師大地理研究報告
第 33 期　民國 89 年 11 月
Geographical Research
No. 33, November. 2000

主成分分析與最小雜訊區段轉換對減少超光譜影像維數之比較

Comparison of Principal Components Analysis and Minimum Noise Fraction Transformation for Reducing the Dimensionality of Hyperspectral Imagery

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中文摘要

超光譜影像通常具有兩百個以上的連續波段，且各波段間存在高度相關，因此在影像分析前常需減少資料量以提昇運算效率，同時消除波段間的相關以減少分析誤差。本研究比較主成分分析與最小雜訊區段轉換這兩種轉換方法對減少超光譜影像資料維數的成效，結果證實最小雜訊區段轉換可正確根據影像品質的高低來排列主成分的次序，且有較高的訊號雜訊比，因此比主成分分析更適用於壓縮超光譜資料。
關鍵詞：超光譜影像，資料維數，主成分分析，最小雜訊區段轉換，訊號雜訊比

INTRODUCTION

Hyperspectral imagery with over two hundred channels provides better target

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detection and identification than broadband imagery, and it allows the flexibility in choosing several narrow bands for specific targets. However, image analyses for hyperspectral data require intensive computation due to the huge amounts of the information content. In addition, spectral bands of hyperspectral data exist high interband correlations and a large amount of redundancy. These disadvantages lead to the needs of efficient methods for information extraction and data compression.

Principal components analysis (PCA) is often applied to determine the underlying statistical dimensionality of the image data set (Ready and Wintz 1973). The process has also been regarded as the information compression in which a smaller number of components could be extracted from the whole data set by discarding redundant information into higher-order components (Singh and Harrison 1985). PCA has become a standard tool for the compression and enhancement for multispectral data (Green *et al.* 1988).

However, several examples show that PCA does not always produce images which show steadily decreasing image quality with increasing component number (Green *et al.* 1988). Another method, minimum noise fraction transformation (MNF), which maximizes the signal-to-noise ratio (SNR) represented by each component, rather than the data variance, could be more effective than PCA to order the components based on the image quality (Lee *et al.* 1990). This method has been tested using 10-band airborne thematic mapper (ATM) simulator data (Green *et al.* 1988). It should be further validated using hyperspectral data.

The objective of this study is to investigate if there is substantial improvement in image enhancement, information extraction and SNR by applying MNF transformation to hyperspectral imagery.

BACKGROUND

Dimensionality Reduction Techniques

Typically, the dimensionality of multispectral / hyperspectral imagery could be reduced by applying a linear transformation, such as principal components transformation or minimum noise fraction transformation. Only significant components would be retained for further processing (Harsanyi and Chang 1994).

Principal Components Analysis. It, also referred to as the Hotelling transformation, the Karhunen-Loève (K-L) transformation, and the eigenvector transformation in the remote sensing and pattern recognition literature, is a multivariate statistical technique for information extraction, SNR improvement, data compression, and change detection (Singh and Harrison 1985). This technique was first developed by Hotelling (1933) for his work in educational psychology. The K-L transformation was introduced to pattern recognition by Watanabe in 1965 and since then research efforts have developed in two parallel directions. In the statistics, interest has been in the area of sampling theory and inference procedures (Kendall *et al.* 1983). In pattern recognition, most interest has been with feature extraction methods such as information compressibility, and the relationship with the Fourier transform (Devijver and Kittler 1982).

Mathematically, if $\mathbf{X}^T = [X_1, \ldots, X_n]$ is a N-dimensional random variable with mean vector **M** and covariance matrix C, then a new set of variables, say, $Y_1, Y_2, \ldots, Y_n$, known as principal components, can be expressed by (Singh and Harrison 1985):

$$Y_j = a_{1j}X_1 + a_{2j}X_2 + \ldots + a_{nj}X_n = a_j^T X$$

Where T denotes transpose of a matrix and $a_j^T X = [a_{1j}, \ldots, a_{nj}]$ are the normalized eigenvectors [i.e. $a_j^T a_j = 1$] of the variance-covariance matrix. By denoting the (N × N) matrix of eigenvectors by **A** and the [N × 1] vector of principal components by **Y**, then

$$\mathbf{Y} = \mathbf{A}^T \mathbf{X}$$

The (N × N) covariance matrix of **Y**, **C**, is given by:

$$C = \begin{pmatrix} \lambda_1 & \cdots & & 0 \\ \cdot & \lambda_2 & & \cdot \\ \cdot & & \lambda_3 & \cdot \\ \cdot & & \cdot & \cdot \\ 0 & \cdots & & \lambda_n \end{pmatrix}$$

Where λ_i are eigenvalues of matrix C. The matrix is diagonal as the components have been chosen to be uncorrelated and $\lambda_1 > \lambda_2 > \ldots \lambda_n$.

Several characteristics of PCA are of special interest in remote sensing. For example, the total variance is preserved in the transformation; the mean square approximation errors were minimized; and it generates uncorrelated coefficients (Moik 1980). Geometrically, it rotates the highly correlated features to the orthogonal space so that the maximum amount of variance is accounted for in decreasing magnitude along the ordered components (Singh and Harrison 1985).

Principal components can be calculated from either a covariance matrix or a correlation matrix. The correlation matrix could be derived by dividing the appropriate standard deviations into the covariance matrix. In the context of remote sensing, a case can be made for using a standardized or non-standardized matrix. The derivation of the components from a non-standardized matrix can be justified because each band would have the same physical units (Singh and Harrison 1985). PCA using the correlation matrix has been used to detect the land cover change. The total variance of multi-temporal images could be decomposed into two parts. These are the substantial sources of variation between the images due to external conditions, such as atmospheric transmission, angle of sun incidence and differences between detector calibration procedures of sensors, and the small variances introduced by the land cover change. One way to minimize the external variances is to standardize all the data from different bands to a standard deviation of one so that the land cover change can be better detected (Byrne *et al.* 1980).

Minimum Noise Fraction Transformation. It, also called maximum noise fraction, is referred to as the noise-adjusted transformation (NAPC). This technique has been used to determine the inherent dimensionality of image data, to segregate noise in the data, and to reduce the computational requirements for subsequent processing (Boardman and Kruse 1994). It was first defined to investigate the improvement by employing MNF transformation compared with PCA in airborne thematic mapper (ATM) ten-band data (Green *et al.* 1988). MNF transformation could be regarded as a two cascaded principal components transformation. The first transformation, based on an estimated noise covariance matrix, decorrelates and rescales the noise in the data so that the noise has unit variance and no band-to-band correlations.

The second step is a standard principal components transformation of the noise-whitened data (ENVI, 1997).

Mathematically, given a multivariate data set of *p*-bands with gray levels,

$$Z_i(x), \quad {}_i = 1, \ldots, p$$

, where x gives the coordinates of the sample. It can be assumed that

$$\mathbf{Z}(x) = \mathbf{S}(x) + \mathbf{N}(x)$$

, where $\mathbf{Z}^T(x) = \{ Z_1(x), \ldots, Z_p(x) \}$, and $\mathbf{S}(x)$ and $\mathbf{N}(x)$ are the uncorrelated signal and noise components of $\mathbf{Z}(x)$. Thus

$$\text{Cov}\{ Z(x) \} = \Sigma = \Sigma_S + \Sigma_N$$

,where Σ_S and Σ_N are the covariance matrices of $\mathbf{S}(x)$ and $\mathbf{N}(x)$, respectively. The noise fraction of the i^{th} band will be

$$\text{Var}\{ N_i(x) \} / \text{Var}\{ Z_i(x) \}$$

the ratio of the noise variance to the total variance for that band. The maximum noise fraction transform chooses linear transformations

$$Y_i(x) = \boldsymbol{a}_i^T Z(x), \; {}_i = 1, \ldots, p$$

such that the noise fraction for $Y_i(x)$ is maximum among all linear transformations orthogonal to $Y_j(x)$, $j = 1, \ldots, i$ (Green *et al.* 1988).

It shows that the vectors $\boldsymbol{a}_i$ are the left-hand eigenvectors of $\Sigma_N \Sigma^{-1}$, and that μ_i, the eigenvalue corresponding to $\boldsymbol{a}_i$, equals the noise fraction in $Y_i(x)$. Therefore, it can be seen that $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_p$, and so MNF components have the potential to show steadily increasing image quality. (Green *et al.* 1988).

The first step in MNF transformation is to calculate the noise covariance matrix which can be estimated from either the dark reference measurements (dark current) or the near-neighbor differences. The former is the signal observed while the foreoptics shutter of the detector is closed. It represents the detector's background data as well as the instrument's noise (Steinkraus and Hickok 1987). In the radiometric calibration processing of hyperspectral data, the dark current could be derived by subtracting each dark current value from the DN values (Vane *et al.* 1987).

The dark image is not available from most instruments. The alternative is using the near-neighbor differences, which can be calculated from a procedure known as minimum/maximum autocorrelation factors (MAF). This procedure assumed that the signal at any point in the image is strongly correlated with the signal at neighboring pixels while the noise shows only weak spatial correlations (Lee *et al.* 1990). The near-neighbor differences could be obtained by differencing adjacent pixels to the right and above each pixel and averaging the results to derive the noise value (ENVI 1997).

METHODS

Data Preparation

The study area is located near Heber City, Utah including Wasatch Mountain National Park, Deer Creek reservoir and Midway town. The water body of Deer Creek reservoir provides a homogeneous spectral reflectance which is required to estimate the noise statistics in MNF transformation (see **Figure 1**).

Figure 1. True-color AVIRIS image of the study area with the red box indicating the subset image used to estimate the

The Airborne Visible/Infrared Imaging Spectrometer (AVIRIS) data was adopted for the investigation because it provides the high quality hyperspectral imagery (i.e., high spectral, spatial resolution and SNR) and meets the requirements for this study. The AVIRIS imagery of the study area was obtained from the Park City flight, scene 2, on 5 August 1998. The data range for this image is from Band 1, with a bandcenter of 369.07 nm, to Band 224, with a bandcenter of 2507.50 nm, and the spatial solution is 20m. In order to save the computation, the original image size, 614 × 512 pixels, was cut to the current image size, 300 × 300 pixels. A spatial subset image, 20 × 20 pixels, over the Deer Creek reservoir was defined to estimate the noise covariance matrix.

Image Processing

PCA and MNF transformations were performed using the ENVI 3.0 software. Both the covariance matrix and the correlation matrix were applied to PCA analysis. The dark current measurements are not available in the 1998 AVIRIS flight so that the MAF procedure was conducted to estimate the noise covariance matrix for MNF transformation.

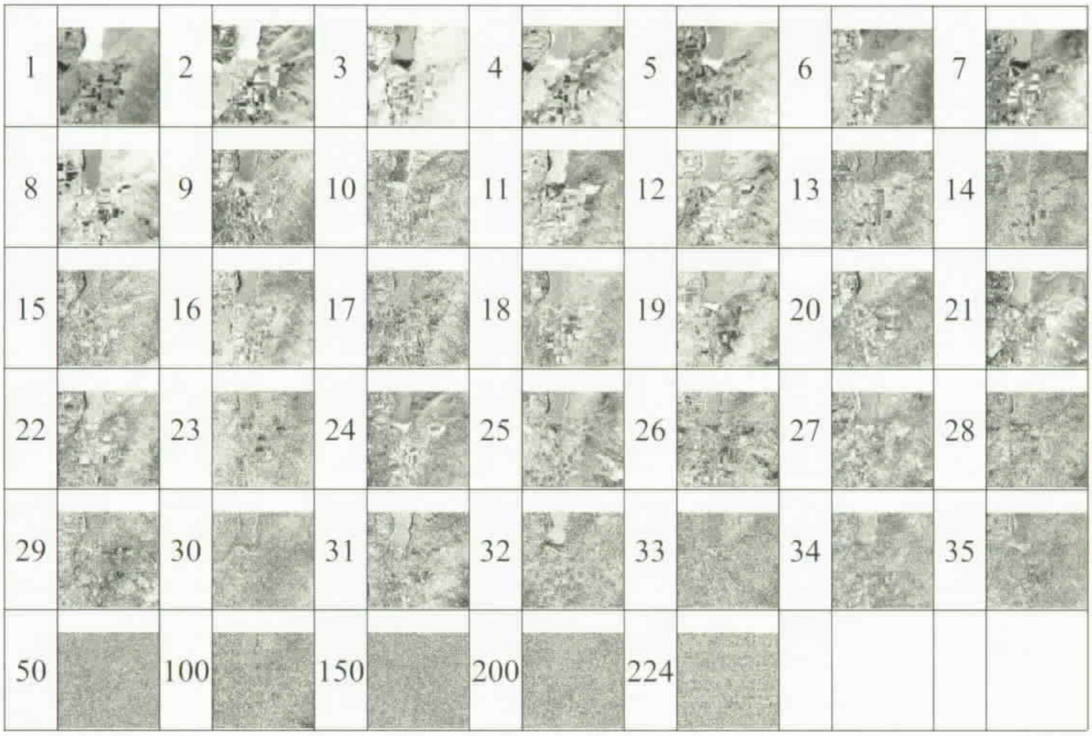
The statistical results of the transformations were exported from ENVI to a text file, which was then imported into Microsoft Excel to calculate the SNR.

RESULTS AND DISCUSSION

Image Enhancement

By applying PCA with the covariance matrix to AVIRIS data, it can be seen that the first few principal components behave much as expected, such as PC1 to PC10, and there is definite trend to increasing noise with increasing component number (see **Figure 2a**). However, PC21 is quite an acceptable image with less noise than PC10, PC14 and PC15. The similar result occurred in PCA with the correlation matrix. For example, the image quality of PC 24, PC 25, and PC26 is much better than that of PC 20, which is a noise-dominated image (see **Figure 2b**). These results reaffirm that PCA could not reliably separate signal and noise components of multispectral image data, especially among aircraft scanner data (Green *et al.* 1988). In contrast, MNF transformation successfully orders components in terms of image quality. MNF component images show steadily decreasing image quality with increasing component number (see **Figure 2c**).

Since each band contributes equal variance , the image quality of the component images using PCA with the correlation matrix becomes much smoother than those of using PCA with the covariance matrix and MNF transformation. The component images with high orders, such as PC100, PC150, PC200, and PC224, are supposed to be dominated by noise. However, the image contrast of those images is not quite low (see **Figure 2b**). For example, the shoreline of the reservoir as well as some crop fields can be easily identified in those higher-order images. This result demonstrates where the main difference lies between using the covariance matrix and the correlation matrix.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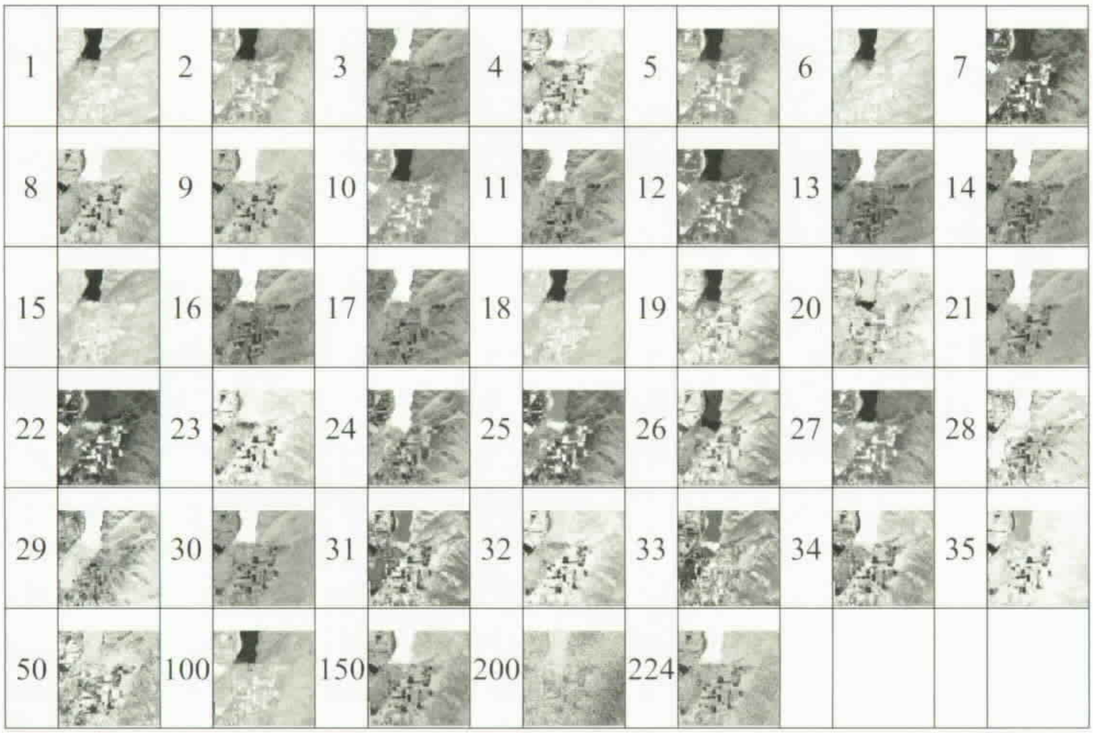
(a)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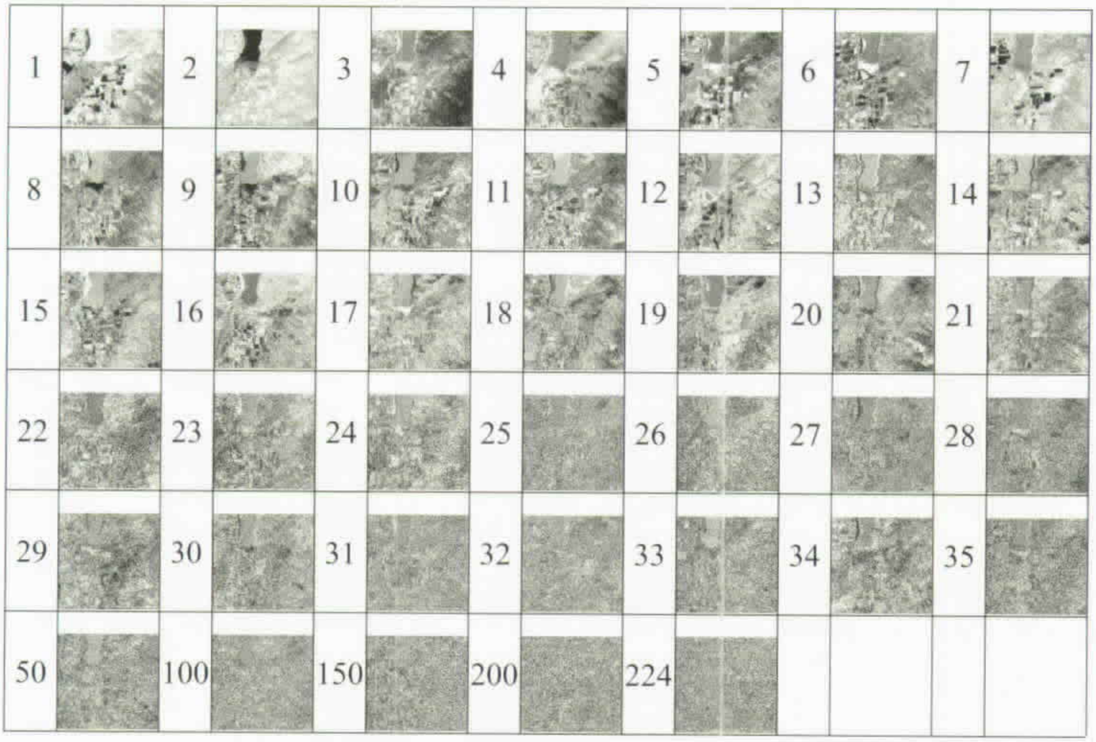
(b)



(c)

Figure 2. (a) Principal component images using covariance matrix
(b) Principal component images using correlation matrix
(c) MNF component images

Information Extraction

The magnitude of eigenvalues shows that by using PCA with the covariance matrix, 84 percent of the total variance is represented in the first principal component (PC1) , and 99.3 percent of the total covariance can be explained by the first three principal components (see **Figure 3**). Comparatively, using PCA with the correlation matrix or MNF transformation, the cumulative percent does not increase as rapidly. To compare the eigenvalues of these three methods in detail, the screen test was used to identify the optimal number of components that can be extracted, and the shape of the resulting curve was applied to evaluate the cutoff point. Using PCA with the covariance matrix, the cutoff point is located at PC4 (see

Figure 4a); using PCA with the correlation matrix, at PC9 (see **Figure 4b**); using MNF, at PC7 (see **Figure 4c**). Visual inspection of the information content in principal component images reveals that more components can be extracted. It should be PC1to PC8 for the covariance matrix, PC1 to PC50 for the correlation matrix, and PC1 to PC12 for MNF transformation (see **Figure 2**).

Eigenvectors, also known as the factor loadings, are the correlation of each band and principal components. Eigenvectors indicate the degree of correspondence between the band and the principal component, with higher eigenvectors making the band representative of the principal component. There is significant difference between PCA and MNF where the latter demonstrates a better basis for carrying out principal components (see **Figure 5**). The major eigenvector (PC1) of PCA is heavily dominated by the high negative values from the red and near infrared bands (see **Figure 5a**). However, the PC1 of MNF is much more uniformly weighted across all bands. Similarly, the rest principal components of MNF are more uniformly weighted across all bands than those of PCA (see **Figure 5b**, **5c**). Visual inspection of the PC1 images shows that the PC1 of MNF has better contrast than those of PCA.

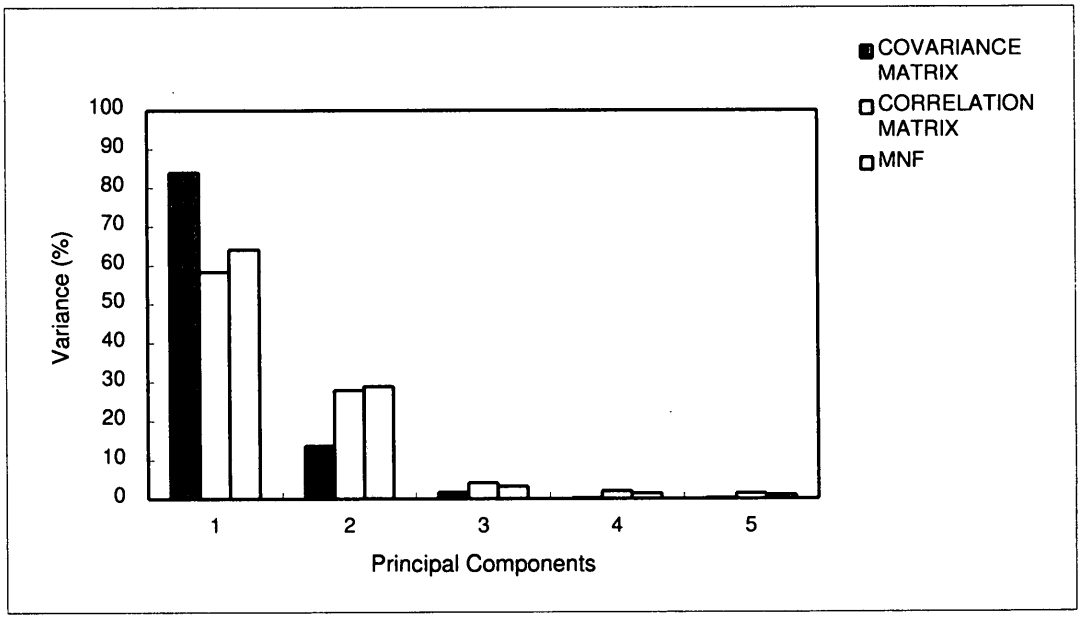


Figure 3. The Magnitude of

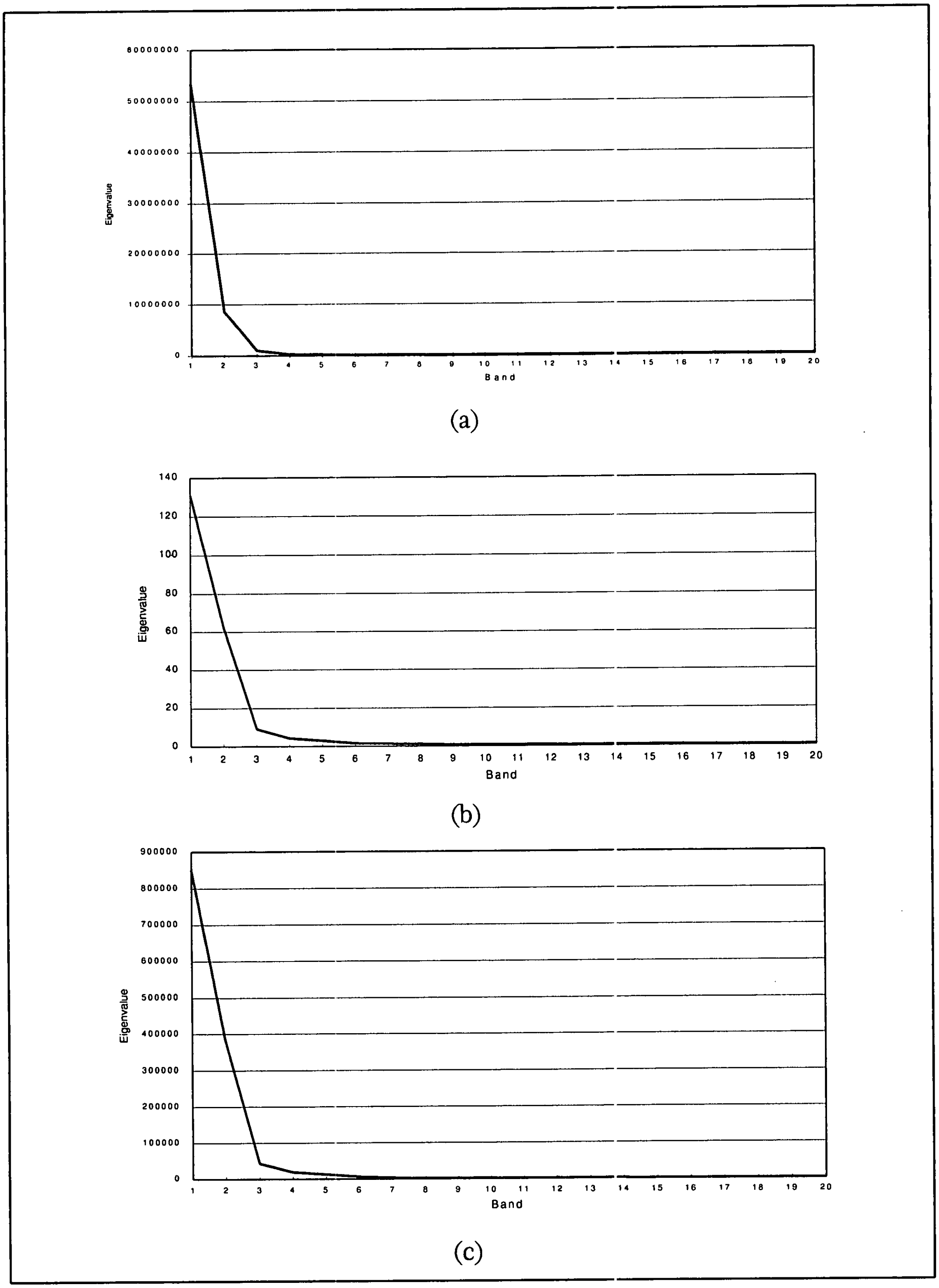


Figure 4. (a) Eigenvalue Plot of PCA (Covariance)
(b) Eigenvalue Plot of PCA (Correlation)
(c) Eigenvalue Plot of MNF

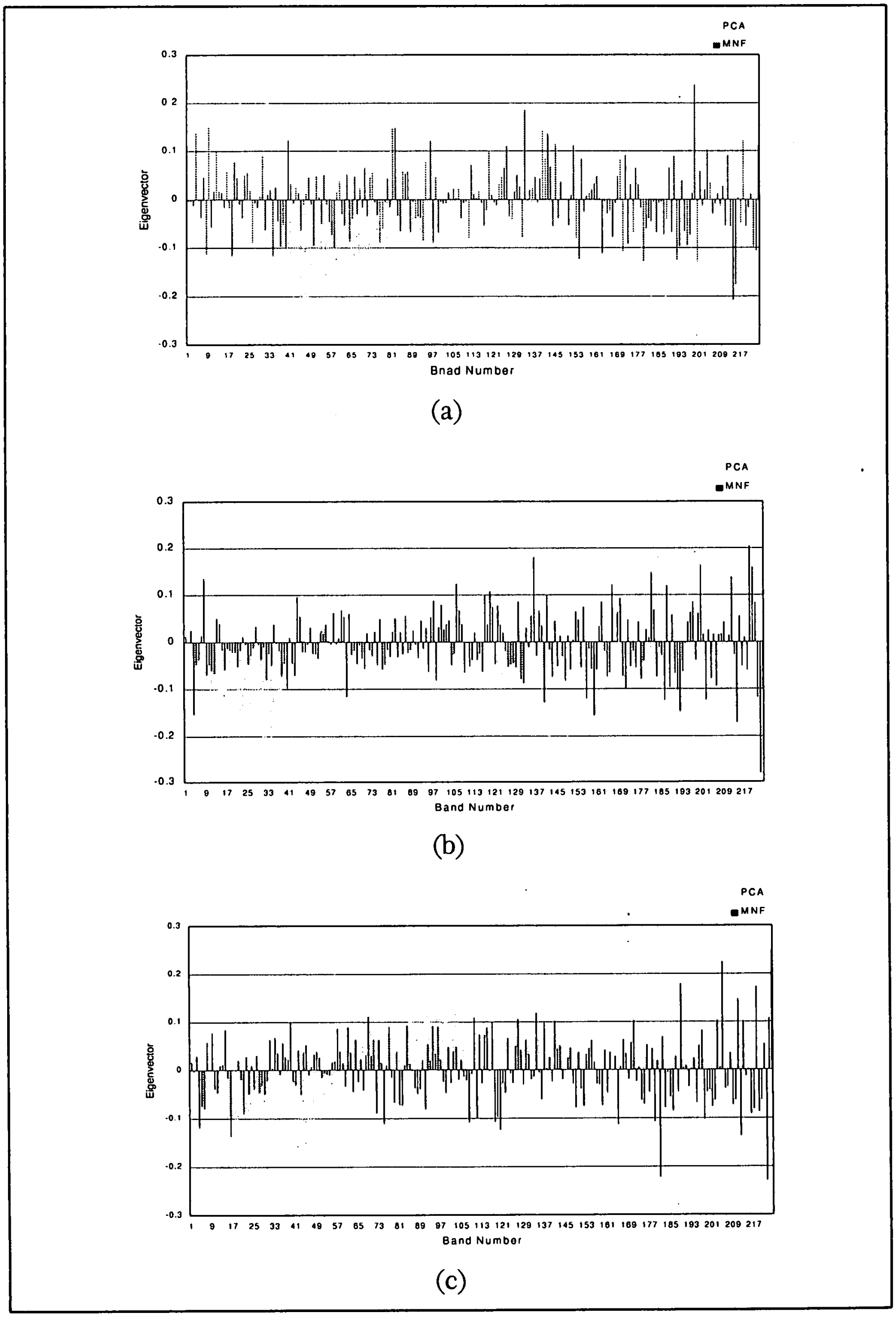


Figure 5. (a) Eigenvector Magnitude of PC1
(b) Eigenvector Magnitude of PC2
(c) Eigenvector Magnitude of PC3

SNR Improvement

The SNR improvement (ΔSNR) achieved by the PCA can be calculated from the eigenvalues of the original spectral band variances (Ready and Wintz 1973).

$$\Delta SNR = \lambda_1 / \delta_x^2$$
$$\text{where } \delta_x^2 = \max\,[\delta_{x1}^2, \delta_{x2}^2, \delta_{x3}^2, \ldots\ldots, \delta_{xn}^2]$$

In PCA using the covariance matrix,
$\Delta SNR = \log_{10}(53398804) - \log_{10}(995305) = 1.73$ dB

In PCA using the correlation matrix,
$\Delta SNR = \log_{10}(130) - \log_{10}(1) = 2.12$ dB

In MNF transformation,
$\Delta SNR = \log_{10}(850378.75) - \log_{10}(1) = 5.93$ dB

A 0.39 dB difference in SNR improvement over the original SNR is therefore realized with eigenvector computed from PCA with the correlation matrix rather than the covariance matrix. Furthermore, a more significant SNR improvement was achieved using MNF transformation, which is 4.2 dB higher than PCA using the covariance matrix and 3.81 dB higher than PCA using the correlation matrix.

CONCLUSION

The difference among using PCA with the covariance matrix, PCA with the correlation matrix and MNF transformation to reduce the dimensionality of hyperspectral data was evaluated statistically in this study. The results reaffirm that MNF transformation is more reliable than PCA when the image quality is the primary concern (Green *et al.* 1998; Lee *et al.* 1990).

By applying PCA and MNF transformation to AVIRIS data, the resulting principal component images illustrate that either using the covariance matrix or the correlation matrix, PCA could not reliably separate signal and noise components of the AVIRIS data. An improvement in image enhancement is achieved by employing MNF transformation, which is capable of steadily decreasing image quality with increasing component number.

The eigenvalues and the principal component images indicate that only 8 components are required for PCA with the covariance matrix, approximately 50 components for PCA with the correlation matrix, and 12 components for MNF transformation. The most efficient compression is using PCA along with the covariance matrix in that 99.3 percent of the total covariance can be explained by the first three principal components. However, this high concentration was partially resulting from the noise variance.

In comparing SNR, MNF transformation enhances SNR better than PCA. The difference between employing the correlation matrix or the covariance matrix for PCA is not significant in this case.

It should be noted that both PCA and MNF transformation are exploratory techniques of constructing new artificial bands, which do not necessarily have any physical meaning or significance. Therefore, the performance of data compression and dimensionality identification cannot be directly assessed by the eigenvalues, but by case studies. The comparison of these techniques needs to be expanded by applying them to extract the information of specific targets in hyperspectral data.

Another application not covered in this study is the investigation of factor loadings for the principal components in hyperspectral data. The results will be useful for the selection of optimal bands to detect the targets of interest.

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收稿日期：89 年 10 月 30 日
修正日期：89 年 11 月 7 日
接受日期：89 年 11 月 20 日