Chemometrics of multichannel imaging

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Introduction

The description of a sample from its proximate composition is often not sufficient to allow its complete characterisation. Some products may have very similar global compositions and behave in different ways in industrial processes. This is the case, for example, for dried samples containing residual water. For practical applications, besides the water content, the distribution of water may be a very important parameter for the control of the process. In the same way, the milling behaviour of wheat grains may not only depend on their proximate composition in protein, starch, fibres… but also on the histological distribution of these components. Near infrared (NIR) spectroscopy is able to give a very accurate global characterisation of samples but is not normally suitable to study the distribution of different constituents in the products.

In order to characterise such distributions, it is necessary to develop devices including a video camera sensible in the near infrared region, which make it possible to record NIR spectra at each point of the surface of the sample. In this way, it would be possible to obtain, for a given sample, a sequence of images, in which each image corresponds to a given illumination wavelength. Each sample is therefore represented by a "cube of data": width × length × wavelength. As an image usually includes a huge amount of data points, it is necessary to find fast chemometric methods for processing multispectral images. Moreover, the usual way of calibration is not applicable on such images, because the proximate composition at each point of the surface is not known, and reference chemical values are therefore not available.

If the studied product is formed of areas of clearly distinct composition, it is possible to label the image, i.e. identify the nature of each picture element (pixel) and map the surface of the sample. Labelling can be obtained either by unsupervised or supervised learning chemometric methods. Unsupervised learning has already been applied to multispectral images.[1] In several studies[2,3] we applied discriminant analysis for labelling NIR video images. In the present communication, a method for applying discriminant analysis to multispectral images is described. The results obtained for artificial and natural samples are presented.

Material and methods

Device for NIR imaging

The imaging system was formed of four elements: a light source, a monochromator for selecting illumination wavelengths, a sample compartment and a NIR sensitive video camera (Figure 1). The light source was a tungsten lamp (Jobin-Yvon) having a maximum power of 170 W and covering the spectral range from 340 to 2000 nm. The monochromator (Jobin-Yvon) was equipped with a grating covering the NIR region up to 2000 nm and was adjusted in order to obtain

From Near Infrared Spectroscopy: The Future Waves

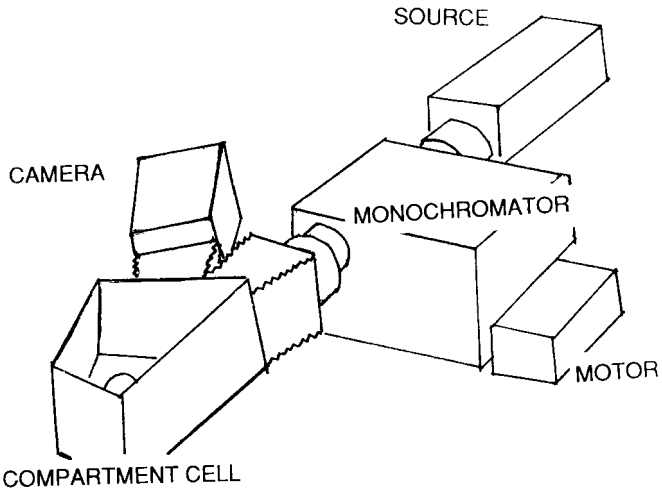

Figure 1. Diagram of the NIR video imaging system.

a band width of 25 nm. The NIR camera (Lhesa, model LH4015) equipped with a Vidicon tube, was fitted with a 55 mm photographic lens (Nikon). The incident and observation angles of the light in the sample compartment were set to 30° and 10° respectively, in relation to the normal of the sample.

The system was driven by an IBM-compatible microcomputer which controlled the acquisition and the storage of images and the movement of the monochromator grating. For each sample, images of 512×512 pixels, coded with 256 grey level values, were recorded from 900 to 1900 nm at intervals of 50 nm. As the images were noisy, it was necessary to average eight images obtained with the same spectral conditions. Moreover, in order to reduce both the size of images and the noise, the four neighbouring pixels were averaged.

Application of discriminant analysis on images

Interactive selection of pixels

The first step of discriminant analysis was to create the learning set and the verification set of pixels from a collection of "known" images. By means of a "mouse", the user selected some representative pixels on images of the samples. He then attributed a given qualitative group to each selected pixel. For example, in a study of sections of wheat grains, the user was supposed to be able to select pixels representative of three qualitative groups "outlayers walls", "starchy endosperm" or "germ".

Chemometrics of discriminant analysis applied on images

The grey level values $p_{i,j,k}$ of a multispectral image $\boldsymbol{P}$ are characterised by three indices: i and j indicate respectively the row and column position of the pixel, and k characterises the channel of the image (i.e. the lighting condition). A pixel $\boldsymbol{p}_{i,j}$ is therefore a vector of grey level values, formed of k elements. By the interactive selection procedure, a small number of pixels (in our case a few hundred) are selected and a qualitative group is attributed to each of them. For computation, the n pixels of the learning set are gathered in a matrix $\boldsymbol{M}$ dimensioned $n \times m$.

A stepwise discriminant analysis[4] is applied to the matrix $\boldsymbol{M}$. In this way, a subset of m relevant spectral conditions, giving the highest number of pixels of the learning set correctly classified, can be obtained. The resulting discriminant model can then be applied to the pixels of unknown multispectral images. By attributing different arbitrary colours to the qualitative groups it is then possible to create a coloured image which represents the spatial distribution of the groups at the surface of the studied sample.

As an image is composed of a huge number of pixels, it was necessary to simplify the mathematical procedure for classification. This was achieved in the following way.

Let $\boldsymbol{X}$ be the centred matrix, dimensioned $n \times m$, of the grey level values of the pixels of the learning set. Let $\boldsymbol{g}_i$ be the vector of the average values of the pixels of the ith qualitative group (i^{th} gravity centre) and suppose there are q qualitative groups.

The classification of an unknown observation $\boldsymbol{x}$ into a qualitative group requires the q so-called "Mahalanobis distances" $d(\boldsymbol{x}, \boldsymbol{g}_i)$ between $\boldsymbol{x}$ and the q gravity centres to be assessed:

$$d(\boldsymbol{x}, \boldsymbol{g}_i) = (\boldsymbol{x} - \boldsymbol{g}_i)\, \boldsymbol{T}^{-1}\, (\boldsymbol{x} - \boldsymbol{g}_i)' \text{ for } i = 1 \ldots q \tag{1}$$

$$\text{with } \boldsymbol{T} = \boldsymbol{X}'\, \boldsymbol{X}.$$

The observation is classified into the group i giving the smallest value of $d(\boldsymbol{x}, \boldsymbol{g}_i)$.
Equation 1 can be rewritten as:

$$d(\boldsymbol{x}, \boldsymbol{g}_i) = \boldsymbol{x}\, \boldsymbol{T}^{-1}\, \boldsymbol{x}' - \boldsymbol{x}\, \boldsymbol{T}^{-1}\, \boldsymbol{g}_i' - \boldsymbol{g}_i\, \boldsymbol{T}^{-1}\, \boldsymbol{x}' + \boldsymbol{g}_i\, \boldsymbol{T}^{-1}\, \boldsymbol{g}_i' \tag{2}$$

The first term of Equation 2, $\boldsymbol{x}\, \boldsymbol{T}^{-1}\, \boldsymbol{x}'$, is constant for a given $\boldsymbol{x}$.
It is therefore equivalent to find the minimum of $d(\boldsymbol{x}, \boldsymbol{g}_i)$ or that of:

$$v(\boldsymbol{x}, \boldsymbol{g}_i) = \boldsymbol{g}_i\, \boldsymbol{T}^{-1}\, \boldsymbol{g}_i' - 2\, \boldsymbol{g}_i\, \boldsymbol{T}^{-1}\, \boldsymbol{x}' \tag{3}$$

The first term of Equation 3 is a number, depending only on the gravity centre studied. The second term of Equation 3 is a scalar product between the vector $2\boldsymbol{g}_i\, \boldsymbol{T}^{-1}$ (which needs to be assessed once for all the observations) and $\boldsymbol{x}$. The assessment of $v(\boldsymbol{x}, \boldsymbol{g}_i)$ therefore requires less computation time than that of $d(\boldsymbol{x}, \boldsymbol{g}_i)$ but leads to the same classification.

Results

Study of pure fraction of wheat

In previous work,[3] pressed pellets of 12 mm diameters were prepared from gluten, bran and starch. Pellets of ceramic were used as reference. Images of the pure fractions were acquired from 900 to 1500 nm, at intervals of 50 nm. For each of the four groups (including ceramic) 120 and 80 pixels were selected as learning and verification sets, respectively. From the initial 21 wavelengths, seven were selected by stepwise discriminant analysis in the following order: 950, 1500, 1450, 1000, 1700, 1600 and 900 nm. These wavelengths allowed the correct classification of 96 percent of the verification set (ceramic : 95; bran : 100; gluten : 90; starch : 100).

The model was then applied to the pixels of all the images and good separation of the groups were still obtained. The percentage of well classified pixels were 92 for bran, 95 for gluten and 99 for starch. The errors were probably due to the shadows in the field of vision.

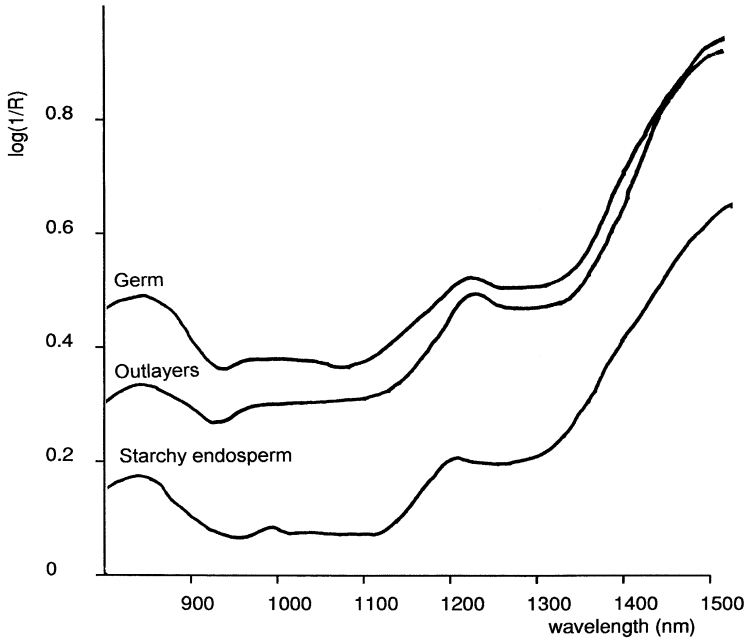

Figure 2. Spectra of three histological areas of section of wheat obtained from NIR imaging.

Sections of wheat grain

Sections of wheat grains were studied in the same way. The images of whole sections were acquired from 800 nm to 1500 nm at intervals of 25 nm. Discriminant analysis was applied to identify three histological regions: “out-layer walls”, “starchy endosperm” and “germ”.

The spectra of the three regions, obtained from video images, are shown in Figure 2. On this graph, the average grey-level values were transformed in absorbances at each wavelength, according to:

$$a = \log(gr/gs)$$

where *gr* and *gs* are the average grey level values of ceramic (reference) and sample, respectively. In the range studied, the spectra were rather similar to those obtained with a classical spectrometer. Discriminant analysis made it possible to efficiently label the images of section of grain (Figure 3), with only six percent of pixels misclassified.

Conclusion

The designed system was able to identify products having large differences in their proximate composition. By means of discriminant analysis, it was possible to label images according to the nature of the apparent surfaces of the samples. The chemometric aspects deserve to be continued, by developing unsupervised approaches.

However, the system was not sufficiently accurate for practical applications. The main problems came from the tube camera which did not give sufficiently stable signals and from the loss of light energy due to the use of a monochromator for selecting wavelengths. In further work, we propose to use a CCD camera and interference optic filters.

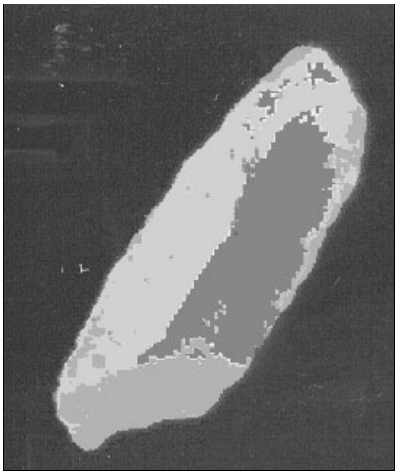

Figure 3. Labelled images of section of wheat. (Pale grey—outlayers walls, Dark grey—starchy endosperm, Mid-grey—germ).

References

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