Chemometrics, Imaging and Spectroscopy Laboratory – Department of Life Sciences, University of Modena and Reggio Emilia

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Following the previous papers of our colleagues from the University of Genova[1] and from the University of Rome "La Sapienza"[2] in the series of articles presenting the Italian research groups active in the field of NIR spectroscopy, this paper aims at introducing the main activities of the Chemometrics, Imaging and Spectroscopy Laboratory (CHIMSLAB) of the University of Modena and Reggio Emilia.

The group is headed by Prof. Alessandro Ulrici, associate professor in Analytical Chemistry and Coordinator of the Research Doctorate School in Food and Agricultural Science, Technology and Biotechnology (STEBA) of the University of Modena and Reggio Emilia. CHIMSLAB team also includes Dr. Giorgia Foca, as assistant professor, and Dr. Rosalba Calvini, as post-doc researcher. We would also like to mention our former PhD students, Dr. Carlotta Ferrari and Dr. Giorgia Orlandi, who gave a fundamental contribution to our recent activities. In addition, in 2017 we had the pleasure to host Prof. Sylvio Barbon Junior (Computer Science Department, Londrina State University) and Dr. Ana Paula A. C. Barbon (Animal Science Department, Londrina State University) as visiting researchers.

CHIMSLAB research group is also affiliated to BIOGEST-SITEIA, the interdepartmental research centre of the University of Reggio Emilia working on the improvement and valorisation of agri-food biological resources.

The keywords in the group name recall our main research activities: the application and development of chemometric methods for data modelling with a specific interest in spectroscopic and imaging data. In particular, the application of near infrared (NIR) spectroscopy, computer vision and NIR hyperspectral imaging (NIR-HSI) in the agri-food sector represents a considerable part of our expertise. However, thanks to collaborations with other research groups, we had the possibility of applying chemometric modelling to a wide range of research fields, including cultural heritage[3], electrochemical sensing[4], microbiology[5,6] and entomology[7,8], among others.

Concerning our research topics of main interest for the readers of NIR News, in the past years we focused on two key aspects of spectroscopic and imaging data analysis: variable selection and data dimensionality reduction.

Feature selection is a crucial aspect in the analysis of spectroscopic signals, since the selection of the spectral regions of interest for the problem at hand usually allows to discard noise and to obtain calibration or classification models with higher performances. For these reasons, starting from the beginning of our research activities, the application of state-of-art variable selection methods and the development of new selection strategies has represented key topic of our work[9-13].

The importance of variable selection methods is even more relevant when dealing with NIR hyperspectral images. Indeed, usually industrial applications require sorting technologies meeting the requirements of fast time of analysis and low costs. Therefore, variable selection is generally applied to hyperspectral data acquired at the laboratory scale in order to find few wavelengths relevant for the problem at hand to be implemented in a faster and cheaper multispectral imaging system. In this context, a recent collaboration with Prof. Jose Amigo (University of Basque Country) and Caffè Molinari S.p.a aimed at simulating the implementation of a multispectral imaging system based on only four wavelengths for the classification of Arabica and Robusta green coffee beans. The four wavelengths were selected through the application of sparse-based variable selection methods to hyperspectral data, and the key aspect of our simulation consisted in the identification of relevant descriptors derived from the reflectance values registered at the four wavelengths in order to obtain classification performances similar to those obtained with the hyperspectral imaging system[14,15].

The second key topic of our research activity concerns the development of data dimensionality methods for the analysis of large datasets of RGB or hyperspectral images. These methods essentially consist in converting the three-dimensional image arrays into one dimensional signals, which in turn can be considered like a sort of fingerprint codifying the properties of interest of the original images. The main advantage of this kind of approach is the possibility of converting large datasets of images into matrices of signals, that can be further analysed using chemometric methods for data exploration and for the development of calibration or classification models.

Considering RGB images, this method consists in transforming each image into a signal, named colourgram, which codifies its colour-related properties. The proposed approach has been successfully applied in several food related applications, including the quantification of pigments and sensory attributes in pesto sauce[16], the detection of skin defects in raw hams[17,18], the determination of grape phenolic ripening[19], the automated identification of defective kernels in maize[20] and hazelnuts[21], and the detection of packaging residuals in former food products[22]. Currently, we are applying the colourgrams approach for the automated in-field determination of grape phenolic

ripening using a smartphone integrated in a portable acquisition case. The satisfactory results obtained in the frame of Research Project SOSTINNOVI[23] allowed us to obtain the Italian patent[24] and at present we are extending the effectiveness of this approach on different typical vines of Emilia-Romagna Italian region.in the frame of the Research Project VITEVEN ("Technological innovation for efficient grape harvest forecast – VITEVEN", Emilia Romagna PSR 2014-2020 Project n° 5111597).

Starting from the colourgrams approach described above for RGB images, we have developed a similar data dimensionality reduction method for NIR-hyperspectral images, which consists in transforming the dataset of hyperspectral images into a matrix of signals, named hyperspectrograms, accounting for spectral and/or spatial features of interest[25]. The hyperspectrograms are obtained by mering in sequence quantities derived from a Principal Component Analysis model, which can be calculated separately for each image of the dataset (Single Space Hyperspectrograms, SSH) or considering all the images altogether (Common Space Hyperspectrograms, CSH). The effectiveness of the hyperspectrograms approach has been tested on different food related issues, such as early bruise detection on apples[26], the characterization of green coffee beans[27], the detection of bacteria in food[28] and the quantification of rind amount in grated Parmigiano Reggiano cheese[29]. The hyperspectrograms approach will be also applied in the frame of the incoming European Research Project HALY.ID ("HALYomorpha halys IDentification: Innovative ICT tools for targeted monitoring and sustainable management of the brown marmorated stink bug and other pests", – EU ERA-NET COFUND ICT-AGRI-FOOD), whose aim is to use NIR-HSI sensors to identify fruit damages caused by the infection of *Halymorpha halys* (L.) and other pests.

In order to simplify the analysis of RGB and hyperspectral images through our data dimensionality reduction approaches, we have developed two graphical user-friendly interfaces (GUIs) in MATLAB environment, namely Colourgrams GUI[30] and Hyperspectrograms GUI, which are freely downloadable from our website[31].

Over the years we have established national and international collaborations with research institutes through research works and funded projects dealing with the application of NIR spectroscopy and NIR-HSI mainly in the agri-food sector. Such collaborations involved the University of Milano, the University of Genova, the University of Rome "La Sapienza", the University of Copenhagen, the University of Basque Country, the Londrina State University and the Institute for Food and Agricultural Research and Technology (IRTA) of the Government of Catalonia, among others.

In addition to research activities, also technology transfer and collaboration with companies represent a crucial part of our work. In the past years, we collaborated with companies producing flour and backed products (East Balt Italia Srl, Molino Quaglia Spa and Buhker AG) to develop strategies to

monitor the quality of their products and to study the relationship between chemical and technological properties of flour doughs and quality parameters of the final products. Recently, we established a collaboration with Parmigiano Reggiano Cheese Consortium to evaluate the possibility of using NIR-HSI to quantify the rind amount in grated Parmigiano Reggiano cheese products. Moving to the recycling sector, we collaborated with MUSA Srl in RICIPLA project for the development of a classification model for the classification of plastic polymers in a waste sorting system based on NIR-HSI[32]. In the frame of this collaboration, we developed a novel version of Partial Least Squares Discriminant Analysis (PLS-DA) classification algorithm, named Soft PLS-DA, which allows to maximise the separation between the classes of interest (as classical PLS-DA) and, at the same time, to reject possible outlier samples. The MATLAB code to apply Soft PLS-DA can be downloaded from our website[31].

Concerning the equipment of our laboratory, we have a Bruker Optic MPA FT-NIR spectrophotometer working in the 4000 – 12500 cm^{-1} spectral range and equipped with three sampling tools: transmission unit, integrating sphere and fiber optic probe. For hyperspectral image acquisition, we have a line-scanning NIR hyperspectral imaging system (NIR Spectral Scanner, DV Optic) working in the 900 – 1700 nm spectral range with a spectral resolution of 5 nm. The hyperspectral system is equipped with a Specim Imspector N17E imaging spectrometer coupled to a Xenics Xeva – 1.7-320 camera (320×256 pixels) embedding Specim Oles 31 f/2.0 optical lens.

CHIMSLAB group is also strongly involved in teaching activities both in institutional courses held at the University of Modena and Reggio Emilia and in schools and pre-conferences courses about NIR spectroscopy and chemometrics.

In the MSc in Food Control and Security of the University of Modena and Reggio Emilia, Alessandro Ulrici holds the courses in “Elaboration of experimental data” and “Chemometrics for food control”. We also supervise MSc students who want to carry out their project thesis in the field of NIR spectroscopy, imaging and chemometrics, frequently in collaboration with agri-food companies of our territory. As an example, some recent thesis projects in collaboration with food companies were related to the application of NIR spectroscopy and chemometrics for quality monitoring of Parmigiano Reggiano cheese and for the development of calibration models able to predict the composition of raw and processed meat products.

We also have courses in the Research Doctorate School in Food and Agricultural Science, Technology and Biotechnology, including “Applications of multivariate analysis in the agri-food context”, “Infrared spectroscopy in food analysis”, “Colour and chemical imaging: RGB and hyperspectral image analysis for food monitoring” and “Introduction to MATLAB environment”.

As mentioned before, our teaching activity is not limited to courses at the University-level, but it also includes the participation and organization of schools and pre-conferences courses. Recently our group was involved in two schools organised by the Italian Society of NIR Spectroscopy (SISNIR): the Summer School on image analysis and hyperspectral imaging, held in Rome in September 2017, and the Winter School—Combining NIR spectroscopy and chemometrics, held in Milano in January 2019. Generally, we are strongly involved in the activities organized by SISNIR such as the organization of conferences and pre-conferences courses, and in 2018 Alessandro Ulrici was elected as member of SISNIR Board.

Our group is also connected with the Italian chemometric community; indeed in 2019 Rosalba Calvini was elected as member of the Board of the Divisional Group of Chemometrics within the Italian Chemical Society, and from 2017 to 2019 this position was covered by Giorgia Foca.

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