



**HAL**  
open science

## **IDC-improved direct calibration. Application to wine ethanol quantification in musts and wines**

Jean Claude J. C. Boulet, Jean-Michel Roger

► **To cite this version:**

Jean Claude J. C. Boulet, Jean-Michel Roger. IDC-improved direct calibration. Application to wine ethanol quantification in musts and wines. NIR2009, Nov 2009, Bangkok, Thailand. pp.1, 2009. hal-02750574

**HAL Id: hal-02750574**

**<https://hal.inrae.fr/hal-02750574>**

Submitted on 3 Jun 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.

# IDC-Improved Direct Calibration. Application to ethanol quantification in musts and wines

Jean-Claude BOULET\*, Jean-Michel ROGER \*\*

\* INRA, UMR-SPO, F-Montpellier

\*\* CEMAGREF, UMR-ITAP, F-Montpellier

## Theory

$$\underbrace{\begin{matrix} \mathbf{x}' \\ \hline \text{P} \end{matrix}}_{\text{Sample spectrum}} = \underbrace{y * \begin{matrix} \mathbf{k}' \\ \hline \text{P} \end{matrix}}_{\text{Useful part}} + \underbrace{\begin{matrix} \mathbf{T}_k \\ \hline \text{Q} \end{matrix} * \begin{matrix} \mathbf{K} \\ \hline \text{P} \end{matrix}}_{\text{Chemical influence factors}} + \underbrace{\begin{matrix} \mathbf{T}_\phi \\ \hline \text{A} \end{matrix} * \begin{matrix} \mathbf{P} \\ \hline \text{P} \end{matrix}}_{\text{Other influence factors}}$$

IDC principle :  
to remove the influences from the useful part

- collect  $X_G$  ( samples with constant  $y$  )
- identify  $P$  with a SVD onto  $X_G$
- project onto  $k$  orthogonally to  $K$  and  $P$

$$R = \begin{bmatrix} K \\ P \end{bmatrix} \quad \Sigma = I - R'(RR')^{-1}R$$

$$b = \Sigma k (k' \Sigma k)^{-1}$$

## Application

Quantification of Ethanol (% vol. ) on clarified grape musts during alcoholic fermentation, using NIR spectrometry (500 to 1900 nm / 2nm)

$k$  = ethanol spectrum

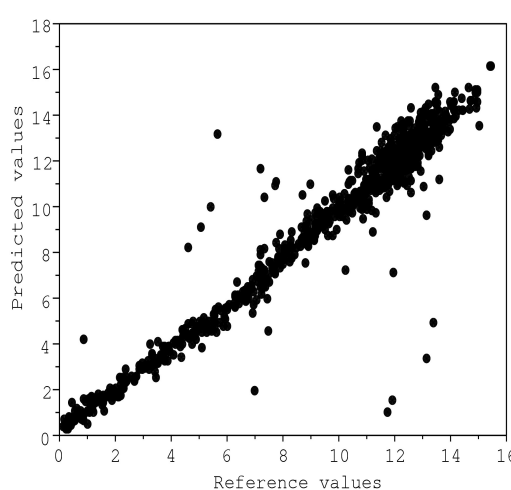
$K = \begin{bmatrix} \text{glycerol} \\ \text{lactic acid} \\ \text{water} \end{bmatrix}$

reference  
= air

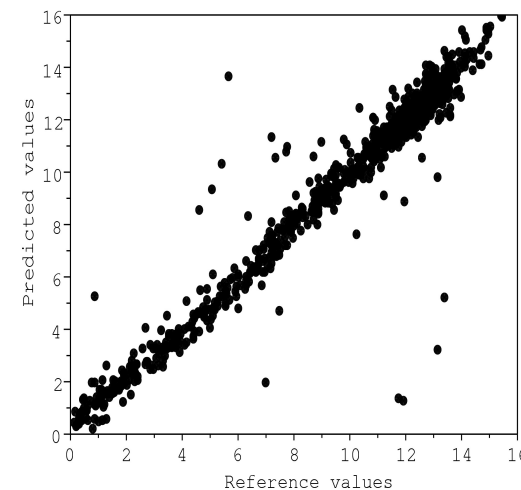
$X_G = 165$  must spectra  
( $y = 0$  %vol.)

$X_{TEST} = 1000$  spectra  
( $0 < y < 16$  %vol)

reference  
= water



IDC RMSEP=0.96 % vol.



PLSR RMSEP=0.89 %vol.

## Discussion and conclusion

### PRACTICAL ASPECTS

- + IDC doesn't need any calibration dataset (contrary to PLSR)  
→ possible application to hyperspectral images
- + IDC is very flexible: chemical compounds whose pure spectra are unknown can be characterised by  $X_G$
- + Different ways to build  $X_G$  (see [1], [2], [3])
- + IDC predictions can be as accurate as PLSR predictions
- when  $X_G$  is calculated according to [2] or [3], constant but not zero influence factors are not taken into account, leading to IDC models with wrong slopes and/or offsets

### THEORETICAL ASPECTS

The term  $\Sigma k$  corresponds to Lorber's definition of the NAS-Net Analyte Signal ([4]):  
« the net analyte signal may be computed as the part of its spectrum orthogonal to other coexisting constituents », extended all other -e.g. physical- influence factors.

Despite similar predictions, IDC and PLSR-b-coefficients vectors are different, and don't converge (not shown).

[1] P.W.HANSEN. Pre-processing methods minimizing the need for reference analyses. *Journal of Chemometrics*, 15:123-131, 2001

[2] J.M.ROGER, F.CHAUCHARD, V.BELLON-MAUREL.EPO-PLS external parameter orthogonalisation of PLS, application to temperature-independent measurement of sugar contents in fruits. *Chemometrics and Intelligent Laboratory Systems*, 66:191-204, 2003

[3] R.MARBACH. A new method for multivariate calibration. *Journal of Near Infrared Spectroscopy*, 13:241-254, 2005

[4] A.LORBER, K.FABER, B.R.KOWALSKI. Net analyte signal in multivariate calibration. *Analytical Chemistry*, 69:1620-1626, 1997