Unmixing of chemical species in hyperspectral imaging

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Nowadays, hyperspectral imaging constitutes a key analytical tool for many diverse applications like material and biosystem characterisation. Hyperspectral images, in fact, provide both structural and chemical insights into complex objects or scenes, with these two types of information being entangled in the multidimensional spatio-spectral data structure yielded by the instrumental platform. In such a context, so-called *spectral unmixing* plays a crucial role: by this term, one refers to the decomposition of hyperspectral imaging data into resolved distribution maps and spectral profiles associated to all the individual chemical species underlying the investigated samples (see Figure 1). Given the nature of this problem and the significant impact that tackling it can have in very disparate domains, spectral unmixing undoubtedly represents a topic of prominence and deep interest. Nonetheless, the fundamentals of the most commonly used approaches to address it may not be straightforward to their potential users. For this reason, this work is aimed at offering a simple overview of spectral unmixing, mainly focusing on the properties of two techniques frequently exploited for the analysis of hyperspectral images: Principal Component Analysis (PCA) and Multivariate Curve Resolution – Alternating Least Squares (MCR-ALS). Their basic principles, pros and cons will be discussed also in the light of their possible utilisation in fields like Fluorescence Lifetime IMaging (FLIM) microscopy.

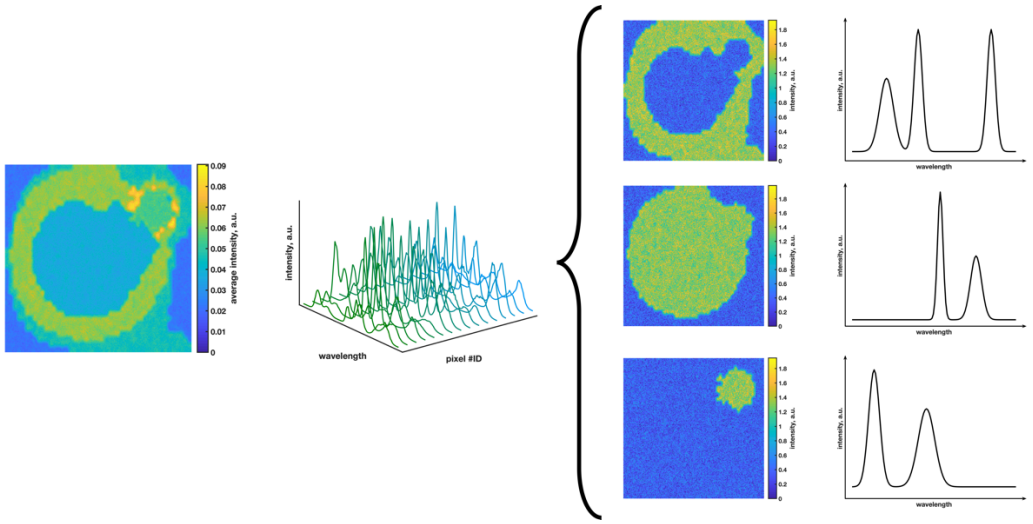

Figure 1. An illustration of the principle of spectral unmixing of hyperspectral images. The spatial and spectral contributions of three "pure" chemical species in the right panel are resolved from the raw data schematically represented in the left panel