

Spectral Image Analysis

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Course Summary: Full Day

The combination of spectroscopy and imaging, known as Spectral (Multivariate or Hyperspectral) Imaging, is a rapidly emerging area of analytical science. Recent advances allow spectral imaging measurements from the ultra-violet into the far-infrared (terahertz) regions of the electromagnetic spectrum. Because the spectral information permits identification of the spatial distribution of chemical analytes, the approach is often referred to as Chemical Imaging. This full day course will address imaging and analysis of images utilizing all of these spectral ranges with industrial, pharmaceutical and agricultural examples for illustration. Spectral Imaging in the near-infrared (NIR) region will be emphasized with additional examples using fluorescence, reflectance, transmission, attenuated total reflectance (ATR) and Raman. Information extraction from the large (e.g., 100 Mbytes) data cubes (x and y spatial coordinates and spectral wavelength along the z direction) is a challenge and several chemometric analysis techniques will be presented. These include unsupervised and supervised pattern recognition techniques, clustering and quantification. Methods will include maximum autocorrelation factors and multivariate curve resolution.

Course Outline

Introduction to Spectral Imaging

Intro to 3-way arrays, Objects and Variables, Example Applications, Structure of Multivariate Images, Comparison to other sources of 3-way data

Types of Spectral Imaging Data

Imaging of water, fluorescence and reflectance imaging in the uv/visible, FT-IR microspectroscopic imaging, attenuated total reflectance (ATR) imaging, Raman, and Near-IR spectral imaging

Spectral Metrics

Histograms, peak area mapping, peak height ratio mapping, and spectral moments

Spectral and Spatial Preprocessing

Baseline Correction, Centering and Scaling, Smoothing and Derivatives, Masking, Filters (convolution), Scatter correction, Image Sharpening (deconvolution)

Unsupervised Pattern Recognition with PCA

Principal Components Analysis (scores, loadings and projections, unusual samples, residuals and T^2), Matricizing of images, Overlays, Score/Score plots: density, Links between scores space and the image plane, Contrast enhancement

Other methods: clustering, maximum / principal autocorrelation factors, maximum / principal difference factors, independent components analysis

Supervised Pattern Recognition

Soft Independent Class Analogy: Image SIMCA. Partial Least Squares Discriminant Analysis: PLS-DA

Quantitative chemical analysis

Classical Least Squares, Extended Least Squares, Weighted Least Squares, Generalized Least Squares, review of signal-to-clutter

Other analysis methods

End-member extraction, multivariate curve resolution and self modeling curve resolution

Texture analysis (FFT, SVD spectrum)

Evolving Window Factor Analysis and Target Factor Analysis

Other emerging spectral imaging measurement capabilities

Spectral imaging using a tunable laser source

Far-infrared (terahertz) spectral imaging

Concluding Remarks and Acknowledgements

Who Should Attend

This course is geared toward chemists and engineers interested in learning about spectral imaging and applying it in an effective manner to industrial, pharmaceutical or agricultural problems. It will provide a general overview of spectral imaging and chemical image analysis with useful information on how to choose the best approach for the specific project or problem.