BOUNDED VARIABLE LEAST SQUARES – APPLICATION OF A CONSTRAINED OPTIMIZATION ALGORITHM TO THE ANALYSIS OF TES EMISSIVITY SPECTRA.
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Introduction: The objective of any linear spectral unmixing procedure is to determine the abundance at which the components represented in a predetermined end-member library are present in the observed target. This is done by modeling an observed spectrum as a linear combination of end-member spectra. Following the work of Ramsey and Christensen [1] and Feely and Christensen [2] linear unmixing has become a fundamental tool for analysis and interpretation of thermal infrared emissivity spectra. This technique was expanded upon by Smith et. al [3] to include inferred Martian atmospheric end-member spectra for the purpose of analyzing Mars Global Surveyor Thermal Emission Spectrometer (TES) data. The simultaneous modeling of atmospheric and surface contributions to the observed TES spectrum in a single linear system has become the most accessible means by which the surface emissivity spectrum and inferred surface mineralogy can be isolated from a given TES spectral observation [4]. In this work we examine the application of an advanced constrained optimization algorithm to the problem of linear spectral unmixing and evaluate its utility in the analysis of TES emissivity spectra.

Constrained Linear Optimization: The fundamental problem to be solved in linear spectral unmixing analysis can be expressed as a matrix equation

$$[\mathbf{G}]\,\mathbf{m} \approx \mathbf{d}$$

where the columns of the n x m design matrix [**G**] consist of the n-channel end-member library spectra, the vector **m** contains the m best-fit model parameters in a least-squares sense, and the vector **d** is the n-channel observed spectrum. In most cases the model parameters are also subject to the linear inequality constraint

$$\mathbf{m}_i \geq 0 \;\;|\;\; 1 \leq i \leq m$$

which is tantamount to requiring that the model disallow the negative presence of an end-member component. In the case of TES data, this constraint may be relaxed for the atmospheric and blackbody end-member spectra [4].

Iterative End-member Ejection. Previous work involving the unmixing of emissivity spectra has exploited the non-negativity parameter constraint as the means by which the minimization algorithm iterates toward a solution [1,2,4]. Iterative End-member Ejection (IEE) relies on the removal of end-member spectra from the design matrix at each iteration to drive the optimization toward a solution. Each iteration begins with the unconstrained calculation of the best-fit linear least-squares model solution for the observed spectrum in terms of the current end-member set. The calculated parameter vector is then reviewed for parameters in violation the non-negativity constraint. Any end-members corresponding to negative parameters are removed from the end-member suite, and the system of equations is solved again with the reduced design matrix. This process continues until the parameter vector contains only non-negative values. By iteratively reducing the rank of the design matrix only end-member components that make a contribution to the solution are retained.

Bounded Variable Least Squares. An alternate optimization method that supports linear inequality constraints is the Bounded Variable Least Squares (BVLS) algorithm of Stark and Parker [5]. This method is a generalization of the Non-Negative Least Squares (NNLS) algorithm of Lawson and Hanson [6] that has been developed for enhanced efficiency and stability. In contrast to the IEE method, the BVLS algorithm does not require the wholesale ejection of end-member spectra from consideration to advance toward the minimum error solution. All of the end-member spectra in the original set are available to the minimization routine at all stages of the procedure. Internally, an active set strategy is used to track the parameters at each iteration with respect to the imposed constraints, while the Kuhn-Tucker theorem is employed to direct the activation and deactivation of end-member spectra as the algorithm moves toward the best-fit solution. The BVLS algorithm is constructed around the QR decomposition method for solving linear least-squares problems, which further enhances the numerical efficiency [6].

Application to TES Spectral Analysis: A total of 64,431 high quality TES radiance spectra for a study area (-10 to +10 E; -5 to +10 N) in the Terra Meridiani region of Mars were extracted from the PDS archive. The data were then converted to apparent emissivity spectra and an unmixing solution was generated for each observation using the IEE and BVLS methods in terms of the end-member suite used by Arvidson et. al [7]. For the majority of the apparent emissivity observations, the solutions generated by the two methods were comparable. However, for a significant fraction of the spectral observations the BVLS algorithm demonstrated a quantifiable improvement over the IEE procedure.

Comparison of Model Error Values. Due to the attrition of end-member spectra over the course of the minimization, the IEE algorithm rarely locates the global model error minimum within the solution space spanned by the original end-member set. A scatter plot comparing the RMS errors associated with the model fits to the spectra using the BVLS and IEE methods is shown in Figure 1. Points that lie on the diagonal represent spectra that were equally modeled by both methods in terms of the model RMS error. All points that lie above the diagonal correspond to observed spectra for which the BVLS algorithm generated a solution with a lower RMS error. While the majority of the observations lie adjacent to the diagonal, the distended shape of the data cloud perpendicular to the diagonal indicates that the BVLS method is generating significant improvement in the model error for a significant number of TES observations.

Inappropriate End-member Ejection. The biggest drawback of the IEE method is the possibility that the algorithm will inappropriately eject a critical end-member component at an early stage of iteration, rendering the system unable to achieve an accurate minimal error solution. Though the occurrence of this breakdown is rare, it is a possibility that needs to be accounted for. An apparent emissivity TES spectrum exemplifying this problem is shown in Figure 2 along with the model spectrum generated by each method. This spectrum was acquired from a surface unit in Terra Meridiani known to host the mineral hematite [8] and a clear hematite spectral signature is present in the 275 to 500 wavenumber region. However, the hematite end-member was ejected from the design matrix by the IEE algorithm in an early iteration. With a critical end-member no longer available to the optimization algorithm the final model fit is necessarily of lower quality than the fit produced by the BVLS algorithm which included a parameter value of 0.14 for the hematite end-member.

Conclusion: From the standpoint of numerical optimization the IEE method for the solution of a constrained liner least-squares problem suffers from two weaknesses: 1) IEE rarely achieves the global minimum error solution with respect to the input end-member suite; and 2) The IEE algorithm is susceptible to the inappropriate and unrecoverable ejection of a critical end-member from consideration. In this circumstance, the procedure is no longer capable of achieving an acceptable model solution. Both of these considerations are accounted for by the BVLS algorithm, as linear inequality constraints are implemented internally without the need to reduce the rank of the design matrix to step toward the minimum model error solution. In light of the stability, versatility, and reliability of the BVLS algorithm as the numerical engine used in linear spectral unmixing analyses, it is the ideal method for use in situations where explicit supervision of the optimization process is not possible.

References: [1] Ramsey M. S. and Christensen P. R. (1998) *JGR*, 103, 577-596. [2] Feely K. C. and Christensen P. R. (1999) *JGR*, 104, 24195-24210. [3] Smith et. al (2000) *JGR*, 105, 9589-9607. [4] Bandfield J. L. (2002) *JGR*, 107, **9**. [5] Stark P. B. and Parker R. L. (1995) *J. Comp. Stat.*, 10, 129-141. [6] Lawson C. L. and Hanson R. J. (1995) Solving Least Squares Problems, SIAM. [7] Arvidson et. al (2003) *JGR*, *in press*. [8] Christensen et. al (2000) *JGR*, 105, 9623-9642.

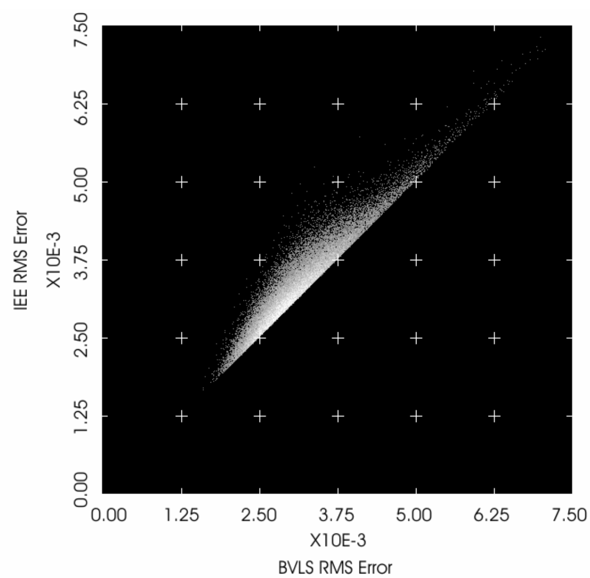

Figure 1 – Comparison of the RMS error values associated with the model spectra generated by the BVLS and IEE optimization methods.

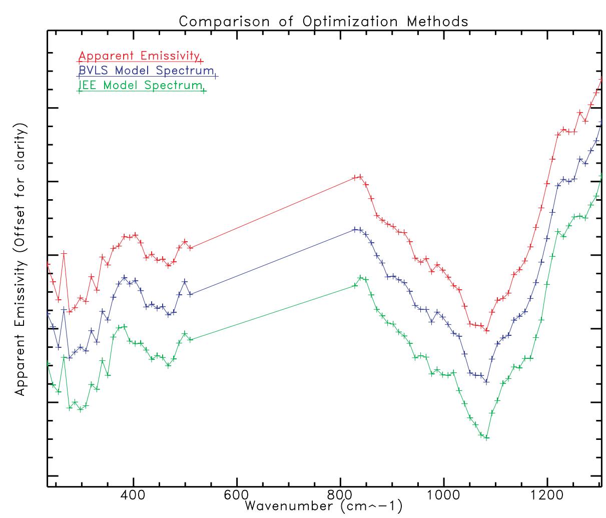

Figure 2 – Example of inappropriate end-member ejection.