Probing Putative Biomarker Assignments in SEM Imagery from BRAILLE Investigations at Lava Beds National Monument (N. CA, USA) Using Machine Learning Tools





Machine Learning 101





Mineral to Microbe Continuum (MMC) Correlations





Mineral-Microbe morphologies in SEM images of lava tubes, sampled from Lava Beds National Monument (LABE), Northern CA, USA

Mineral to Microbe Continuum (MMC): gradient of life activity across mineral/biomineral features

LABE Proposed Continuum



Unsupervised Clustering Techniques



- **Principal Component Analysis** (PCA)
 - Used to visualize low dimensionality representation of data variance
 - Limited to linear projections
- t-Distributed Stochastic Neighbor Embedding t-SNE)
 - Probabilistic characterization of local structure
 - Prevents low dimensional "crowding problem"
 - Well suited for visualization of highdimensionality
- K-Means Clustering
 - Optimizes grouping of data into user specified number of groups ("K")
 - Reassigns data points to new group means with every round until no changes are made



First and Second Principal Components colored by digit

tSNE dimensions colored by digit





PCA & tSNE – MMC Features (n = 770)





PCA & tSNE – Detector Bias





Magnification vs. Morphology













4000x



tSNE – Magnification Plots



Boundary Magnification Ranges (40% of Images) Median Magnification Ranges (60% of Images)





Magnification tSNE Comparison



All Images (n = 770)



Magnification Subset (n = 401)



K-Means Clustering on TSNE





K-Means Cluster vs. MMC Category Corrected Rand Index: **0.006367637** K-Means Cluster vs. MMC Category Chi-Squared P-Value: **2.721e-07** MMC vs. TSNE-X + TSNE-Y MANOVA P-Value: **8.545e-08** Response TSNE-X P-Value: **0.03237** Response TSNE-Y P-Value: **1.421e-**



K-Means Cluster vs. MMC Category Corrected Rand Index: **0.02526194** K-Means Cluster vs. MMC Category Chi-Squared P-Value: **7.529e-08** MMC vs. TSNE-X + TSNE-Y MANOVA P-Value: **8.177e-07** Response TSNE-X P-Value: **6.703e-**

Convolutional Neural Networks (CNNs) for Image Classification









Low-level features

Mid-level features

High-level features

Convolution Layers





Input layer

CNN Results



- Binary vs. multiclass vs. multilabel
- Overfitting/Biased Classes
- Possibly insufficient training data

Accuracy

	Binary	Multiclass
Cross-Validation	75%	80%
Hold-Out Testing	55%	50%

Generative Adversarial Networks







- Strengthen supervised classification
 - Generative Adversarial Networks
 - Leverage pre-built models
- Develop methodology for generating unbiased datasets
 - Raster scans
 - Random fields
- Applications
 - Automatically detect microscopic life
 - Correlate morphology with distinct taxonomies
 - Automatically detect biomineralization features/extinct life

Acknowledgements









