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Chemometrics of Multivariate Images in Food Science

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Most of the classical spectroscopic techniques are nowadays adapted in order to allow the acquisition of multivariate images (Geladi and Grahn, 1996). Multivariate digitised images can basically be represented by a data cube, D . The three dimensions of this cube, x,y,z are respectively associated with the two spatial dimensions x and y and with a spectral dimension z. A given element of D, dxyz is the value of the pixel at position [x,y] for the channel of index z. Moreover, in a given experiment, many data cubes, associated with different studied objects, are gathered. It is thus necessary to have relevant chemometrics tools dealing with such complex structures of data. In the present communication, we will give simple examples of typical chemometric methods that can be used for analysing collections of multivariate images. An important step in the analysis of multispectral images is pre-treatment. After these possible pre-treatments, unsupervised or supervised methods can be applied on the images in order to extract the more relevant information. Among the unsupervised methods, Principal component analysis (PCA) allows to summarise the information by the construction of images of latent variables which are linear combinations of the original image channels. Examples of application of PCA for characterising the frame of collagen using fluorescence imaging will be shown. Supervised techniques such as discriminant analysis can also valuably be applied on multivariate images. Such approaches give a way to label the pixels, but also to take into account both of the spatial and spectral information. When collection of multivariate image are available, it is possible to use multiblock statistical techniques on the collection of unfolded images. The practical interest of this data processing will be discussed.

References

Geladi P, Grahn H (1996). Multivariate image analysis. John Wiley & Sons Publisher.