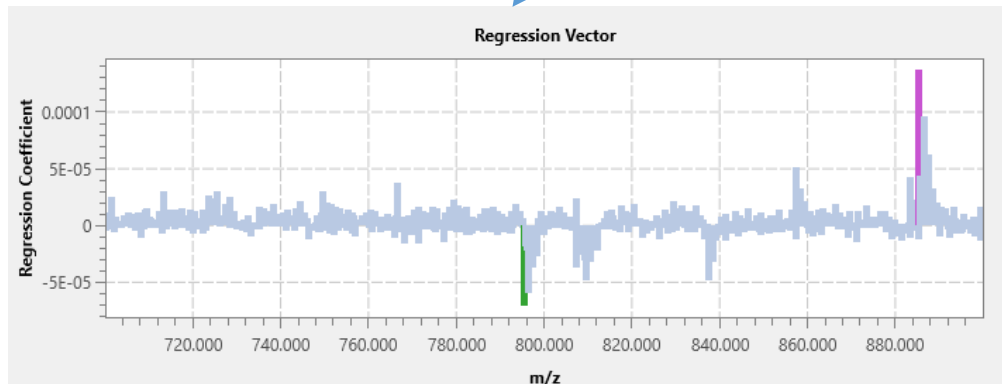
PLS Parameter

Number of Latent Variables: Auto Manual (5)

Pre-processing: Pareto Scale

ROI List

No.	File Name	ROI Name	Attribute	Y value
1	Testicle_9AA_Pi_SL_5x_1...	ROI001	Group A	1.00000
2	Testicle_9AA_Pi_SL_5x_1...	ROI002	Group B	0.00000
3	Testicle_9AA_Pi_SL_5x_1...	ROI003	Group C	0.00000



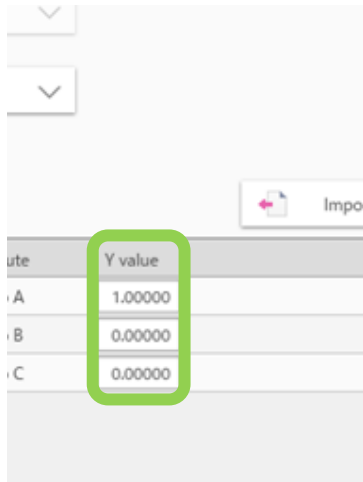
Data Matrix Table

No.	Use	Tag	Label	m/z	ROI001	ROI002	ROI003
1	<input checked="" type="checkbox"/>		699.9849-700.1849	700.0849	1335.372	955.008	719.154
2	<input checked="" type="checkbox"/>		700.1849-700.3849	700.2849	3233.055	2285.856	4259.140
3	<input checked="" type="checkbox"/>		700.3849-700.5849	700.4849	7135.789	6658.481	6215.483
4	<input checked="" type="checkbox"/>		700.5849-700.7849	700.6849	350.186	557.643	704.661
5	<input checked="" type="checkbox"/>		700.7849-700.9849	700.8849	599.713	535.929	1297.413
6	<input checked="" type="checkbox"/>		700.9849-701.1849	701.0849	1603.896	1003.419	1719.029
7	<input checked="" type="checkbox"/>		701.1849-701.3849	701.2849	3562.864	3135.136	6112.206
8	<input checked="" type="checkbox"/>		701.3849-701.5849	701.4849	4053.940	4716.231	11056.985
9	<input checked="" type="checkbox"/>		701.5849-701.7849	701.6849	364.000	440.763	147.480
10	<input checked="" type="checkbox"/>		701.7849-701.9849	701.8849	547.404	453.994	1172.073
11	<input checked="" type="checkbox"/>		701.9849-702.1849	702.0849	1298.887	1064.758	1399.292
12	<input checked="" type="checkbox"/>		702.1849-702.3849	702.2849	2988.290	1353.019	2972.140
13	<input checked="" type="checkbox"/>		702.3849-702.5849	702.4849	2129.094	2368.437	5835.236
14	<input checked="" type="checkbox"/>		702.5849-702.7849	702.6849	205.491	299.329	127.194
15	<input checked="" type="checkbox"/>		702.7849-702.9849	702.8849	254.150	323.080	207.405
16	<input checked="" type="checkbox"/>		702.9849-703.1849	703.0849	1143.333	1304.598	1899.105
17	<input checked="" type="checkbox"/>		703.1849-703.3849	703.2849	2979.481	2536.971	3065.977
18	<input checked="" type="checkbox"/>		703.3849-703.5849	703.4849	4640.529	3625.504	6333.597
19	<input checked="" type="checkbox"/>		703.5849-703.7849	703.6849	383.706	380.487	874.887
20	<input checked="" type="checkbox"/>		703.7849-703.9849	703.8849	476.825	328.199	732.437

IMAGEREVEAL MS内では

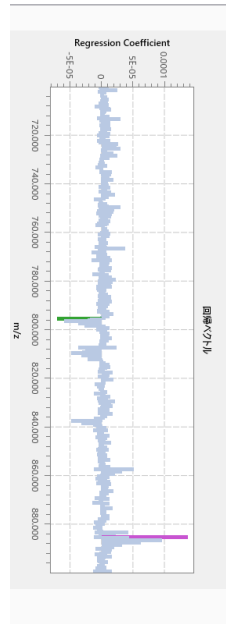
y : ユーザー入力
X: 各m/zの信号強度
B: 計算される

$$y = X B$$



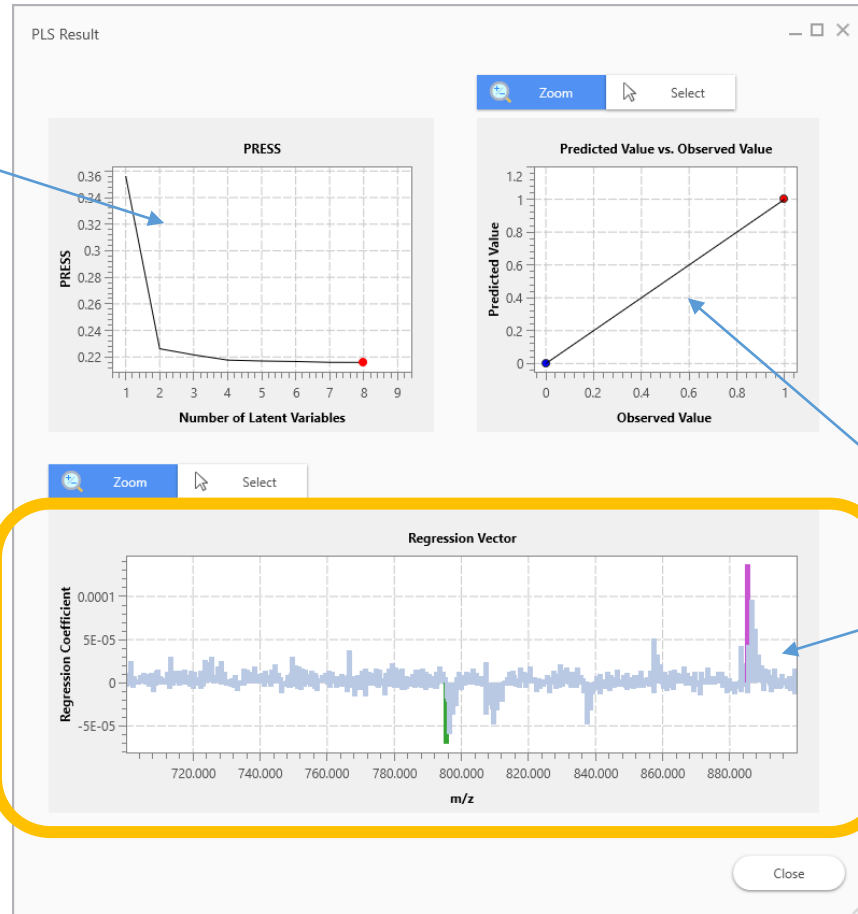
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m/z	Signal Intensity
107.0846	44.0243
107.0846	38.1288
107.0846	25.5204
107.0846	18.4781
107.0846	11.0733
107.0846	7.00728
107.0846	3.87131
107.0846	3.02723
107.0846	1.12044
107.0846	0.88828
107.0846	0.71020
107.0846	0.58781
107.0846	0.41033
107.0846	0.24344
107.0846	0.16700
107.0846	0.10273
107.0846	0.06379
107.0846	0.03524
107.0846	0.02113
107.0846	0.01208
107.0846	0.00700
107.0846	0.00384
107.0846	0.00208
107.0846	0.00110
107.0846	0.00058
107.0846	0.00030
107.0846	0.00016
107.0846	0.00008

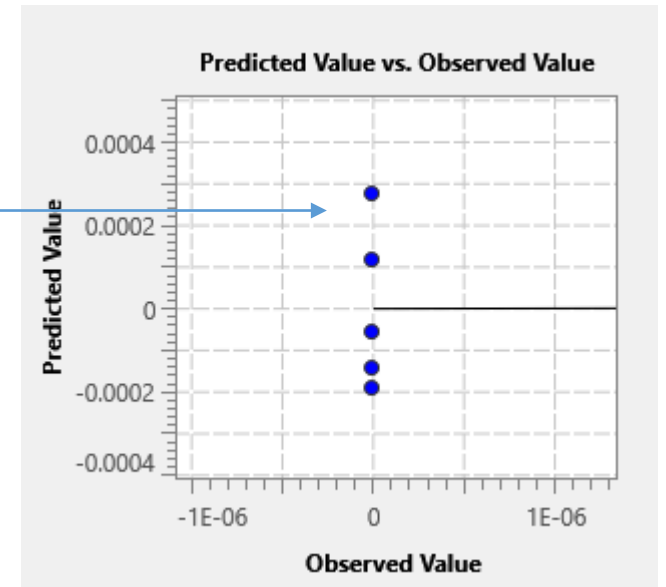


PLS の結果

幾つの潜在変数が予測
にいいか



“予測” は “計算結果” です



“観測値” は “入力値” です

$$Y = XB$$

回帰係数は“データ行列テーブル”にも表示されます。

データ行列テーブル

No.	使用	タグ	ラベル	m/z	PLS係数	<input checked="" type="checkbox"/> ROI001	<input checked="" type="checkbox"/> ROI006	<input checked="" type="checkbox"/> ROI007
1	<input checked="" type="checkbox"/>		699.9849-700.1849	700.0849	-1.031e-005	3826.025	7539.937	7142.123
2	<input checked="" type="checkbox"/>		700.1849-700.3849	700.2849	-1.036e-005	16109.992	23400.471	19211.543
3	<input checked="" type="checkbox"/>		700.3849-700.5849	700.4849	-1.959e-005	21877.961	42638.046	33311.234
4	<input checked="" type="checkbox"/>		700.5849-700.7849	700.6849	6.367e-006	1467.580	190.273	111.123
5	<input checked="" type="checkbox"/>		700.7849-700.9849	700.8849	-2.211e-006	1273.433	1008.485	201.123
6	<input checked="" type="checkbox"/>		700.9849-701.1849	701.0849	7.801e-006	7208.971	6658.819	301.123
7	<input checked="" type="checkbox"/>		701.1849-701.3849	701.2849	-2.411e-005	22713.335	30928.034	56211.123
8	<input checked="" type="checkbox"/>		701.3849-701.5849	701.4849	-1.822e-005	14148.507	55911.353	21411.123
9	<input checked="" type="checkbox"/>		701.5849-701.7849	701.6849	1.407e-006	2301.442	3029.906	1311.123
10	<input checked="" type="checkbox"/>		701.7849-701.9849	701.8849	-1.144e-005	855.183	5883.234	4911.123
11	<input checked="" type="checkbox"/>		701.9849-702.1849	702.0849	-4.200e-006	7153.956	20282.529	3811.123