

Entropy, priors and fusion in spectroscopic mapping techniques

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We define a spectroscopic map as a 3 dimensional data set which contains 2 dimensional spatial information in a plane, with spatially correlated spectra in the orthogonal direction. A map sequence is a 4 dimensional (at least) data set which consists of a stack of spectroscopic maps, following their evolution through a further dimension. Because different physical conditions (e.g. temperature) cannot be applied to the same system simultaneously, the most usual form of a map sequence is a time series with the 4th independent variable also being a known (or assumed) function of time. Conventional data fusion can be defined as the use of statistical and other data analysis tools for combining output from different sensors into a common format, usually with the objective of taking automatic or semiautomatic decisions based on the sensoria. An example would be the fusion of data from globally distributed fire detection systems in a city with the real-time distribution of fire fighting equipment, the availability of personnel, the status of hospital casualty departments, police, military units and etc. to form an effective decision making system for civil defence. In this case, the data are relatively simple, but the logistical problem is complex.

This project considers overall the application of principles similar to those above to data from chemical mapping techniques. These have the capability to provide, through the use of spectroscopy, information on the spatial distribution of chemical species on (or in) a sample. However, no known single spectroscopy can provide a complete picture: For example, x-ray diffraction and x-ray absorption tell us, respectively, about long and short range order; x-ray fluorescence tells us about atomic composition. To make it interesting, the sampling volumes of the three techniques are different. Similar considerations apply to combinations of electron spectroscopy, electron microscopy, and mass spectrometric mapping techniques. Moreover, two factors determine the resolution of the data: (i) the technique response (i.e. a function which, if determined, could be convolved with the “truth” to simulate a noise-free measurement) and (ii) the fluctuation in the data. In this context, then, the resolution is a parameter which determines the mismatch between truth and measurement. e.g. In a photograph taken through cheap lenses exhibiting spherical aberration, intensity from a point in the object is distributed over a finite region in the image. Additionally, at low light levels, features appear grainy because of statistical fluctuations in the numbers of photons arriving in adjacent parts of the image. These two effects combine to give a blurred photograph, but note that the latter effect inhibits the correction of the former. Here, the data are complex, but the problem, determining chemical and structural evolution of a sample, is simple.

In fact, this is where this project starts: At the MSc level, given a noisy data set, how can we apply corrections relevant to different techniques and different dimensions (spectral resolution, spatial resolution, sampling volume ...) so that data taken with different mapping tools on the same region of sample become comparable? Can maximum entropy techniques combined with deconvolution and correlation help us make a reasonable guesstimate of the truth in each case? To give context, the data involved will come from secondary ion mass spectrometry depth profiles where the response is known, and from new x-ray excited optical luminescence maps, where it is not, although methods do exist for constructing priors where the chemical structure of a sample is known. As a PhD, the project would encompass inter technique comparisons and fusion of different spectroscopies for a complete picture of the chemistry and structure of a sample. The student should be prepared to develop user-friendly, object oriented, code for Windows[®] using Visual C++ or Visual Basic.