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An Overview of Chemometric Methods for Analysis of Multivariate Images

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Images have been used in the sciences for a long time, and due largely to improvements in digital Imaging technology, their use is expanding. Large amounts of data representing complex systems can often only be represented by visualization as images.
Multivariate images arise from a surprising varietyof sources. Some are images in the conventional sense (such as satellite data) while others are not (secondary ion mass spectroscopy, SIMS).
Almost all physical units can be used to make images and multivariate images: temperature, gravitational field, impedance, magnetic field, electrical field, mass, wavelength, ultrasound wavelength, polarization, electron energy etc. The simplest meaningful multivariate image has two pixel indices (e.g. width and height in the image plane) and a variable index, making up a threeway array. An important aspect in going from analog scenes or objects to digital images is resolution. Multivariate images have spatial, intensity, spectral and time (temporal) resolution. A typical older satellite image would have 512x512 pixels, in 7 wavelength bands and an intensity resolution of 256 gray levels. High spatial and intensity resolution is desirable and this makes the arrays rather large, making computational speed and memory issues challenging. The traditional field of univariate image analysis works in the spatial domain in 2D or 3D image arrays. When images become multivariate or multitemporal, the spectral or time domain becomes a higher priority than spatial considerations. When this is the case, the tools of Multivariate Image Analysis (MIA) become very useful.
This talk introduces the main tools of MIA and gives examples of their use. Principal Component Analysis (PCA), a fundamental tool of MIA, is discussed. PCA allows the variable dimension of images to be compressed. This allows for variables to be combined in a way that produces images that clearer than any individual variable. PCA score images can be combined in different colors to describe the largest possible amount of variation in the data. Besides viewing PCA scores in the image plane, they can also be viewed as cross plots in PCA space. This allows for a better understanding of distribution of features in an image and the relationship between the types of features on the surface. Linking between score space and image space is demonstrated, allowing interactive exploration of images.