



Contribution ID: 71

Type: **Poster**

Self-Organising Maps with Relational Perspective Mapping (SOM-RPM); A practical tool for the evaluation hyperspectral data sets

Monday 1 December 2025 16:00 (1 hour)

Unsupervised machine learning, specifically self-organizing maps with relational perspective mapping (SOM-RPM), is a practical tool for thoughtful and considered analysis of complex hyperspectral data sets. The SOM-RPM approach treats each pixel in a hyperspectral image as a sample, clustering spectra based on similarity. This method creates a colour-coded similarity map in which changes in colour are specifically graded to accord with changes in the spectral dimension, by examining the entire data set. The SOM-RPM toolbox allows for interactive selection and exploration of the data, regardless of the data source. This methodology has proven to be a robust technique that has so far been demonstrated mostly on Time-of-flight secondary ion mass spectrometry (ToF-SIMS) data.

ToF-SIMS is a mass spectral imaging technique, which can be extended into a three-dimensional depth profiling using a secondary sputtering gun. ToF-SIMS images and depth profiles are large and complex hyperspectral data sets. Interpretation requires that the complexity of these data sets is reduced. For two-dimensional data, individual ion peaks are often extracted and overlaid or for three-dimensional data, a handful of peaks are plotted in one dimension as a function of depth. These simple methods work well for known or simple samples, however for complex or unknown samples, these methods struggle to convey the depth of information captured within the data set. Furthermore, the choice of displayed ion peaks has the potential to impart user bias and make a significant difference to the interpretation of results.

By pairing ToF-SIMS and SOM-RPM, the complete hyperspectral data set in 2D or 3D can be intuitively visualized, providing a unique picture of the local and global mass spectral relationships between individual pixels. This work will present several case studies across a broad range of sample types.

Author: BAMFORD, Sarah (La Trobe University)

Co-authors: Prof. WINKLER, David (La Trobe University); Prof. PIGRAM, Paul (La Trobe University); Dr GARDNER, Wil (La Trobe University)

Presenter: BAMFORD, Sarah (La Trobe University)

Session Classification: Poster Session

Track Classification: Topical Groups: Condensed Matter & Materials