Partial Least Squares Algorithms for PCA, Component-Based Regression and Predictive Path Modeling: the joining ring and their Non-Metric extension.

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What is PLS?

 \rightarrow It is an acronym standing for Partial Least Squares

 \rightarrow It refers to a family of ALGORITHMS implementing a suite of METHODS of multivariate analysis for analyzing one, two or several blocks of variables

 \rightarrow All these algorithms are iterative algorithms

 \rightarrow These algorithms consist of various extensions of the Nonlinear estimation by Iterative PArtial Least Squares (NIPALS) algorithm

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Nonlinear Iterative Partial Least Squares

- **NIPALS** (Wold H., 1966), algorithm is an iterative algorithm for implementing a PCA to a block **X** of variables.
- The peculiarity of this algorithm is that it calculates principal components by means of an iterative sequence of simple ordinary least squares (OLS) regressions.
- This feature enables us to overcome computational problems due to missing data or landscape data matrices, i.e. matrices having more columns than rows.





Deflation: Find $\mathbf{E}_{1(1)}$ as the residual matrix of the regression of \mathbf{X} on $\mathbf{t}_{(1)}$

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The PLS family

- By using NIPALS-based algorithms, i.e. PLS algorithms, applied on one or several blocks of variables is possible to perform a large number of well known MDA methods, such as:
 - \rightarrow PCA (Hotelling, 1933)
 - \rightarrow CCA (Hotelling, 1936)
 - → Tucker Interbactery Analysis (Tucker, 1958)
 - → Redundancy Analysis (Van de Wollenberg, 1977)
 - → Horst and Carroll GCCA (Horst, 1965; Carroll, 1968)
 - → Multi-tables analysis (Kettenring, 1971)
 - → Analyse Factorielle Multiple (Escofier, 1994) among others

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The two PLS cultures

PLS Regression models (PLS-R)

- 2 blocks of variables (X₁, X₂)
 (at least originally, then
 L-PLSR, U-PLSR, etc.)
- Component-based Regularized regression tool
- Chemometrics and related areas, Biometrics, Anthropology
- Some references:

(non exhaustive list)

- Wold S., Martens H. and Wold H., 1983
- Martens H. and Næs T., 1991
- Tenenhaus M., 1998

PLS Path Modeling (PLS-PM)

- Several blocks of variables $(X_1, ..., X_Q)$ linked by interdependent regressions
- Predictive approach to network of dependence relationships (SEM), hierarchical models (MTA)
- Econometrics, Social Sciences, Marketing, Strategic Management
- Some references: (non exhaustive list)
 - Wold H., 1982, 1985, 1966, 1975, 1977
 - Fornell C., Bookstein F.L., 1982
 - Lohmöller J.B., 1987, 1989
 - Chin W.W., 1998
 - Tenenhaus M. et al., 2005
 - Esposito Vinzi V. et al., 2010

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PLS Regression criterion

Research of *H* (chosen by **cross-validation**) **orthogonal** components $\mathbf{t}_{1(h)} = \mathbf{X}_1 \mathbf{w}_{1(h)}$ and $\mathbf{t}_{2(h)} = \mathbf{X}_2 \mathbf{w}_{2(h)}$ as **correlated** between them as possible **and explanatory** of their own groups.

 $Cov^{2}(t_{1(h)}, t_{2(h)}) =$ $Cor^{2}(t_{1(h)}, t_{2(h)}) * Var(t_{1(h)}) * Var(t_{2(h)})$

PLS2 regression leads to a compromise between a canonical correlation analysis between Y and X and two principal component analyses of X (orthogonal) and Y (oblique = non orthogonal components).

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PLS-R is useful for..

- 1. Prediction (Regression equation)
- 2. Visualization (PLS = Projection on Latent Structures)
- 3. Regularization (Full component PLS1 coefficients = OLS coefficients)

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Structural Equation Models: inner model

ξ₂

β₁₃

β₂₃

The structural model describes the causations among the latent variables.



$$\boldsymbol{\xi}_{j} = \sum_{m=1}^{M} \beta_{mj} \boldsymbol{\xi}_{m} + \boldsymbol{\zeta}_{j}$$

where:

- B_{mj} is the path-coefficient linking the *m*-th LV to the *j*-th endogenous LV

- *M* is the number of the explanatory LVs impacting on ξ_i

Structural Equation Models: outer model



Mode A

$$\mathbf{x}_{pq} = \lambda_{pq} \boldsymbol{\xi}_q + \boldsymbol{\varepsilon}_{pq}$$

- **OLS simple regressions** not affected by multicollinearity
- LV is a principal component of its MV's (minimizes outer residual variances) under the constraint of being the best neighbor of its adjacent LV's (minimizes inner residual variances)

$$\xi_q = \sum_{p=1}^{p_q} \omega_{pq} \mathbf{x}_{pq} + \delta_q$$

- **OLS multiple regression** affected by multicollinearity
- LV is the best predictor of its MV's under the constraint of minimizing the trace of the residual variances in the structural model
- Aim at **minimizing residuals** in structural relationships (explanation of unobserved variance)

Mode B



After convergence: OLS simple/multiple regressions on LV scores for path coefficients

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After convergence: OLS simple/multiple regressions on LV scores for path coefficients

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Three PLS Criteria

- NIPALS: $\underset{\|\mathbf{w}\|=1}{\operatorname{argmax}} \{\operatorname{var}(\mathbf{X}\mathbf{w})\}$ • PLS-R: $\underset{\|\mathbf{w}_1\|=\|\mathbf{w}_2\|=1}{\operatorname{argmax}} \{\operatorname{cov}^2(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)\}$
- Full Mode A PLS-PM
- Full New Mode A PLS-PM (Wold algorithm): $\arg \max_{\|\mathbf{w}_q\|=1} \left\{ \sum_{q \neq q'} c_{qq'} g\left(\operatorname{cov} \left(\mathbf{X}_q \mathbf{w}_q, \mathbf{X}_{q'} \mathbf{w}_{q'} \right) \right) \right\}$ (*T* = 1 = 0, *T* = 1 = 2000)

(Tenenhaus & Tenenhaus, 2009)

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PLS algorithms: the joining ring (1)

Each iteration of a PLS algorithm can be resumed in three steps:

- 1. Compute weights
- 2. Normalize weights
- 3. Calculate the score vector(s)

NIPALS iteration	PLS-R iteration	new Mode A PLS-PM iteration
$\mathbf{w} = \mathbf{X}'(\mathbf{X}\mathbf{w})$	$\mathbf{w}_q = \mathbf{X}'_q(\mathbf{X}_{q'}\mathbf{w}_{q'})$	$\mathbf{w}_q = \mathbf{X}'_q(\sum_{q'} e_{qq'} \mathbf{X}_{q'} \mathbf{w}_{q'})$
$\operatorname{norm}(\mathbf{w})$	$\operatorname{norm}(\mathbf{w}_q)$	$\operatorname{norm}(\mathbf{w}_q)$
$\mathbf{t} = \mathbf{X}\mathbf{w}$	$\mathbf{t}_q = \mathbf{X}_q \mathbf{w}_q$	$\mathbf{t}_q = \mathbf{X}_q \mathbf{w}_q$
	$q \in \{1,2\}; \ q \neq q'$	$q \in \{1,2,\ldots,Q\}; \ q \neq q'$ $e_{qq'}$ is the generic element of a squared matrix of order Q that is null if $x_{q'}$ is connected to x_{q} ; otherwise, it represents the corresponding inner weight.
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PLS algorithms: the joining ring (2)

- In all of the previously showed PLS methods, when working on standardized variables, weights are calculated as Pearson's product-moment correlation coefficients between each variable and a latent construct.
- In homage to what Hayashi called *External Criterion* in its quantification methods, we call this latent construct *Latent Criterion* (LC, noted as γ)

$$W_{pq} \propto \operatorname{cor}(\mathbf{x}_{pq}, \boldsymbol{\gamma}_{q})$$

For each PLS method different LCs are considered:

- In NIPALS, the LC to bear in mind is the first PC.
- In PLS-R, we have to keep into account two LCs: the vector scores in predictor space for the response variables and the vector score in response space for the independent variables.
- In new Mode A PLS-PM, a LC is considered for each block of manifest variables, i.e. the corresponding inner estimate.

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A limit of PLS methods

This leads to two basic hypotheses underlying PLS models:

- Each variable is measured on a interval (or ratio) scale.
- **Relations** between variables and latent constructs **are linear and**, consequently, **monotone**.

As a consequence, standard PLS methods cannot handle data which are measured on a scale which does not have metric properties, nor non-linear relations.



Solution: the Non-Metric approach

A new class of PLS algorithms making the PLS iteration able to work as optimal scaling algorithms, calculating iteratively both scaling and model parameters: we name them

Non-Metric Partial Least Squares (NM-PLS) algorithms

because they are able to provide optimally scaled data $(\hat{\mathbf{X}})$ with a new metric structure, which does not depend on the metric properties of the raw data (\mathbf{X}^*) . In other words, NM-PLS methods yield a metric to non-metric data, and a new metric to metric data, linearizing the relations between variables and latent constructs, as required by the hypothesis of standard PLS models.

These methods could be named non-linear PLS methods as well, since they discard the intrinsic linearity hypothesis of standard PLS methods.

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Optimal Scaling

According to Young [1981], "Optimal scaling (OS) is a data analysis technique which assigns numerical values to observation categories in a way which maximizes the relation between the observations and the data analysis model while respecting the measurement character of the data"

- Hence, scalings provided by OS methods are optimal, if they satisfy two conditions:
- they optimize the same criterion of the analysis in which the Optimal Scaling is involved
- they respect the constraints defining which properties of the original measurement scale we want to preserve.

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Non-Metric PLS criteria

- NM-PLS algorithms optimize NIPALS, PLS-R and New Mode A PLS-PM criteria under two sets of parameters: the model parameters and the scaling parameters, constrained to the restrictions due to the scaling level chosen for each raw variable **X**^{*}
- **NM-NIPALS**:
- **NM-PLSR:**
- Full New Mode A NM-PLSPM (Wold algorithm):

$$\operatorname{arg\,max}_{\substack{\|\mathbf{w}\|=1, \\ \operatorname{var}(\hat{\mathbf{x}}_{p}=1)}} \left\{ \operatorname{var}(\hat{\mathbf{X}}\mathbf{w}) \right\} \\
\operatorname{arg\,max}_{\substack{\|\mathbf{w}_{1}\|=\|\mathbf{w}_{2}\|=1, \\ \operatorname{var}(\hat{\mathbf{x}}_{p1})=\operatorname{var}(\hat{\mathbf{x}}_{p2})=1}} \left\{ \operatorname{cov}^{2}(\hat{\mathbf{X}}_{1}\mathbf{w}_{1}, \hat{\mathbf{X}}_{2}\mathbf{w}_{2}) \right\} \\
\operatorname{arg\,max}_{\substack{\|\mathbf{w}_{q}\|=1, \\ \operatorname{var}(\hat{\mathbf{x}}_{pq})=1}} \left\{ \operatorname{cq}_{qq'}g\left(\operatorname{cov}(\hat{\mathbf{X}}_{q}\mathbf{w}_{q}, \hat{\mathbf{X}}_{q'}\mathbf{w}_{q'})\right)\right) \right\} \\
\operatorname{var}_{\substack{\{\mathbf{w}_{q}\|=1, \\ \operatorname{var}(\hat{\mathbf{x}}_{pq})=1 \\ \forall p, q}}} \left\{ \operatorname{var}_{qq'}g\left(\operatorname{cov}(\hat{\mathbf{X}}_{q}\mathbf{w}_{q}, \hat{\mathbf{X}}_{q'}\mathbf{w}_{q'})\right)\right) \right\}$$

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Non-Metric PLS scaling levels

NM-PLS methods satisfy model criteria under three possible levels of scaling analysis:

Nominal Ordinal Polynomial

To each level of scaling analysis, it corresponds an *ad hoc* scaling function.

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Nominal scaling and its properties

In a nominal analysis, a variable is quantified as orthogonal projection of γ in the space spanned by the columns of the indicator matrix X
_n (Richardson & Kuder, 1933):

$$Q(\tilde{\mathbf{X}}^{n},\gamma) = \tilde{\mathbf{X}}^{n} (\tilde{\mathbf{X}}^{n'} \tilde{\mathbf{X}}^{n})^{-1} \tilde{\mathbf{X}}^{n'} \gamma$$

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• Quantification function $Q(\tilde{\mathbf{X}}^n, \gamma)$ optimizes model criterion while respecting the grouping constraint that, for each pair of observations i and i':

$$\left(x_{i}^{*} \sim x_{i'}^{*}\right) \Longrightarrow \left(\hat{x}_{i} = \hat{x}_{i'}\right)$$

→ Relation between γ and x^* in terms correlation ratio can be expressed as Pearson's correlation coefficient between the scaled variable and γ : $\operatorname{Cor}(\mathbf{x}, \gamma) = \eta_{\gamma|\mathbf{x}^*}$

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Ordinal scaling and its properties

• In a ordinal analysis, a variable is quantified as orthogonal projection of γ in the space spanned by the columns of the indicator matrix \tilde{X}_{o} , built by Kruskal's secondary least squares monotonic transformation

$$Q(\tilde{\mathbf{X}}^{\circ},\gamma) = \tilde{\mathbf{X}}^{\circ} (\tilde{\mathbf{X}}^{\circ'}\tilde{\mathbf{X}}^{\circ})^{-1} \tilde{\mathbf{X}}^{\circ'}\gamma$$

• Quantification function $Q(\tilde{\mathbf{X}}^{\circ}, \gamma)$ optimizes model criterion under the order constraint that, for each pair of observations *i* and *i*':

$$\left(x_i^* \sim x_{i'}^* \right) \Longrightarrow \left(\hat{x}_i = \hat{x}_{i'} \right) \quad \text{and} \quad \left(x_i^* \prec x_{i'}^* \right) \Longrightarrow \left(\hat{x}_i \le \hat{x}_{i'} \right)$$

→ Relation between γ and $\hat{\mathbf{x}}$ in terms of linear correlation can be interpreted as a measure of the approaching monotonicity of the relation between \mathbf{x}^* and the LC, as it is strictly related to Kruskal's STRESS index

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Polynomial scaling and its properties

- In functional scaling we suppose that we know the degree *D* of a polynomial relation between a raw numerical variable and the LC.
- Optimal parameters for the polynomial transformation (Young, 1981) are found by projecting γ in the conic space spanned by the columns of matrix $\tilde{\mathbf{X}}^{\text{p}}$, built with a row for each observation and with (D + 1) columns, each column being an integer power of the vector \mathbf{x}^{*}

$$Q(\tilde{\mathbf{X}}^{\mathrm{p}},\gamma) = \tilde{\mathbf{X}}^{\mathrm{p}} \left(\tilde{\mathbf{X}}^{\mathrm{p}'} \tilde{\mathbf{X}}^{\mathrm{p}}\right)^{-1} \tilde{\mathbf{X}}^{\mathrm{p}'} \gamma$$

• If we suppose that the variable and the LC are linked by a linear relation, we just have to put D = 1. If this is the case for all of the variables, NM-PLS methods provide the same results of the standard PLS methods.

How to implement all of these scaling functions?



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Problem:

As previously shown, scaling are obtained as a function of LCs.. But LCs, on their turn, are functions of scaling values!

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Solution:

Non-Metric PLS algorithms



How do NM-PLS algorithms work?

- In NM-PLS algorithms, model and scaling parameters are alternately optimized in a modified PLS loop where a quantification step is added.
- In standard PLS steps the model parameters are optimized for given scaling parameters.
- In the quantification step, instead, the scaling parameters are optimized for given model parameters: raw variables are properly transformed through scaling functions Q, then they are normalized to unitary variance



 $e_{qq'}$ is the generic element of a squared matrix of order Q that is null if $x_{q'}$ is connected to x_{q} ; otherwise, it represents the corresponding inner weight.



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Non-Metric PLS features

Optimality: NM-PLS algorithms optimizes NIPALS, PLS-R and New Mode A PLS-PM criteria under two sets of parameters: the model parameters and the scaling parameters, constrained to the restrictions due to the scaling level chosen for each raw variable \mathbf{x}^*

Flexibility: NM-PLS satisfies model criterion under several levels of scaling, depending on the properties of the raw variable we want to retain.

Interpretability: The weight of a scaled variable can be interpreted as a measure of the statistical relation between \mathbf{x}^* and the LV





Sensorial data: the Tea dataset

Obs	J1	J2	J3	J4	J5	J6	Temp	Sugar	Strength	Lemon
1	4	2	4	3	13	5	Hot	No	Str	Y
2	2	8	1	9	10	8	Hot	One	Med	Y
3	6	10	13	18	5	6	Hot	Two	Light	Ν
4	13	13	10	5	2	12	LW	No	Med	Ν
5	14	16	17	12	16	9	LW	One	Light	Y
6	15	18	12	15	8	16	LW	Two	Str	Y
7	7	3	14	2	18	2	Cold	No	Light	Y
8	11	6	5	7	3	17	Cold	One	Str	Ν
9	10	11	6	13	12	7	Cold	Two	Med	Y
10	3	1	11	4	6	4	Hot	No	Light	Ν
11	1	7	2	10	7	14	Hot	One	Str	Y
12	5	12	3	17	9	13	Hot	Two	Med	Y
13	17	14	16	6	11	18	LW	No	Str	Y
14	18	15	9	11	1	11	LW	One	Med	Ν
15	16	17	18	16	15	10	LW	Two	Light	Y
16	8	4	8	1	14	1	Cold	No	Med	Y
17	9	5	15	8	17	3	Cold	One	Light	Y
18	12	9	7	14	4	15	Cold	Two	Str	N

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The regression coefficients matrix

_						
Var	J1	J	J3	7	J5	J6
Temp(H)	-0.35	-0.	0.35	٥	-0.15	-0.08
Temp(LW)	0.49	0.51	.36	31	-0.01	0.26
Temp(C)	-0.15	-0.18		0.15	0.15	-0.18
Sugar(0)	-0.21	-0.27		-0.22	0.23	-0.26
Sugar(1)	-0.03	-0.02		0.01	-0.08	0.04
Sugar(2)	0.25	0.29		0.21	-0.15	0.23
Strenght(S)	0.01	0.05		0.10	-0.24	0.16
Strenght(M)	-0.07	-0		0.01	-0.14	0.05
Strenght(L)	0.07	-	0	0.11	0.38	-0.21
Lemon(Y)	-0.00		0.18	.11	0.29	-0.19
Lemon(N)	0.00		-0.18	.11	-0.29	0.19
Var	J1	J2	J3	J4	J5	J6
Temp	0.70	0.83	0.50	0.5	0.01	0.35
Sugar	0.43	0.49	0.11	0.38	-0.30	0.45
Strenaht	0.01	-0.02	-0.36	-0.15	-0.57	0.44

-0.29

-0.15

-0.48

0.39

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0.01

0.03

Lemon

Mapping the observations on the **Correlation Circle: the Biplot**



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Mobile Data – ECSI model





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Latent variables	Manifest variables	R
Image (ξ1)	 (a) It can be trasted in what it says and does (b) It is stable and firmly established (c) It has a social contribution for the society (d) It is concerned with customers (e) It is innovative and forward looking 	ussolil
Customer expectations of the overall quality (ξ_2)	 (a) Expectations for the overall quality of "your mobile phone provider" at the moment you became customer of this provider (b) Expectations for "your mobile phone provider" to provide products and services to meet your personal need (c) How often did you expect that things could go wrong at "your mobile phone provider" 	lo
Perceived quality (\$3)	 (a) Overall perceived quality (b) Technical quality of the network (c) Customer service and personal advice offered (d) Quality of the services you use (e) Range of services and products offered (f) Reliability and accuracy of the products and services provided (g) Clarity and transparency of information provided 	
Perceived value (ξ_4)	 (a) Given the quality of the products and services offered by "your mobile phone provider" how would you rate the fees and prices that you pay for them? (b) Given the fees and prices that you pay for "your mobile phone provider" how would you rate the quality of the products and services offsered by "your mobile phone provider"? 	
Customer satisfaction (§5)	 (a) Overall satisfaction (b) Fulfillment of expectations (c) How well do you think "your mobile phone provider" compares with your ideal mobile phone provider? 	
Customer complaints $(\xi \epsilon)$	(a) You complained about "your mobile phone provider" last year. How well, or poorly, was your most recent complaint handled or (b) You did not complain about "your mobile phone provider" last year. Imagine you have to complain to "your mobile phone provider" because of a bad quality of service or product. To what extent do you think that "your mobile phone provider" will care about your complaint?	36/4
Customer loyalty (\$7)	 (a) If you would need to choose a new mobile phone provider how likely is it that you would choose "your provider" again? (b) Let us now suppose that other mobile phone providers decide to lower their fees and prices, but "your mobile phone provider" stays at the same level as today. At which level of difference (in %) would you choose another mobile phone provider? (c) If a friend or colleague asks you for advice, how likely is it that you would recommend "your mobile phone provider? 	

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- Stanuaruizeu ivivs
- -> All reflective blocks
- -> Centroid scheme has been used







Ordinal and Nominal Quantification: the case of "Ratio Quality-Prize" variable



Flashback

Power methods involve a suite of iterative algorithms, well known from the first half of the 20th century, used for extracting the greatest eigenvalue (in absolute value) of a matrix.

Two classes of algorithms of this type have been greatly used in Statistics to solve different problems: PLS algorithms and ALSOS algorithms.



- A suite of algorithms (NIPALS, PLS-R, PLS-PM, etc.) aiming to:
 - easily handle in presence of missing data
 - Perform multidimensional analyses of landscape matrices
- perform a regression analysis of data affected by multicollinearity problems
- (H. Wold)
- estimate SEM parameters without making strong distributional assumptions (PLS-PM)



A suite of algorithms (Princals, Ascal, Morals, Corals, Overals, etc.) for multivariate analysis on one, two or several blocks of variables measured at different scale levels.

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Conclusion

Quoting F. W. Young (Psychometrika, vol. 46, n. 4, 1981):

"Certain strong correspondences exist between an ALSOS procedure and the NILES approach developed by Wold and Lyttkens.

The main difference between these metric algorithms and the nonmetric ALSOS algorithms is the optimal scaling features of the ALSOS algorithm.

The scaling feature permits the analysis of qualitative data, whereas the previous procedures can only analyze quantitative data."

This ultimate statement is no more true!

It is possible to exploit the iterative nature of PLS algorithms to transform PLS methods in optimal scaling methods

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Thank you for your attention.

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