MULTIVARIATE AND ENSEMBLE MANGANESE CALIBRATION MODELS FOR SUPERCAM. Patrick J. Gasda (gasda@lanl.gov)[1], Ryan Anderson[2], Mohit Dubey[1], Diane Oyen[1], Agnes Cousin[3], Olivier Forni[3], Samuel Clegg[4], Ann Ollila[1], Nina Lanza[1], Roger C. Wiens[1], Sylvestre Maurice[3], Olivier Gasnault[3], Adriana Reyes-Newell[1], Dorothea Delapp[1]. 1) LANL, NM, USA; 2) USGS, Flagstaff, AZ, USA; 3) IRAP, Toulouse, France

Introduction: Enrichments of manganese can be used to understand past habitability, pH, and redox, of water on ancient Mars [1]. In addition, measurements of MnO in situ in primary igneous rocks can shed light on the composition of Mn in bulk silicate Mars [2]. The SuperCam instrument suite, which includes a Laser Induced Breakdown Spectroscopy instrument, onboard the NASA *Perseverance* rover measures the elemental composition of targets on Mars [3–5]. We have produced a multivariate model using Partial Least Squares (PLS) and Least Absolute Shrinkage and Selection Operator (LASSO) multivariate techniques with blended submodels; similar to the calibration model used from ChemCam [6], and then compared this model to ensemble methods [5,7].

Blended submodels split the data into smaller portions, trains linear models on these portions, and then optimizes the blend ranges of the submodels to cover the full data range [8]. The process of creating optimized submodels is time consuming, and may not yield the best model possible. Ensemble methods are non-linear, and would negate the need to train and optimize submodels. The response of the instrument to atomic emission is likely non-linear, and thus ensemble methods are likely to have better success in calibration than our previous attempts using LASSO, PLS, etc. Ensemble methods tested include Gradient Boosting, Random Forests, and Extra Trees [9].

Methods: *Data Collection and Pre-processing.* A standard set, for which MnO content is known, consisting of 252 training and 70 test standards, was analyzed using the SuperCam flight model from 1.6 m distance (3 average spectra were collected on each standard consisting of 50 shots averaged in each point) under a Mars-like atmosphere [5]. The standard set covers a range of Mn compositions from 0.0009–76 wt% MnO and contains a variety of rock matrices (e.g., rock, mineral, Mn ores). No outliers were removed. We use the Python Hyperspectral Analysis Tool [10] and the associated graphical interface for point spectra analysis [10] to preprocess the data and evaluate multivariate regression models. Ensemble methods were trained using Python scikit-learn [7,9]. Each spectrum is normalized by the sum of the total emission for each detector [5]. A "peak area" (PA) preprocessing technique is used [6], where local minima and maxima of the average spectra of the dataset is determined. The process then bins the emission between each pair of minima and assigns the result to the wavelength of the corresponding maximum. We compared full spectra with peak area spectra for this work. Based on preliminary work, we masked wavelengths ≥750 nm, where there are no Mn emission lines, to remove lines from alkali, minor elements, and oxygen, all of which had some influence on the LASSO model.

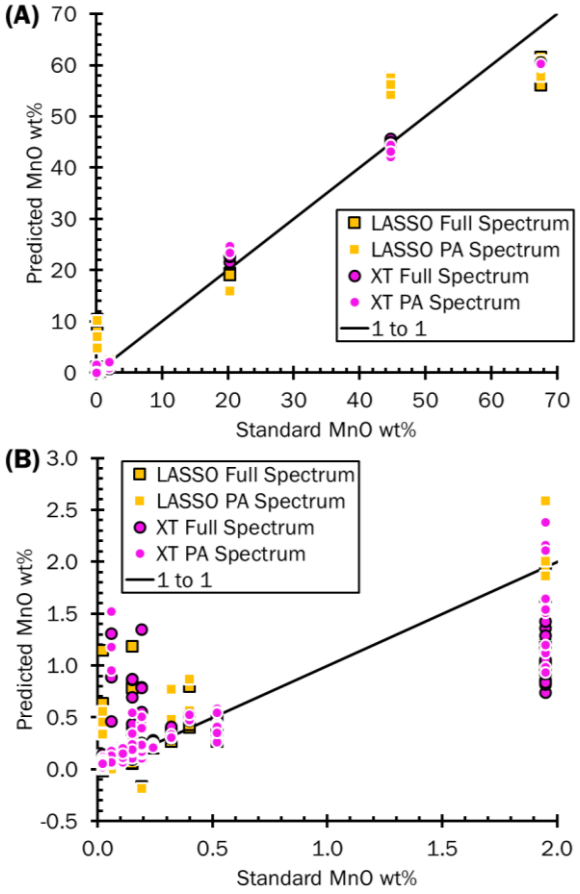

Fig 1: Test Set predictions of the LASSO blended submodels and Extra Trees (XT) models compared to a 1:1 line for A) the full data range and B) up to 2 wt% MnO.

Models. The dataset was split into 5 stratified folds of similar distributions of MnO content, and fold 3 was held out as the test set while the other 4 were used for cross validation and the training set. We cross validated PLS and LASSO models to find optimal parameters [see 6] for submodels that cover the full range of data (PLS and LASSO), 0–10 wt.% MnO (LASSO only), and 0–1 wt.% MnO (LASSO only). The blending of the submodels are optimized on the training set. A "double blending" model was used [6].

Grid search cross validation [9] is used to find optimal model parameters for ensemble methods, and the following initial parameters were determined by tests on ChemCam data [7]. For Random Forests and Extra Trees, bootstrapping was set to true and a minimum depth of 20 was used. For Gradient Boosting, a depth of 3 was used. For Extra Trees, the default number of estimators were used (100). Otherwise, the parameters for number of es-

timators, maximum features (i.e., wavelength channels), and learning rate were tuned during cross validation.

The same test set is used to evaluate the accuracy of all the models in this study, and accuracy is quantified using root mean squared error of prediction (RMSEP). The performance of the best models were then evaluated using the MnO predictions of the SuperCam onboard calibration targets (SCCTs).

Results: Test set RMSEP are listed in Table 1 for the models before masking ≥750 nm. Based on the analysis of the LASSO submodel regression vectors, the spectra were masked ≥750 nm, then the best models were re-optimized (Table 2; Figure 1).

Analysis of the Mars SCCTs. The PA LASSO blended and PA Extra Trees models were used to predict the SCCTs to evaluate performance on Mars targets (Fig 2). LASSO tends to underpredict at high MnO wt% and overpredict at low MnO wt%. Extra Tress tends to predict the SCCTs more accurately than LASSO.

Discussion: Peak Area spectra tend to yield better results, especially for the ensemble methods. The largest difference between full spectra and PA spectra are observed in Fig 1B, where scatter occurs near the origin. Potentially, this occurs when the ensemble method uses noise/baseline rather than an Mn emission line to predict MnO from a spectrum. PA processing should remove areas of the spectrum that contain only baseline, and mitigate this issue to some extent. PA spectra are also robust to small shifts in the wavelength calibration due to drift or other factors. LASSO is a sparse technique (the model relies on single channels to predict MnO), and so it is especially sensitive to wavelength shifts. We do not observe a large difference between the full and PA spectra RMSEP for SuperCam as we did for ChemCam [6], and potentially due to the relative ages of the instruments and length of time over which ChemCam data was collected in the lab.

Conclusions & Future work: The Extra Trees peak area spectrum model is the best MnO calibration model so far, based on the test set RMSEP and its tendency to accurately predict low MnO composition values. To better assess the ensemble methods and help develop improved models, feature importance for ensemble methods will be explored [7]. Masking empty parts of the spectrum could yield improvements to the models.

Acknowledgements: NASA Mars Exploration program, CNES, France; Carlsberg Foundation. LANL LDRD 20210043DR **References:** [1] Lanza et al. (2014) GRL, 41(16), 5755–63. [2] Taylor (2013) Geochem. 73(4), 401–420. [3] Wiens et al. (2021) SSR, 217(1). [4] Maurice et al. (2021) SSR, 217(3). [5] Anderson et al. (2021) Spectrochim B, *in press*. [6] Gasda et al. (2021) Spectrochim B, 181. [7] Dubey et al (2021) *this meeting*. [8] Anderson et al. (2017) Spectrochim B, 129, 49–57. [9] https://scikit-learn.org/stable/modules/ensemble.html [10] https://github.com/USGS-Astrogeology/PyHAT; https://github.com/USGS-Astrogeology/PyHAT_Point_Spectra_GUI

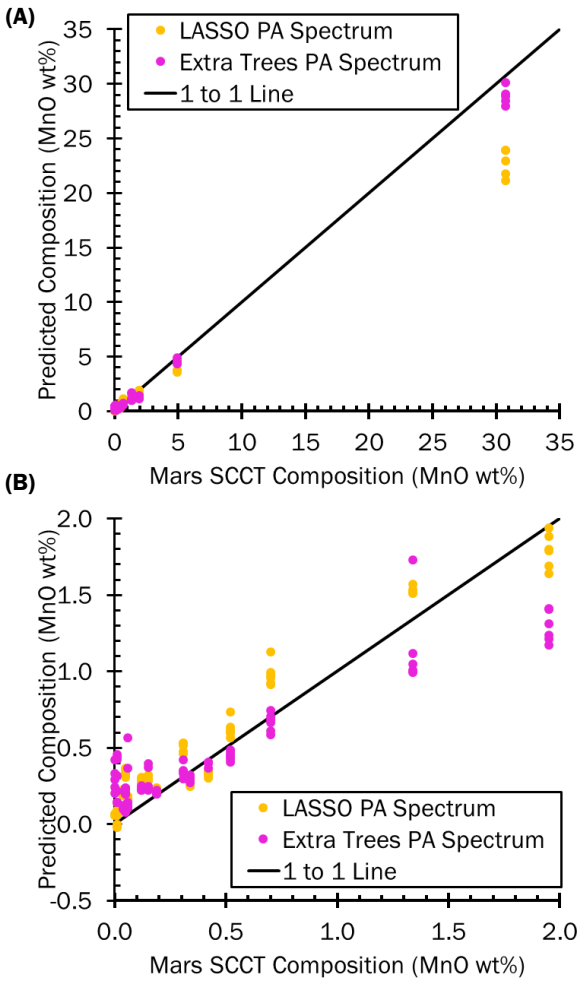

Fig 2: Predictions of SCCTs using LASSO blended submodels and Extra Trees models compared to a 1:1 line for A) the full data range and B) up to 2 wt% MnO.

Table 1: Summary of Root Mean Square Error of Prediction (RMSEP) for models tested before masking.

Method	*RMSEP wt% MnO Full Spectrum*	*RMSEP wt% MnO PA Spectrum*
PLS	2.09	2.11
LASSO	2.01	1.94
LASSO blend 1	1.85	1.82
LASSO blend 2	1.85	1.82
Random Forests	1.15	1.06
Extra Trees	1.07	0.91
Gradient Boosting	1.77	1.56

Table 2: Summary of Root Mean Square Error of Prediction (RMSEP) for models tested after masking ≥750 nm.

Method	*RMSEP wt% MnO Full Spectrum*	*RMSEP wt% MnO PA Spectrum*
LASSO blend 2	1.86	1.84
Extra Trees	0.89	0.98