Simultaneous decomposition of multivariate images: Application to near infrared hyperspectral images of wheat

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Abstract
We present here a three-way data analysis method able to reveal common latent components in a collection of multivariate images observed for different objects or scenes. The main objective is to follow the water diffusion in single wheat sections over time using Near-Infrared Hyperspectral Imaging (NIR-HSI). The study is mainly descriptive and data treatments were investigated to find the tissues common to different grains as well as to provide tissues specific to one or more samples. The algorithm proposed is based on the simultaneous decomposition of the covariance matrices calculated for each NIR image supposing that common loading vectors exist and can be weighted differently for each multivariate image. The method is illustrated by the analysis of NIR hyperspectral images acquired at regular time interval for five wheat kernel sections exposed to water. These results show that the kinetics of propagation of water and thus the germination are grain specific.

Keywords: Imbibition, Water, Wheat, NIR hyperspectral imaging, Chemometrics

Résumé
Nous présentons ici une méthode d'analyse de données trois voies en mesure de trouver les composants latents communs d’une collection d'images multivariées observées pour différents objets ou scènes. L'objectif principal est de suivre la diffusion de l'eau dans des sections de blé au fil du temps en utilisant l’imagerie hyperspectrale Proche-Infrarouge (NIR-HSI). L'étude est principalement descriptive et les traitements de données ont été développés pour trouver des tissus communs à différents grains ainsi que de fournir des tissus spécifiques à un ou plusieurs échantillons. L'algorithme proposé est basé sur la décomposition simultanée des matrices de covariance calculées pour chaque image NIR supposant que les vecteurs propres communs existent et peuvent être pondérées différemment pour chaque image. La méthode est illustrée par l'analyse d’images hyperspectrales NIR acquises à intervalle de temps régulier pour cinq sections de blé exposées à l'eau. Ces résultats montrent que la cinétique de la propagation de l'eau et ainsi la germination sont grain spécifique.
Mots-clés : Imbibition, Water, Blé, Imagerie Hyperspectrale Proche Infrarouge, Chimiométrie

1. Introduction

Multivariate images can be represented as cube-images constituted by two spatial dimensions and one third spectral. The extraction of information in such a structure is possible by unfolding the cube into a large matrix: each image-plane is unfolded into a column of the resulting matrix (Esbensen et al, 1989) Chemometrics such as principal components analysis (PCA) or Partial Least Squares (PLS) regression can be applied on this matrix. But a two-way data can be extended to a three-way data array, when the same variables are measured on the same samples under different circumstances, for example time or temperature. In this way, the data structure is no longer a two-way data matrix. To process data, PCA can be applied on each cube or on a very large matrix obtained by merging all the cubes. These approaches exhibit common features but would not take into account the structure inside each scene (Courcoux et al, 2002). Pixels are not homologous and we have to modify the three-mode principal component analysis (Kroonenberg, 1983). The algorithm assigns a weight to the common loading which is related to each multivariate image. The parameters (common loading vectors, weights, scores) for the three modes were estimated by simultaneously decomposing the cross product matrices of each hyperspectral image (Qannari et al, 2000).
This approach is particularly suitable for following the imbibition of single wheat sections over time by Near-Infrared hyperspectral imaging. Indeed, one of the major seed qualities is the potential of the seed to germinate. The first phase of germination, so-called "imbibition phase", consists in water absorption and is a critical step in the development of the plant. Due to some abiotic and morphologic criteria such as climate, kernel position in spikelet, the history of seeds is depending of the kernel itself. The kinetics of germination can be different between seeds and a good understanding of this phenomenon is crucial.
The most used technique for determining the imbibition rate is the ponderal method (ISTA 1985) (Wiwart et al, 2006). This technique is quantitative, simple to perform, and nondestructive; however, the way of water diffusion inside the grain cannot be observed. Due to the properties of absorption of water in the Near-Infrared range, NIR hyperspectral imaging (NIR-HSI) is particularly indicated to track diffusion of water in single wheat kernels. However, the pathway used by water to penetrate into the grains was not yet described and the imbibition process still remains misunderstood (Manley et al, 2011).
As the seeds must be generally completely immerged in water for hours to observe imbibition, we propose here a different method to provide an accurate description of water uptake and distribution in wheat grain tissues using NIR-HSI in real time.

2. Material and Methods

2.1 Sample description

A specific Teflon holder has been produced (105X40X10 mm) with five holes of 3 mm diameter connected to a tank that can be filled with water. Five seeds (TURDA-81-77, Triticum aestivum aestivum, number 7085 in database SIREGAL, https://urgi.versailles.inra.fr/siregal/siregal/) are transversely cut to about 80%, slightly underneath the germ and are placed in the holes, the germ below and the cut surface above as shown in Figure 1. Preliminary studies have been necessary to optimize the design of the water tank and to choose the best seed cutting height, giving a cross-section with the following tissues: radicle, coleoptile, scutellum. At the beginning of the experiment, the tank is empty, and reference NIR absorbance images of each surface are acquired individually. Then water is added into the tank (giving the zero-time) and NIR hyperspectral images of the five surfaces are then acquired at regular intervals for 33 hours, except during the night. Twenty images were collected for each seed but only the nine most interesting are presented, namely those obtained at time 0, 30min, 1h, 5h, 9h, 24h, 28h, 33h and the reference. The lab temperature was set at 22°C nevertheless, it was necessary to add frequently some drops of water into the tank to avoid evaporation.

Figure 1: Teflon holder with five seeds cut at 50%, placed in holes linked to a water tank

2.2 Hyperspectral NIR imaging system

Hyperspectral images were acquired with a pushbroom hyperspectral imaging system (BurgerMetrics, SIA, Riga, Latvia) consisting of a SWIR Xeva MCT camera (Xenics) combined with a Hyperspec SWIR imaging spectrometer (Headwall photonics) covering the spectral range of 950-2500nm with a spectral resolution of about 7nm. All images are acquired in absorbance and the final image size for each kernel is 231(x) × 318(y) × 212(λ), the first two values representing pixel dimensions in the x and y directions (field of view of 6 × 8.2mm mm, with a spatial resolution of 26µm) and the third value accounting for the number of spectral channels.

2.3 Data processing

The method is based on the assumption that common loading vectors exist that can possible be weighted differently for each multivariate image. The loading vectors and weights are estimated from the set of covariance matrices issued from the unfolded multivariate images.

For all multivariate images $\mathbf{X_i}$, the common loadings $\mathbf{P}$ and the specific weights $\boldsymbol{\lambda_i}$ are computed iteratively. Scores are then obtained by multiplying the unfolded image matrix $\mathbf{X_i}$ by $\mathbf{P}$ matrix. These scores can be refolded in the initial dimension of images and displayed with false colors related to the intensity of pixels on the scores component: blue for low and red for high.

3. Results and discussion

The positive part of the first loading (not shown) is made with wavelengths of starch and we can see in the PC1 scores-images (Figure 2, left part) that some parts of seed, in red, stay dry during the imbibition (high signal of starch). The positive part of the second loading (not shown) is constituted by wavelengths specific of water, and the scores-images mainly exhibit the water in yellow and red (Figure 2, right part).

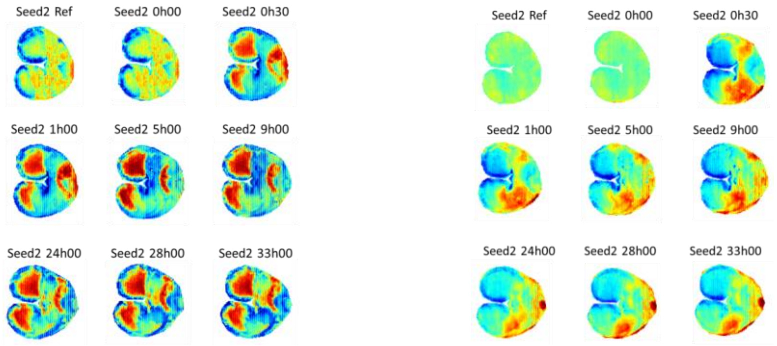
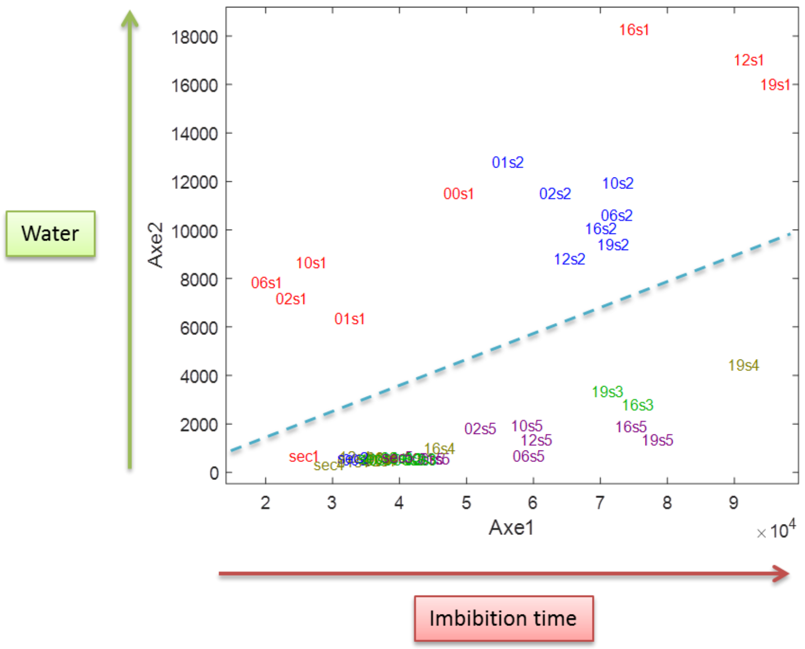


Figure 2: Simultaneous decomposition for the seed N°2: PC1 scores-images (left) and PC2 scores-images (right).

Weights were plotted on a factorial plot and those associated to images of seeds 1 and 2 exhibit the relative abundance of the common structure in the original images, i.e. the water.



4. Conclusion

A new approach has been developed to provide a detailed mapping of absorption and distribution of water in the tissues of the wheat grain using Near-infrared hyperspectral imaging and chemometrics. Unsupervised chemometrics used, e.g. simultaneous decomposition, are useful to obtain intensity images in false colors that bring out the spatial organization of the different components of the grains.
Moreover, the results obtained by simultaneous decomposition show that the kinetics of propagation of water is grain specific. Beginning of imbibition process is sometimes extremely rapid (few minutes) but can also take hours. It depends on the dormancy release.

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