MACHINE LEARNING METHOD FOR METEORITE CLASSIFICATION BASED ON REFLECTANCE SPECTROSCOPY. Sydney M. Wallace[1,2], M. Darby Dyar[2], Thomas H. Burbine[2], and Daniel Sheldon[3]. [1]Harvey Mudd College, 301 Platt Blvd., Claremont, CA 91711 (smwallace@hmc.edu); [2]Dept. of Astronomy, Mount Holyoke College, 50 College St., South Hadley, MA 01075; [3]College of Information and Computer Sciences, University of Massachusetts Amherst, Amherst, MA 01003.

Introduction: Meteorite classification currently involves preparation of a thin section and careful petrographic and chemical analyses. Development of a field method for rapid classification would be useful for preliminary taxonomy. Moreover, a spectroscopy-based meteorite classification would enable relationships to be drawn between meteorites and their parent bodies. This project uses modern machine learning (ML) methods to develop an automated meteorite classifier using visible and near-infrared (VNIR) spectra from particulate meteorite samples that had been previously classified by conventional methods.

Data: This project uses 1,623 meteorite spectra obtained from archives and unreleased data from meteorite samples generously made available to us by the Keck/NASA Reflectance Experiment Laboratory (RELAB) at Brown University [1]. VNIR spectra were acquired there using the bi-directional reflectance spectrometer. Meteorite classifications were obtained from file headers on RELAB files and from the *Meteoritical Bulletin Database* [2]. Consistent headers containing metadata fields were created for all files and individual spectra files were reformatted to conform to a consistent file format. Prior to classification, all data were resampled to cover 0.3 to 2.5 µm at 0.01 nm resolution.

Although 30 different meteorite groups were represented in the initial database (Figure 1), some groups were combined due to the small number of spectra available. Classes that were spectrally similar and closely related in the taxonomy were merged: CV and CK became CV-CK, EH and EL combined to EH-EL, and IAB, IIAB, and IVB represent irons.

For statistical testing, the large data set was separated into three groups: *training data* (53.3% of spectra) to build the models, *validation data* (13.3%) to choose which model had the best performance, and *test data* (33.3%) to evaluate the accuracy of the best-performing classification algorithm. Selection of spectra for each group was stratified such that the number of spectra from the same group represented in each dataset reflected these same proportions.

Methods: Data were analyzed with an in-house tool written in Python and utilizing the SciKit-learn library [4]. Two types of classification algorithms were tested. *Logistic regression* (LR) is a machine learning technique that uses binary values to predict the probability that an input value (X) belongs to a default class (Y). The X values are combined using coefficients, but the outputs are binary values (0 or 1) instead of predictions (as would be the case in linear regression). The regularization parameter (C) is varied to penalize the variance allowed in our model. This helps control overfitting, reduces how much the model is affected by noisy data, and can encourage construction of generalizable models that might be appropriate for asteroid classification.

A *Gaussian Kernel Support Vector Machine* (SVM) creates a hyperplane in n-dimensional space that can be used for classification based on the distance to the nearest training-data point in any class. The Gaussian kernel defines the shape used to surround our classes. SVM can be fine-tuned by adjusting the C and γ parameters. A high γ will allow high variance within the model, which

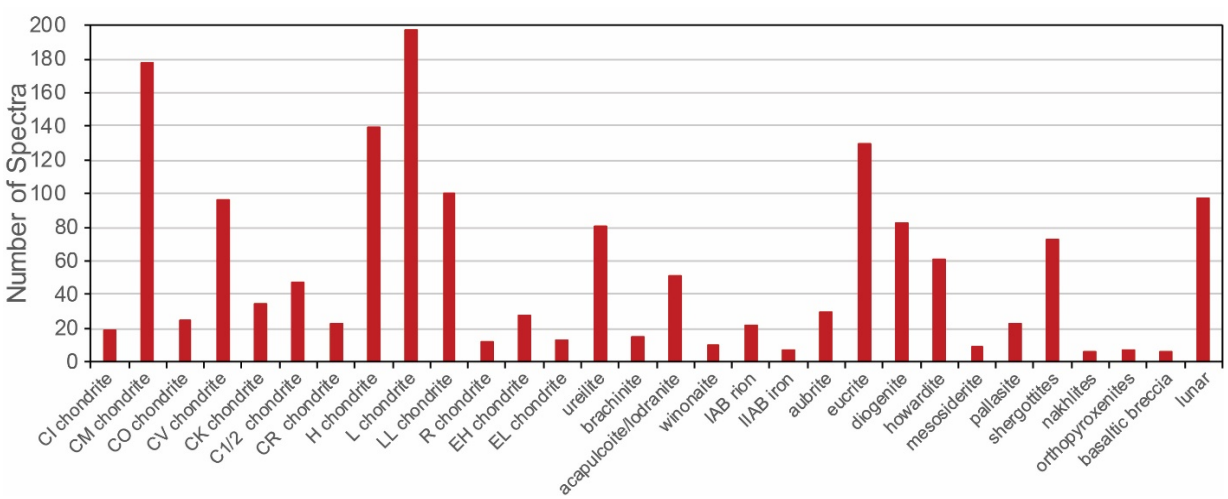

Figure 1. Distribution of 1623 samples for each meteorite group represented from RELAB.

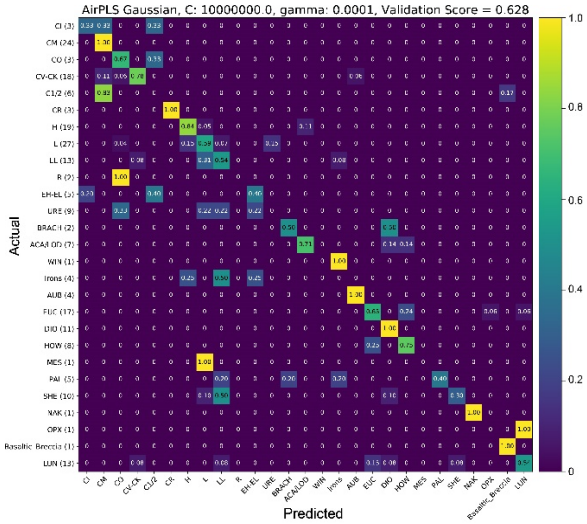

Figure 2. A confusion matrix showing the number of samples in each class of the validation set that were correctly classified. Numbers in each square indicate the extent to which each pair of classes was accurately identified (e.g., 1.0 implies 100% accuracy). Colors shading to purple indicate classes that were not confused with each other.

could lead to overfitting. For this reason, models with high C and a low γ were used.

Spectra of samples from a single meteorite class often were not identical due to instrumentation, acquisition parameters, and slope changes resulting from terrestrial weathering. This study used only RELAB data to mitigate instrument differences, though spectra from other labs are available and can be used in the future. Additionally, preprocessing of spectra data (e.g., baseline removal, normalization, smoothing, and squashing) has been shown in other types of spectroscopy [5,6] to ameliorate spectral differences not related to the sample. Thus this study investigated the effect of pre-processing on classification accuracy using trial and error.

Baseline removal (BLR) was tested using Fully Automated Baseline Correction (FABC) [7], Kajfosz-Kwiatek (K-K) [8], Adaptive Iteratively Reweighted Penalized Least Squares (AirPLS) [9], Asymmetric Least Squares (ALS) [10], and Morphologically Weighted Penalized Least Squares (MPLS) [11]. These were found to improve LR model matching accuracy only slightly, from ~55% for non-BLR to ~60%. SVM models were relatively insensitive to pre-processing because they utilize projection into the hyperplane; they performed comparably to non-BLR models with a classification accuracy of ~63%. Normalization, squashing, and smoothing also affected accuracy in different ways depending on which baseline removal algorithm was used. In this preliminary study, model performance either remained the same or was worse when these methods were applied. Further study and work are needed to optimize preprocessing and more carefully and thoroughly characterize its effects on model accuracy.

Results: Models trained with the SVM were on average 5% more accurate than LR models for the validation set data. The top three baseline removals for SVM models were AirPLS (63.8% accuracy), non-BLR (62.8%), and K-K (63.3%) with $C = 10^6$ and $\gamma = 0.0001$. Prediction accuracies for each meteorite group within the validation set are seen in Figure 2. The AirPLS SVM model classified the held-out test data for the meteorites across all 27 groups with an overall 58.2% accuracy. However, many of the "inaccurate" predictions are actually misclassifications to closely related classes (e.g., most of the >0% matches lie close to the diagonal of the plot). For this reason, classification accuracy should significantly improve with use of more sophisticated ML models that have lower penalties for near mismatches.

Discussion: Representation of each group varied depending upon how many spectra were available for each class. Data are abundant for ordinary chondrites (H, L, and LL) but lacking for Martian samples (OPX, SHE, NAK, etc.) as well as rarer meteorite groups (e.g., R group, winonaites). Smaller groups do not perform well because there are fewer spectra to train on and thus models have larger opportunities to miss diagnostic characteristics of the group. Small groups drag down the accuracy of the overall classifications. Of course, this problem can be fixed by adding more spectra of these rare groups to the database; that work has been proposed.

Summary: This project demonstrates the great potential of using spectroscopic data and ML techniques to classify meteorites. A more principled study of preprocessing methods is needed to accommodate spectra from multiple instruments/laboratories. Vector-based ML methods that can utilize the ordered nature of the spectral data will likely improve results. Finally, models with lower penalties for near mismatches should be explored. A more complex and fine-tuned model will one day accurately classify meteorites using only their spectra. This will not only make meteorite classification more efficient but also allow extension of the model to asteroid classification. Additional reflectance spectra of under-represented meteorite classes are needed to improve overall model accuracy.

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References: [1] Pieters C.M. & Hiroi T. (2004) *LPS XXXV*, Abstract #1720. [2] *Meteor. Bull. Datab.*, https://www.lpi.usra.edu/meteor/ [3] Parente M. (2008) *LPSC XXXIX*, Abstract #2528. [4] Carey C. et al. (2017) *LPSC XLVIII*, Abstract #1097. [5] Carey C. et al. (2015) *J. Raman Spectrosc.*, *46*, 894-893. [6] Dyar M. et al. (2016) *Spectrochim. Acta B*, *123*, 93-104. [7] Cobas J.C. et al. (2006) *J. Mag. Reson.*, *183*, 145-151. [8] Kajfosz J. & Kwiatek W.M. (1987) *Nucl. Instrum. Methods Phys. Res.*, *22*, 78-81. [9] Zhang Z.-M. et al. (2010) *Analyst*, *135*, 1138-1146. [10] Eilers P.H.C. & Boelens H.F.M. (2005) http://www.science.uva.nl/~hboelens/. [11] Li et al. (2013) *Analyst*, *138*, 4483-4492.