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Poster Presentations

P01
THE EFFECT OF IMAGE PROCESSING CONSTRAINTS ON ROTATIONAL AMBIGUITY IN MULTIVARIATE CURVE RESOLUTION OF HYPERSPECTRAL IMAGES

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Hyperspectral imaging refers to the collection of a spectrum for each pixel in the image of scene. It is now being used in many different fields of industry and research; and the number of applications keeps growing. The main interest of hyperspectral imaging is that it combines spatial and spectral information about a sample or a scene. However, to extract this information, spectral unmixing of some kind has to be performed. Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS) is one of the techniques that can provide pure spectra and distribution maps of different components in the samples [1]. MCR-ALS is very useful and probably the most commonly used technique in chemistry for this purpose. However, as for any two-way factor analysis technique, it inherently suffers from non-uniqueness of the pure component decomposition, known as rotational ambiguity. Rotational ambiguity can be alleviated and sometimes totally avoided by a judicious use of the data structure or by incorporating well-suited constraints [2].

In this contribution, we aim to visualize and investigate the reduction effect of some image processing constraints on the extent of rotational ambiguity in MCR-ALS of hyperspectral imaging data [3, 4]. For this purpose, Borgen plots of three component simulated systems are used. Different spatial information, such as 2D-Gaussian fitting (hard-modeling), image segmentation and sparse image recovery are investigated. In each case, the extent of rotational ambiguity is evaluated. We discuss how these spatial constraints can reduce uncertainty and improve results accuracy. Hard-modeling, and to a certain extent sparse image fitting, can lead to unique solution, but their applications of spatial hard modeling constraint in real scenario can be questioned. Image segmentation, on the other hand, is more widely applicable, and its application result in less ambiguous solutions. Lastly, a couple of real examples such as remote sensing data sets and FTIR imaging are taken.

To recap: we visualize rotational ambiguity before and after applying constraints and discuss the importance of using proper and chemically meaningful constraints.

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P02
CONTRAST ENHANCEMENT AND TOTAL VARIATION IMAGE PROCESSING CONSTRAINTS: COMPLEMENTARY APPROACHES FOR MCR-ALS OF HYPERSPECTRAL IMAGES

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MCR-ALS [1] has demonstrated to be a valuable tool to resolve hyperspectral images (HSI). However, traditional MCR-ALS analysis of an HSI requires the unfolding of the hyperspectral data cube into a two-way array, which causes the loss of information on adjacency between pixels. In such cases, exploiting the spatial structure of HSI to improve the corresponding MCR-ALS solutions is unfeasible [2]. Several approaches have been developed to overcome this issue. The angle constraint (also known as contrast enhancement constraint) proposed by Winding et al. [3, 4] takes advantage from the duality of the spectral and spatial domain to enhance the selectivity of one of the two. Alternatively, a refolding step can be added in the least squares loop of the MCR-ALS decomposition [2]. This allows image processing constraints like sparsity, segmentation or total variation [2, 5-7] to be employed for improving the visualisation of regions of interest with sharp edges.

The aim of this work is to compare the outcomes resulting from the MCR-ALS analysis of hyperspectral images when contrast enhancement and total variation constraints are applied. Three simulated and a real dataset are here investigated, with the aim of exploring different experimental scenarios in which their effect is tested. The resolution of each dataset is discussed and the pros and cons of the two approaches are highlighted. Particular attention is given to how overlap among components (both in the spectral and spatial domain) can affect the possibility of achieving a physico-chemical meaningful MCR-ALS solution. Overall, contrast enhancement led to more *orthogonal* MCR-ALS components: for this reason, it may represent an optimal approach when such components are scarcely overlapped in one of the two aforementioned domains (e.g. overlapping distribution maps but independent spectra). On the other hand, for datasets clearly structured in the spatial domain, total variation was found to be able to retrieve even largely overlapping components.

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P03
ITERATIVE TARGET DETECTION FOR DETECTION AND CLASSIFICATION IN HYPERSPECTRAL IMAGES WITH AN APPLICATION TO A LANDSAT 8 IMAGE OF LAKE CHELAN, WA USA

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Classical least squares (CLS) is the tool of choice for detection and classification in hyperspectral images because often target spectra are known but reference values for each pixel are rarely available. Generalized least squares (GLS) is a weighted CLS model used to suppress clutter signal (interferences and noise) while enhancing minor target signal. (GLS is also known as the matched-filter.) An iterative target detection approach exhibits synergy between GLS and the extended mixture model (extended least squares, ELS) to further improve discrimination. The approach is relevant for chemical imaging, medical imaging and remote sensing. An example is shown for a Landsat 8 image of Lake Chelan, WA USA. GLS was used iteratively in a hierarchical approach to classification and GLS combined with ELS was used to further split a single class that was otherwise difficult to classify.
The first task used GLS iteratively to create global classes in the image associated with Water, Green (orchards, vineyards and lawn), Bare Earth, three types of forest, Road, Buildings and Other (corresponding to no specific class). The second task used GLS/ELS to split Class Green into signal attributable to lawn (e.g., associated with the municipal golf course) from cherry orchard (and other agricultural land including vineyards and other orchard types). Both objectives were complicated by the presence of a large number of pixels associated with water, forest, rough terrain, dry scrubland, homes, roads and buildings. The local GLS/ELS model showed good results that were verified in many cases using ground truth.

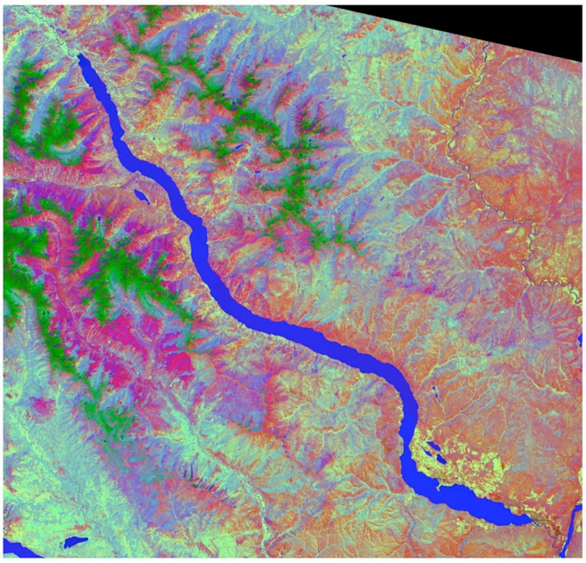

Figure 1 PCA Image of Lake Chelan Landsat8 – False color image of components 1, 2 and 3.

P04
REAL TIME AIRBORNE GAS DETECTION USING THERMAL HYPERSPECTRAL IMAGING

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Gas leaks and air pollution sources present to a certain extend health, safety and environmental risks. A history of crisis management in the Upstream has shown the value of efficient and accurate tools for detecting gas leakages and/or the characterization air pollution agents. Knowing about the existence of a leak or the existence of an environmental thread is not always enough to launch a corrective action. Additional critical inputs such as the leak source, the chemical nature of the gas cloud, its direction and speed and as well as the gas concentration must most of the time be gathered in a short amount of time to help securing the hazardous areas. Most of the time gas identification for gas leaks surveys or environmental monitoring purposes involve explosives and/or toxic chemicals. In such situations, airborne measurements present particular advantages over ground based-techniques since large areas can be covered efficiently from a safe distance. In this work, we present our recent results on real time airborne gas detection up to 4600 feet above the ground using thermal hyperspectral Imaging technology. The Fourier transform technology used in the longwave (8-12 mm) hyperspectral camera on an airborne platform allows recording of airborne hyperspectral data using mapping and targeting modes. These two acquisition modes were used for gas imaging a ground-based ethylene, Methanol and acetone gas release experiment. Real time quantitative airborne chemical images of the three gas clouds were obtained paving the path toward a viable solution for gas leak surveys and environmental monitoring.

P05

COMBINATION OF MALDI IMAGING MASS SPECTROMETRY WITH CHEMOMETRIC TOOLS FOR INVESTIGATION OF TUMOR HETEROGENEITY

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Tumor heterogeneity could help to explain, why some patients that initially respond positively to a cancer drug eventually relapse, often with new tumors that no longer respond to the therapy. Understanding tumor heterogeneity is therefore a key factor in cancer science. Differences between cells types within a tumor tissue can have profound implications during the diagnosis and treatment of cancers [1-2].

Matrix-assisted laser-desorption ionization-Mass spectrometry imaging (MALDI-MSI) is very well suited to study molecular distribution patterns within CRC tissues. The aim of this study is to demonstrate that the combination of MALDI Imaging mass spectrometry with chemometric tools allows investigation of tumor heterogeneity and identification of relevant tumor populations within the cancer tissues. With this purpose and as a preliminary study, human colon adenocarcinoma cell lines sensitive HCT116 (S) and resistant HCT116-SN50 (R) to irinotecan (chemotherapy drug) were used as a model of experimental tumors. Clonogenic tumor xenographs were generated by subcutaneous injection of both unique cell line on athymic mice whereas a model of heterogeneity was created injecting various mixture of (R) and (S) HCT116 clones. Tumors were then collected, sliced, and analyzed by MALDI Imaging mass spectrometry. Potential discrimination of R and S populations will be tested by classification methods such as Least Squares Dicscriminant Analysis (PLS-DA), k-Nearest Neighbors (kNN) and Soft independent modelling by class analogy (SIMCA)

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P06
HSI-NIR: SIMPLY A SURFACE-ANALYSIS TECHNIQUE? INSIGHTS ON PENETRATION DEPTH AND TRANSMISSION MODE

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Hyperspectral imaging is usually considered as a surface analysis method. Nevertheless, electromagnetic rays may penetrate in depth, inside the upper layers of the sample, including information from the inner parts in the recorded spectra. Moreover, such an effect depends on the matrices analysed and on the specific wavelengths at which spectra are recorded.
In the present study, penetration depth was evaluated for a near infrared hyperspectral imaging system working in the 1000–2500 nm spectral range, at 8 nm spectral resolution (HSI-NIR SWIR3 camera equipped with a LabScanner 40x20).
To the aim, a chessboard background was assembled using two polymeric materials characterised by different total reflectance values (about 0% and 90%, respectively) and with different and characteristic spectral profiles. The use of a geometrical pattern, in comparison with uniform backgrounds, adds spatial information to the penetration depth evaluation. Images were recorded placing samples (sliced cheese), both sliced at different thickness and wedge-shaped, between the source and the chessboard background.
Univariate and multivariate image analysis was carried out in order to highlight both spatial and spectral features, allowing to evaluate the penetration depth. First of all, a region of interest (ROI) within the hyperspectral image, including a representative portion of the sample was selected. Then, principal component analysis (PCA) was carried out, reducing data dimensionality and removing non-useful information to confirm the level of penetration on the basis of score images.
On the basis of these outcomes, in many practical applications, hyperspectral imaging should be regarded as a transflectance approach, depending, of course, on the physico-chemical characteristics of the matrix, such as the chemical composition and the physical microstructure, and on characteristics of the electromagnetic radiation involved (wavelengths and intensity).
A further interesting topic concerns the possibility of acquiring hyperspectral images in the transmission mode. To this aim, an in-house instrumental setup was adopted, allowing to transmit electromagnetic radiation across samples. Particular strategies for focusing and normalising image intensities were developed. Transmittance images obtained on samples of biological interest allowed capturing important chemical information on the internal structures of biological tissues, complementary to information acquired in the reflection mode.

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P07
THE HIGH-POWERED EYE OF HSI-NIR: A DECISIVE TOOL IN FORENSIC SCIENCES

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During the last decade, there has been an increasing interest in the development of customised analytical methods based on non-destructive chemical imaging in several fields of application. This is of particular interest when it is important to spatially visualise the results as an unequivocal proof of a crime and without damaging the evidences, because further investigations could be required during legal inquiries. For these reasons, the present work aims at developing a reliable method for the application of hyperspectral imaging in the near infrared region (HSI-NIR) to detect biological traces on the crime scene; in this way, a screening procedure is proposed to detect areas of interest in which collecting micro-samples for applying the conventional more targeted DNA analyses. In more detail, this work will give a fundamental contribute to forensic scientists in identifying biological traces directly on specimens, recognising the type of trace (e.g. blood, urine, semen and their mixtures as well as food traces) regardless of the material constituting the collected evidences (e.g. paper, glass and cloth).

HSI-NIR is one of the newest technologies developed in the field of NIR spectroscopy; it is based on the interaction between radiation – in the region of the electromagnetic spectrum between 1000 and 2500 nm – and the sample, to obtain chemical information about its composition, thanks to the spectroscopic absorption of characterising compounds. The advantages of this approach are exploited when samples to be evaluated are characterised by a non-uniform distribution of chemicals inside the whole matrix. In this situation, the validity of traditional chemical analyses is strictly dependent upon the design of a correct sampling plan; the extent of sampling required to account for such a variability of distribution is necessarily quite large and the method of collecting samples is also critical. All these limits become serious when data collected have to be used for drawing conclusions at the service of law. In fact, sampling limitations leave an analytical crack in which crime may act.

Often, HSI-NIR equipment setup is not directly applicable, since optimisation steps are required, in terms of both instrumental parameters and image acquisition; furthermore, the acquisition of images is not sufficient for extracting reliable information from samples in a robust way. For these reasons, in this work, HSI-NIR is supported by a proper chemometric strategy particularly suited to account for the spatial information, allowing to define a customised method for the specific application.

P08
DEVELOPMENT OF A HAND-HELD HIGH RESOLUTION HYPERSPECTRAL IMAGING CAMERA

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HinaLea Imaging developed a unique low-cost high-resolution hyperspectral reader platform to read and decode objects labelled with its microscopic silica tags which are edible memories sparsely embedded in a wide variety of objects. These readers can be readily adapted to Hyperspectral Imaging and offers a unique cost, size, spatial-resolution and spectral-resolution combination.

Although their application space is broad, these instruments can revolutionize the space of sample analysis. Whereby most current instruments analyze the bulk properties of samples, the new imager cannot only analyze spectral content with spectral resolutions approaching that of state-of-the-art spectrometers but can also provide high spatial resolution.

At the heart of the imager is an optical engine using HinaLea Imaging's proprietary Fabry-Perot Interferometer and embedded technology which has been adapted into a mass-manufacturable solution. This optical engine can be adapted to other applications and instruments. HinaLea Imaging is currently collaborating with and is looking for new collaboration partners for harnessing the power of this technology to new application areas.

Figure 1: HinaLea Imaging's Solid-State Tunable Filter Production and the Model 4100H

P09
PROS AND CONS OF IMAGE TEXTURE ANALYSIS ON HYPERSPECTRAL DATACUBES: THE FLOUR CASE-STUDY

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Surface texture is an important feature for evaluating physical nature of analytical samples, allowing to highlight differences between matrices with a very similar chemical composition. To measure such a property, several algorithms of image texture are available in literature and are typically applied on mono-layer images, usually the grey scale ones.

The aim of the work is to compare and evaluate the ability of three different approaches of image analysis on hyperspectral data; the fact that these data are organised in three-dimensional data cubes may constitute a limiting factor in applying image texture algorithms directly on the hypercube. In more detail, two algorithms typically applied on mono-layer images are taken into consideration: GLCM (Grey Level Co-occurrence Matrix) and AMT (Angle Measure Technique), while for multivariate approaches an algorithm proposed by Bharati e MacGregor and based on PCA was considered [1]. Different types of data compression, such as integral images and PCA, were applied to extract the information related to physical properties of the samples, before performing the procedures under study.

In the flour case study, images of 5 types of flour (durum wheat flour, strong flour – Manitoba, wholemeal, plain flour and soft flour) were recorded by a hyperspectral camera SWIR3 (SPECIM Ltd, Finland), working in the spectral range 1000-2500 nm. These images were submitted to combinations of data compression and image texture algorithms to distinguish between the five commercial types of flour.

This work allows to deeply evaluate the reliability of well-known image texture approaches on HSI-NIR images; pros and cons of each procedure were highlighted.

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