Automatically Identifying Rock Coatings in Laboratory LIBS Data Using Machine Learning Algorithms

Diane Oyen and Nina Lanza; Intelligence and Space Research, Los Alamos National Laboratory

Rock Coatings in Laboratory LIBS Data

- Surface composition, such as rock coatings and weathering rinds provide information about past aqueous environments
- Can we automatically identify these features from LIBS data?

Results: Exterior of Basalt Sample

The exterior of the basalt displays a chain-like structure in the Gaussian graphical model (right) indicating that the chemistry is changing systematically along these shots as seen in the LIBS plot.

Results: Interior of Basalt Sample

The interior of the basalt displays a blob-like structure in the Gaussian graphical model (right) indicating that the chemistry is homogeneous after the first two shots as shown in the LIBS plot.

Background

Gaussian graphical model
- Dependencies between samples as partial correlations
- Partial correlation is the degree of association between two variables, after effects of other variables is removed
- No link (partial correlation = 0) is conditional independence
- Example graph:

Depth trends from LIBS spectral data
- Data: Spectra from sequence of shots in single location
- Shots are nodes and associations are links in graph

Methods

Depth trends as shot association graph
- Surface layer: early shots linked but not later shots
- Gradual changes: graph will form chain
- Abrupt changes: graph will cluster

Estimating a graph from data
- Data matrix $X$ with sample covariance matrix $\Sigma$
- $X_j = \text{shot } j$ with spectral values $X_{ij}$ for $i \in \{1, \ldots, n\}$ wavelengths
- Estimate sparse matrix $\Theta$ given sparsity constraint $\lambda$:
  $$||\Theta||_1 = \sum_{ij} |\Theta_{ij}|$$

Discussion

Graphs are informative models of ChemCam data
- Shot-to-shot associations follow expected patterns
  - Exterior of rock shows systematically-changing chemistry
  - Interior of rock shows homogeneous chemistry

Automated data mining aids interpretation of data
- Graphs model dynamic nature of observations
- Associations summarize high dimensional data

Future Work
- Wavelengths of interest, rather than full spectrum
- Search for samples indicative of surface coatings
- Characterize surface and interior features