

**FOURIER DOMAIN TARGET TRANSFORMATION ANALYSIS IN THE THERMAL INFRARED;** *D. L. Anderson*, Department of Geology, Arizona State University, Tempe, AZ 85287-1404.

Remote sensing uses of principal component analysis (PCA) of multispectral images include band selection and optimal color selection for display of information content [1,2]. PCA has also been used for quantitative determination of mineral types and abundances given endmember spectra [3,4]. This abstract reports on the preliminary results of the investigation of target transformation PCA (TTPCA) in the fourier domain to both identify endmember spectra in an unknown spectrum, and to then calculate the relative concentrations of these selected endmembers.

Identification of endmember spectra in an unknown sample has previously be performed through bandmatching [5], expert systems [6], and binary classifiers [7]. Both bandmatching and expert system techniques require the analyst to select bands or combinations of bands unique to each endmember. Thermal infrared mineral spectra have broad spectral features which vary subtly with composition. This makes identification of unique features difficult. Alternatively, whole spectra can be used in the classification process, in which case there is no need for an expert to identify unique spectra. Use of binary classifiers on whole spectra to identify endmember components has met with some success [8]. These techniques can be used, along with a least squares fit approach on the endmembers identified, to derive compositional information.

An alternative to the approach outlined above uses target transformation in conjunction with PCA to both identify and quantify the composition of unknown spectra [9]. Preprocessing of the library and unknown spectra into the fourier domain, and using only a specific number of the components, allows for significant data volume reduction while maintaining a linear relationship in a Beer's Law sense [10]. The most serious problem with the PCA method is the determination of the proper number of factors in a set of unknown spectra in the presence of noise and other effects. The noise associated with laboratory spectra is the only effect incorporated in this preliminary study. Many statistical techniques attempt to determine the number of factors in an unknown spectral matrix, with limited success. The approach taken here is to iteratively calculate concentrations, reducing the number of endmember components until only non-negative concentrations remain. This technique, though computationally intense, is an unequivocal method for determining the number of components. Through this iterative process it is possible to determine both the number of components and the identity of those components from the spectral library that best match the target transformed unknown spectra. Once the proper spectral library components have been determined, PCA is used to calculate both concentrations and spectra. Least-squares errors (LLE) of calculated vs. true concentrations can be used to estimate the error associated with the technique. No such error can be determined for remotely sensed data with no ground truth. The LLE of calculated vs. library spectra can give an estimate of the error associated with the separation of imbedded verses extracted error in the unknown data matrix.

Mineral mixtures of quartz, enstatite, and calcite have been analyzed using linear least squares (LLS) analysis to determine mineral compositions for application to analysis of TIMS images of Meteor Crater [11]. Five samples varying in approximate percent composition of the three endmembers, using large crystals to minimize particle size effects, were run by Ramsey and Christensen (see also Table I). The spectra where sampled at one wavenumber (wn) resolution from 400 to 1600 wn. The first pair of each column in Table I is the percent of the component in the sample and the second column is the LLS best fit ratio.

TTPCA was run on the samples in the fourier domain for comparison to the LLS technique. A spectral library consisting of calcite, enstatite, kyanite, pyrophyllite, quartz, gypsum, and

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tourmaline was used. Three components were found for all TTPCA runs (i.e., quartz, enstatite, and calcite were the spectra having the closest matches to the unknown samples). Table II compares the LLS concentration of sample number one with those calculated with TTPCA.

As seen in Table II, the Fourier domain TTPCA technique does as well as the LLS technique with as few as 20 Fourier coefficients. Thus, low frequency information is what distinguishes mineral spectra in the thermal infrared. Both LLS and PCA should calculate approximately the same results as both are least-squares types of analysis. TTPCA can separate out some of the imbedded error in the spectra through determination of the true number of components. Thus, it has the potential for being more accurate than LLS in the analysis of remotely sensed spectra. TTPCA can also be a fast semi-quantitative technique using a minimum number of Fourier coefficients.

**Table I**  
Comparison of Laboratory to Linear Least Squares Analysis  
of Quartz, Enstatite, Calcite Mixtures

	Sample 1		Sample 2		Sample 3		Sample 4		Sample 5	
Calcite	5	4	20	25	33	30	10	10	10	11
Enstatite	90	91	60	58	33	40	50	52	30	27
Quartz	5	5	20	18	33	30	40	38	60	62

(First of each pair is the percent volume, the second is the best fit ratio)

**Table II**  
Comparison of Laboratory to Linear Least Squares Analysis and  
Fourier Domain Target Transformation Principal Component Analysis  
of Quartz, Enstatite, Calcite Mixtures

	Sample 1	LLS	TTPCA 50pts	TTPCA 20pts	TTPCA 4pts
Calcite	5	4	4	4	5
Enstatite	90	91	91	91	88
Quartz	5	5	5	5	7

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