Lunar and Planetary Science Conference, March 16th, 2014

COMMUNITY USER WORKSHOP ON PLANETARY LIBS (CHEMCAM) DATA

Additional LIBS Data Processing

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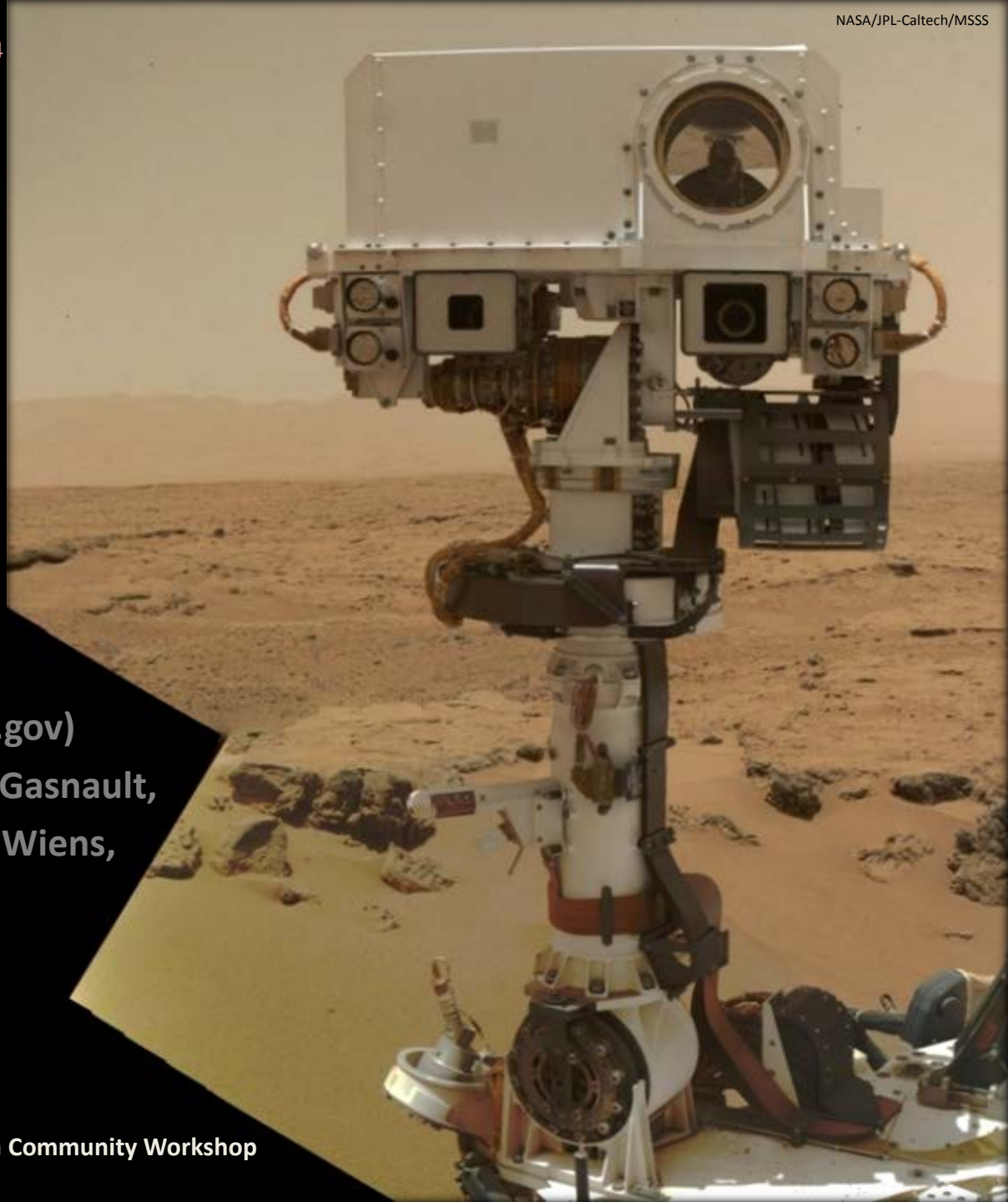
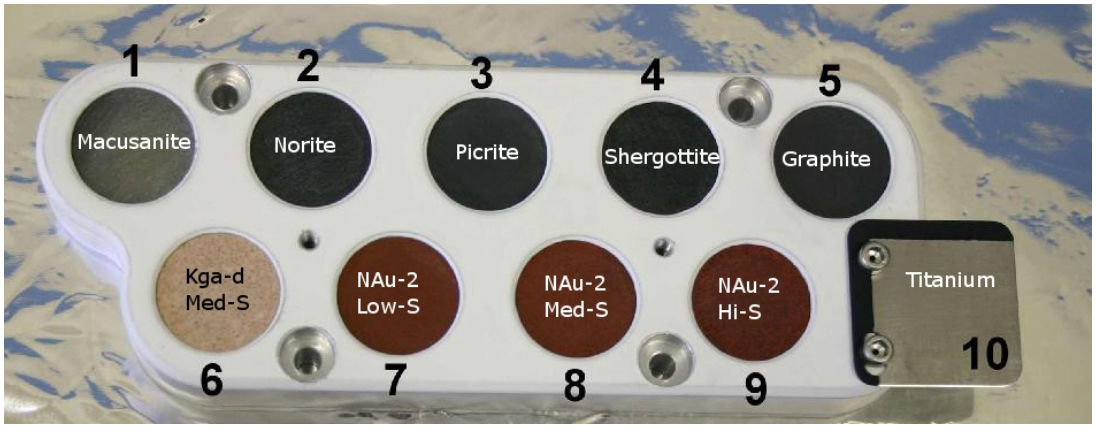
Agnes Cousin, Cecile Fabre, Olivier Gasnault, Olivier Forni, Jeremie Lasue, Roger Wiens, and the ChemCam Team



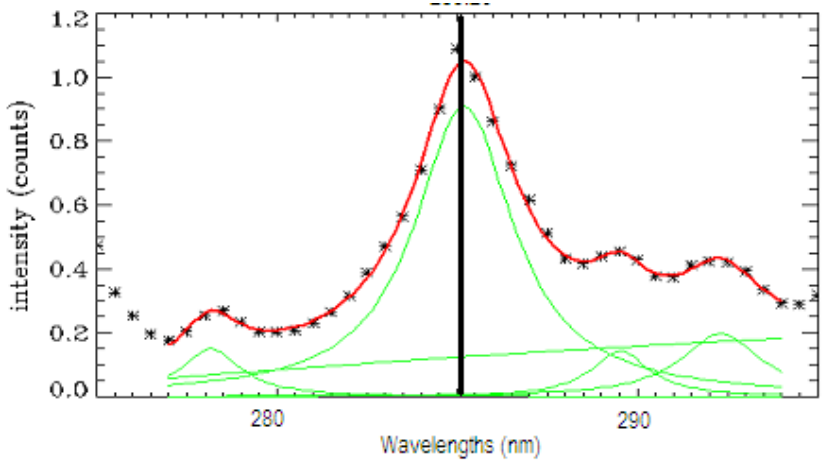
Univariate Calibration

- Use strength of a single emission line to predict compositions for that element
- Useful alternative to multivariate methods, especially for minor/trace elements
- Use calibration targets on the rover to build the model
  - Different laser energies require different models



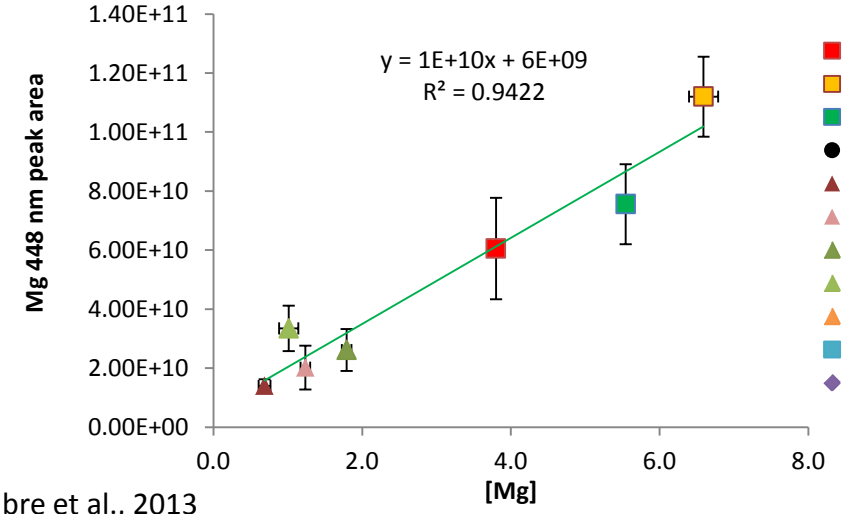
Univariate Calibration

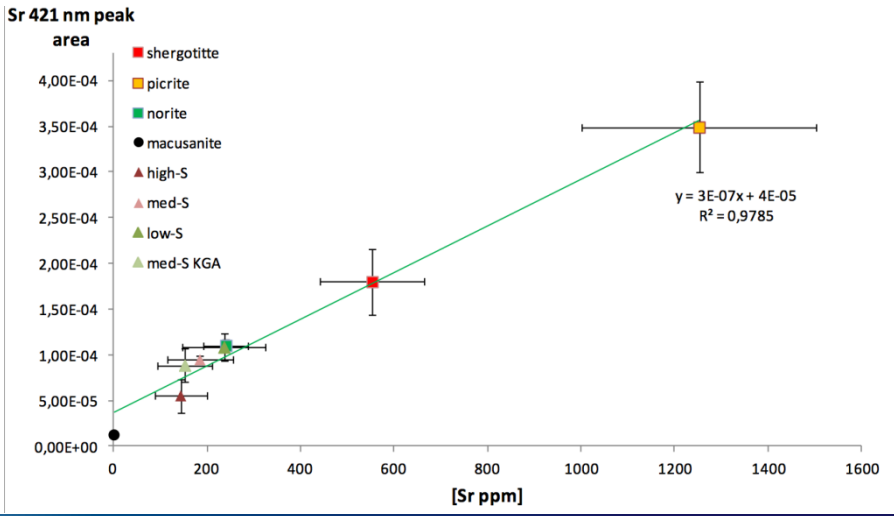
Peak Fitting is Necessary:



- Use “cleaned calibrated spectra” (CCS)
- Peak fitting is necessary to isolate the emission line of interest, so that calculated peak area is accurate
- Calibration curves plot peak area vs known composition
- Taking ratios of lines can help correct for differences in intensity from different targets

Example Calibration Curves:

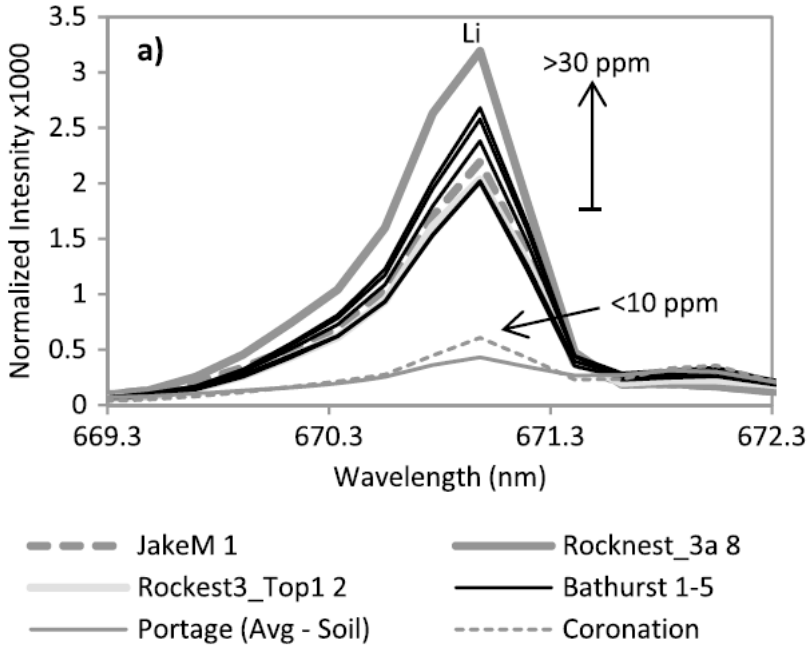




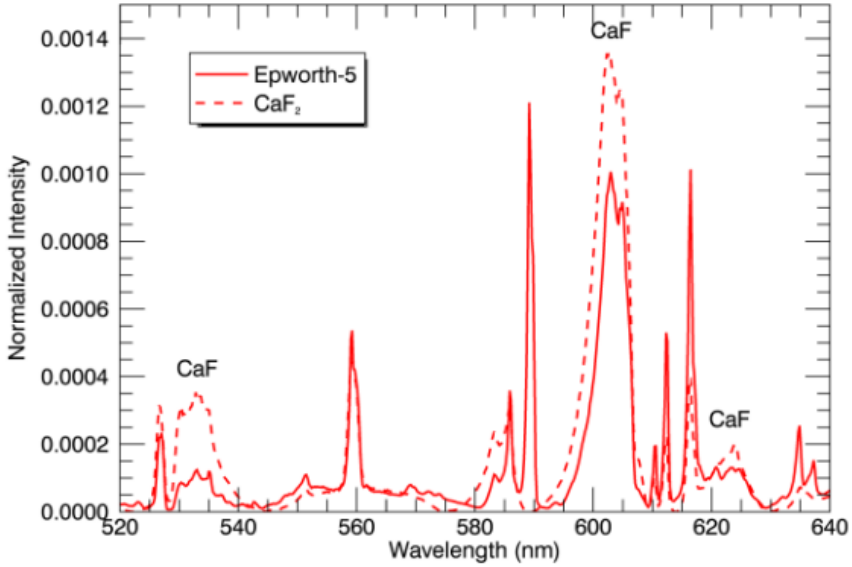
Fabre et al., 2013

Trace Elements

- ChemCam can detect minor and trace elements, including: Li, Ba, Sr, Rb, Mn, F
- Univariate models and/or restricted-range PLS can be used to get approximate quantitative measurements
- Using the full wavelength range in PLS doesn't perform as well: strong lines dominate
- Also see presentations from Forni (CF detection - #1328), Lanza (Mn detection - #2599), and Ollila (Li, Ba, Sr, Rb - #2490) this week



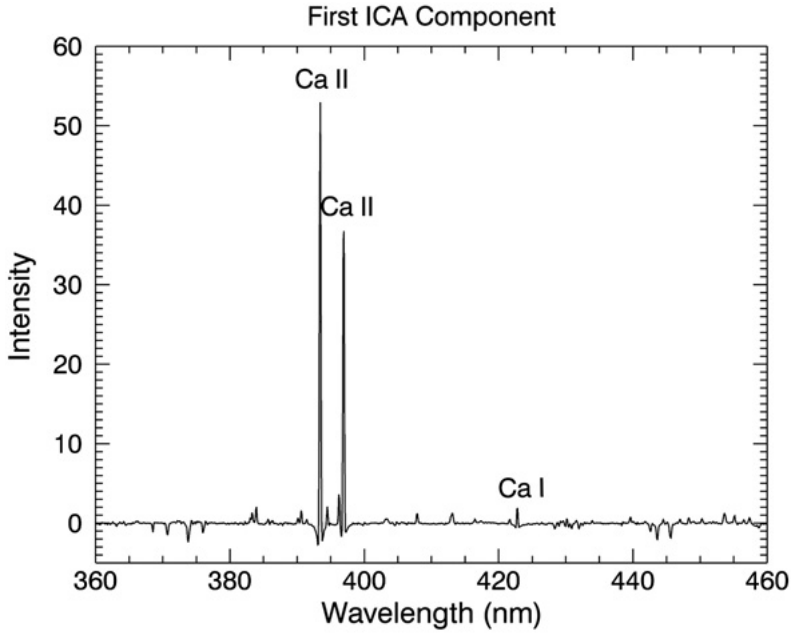
Ollila et al, 2013; this meeting



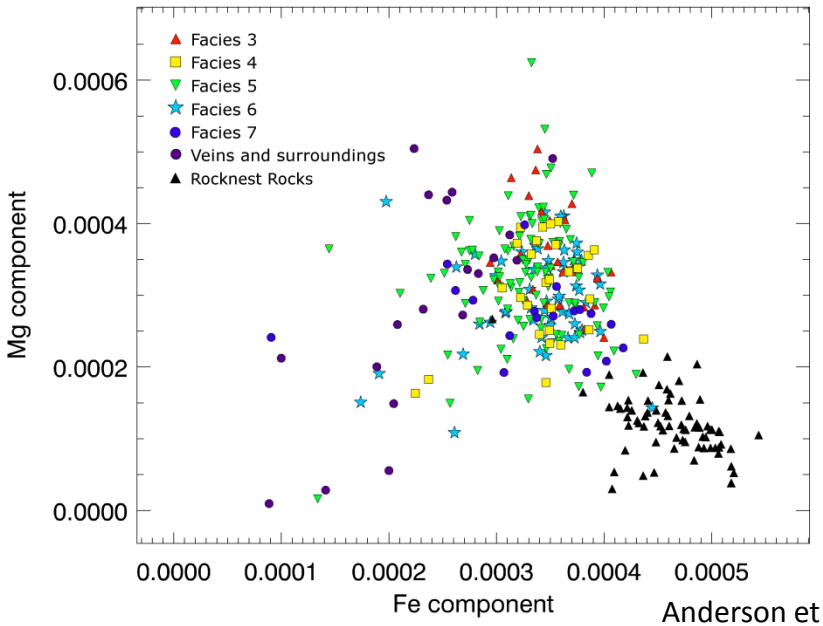
Forni et al. (this meeting)

Independent Component Analysis

- Similar to PCA, but seeks to minimize statistical dependence between components
  - Does not assume a Gaussian distribution as PCA does
  - Results in loadings that isolate individual elements→ easier to read scores plots than PCA
    - Axes are a qualitative measure of signal from one element



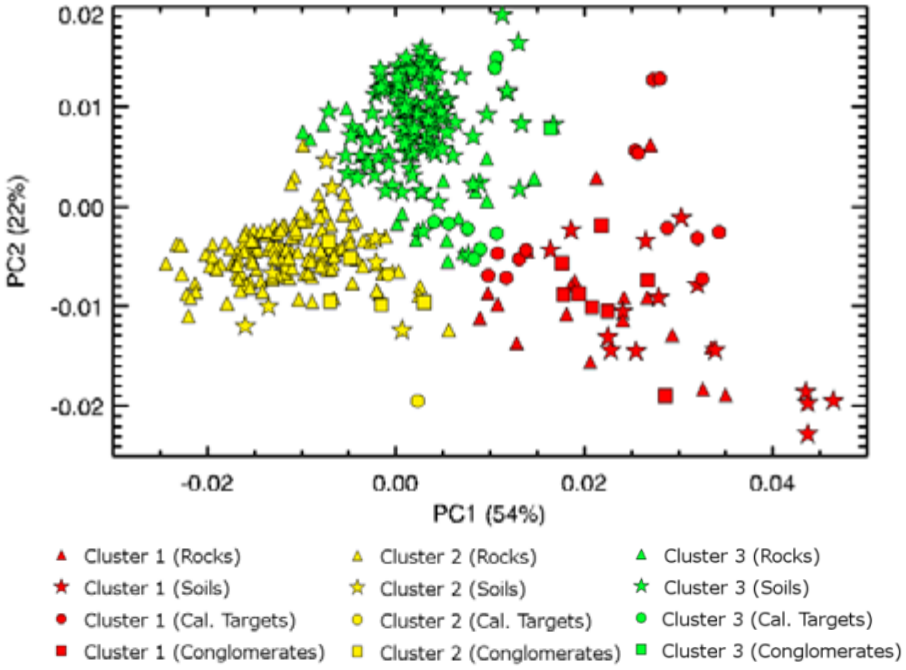
Forni et al., 2013



Anderson et al., 2014

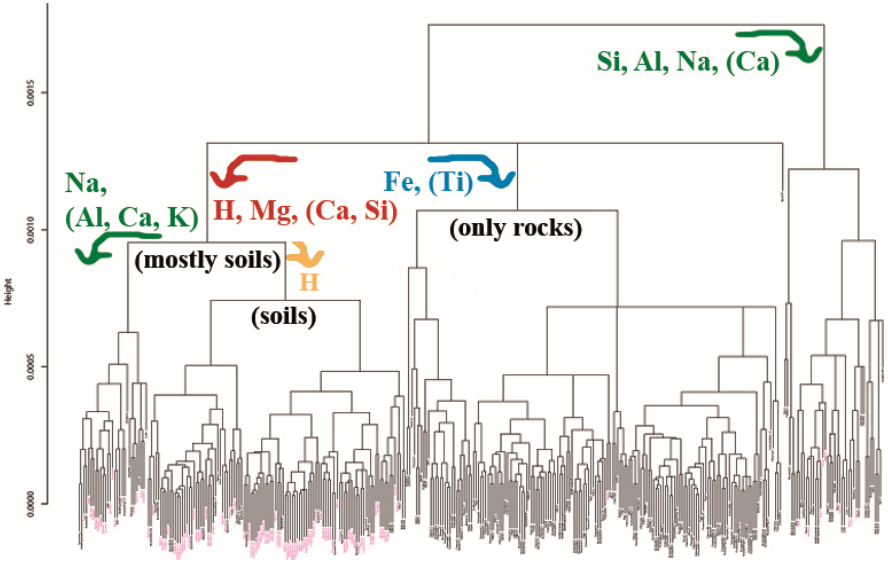
Clustering / Classification

- Many different methods!
- Many use ICA or PCA scores as input



Anderson et al., 2013 LPSC

- Unsupervised:
  - Hierarchical clustering
  - K-means clustering
- Supervised:
  - SIMCA
  - PLS-DA



Gasnault et al., 2013 LPSC

Software Options

- Unscrambler
  - Pro: capable of most multivariate analysis methods, relatively user-friendly
  - Con: proprietary, expensive, not scriptable
- Programming languages:
  - IDL
    - **Primary language currently used by the CCAM team**
    - Pro: scriptable, has functions for some methods described
    - Con: expensive, learning curve, doesn't have functions for all methods
  - Python/Numpy/SciPy
    - Pro: free, scriptable, many libraries for multivariate analysis, widely used
    - Con: learning curve
  - R
    - Pro: very large library of statistical functions, free, widely used
    - Con: learning curve
- Many others!
- Questions? Ask a CCAM team member!

  My Email: rbanderson@usgs.gov

References

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- Lanza et al., (2014) “Manganese Trends with Depth on Rock Surfaces in Gale Crater, Mars”, 45th LPSC, #2599
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