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

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## 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 useful information from  $X$

#### (1) NIPALS

Known properties:  
 $T = XW(P'W)^{-1}$   
 $b = W(P'W)^{-1}c$

#### (2) a new writing of NIPALS

New properties:

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

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

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

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

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

(simplified)

Definitions:

$T$  NxA scores  $\{t_1 \dots t_A\}$   
 $W$  PxA weights  $\{w_1 \dots w_A\}$   
 $P$  PxA loadings of  $X$   $\{p_1 \dots p_A\}$   
 $c$  Ax1 loadings of  $y$   
 $b$  Px1 regression vector

New definitions:

$\Sigma$  PxP  $\Sigma = (X'X)^+$  (Moore-Penrose)  
 $P_i$  Pxi loadings of  $X$   $\{p_1 \dots p_i\}$   
 $Q_i$  PxP  $Q_i = I_P - \Sigma P_i (P'_i \Sigma P_i)^{-1} P_i$   
 $r$  Px1  $r = X'y$

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

#### 3-1: a new calculation of $P$ :

$$p_1 = (X'X)(r)$$

loop:  $p_{i+1} = (Q'_i X'X) (Q'_i r)$

#### 3-2: choice of $r$

- (1)  $r = X'y \Rightarrow$  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

Validation: RMSEP

Calibration		
Model	r choice	Notes
$m_1$	$1_P$	
$m_2$	$X'1_N$	Mean of $X$ spectra
$m_3$	$X'y$	NIPALS
$m_4$	$k$	Pure spectra
$m_5$	NAS	Net analyte signal
$m_6$	$X'_c y_c$	NIPALS centered

LV5	LV6	LV7	LV8	LV9	LV10	LV11	LV12	LV13	LV14
2.30	2.94	1.43	1.12	1.09	1.08	0.99	0.96	0.97	0.96
2.22	2.50	2.23	1.46	0.94	0.93	1.02	0.97	1.01	1.00
1.26	1.04	1.03	1.34	1.02	1.38	1.19	1.08	1.19	1.18
1.93	2.42	1.88	1.21	1.02	1.01	1.02	1.03	1.03	1.02
0.94	0.92	0.92	0.93	0.97	0.99	1.02	1.04	1.04	1.01
1.05	1.00	0.95	1.25	1.02	1.40	1.20	1.11	1.23	1.22

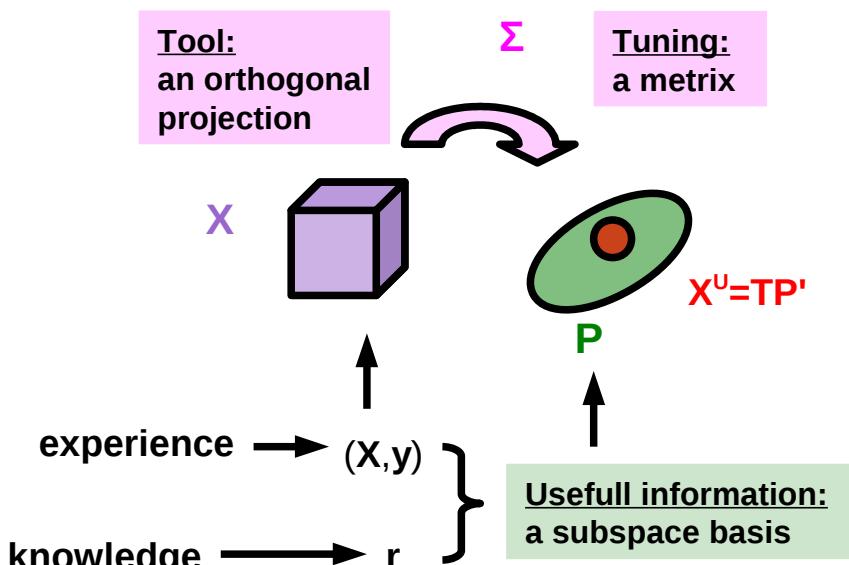
$m_2$  and  $m_5 \rightarrow$  better predictions than NIPALS

## 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

### VODKA-PLSR synopsis



### Theoretical aspects

- A more general model depending on the choices of  $P$  and  $\Sigma$