HAL
open science

VODKA-PLS : a family of PLS models based on the NIPALS algorithm

J.C. Boulet, D. Bertrand, Gérard Mazerolles, Rodolphe Sabatier, J.M. Roger

To cite this version:

J.C. Boulet, D. Bertrand, Gérard Mazerolles, Rodolphe Sabatier, J.M. Roger. VODKA-PLS : a family of PLS models based on the NIPALS algorithm. 12th CAC meeting, Oct 2010, Antwerp, Belgium. 2010. hal-02595676

HAL Id: hal-02595676

https://hal.inrae.fr/hal-02595676v1

Submitted on 15 May 2020

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

VODKA-PLSR, a family of PLS models based on the NIPALS algorithm

J.C. BOULET [1], D. BERTRAND [2], G. MAZEROLLES [1], R. SABATIER [3], J.M. ROGER [4]
[1] INRA, UMR1083, F-Montpellier
[2] INRA, Bioinformatique, F-Nantes
[3] UM1, EA2415, F-Montpellier
[4] CEMAGREF, UMR1201, F-Montpellier

Theory

Including expert information into regression models using NIPALS

A re-writing of NIPALS puts forwards a new parameter, a vector r chosen by the operator. This vector allows the extraction of usefull information from X

(1) NIPALS

Known properties:

$\mathbf{T} = \mathbf{X}\,\mathbf{W}\,(\mathbf{P}'\,\mathbf{W})^{-1}$

$\mathbf{b} = \mathbf{W}\,(\mathbf{P}'\,\mathbf{W})^{-1}\,\mathbf{c}$

(2) a new writing of NIPALS

New properties:

$\mathbf{T} = \mathbf{X}\,\Sigma\,\mathbf{P}\,(\mathbf{P}'\,\Sigma\,\mathbf{P})^{-1}$

$\mathbf{c}' = \mathbf{y}'\,\mathbf{T}\,(\mathbf{T}'\,\mathbf{T})^{-1}$

$\hat{\mathbf{y}} = \mathbf{T}\,(\mathbf{T}'\mathbf{T})^{-1}\,\mathbf{T}'\,\mathbf{y}$

$\mathbf{b} = \Sigma\mathbf{P}(\mathbf{P}'\,\Sigma\,\mathbf{P})^{-1}(\mathbf{T}'\mathbf{T})^{-1}\mathbf{T}'\,\mathbf{y}$

$\mathbf{b} = \Sigma\mathbf{P}(\mathbf{P}'\,\Sigma\,\mathbf{P})^{-1}\,\mathbf{P}'\,\Sigma\,\mathbf{X}'\,\mathbf{y}$

(simplified)

Definitions:

T	NxA	scores	$\{\mathbf{t}_1 \ldots \mathbf{t}_A\}$
W	PxA	weights	$\{\mathbf{w}_1 \ldots \mathbf{w}_A\}$
P	PxA	loadings of **X**	$\{\mathbf{p}_1 \ldots \mathbf{p}_A\}$
c	Ax1	loadings of **y**	
b	Px1	regression vector	

New definitions:

Σ	PxP	$\Sigma = (\mathbf{X}'\mathbf{X})^{+}$ (Moore-Penrose)
$\mathbf{P}_i$	Pxi	loadings of **X** $\{\mathbf{p}_1 \ldots \mathbf{p}_i\}$
$\mathbf{Q}_i$	PxP	$\mathbf{Q}_i = \mathbf{I}_P - \Sigma\,\mathbf{P}_i\,(\mathbf{P}'_i\,\Sigma\,\mathbf{P}_i)^{-1}\,\mathbf{P}_i$
r	Px1	$\mathbf{r} = \mathbf{X}'\,\mathbf{y}$

(3) Vector Orientation Decided through Knowledge Assessment: VODKA- PLSR

3-1: a new calculation of P:

$\mathbf{p}_1 = (\mathbf{X}'\,\mathbf{X})\,(\mathbf{r})$

loop: $\mathbf{p}_{i+1} = (\mathbf{Q}'_i\,\mathbf{X}'\,\mathbf{X})\,(\mathbf{Q}'_i\,\mathbf{r})$

3-2: choice of r

(1) $\mathbf{r} = \mathbf{X}'\mathbf{y}$ => NIPALS (postulate)

(2) **r** = any vector of dimension P

Expert knowledge can be used for the choice of r

Application

Ethanol quantification in wines and musts

Spectra: 500-1900nm

$\mathbf{k}, \mathbf{k}_W, \mathbf{k}_G, \mathbf{k}_L$: pure spectra of ethanol, water, glycerol, lactate

$\mathbf{X}_G$ 165 spectra (EtOH=0)

$\mathbf{X}$ 315 spectra (EtOH ≠ 0)

$\mathbf{X}_V$ 1000 spectra (EtOH≠ 0)

Processing:

$\mathbf{X}_G \rightarrow$ PCA $\rightarrow$ **G**= 1-4 PCs

$\mathbf{R} = [\mathbf{G}\ \mathbf{k}_W\ \mathbf{k}_G\ \mathbf{k}_L]$

$\mathrm{NAS} = (\mathbf{I} - \mathbf{R}\,(\mathbf{R}'\mathbf{R})^{-1}\,\mathbf{R}')\mathbf{k}$

Calibration / Validation: RMSEP

Model	r choice	Notes	LV5	LV6	LV7	LV8	LV9	LV10	LV11	LV12	LV13	LV14
m_1	$\mathbf{1}_P$		2.30	2.94	1.43	1.12	1.09	1.08	0.99	0.96	0.97	0.96
m_2	$\mathbf{X}'\mathbf{1}_N$	Mean of **X** spectra	2.22	2.50	2.23	1.46	**0.94**	**0.93**	1.02	0.97	1.01	1.00
m_3	$\mathbf{X}'\mathbf{y}$	NIPALS	1.26	1.04	1.03	1.34	1.02	1.38	1.19	1.08	1.19	1.18
m_4	**k**	Pure spectra	1.93	2.42	1.88	1.21	1.02	1.01	1.02	1.03	1.03	1.02
m_5	NAS	Net analyte signal	**0.94**	**0.92**	**0.92**	**0.93**	0.97	0.99	1.02	1.04	1.04	1.01
m_6	$\mathbf{X}'_c\,\mathbf{y}_c$	NIPALS centered	1.05	1.00	**0.95**	1.25	1.02	1.40	1.20	1.11	1.23	1.22

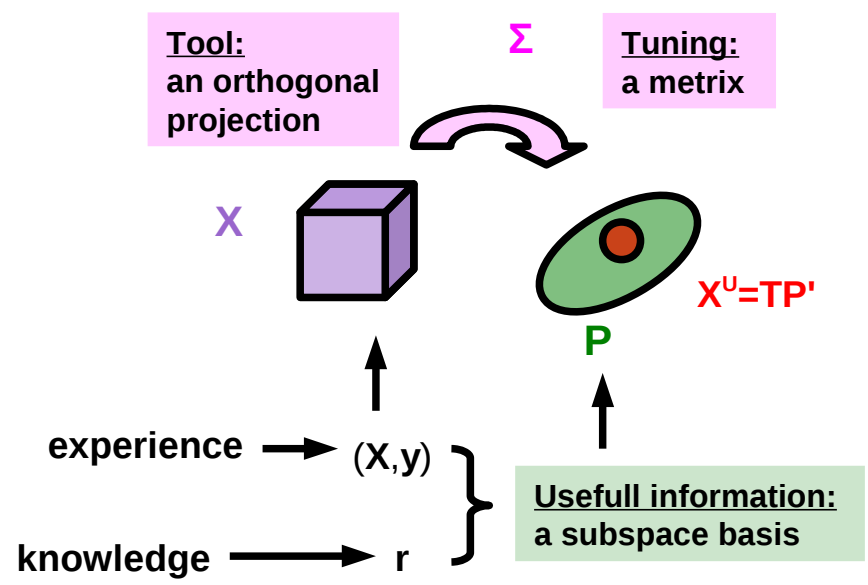
m2 and m5 → better predictions than NIPALS

Discussion and conclusion

Practical aspects

- An infinity of regression models based on NIPALS
- Expert information (e.g. NAS) can be directly introduced into regression models through **r**
- NIPALS (**r**= **X'y**) isn't always the best choice

Theoretical aspects

- A more general model depending on the choices of **P** and **Σ**

VODKA-PLSR synopsis