Independent Component Analysis and Nonnegative Linear Model Analysis of Illuminant and Reflectance Spectra

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Abstract
Principal Component Analysis (PCA), Independent Component Analysis (ICA), Non-Negative Matrix Factorization (NNMF) and Non-Negative Independent Component Analysis (NNICA) are all techniques that can be used to compute basis vectors for finite-dimensional models of spectra. The two non-negative techniques turn out to be especially interesting because the pseudo-inverse of their basis vectors is also close to being non-negative. This means that after truncating any negative components of the pseudo-inverse vectors to zero, the resulting vectors become physically realizable sensors functions whose outputs map directly to the appropriate finite-dimensional weighting coefficients in terms of the associated (NNMF or NNICA) basis. Experiments show that truncating the negative values incurs only a very slight performance penalty in terms of the accuracy with which the input spectrum can be approximated using a finite-dimensional model.

1. INTRODUCTION

Finite-dimensional models of spectra based on PCA have been widely used since Judd's model of daylight and Cohen's analysis of Munsell chips. Previous studies have applied ICA to surface reflectance [4] and daylight spectra [3]. In this paper, we extend this analysis to a larger set of illuminants and to colour signal spectra. The colour signal is defined as the product of surface reflectance and spectral power distribution of the illuminant incident on it. We compare the PCA and ICA bases to the entirely non-negative bases obtained via NNICA and NNMF in terms of the accuracy with which full spectra can be modeled using the various bases.

For any finite-dimensional model, a spectrum is modeled by projecting it onto the pseudo-inverse of a set of basis vectors. This projection yields the weighting coefficients of the model as described in more detail below. The output of an optical sensor can also be described as the result of a projection of the incoming spectrum on the sensor's spectral sensitivity functions. The leads to the question: Is there a good basis for modeling spectra that also has the property that the pseudo-inverse of the basis might be used as physically realizable sensors?

PCA is a standard technique for calculating a good orthogonal basis from a training set of spectra. However, being orthogonal, the PCA basis vectors contain significant negative components. The pseudo-inverse of this basis is also orthogonal and similarly contains significant negative components. As a result, the PCA basis is unlikely to yield physically realizable sensors; however, we hypothesize that perhaps NNICA and NNMF which yield non-negative basis vectors might. Such a sensor would directly output the weighting coefficients of a finite-dimensional model of the incident light's spectrum.

2. METHOD

It is convenient to express a finite-dimensional linear model of spectra as: $X = AB$ where X is an m-by-d matrix of m spectra each uniformly sampled at d wavelengths; B is an n-by-d matrix of n basis vectors; and A is the m-by-n mixing matrix of weighting coefficients. Since the intent of the dimensionality reduction techniques is to identify a basis of reduced dimension that approximates the original data well, n is generally less than m. Each of the four dimensionality reduction techniques finds a basis B minimizing (possibly subject to additional constraints):

$$\sum_{i=1}^{m} \left\| X_i - A_i B \right\|^2 \qquad (1)$$

PCA finds basis vectors that are uncorrelated and orthogonal. ICA finds basis vectors that are uncorrelated and in addition are independent but not orthogonal. There are many different ICA algorithms [6]. Here we used the JADE [7] (Joint Approximate Diagonalization of Eigenvalues) implementation. NNICA [2] carries out ICA subject to the additional constraint of non-negativity in the resulting basis vectors. Non-negative Matrix Factorization solves (1) subject to all entries in both A and B being nonnegative. An iterative algorithm [1] to do this is based on the following pair of equations:

$$B_{ij} = B_{ij} * \frac{(A^T X)_{ij}}{(A^T AB)_{ij}} \qquad A_{ij} = A_{ij} * \frac{(XB^T)_{ij}}{(ABB^T)_{ij}} \qquad (2)$$

3. RESULTS

We used the 1781 surface reflectances and 102 illuminant sources described in [5]. The wavelength range is from 380nm to 780nm with a sampling 4nm interval. The reflectance and illumination data sets are each broken into two random subsets for training and testing. Color signal training and test sets are constructed from the respective training and test reflectance and illumination datasets. The first 3 basis vectors obtained by each of PCA, ICA, NNMF and NNICA for training sets of surface reflectances, illuminations, and colour signals are shown in the Figure 1.

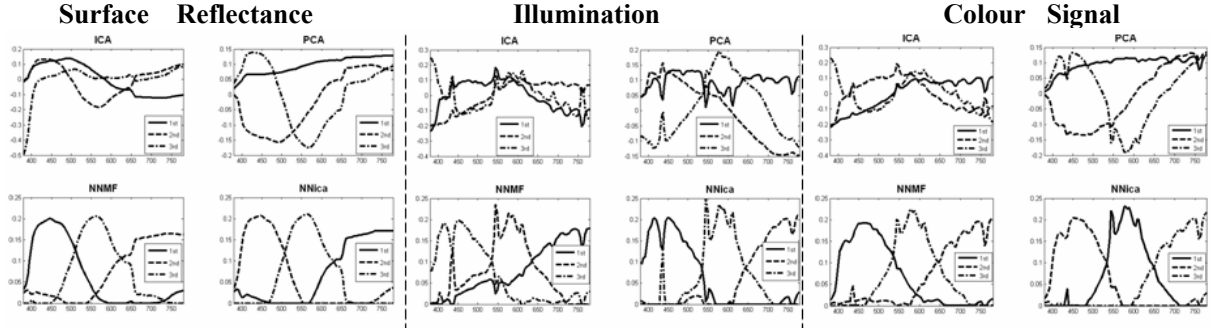
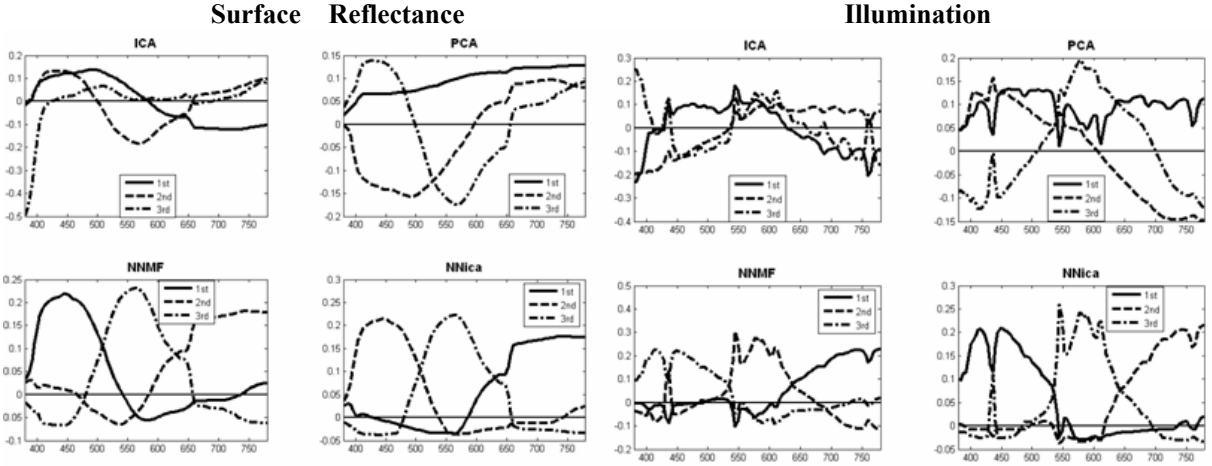


Figure 1: First 3 basis vectors for surface reflectance, illumination and colour signal spectra as obtained by ICA, PCA, NNMF and NNICA. The horizontal axis is wavelength. The vertical axis is in terms of normalized power (illumination and colour signal) or fractional reflectance.

Given a set of basis vectors, a spectrum written as a column vector, x, can be represented by the weighting coefficients, $w = x^T \times B^{-1}$. The PCA basis vectors are orthogonal so $B^{-1} = B^T$. However, for the other methods the basis vectors are not orthogonal so the pseudo-inverse of matrix B, B^+, is used to obtain the coefficients instead. Figure 2 shows the corresponding pseudo-inverse for each of basis vectors sets from Figure 1.



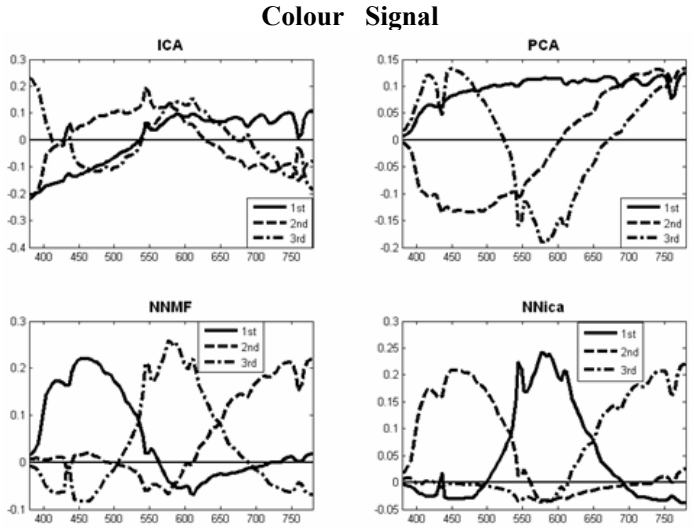


Figure 2: The pseudo-inverse of the surface reflectance, illumination and colour signal basis vectors. The horizontal axis is wavelength. The horizontal line at zero. Physically realizable sensors approximating these pseudo-inverses can be based on the portion of each curve on or above the zero line. Clearly, the approximation is likely to be best in the case of NNICA and NNMF.

Setting all the negative values in the pseudo-inverse vectors to zero results in a new set of vectors we will call the truncated pseudo-inverse, B_T^+. The weighting coefficients are then obtained as $w = x \times B_T^+$. An approximation, x_a, to the original spectrum is reconstructed from the weights and basis as $x_a = w \times B$. The root mean square distance is one the measure of the accuracy of the approximation of x_a to x:

$$e_{RMS} = \sqrt{\frac{1}{M}\sum_{\lambda=1}^{M} | x_a(\lambda) - x_s(\lambda) |^2} \qquad (3)$$

We found that the L1 norm yielded qualitatively similar results to the RMS error and therefore report only the RMS error. For *N* spectra the mean RMS error is then simply the mean of the individual RMS errors:

$$MRMS = \frac{1}{N}\sum_{i=1}^{N} e_{RMS\_i} \qquad (4)$$

When the true pseudo-inverse of basis vectors is used, ICA always results in the least error. Figure 3 shows the mean approximation error as a function of the number of basis vectors used. Plots of the median RMS error are qualitatively similar.

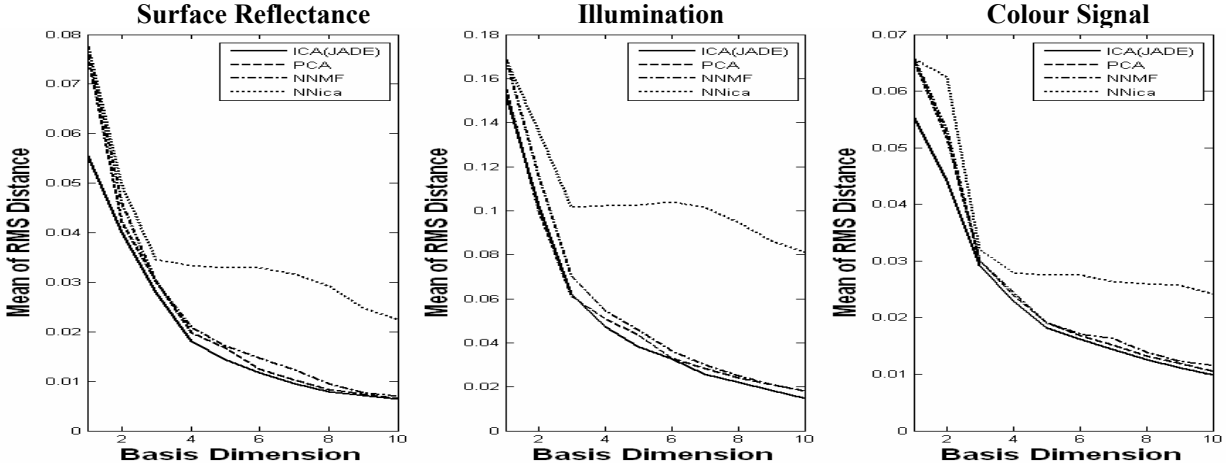
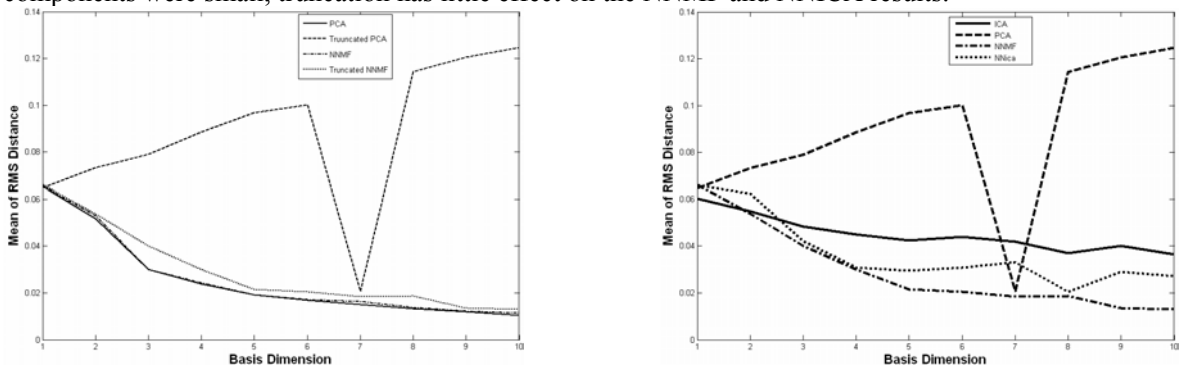


Figure 3 Mean RMS error in spectral approximation (MRMS error) for surface reflectances, illuminations, and colour signals in the test set for each of the four methods as a function of the number of basis vectors used.

When the actual pseudo-inverse vectors are replaced with the truncated pseudo-inverse vectors, the approximation error necessarily increases. Figure 4 compares the mean RMS errors for colour signal reconstruction based on truncated versus un-truncated pseudo-inverse vectors. Since the negative components were small, truncation has little effect on the NNMF and NNICA results.



(a) (b)

Figure 4 (a) A comparison of the mean RMS error in reconstructing the colour signal spectra with the actual and truncated pseudo-inverse vectors for the case of NNMF and PCA. Without truncation the NNMF and PCA results overlap (lowest curve); however, with truncation the PCA error increases substantially (with the exception of dimension 7) while the NNMF error increases marginally. **(b)** A comparison of the mean RMS error approximating colour signal spectra for all four methods using the truncated pseudo-inverse.

4. CONCLUSION

Whether for reflectances, illuminants or colour signals, ICA consistently yielded the lowest mean RMS error in spectral approximation followed by PCA, NNMF and NNICA. The errors, however, for ICA, PCA and NNMF were all qualitatively very similar. NNMF and NNICA have the advantage that the basis vector components are all nonnegative. Although for NNMF and NNICA, the fact that the basis vectors are all nonnegative does not mean that and their pseudo-inverses necessarily will also be nonnegative, we found that in practice the negative components are relatively small. Setting the negative components to zero results in functions that could be realized by actual optical sensors. Such sensors would have the advantage that their output would correspond directly to the weighting coefficients of a finite-dimensional model of the incident spectra. As such, they could be considered optimal (ignoring the influence of noise) in terms of the information they capture about the incident spectra.

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