Journal of Imaging Science and Technology® 54(1): 010508–010508-8, 2010.

Reconstruction of Spectral Transmission of Colored Solutions Using a Conventional Digital Camera

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Abstract. *In this study, the red-green-blue (RGB) color values of colored solutions captured from a digital camera are employed for reconstruction of spectral transmission of the transparent solutions. A capturing box is assembled and a spectral data set gathered from colored solutions prepared for this purpose. Principal component analysis (PCA), pseudoinverse, and matrix R methods are employed to reconstruct the spectral transmission of clear solutions from their RGB data. Two different illuminants are employed to achieve two sets of RGB data. According to the results, the PCA method led to inadequate accuracy when a set of RGB data and three eigenvectors are used, while results are improved by using first six basis functions. On the other hand, pseudoinverse leads to the worse results in comparison with PCA by using the first six basis functions. However, the results obtained from matrix R method shows considerable improvement in terms of the root mean square error between the actual and reconstructed spectral transmission curves. In fact, matrix R method diminishes the spectral errors in the two ends of spectrum in relation to other methods. © 2010 Society for Imaging Science and Technology.*
[DOI: 10.2352/J.ImagingSci.Technol.2010.54.1.010508]

INTRODUCTION

The measurement of spectral behavior of an object, i.e., reflectance or transmission behavior, is a routine technique for identification and analyzing of materials. Spectrophotometers are the most classical instruments usually employed to collect accurate data for this purpose, but they are not always available. There has been tremendous interest during the past decade to employ the outputs of more popular color measurement devices, such as scanners and/or digital cameras, for some scientific applications. Such devices are able to provide colorimetric data with higher spatial resolution, while the classical instruments, such as colorimeters, average the results over the region of measurement. Several processing methods with different computational complexities and accuracies have been introduced to extract valuable spectral data from device dependent RGB colorimetric information. Ideally, this approach could replace the classical color measurement instruments, such as spectrophotometers and colorimeters, with more accessible one, i.e., digital image capturing devices. The efforts can be broadly categorized into two groups: colorimetric and spectral characterization of image capturing devices. By the colorimetric characterization method, device dependent RGB data are converted to one of the classical color specification systems[1] most often CIEXYZ or CIELAB color systems. Different methods have been suggested for data transformation between dependent and independent spaces, and the most popular one is the nonlinear regression using a standard color chart.[2–7] In the spectral domain, some methods have been presented for the determination of spectral responses of digital image capturing devices. Basically, the methods can be divided into two groups: pseudoinverse and principal eigenmethods. These methods have been improved by several modification approaches.[5,8–13]

Hyperspectral and multispectral imaging devices are also used for data gathering. However, such devices are expensive and less accessible. There is no doubt that these devices would effectively change the camera into an imaging spectrophotometer. Owing to the smoothness of spectral properties of objects within the visible spectrum, the application of a multispectral camera with limited number of filters has been also reported.[14]

In multispectral imaging methods, the response of an object, which can be described by the product of spectral reflectance of its surface and the illuminant spectrum, can be represented by low-dimensional models based on principal component analysis (abbreviated as PCA)[8,9] or independent component analysis (abbreviated as ICA)[15,16] techniques. So, for a given linear model, if the number of PCA or ICA coefficients of a particular set of spectra is equal to the number of camera responses, then the spectra can be easily estimated by an inverse transformation of the set of camera responses, with the forward transformation being estimated from a representative "training" data set.[5,10,14,17–22] If the numbers of coefficients are more than the numbers of device responses, then the number of responses may need to be increased by imaging the scene under different illuminants or by introducing suitable filters in front of the camera to modify the sensor spectra. A conventional trichromatic digital camera combined with either absorption filters[23,24] or different light sources[20,25] has been recommended for capturing multispectral images.

In the field of spectral recovery from colorimetric data, most research has been focused on the reconstruction of spectral reflectance of opaque surface color and did not con-

Received Apr. 27, 2009; accepted for publication Aug. 27, 2009; published online Dec. 14, 2009.
1062-3701/2010/54(1)/010508/8/$20.00.

sider the transparent media, which are important in identification and quantitative analysis of materials in chemistry and physics.

This article presents the results of the recovery of spectral transmission of a set of transparent colored solutions from the RGB data obtained by a Canon EOS D350 commercial still camera. A wide range of colored solutions has been prepared, different reconstruction techniques are employed, and the recovery results compared with each other. More specifically, the PCA, pseudoinverse, and matrix R methods[26] are employed with some modification to recover spectral transmission of different examples of colored solutions.

RECONSTRUCTION OF SPECTRAL DATA FROM COLORIMETRIC INFORMATION

PCA

Principal component analysis has been the most successful method for the reconstruction of reflectance data from the corresponding standard tristimulus values as exemplified by CIEXYZ color space.[8,9] The method was employed by many researchers and simply formulated by Fairman and Brill.[8] Since the reflectance spectra of natural color and most nonfluorescent surfaces are smooth functions of wavelength, the reflectance curve could be represented by a limited number of the most significant eigenvectors. Hence, a linear model, as shown in Eq. (1), can be implemented for reflectance spectra reconstruction

$$\hat{R}_\lambda = V_{0,\lambda} + V_\lambda C, \tag{1}$$

where $\hat{R}$ shows the estimated reflectance value and $V_{0,\lambda}$ and V_λ, respectively, represent the mean of spectral reflectance and the selected eigenvectors of a suitable reflectance data set. The selected eigenvectors correspond to the highest eigenvalues. Accordingly, C is a column vector of k elements, which contains the principle component coordinates, and it can be calculated from Eq. (2),

$$C = T^{-1}(Q - Q_0), \tag{2}$$

where T^{-1} is a 3×3 matrix and contains the tristimulus values of the first three selected eigenvectors; Q and Q_0 show the color coordinates of proposed sample and the mean vector of the database, respectively. So, $\hat{R}$ may be easily calculated from Eq. (1). When a set of tristimulus values i.e., CIEXYZ under a given viewing condition are available, three eigenvectors can be considered and a fully defined equation is employed. Obviously, in such cases the recovery of the reflectance factor cannot be ideal, and the reproduced spectra would be improved by introducing additional coordinates, such as another set of tristimulus values, under a second illuminant. Accordingly, the size of the matrix in such condition increases to six, as shown in Eq. (3),

$$T = \begin{bmatrix} X_{1,1} & X_{1,2} & X_{1,3} & X_{1,4} & X_{1,5} & X_{1,6} \\ Y_{1,1} & Y_{1,2} & Y_{1,3} & Y_{1,4} & Y_{1,5} & Y_{1,6} \\ Z_{1,1} & Z_{1,2} & Z_{1,3} & Z_{1,4} & Z_{1,5} & Z_{1,6} \\ X_{2,1} & X_{2,2} & X_{2,3} & X_{2,4} & X_{2,5} & X_{2,6} \\ Y_{2,1} & Y_{2,2} & Y_{2,3} & Y_{2,4} & Y_{2,5} & Y_{2,6} \\ Z_{2,1} & Z_{2,2} & Z_{2,3} & Z_{2,4} & Z_{2,5} & Z_{2,6} \end{bmatrix}, \tag{3}$$

where the first subscript refers to the illuminant-observation and the second shows the index of the selected eigenvectors.

Pseudoinverse Method

The simplest approach for the determination of spectral data from colorimetric information can be the pseudoinverse method. Recently, the method was implemented by Berns and Zhao using a six-channel camera signal. In this work, the transformation matrix was constructed by the Moore-Penrose pseudoinverse method.[26]

The spectral transformation was derived to convert multichannel camera signals D of color targets to spectral transmission factors N, as shown in Eqs. (4) and (5),

$$N = T_S D, \tag{4}$$

$$T_S = N \times PINV(D). \tag{5}$$

They employed two different light sources to provide two sets of RGB data for each sample. Hence, six-dimensional colorimetric data were converted to 31 dimensional reflectance spectra by this method.

Matrix R Method

In 1953, Wyszcki[27] presented his hypothesis that each spectrum can be decomposed into a fundamental stimulus and a metameric black. Later, a mathematical method was developed by Cohen and Kapuff[28–31] for performing such decomposition idea. Finally, Fairman[32] suggested a correction compensation technique for parametric pairs based on Wyszecki decomposition hypothesis.

Recently, Zhao and Berns[26] offered a new technique for the reconstruction of spectral reflectance based on the implementation of the matrix R method. As Cohen and Kapuff showed, matrix R can be calculated from matrix A. Matrix A can be formed from the inner products of spectral color matching functions of a standard observer and the relative spectral power of the applied light source. Matrix A is an n-by-3 matrix, where n is the number of wavelength, i.e., $n=31$ in the visible spectrum, and the three columns are three independent primaries. Matrix R, an n-by-n symmetric matrix, can be mathematically defined as shown in Eq. (6),

$$R = A(A'A)^{-1}A'. \tag{6}$$

Zhao and Berns first computed the spectral reflectance of the sample from camera signals using the pseudoinverse method. Then, as shown by Eq. (7), the metameric black, denoted by B, was calculated from spectral reflectance data

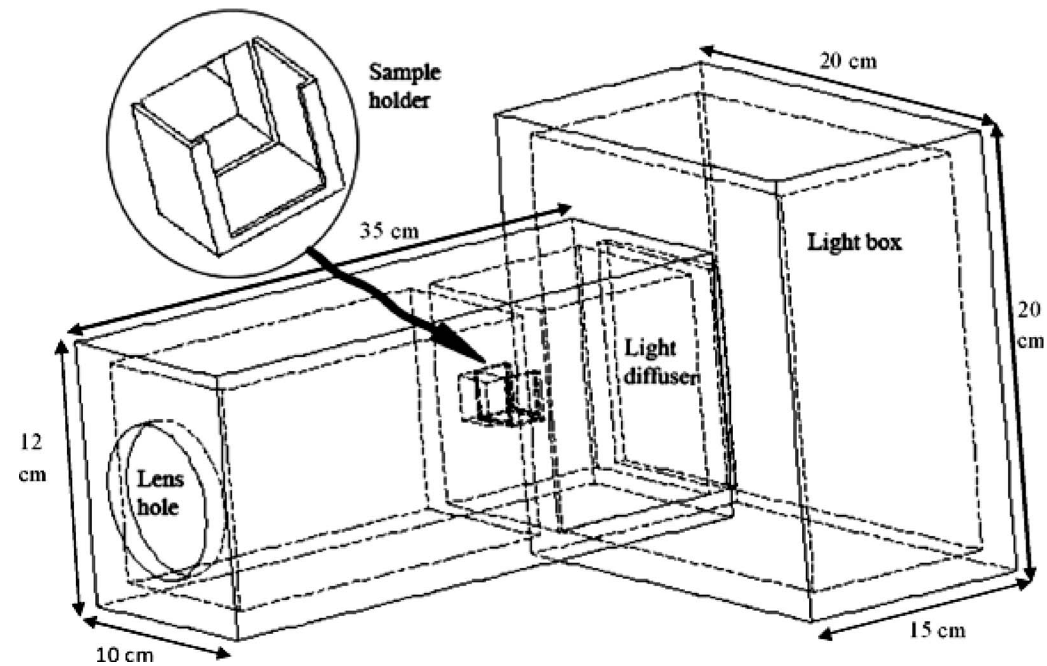

Figure 1. A schematic diagram of the image capturing box.

$$B = (I - R)N, \quad (7)$$

where I is an n-by-n identity matrix and N is the estimated spectral reflectance factor determined from the pseudoinverse method. The second set of tristimulus values was predicted from camera signals by employing the classical characterization method.[2–4] The proposed transformation matrix designated by T_C can be calculated by Eq. (8)

$$T_C = N_C \times PINV(D_L), \quad (8)$$

where D_L represents the linearized camera signals and N_C shows the tristimulus vector. Then, fundamental stimulus (N^*) can be calculated from estimated values using Eq. (9),

$$N^* = A(A'A)^{-1}T. \quad (9)$$

Finally, the metameric black from predicted spectral reflectance factors B was fused with the fundamental stimulus from estimated tristimulus values N^* to get the spectral reflectance factors $\hat{R}$, as shown in Eq. (10)

$$\hat{R} = N^* + B. \quad (10)$$

EXPERIMENTAL

A Canon EOS D350 single-lens-reflex digital still camera equipped with a 100 mm $f/2:8$ Canon macro lens EF was used in this research. The camera uses complementary metal oxide semiconductor (CMOS) image sensors in an 8 megapixel array; a UV filter (Sigma DG) was placed in front of the lens to remove any ultraviolet radiation. The captured data were saved in CR2 (RAW) format.

A suitable box was assembled to capture the images of test solutions. The schematic diagram of the image capturing box is shown in Figure 1. The inner layers of box were made of matt white acrylic sheets. In order to avoid the effect of unwanted ambient light, the outer faces of the box were covered with thick black acrylic sheets. A suitable aperture for the camera lens was arranged at one end of the box, while two fluorescent lamps (Philips, TL 8W/965) with 7000 K correlated color temperature and two halogen lamps (Osram, 41870 WFL, 12 V, 50 W) with 2500 K color temperature were placed in the other end. To prevent direct illumination of solutions and prepare a uniform lighting condition, a light diffuser sheet was fixed in front of the lamps. The spectral energy distributions of these lamps were measured using a GretagMacbeth Eye-One Pro™ spectrophotometer from 380 to 730 nm at 10 nm intervals, while the measurement aperture was 4.5 mm. Figure 2 shows the relative spectral energy distribution of the light sources employed.

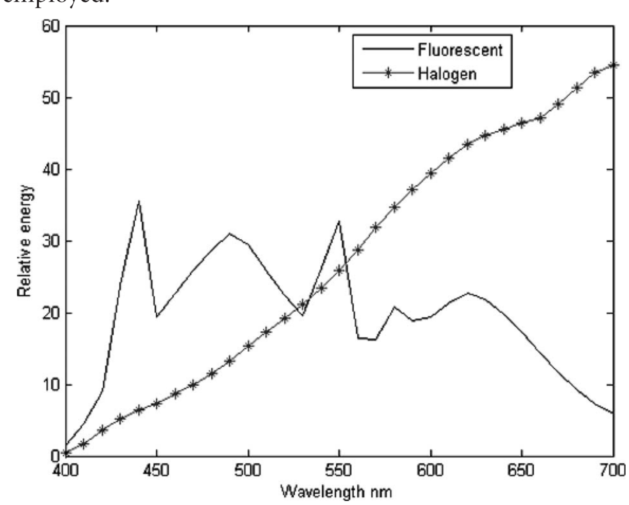

Figure 2. The spectral energy distributions of fluorescent and halogen lamps.

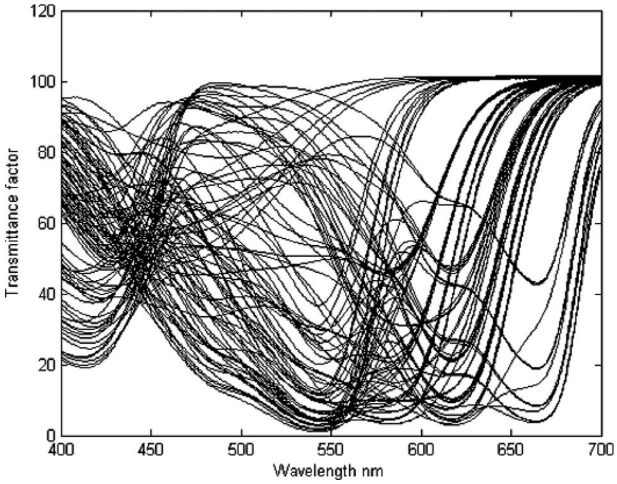

Figure 3. Spectral transmission of prepared transparent colored solutions.

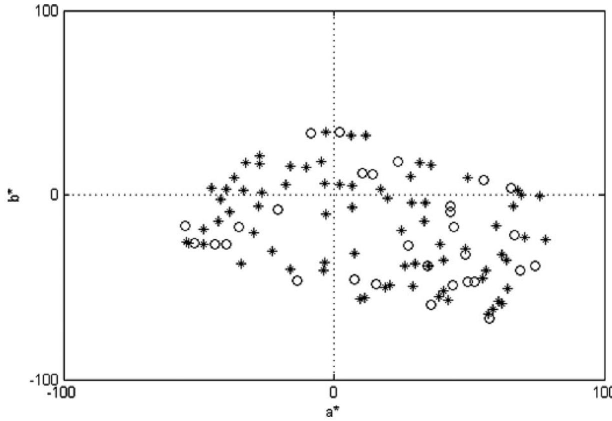

Figure 4. Color distributions of prepared transparent colored solutions and the selected samples in training sequence in a*b* chromaticity coordinates along with the samples which were used in testing step (training and testing samples are shown with "o" and " *," signs, respectively).

As Fig. 1 shows, the sample was placed between the diffuser and lens over a black separator, so that no light could reach to the camera except that which passed through the sample holder. A standard glass sample holder with the size of 2 cm width, 1 cm depth, and 3 cm height was used in the hole arranged in the black separator. Commercial samples of methyl violet, methylene blue, malachite green, bismark brown, magenta, and auramine were used as primaries. Different tertiary combinations of these dyes were used for preparation of different colored solutions. To prepare a variety of transparent samples, dye solutions were mixed in different concentrations. The spectral transmissions of samples were measured using a Varian Cary 50 double beam absorption spectrophotometer. Samples were measured from 400 to 700 nm at 1 nm intervals. The spectral transmissions of the experimental samples are shown in Figure 3. The CIEXYZ and CIELAB color specifications of the samples under D65 illuminant and 1964 standard observer were also computed from these data. Figure 4 shows the a*b* chromaticity coordinates of samples in the CIELAB color spaces.

All computations were conducted with MATLAB 7 from the Mathworks. The captured images in raw CR2 format were converted to a readable MATLAB file using public domain software named DCRAW.C[33]; the CR2 data format was changed into 16-bit PPM (Portable PIXMAP) format by this code.

To balance the camera responses to gray samples, gray patches of a Kodak Q_60 color chart (IT8.7/2) were used. Camera signals corresponding to these patches are illustrated in Figure 5. As this figure shows, responses of the Canon digital camera to these patches were adequately linear. Hence, linearization was not conducted and the raw data were directly used in subsequent processing.

RESULTS AND DISCUSSION

Colorimetric Characterization of Camera

A nonlinear regression method was performed to convert RGB raw data to CIELAB values with a precorrection, involving the cube root function of the RGB data. Different

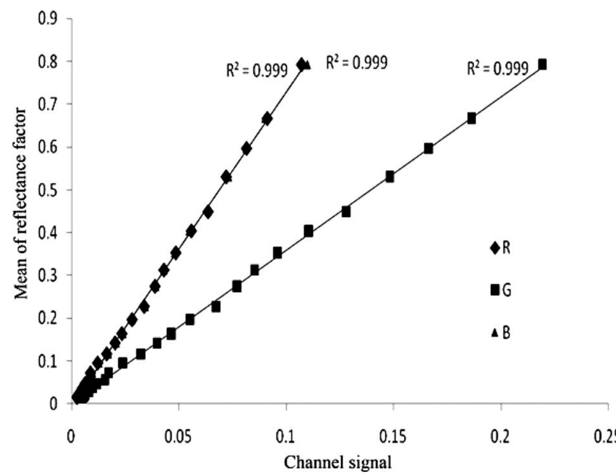

Figure 5. The results of camera signals into gray patches of Kodak Q_60 (IT8.7/2) chart.

transformation matrixes were examined and a 17 term polynomial led to the best results. As training and testing sets during the optimization process 105 clear solutions were used. To select the most suitable samples for the training step, the technique suggested by Hardeberg[5] was employed and the optimal samples were determined. Fig. 4 shows the distributions of selected samples in a*b* chromaticity coordinates along with the samples, which were used in testing step. Results of colorimetric characterization of the digital camera with the training and testing sets of colored solutions were evaluated by the color difference values using CIEDE2000 under fluorescent and halogen illuminants and presented in Tables I and II for the training and testing steps, respectively.

As the tables show, the accuracy of colorimetric characterization of captured images under the fluorescent lamp is higher than under the halogen light source for both the training and testing groups. The CIEDE2000 values were, respectively, 3.38 and 3.95 for fluorescent and halogen light sources in the testing set.

Table I. Statistical results of colorimetric characterization in training step.

Mean Δb^*	Mean Δa^*	Mean ΔL^*	STD CIEDE2000	Max CIEDE2000	Mean CIEDE2000	Polynomial parameters number	Samples number	Illuminant
0.95	1.01	1.84	1.64	7.71	1.78	17	30	Fluorescent
1.33	0.91	2.33	1.75	8.56	2.11	17	30	Halogen

Table II. Statistical results of colorimetric characterization in testing step.

Mean Δb^*	Mean Δa^*	Mean ΔL^*	STD CIEDE2000	Max CIEDE2000	Mean CIEDE2000	Polynomial parameters number	Samples number	Illuminant
1.90	2.34	3.24	1.57	7.59	3.38	17	75	Fluorescent
2.01	2.42	3.48	1.75	8.68	3.95	17	75	Halogen

Recovery of Spectral Transmission

The first six most significant basis functions to describe spectral transmission of solutions were extracted and are shown in Figure 6, while Table III shows the corresponding cumulative variance of the database. As the figure shows, the cumulative variance for the first three eigenvectors is 93.24 and suggests that three eigenvectors may be inadequate for spectral recovery; the corresponding result for six basis functions is 99.45.

To provide two sets of *XYZ* tristimulus values, the RGB data of samples obtained under fluorescent illumination were converted to $L^*a^*b^*$ color coordinates under D65 and A illuminants and 1964 standard observer. The $L^*a^*b^*$ data were then converted to *XYZ* values and used for spectral reconstruction.

In order to investigate the effect of the number of selected eigenvectors on results, the reconstruction of spectral transmission was also conducted under D65 and A illuminants individually by using three basis functions. The RGB values captured under the fluorescent illuminant were converted to CIELAB values under D65 illuminant. Table IV shows the results of reconstruction of spectral transmission in terms of the root mean square error (RMS) between the actual and reconstructed spectra and the color difference values under different illuminants. Obviously, poor recovery results were achieved when three eigenvectors were used and a noticeable improvement could be realized when the number of eigenvectors was increased to six. In this approach, the RGB values captured under one illuminant (fluorescent lamp) were converted to two sets of CIELAB values under D65 and A illuminants. However, the results indicate that further improvements are still needed for acceptable recovery results.

For better analysis of results, the residue of differences between the actual and the reconstructed spectra, using three and six eigenvectors, was calculated and shown in Figures 7 and 8, respectively. As these figures show, the residuals become smaller when six eigenvectors are employed; the errors are more noticeable at the two extrema of the spectra.

Apparently, the recovery errors are greater in comparison with those reported in articles on reconstruction of reflectance spectral from CIEXYZ tristimulus values. So, other modification methods were examined to enhance the results.

To improve the recovery results, the pseudoinverse as well as matrix *R* methods were employed as suggested by Zhao and Berns.[26] In this case, two sets of RGB data, which were gathered under fluorescent and halogen lamps, were converted to spectral transmission by the pseudoinverse method. Because of good linear response of the camera, the linearization step was omitted and the raw RGB data under fluorescent illuminant were directly transformed to CIELAB

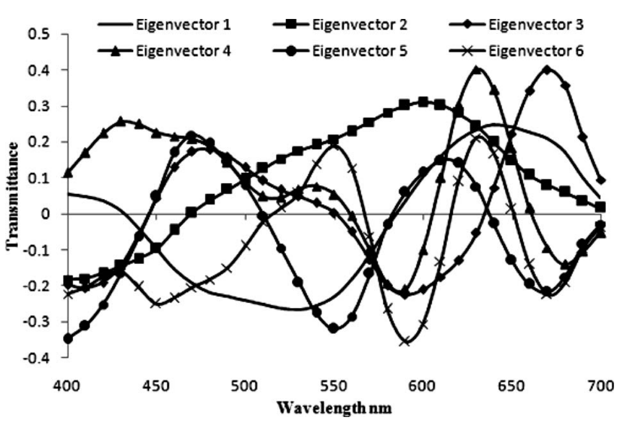

Figure 6. The first six most significant eigenvectors of spectral transmission data of colored solutions.

Table III. Cumulative variances of spectral transmissions of dye solutions.

Eigenvalues	1	2	3	4	5	6	7	8	9	10	11	12
CV%	47.10	82.10	93.24	96.34	98.54	99.45	99.77	99.86	99.91	99.96	99.98	99.99

Table IV. Statistical results of recovery using PCA with three and six basis functions, pseudoinverse, and matrix R methods.

Methods	Mean RMS (%)	Median RMS (%)	Min RMS (%)	Max RMS (%)	Std RMS	Mean ΔE2000 (D65)	Std ΔE2000 (D65)	Max ΔE2000 (D65)	Mean ΔE2000 (A)	Std ΔE2000 (A)	Max ΔE2000 (A)
PCA (3eigs)	17.78	16.10	4.90	47.88	8.97	2.50	2.82	8.53	4.20	1.77	12.90
PCA (6eigs)	10.88	10.08	4.18	19.05	3.87	2.42	1.54	8.42	2.44	1.40	8.97
Pseudoinverse	11.31	10.28	5.20	31.50	4.34	5.76	3.77	27.64	5.62	4.08	31.84
Matrix R	3.24	3.09	0.17	8.10	1.90	2.96	1.71	11.32	2.75	1.54	10.92

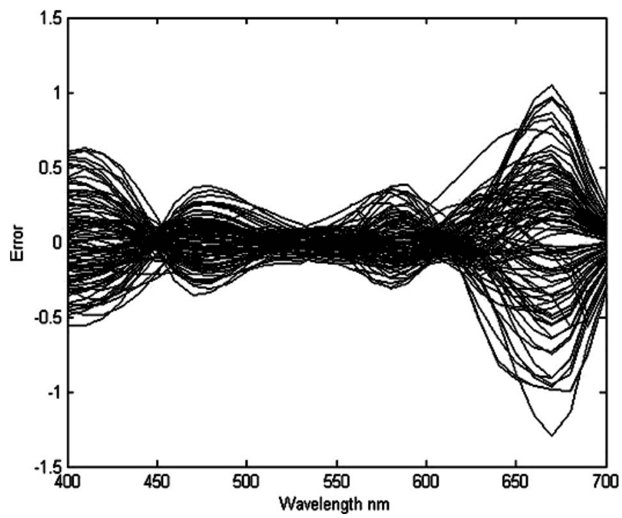

Figure 7. The recovery errors ($T_\lambda - \hat{T}_\lambda$) vs wavelengths for PCA method. Three eigenvectors have been used.

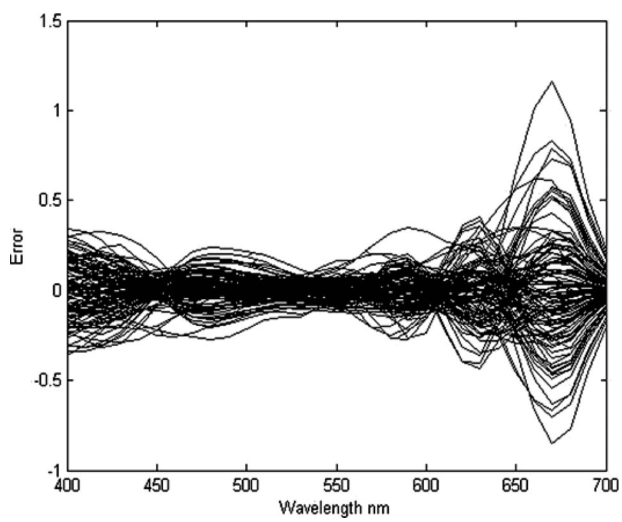

Figure 8. The recovery errors ($T_\lambda - \hat{T}_\lambda$) vs wavelengths for PCA method. Six eigenvectors have been used.

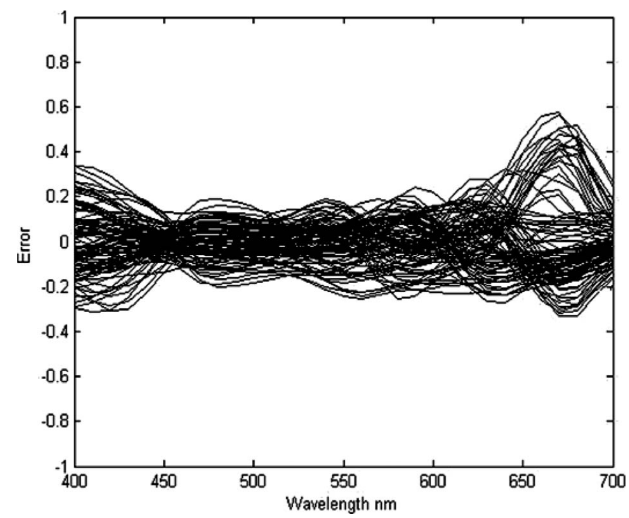

Figure 9. The recovery errors ($T_\lambda - \hat{T}_\lambda$) vs wavelengths for pseudoinverse method.

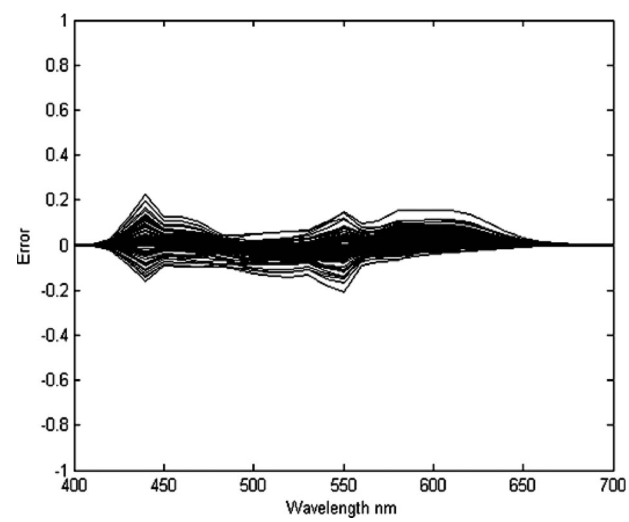

Figure 10. The recovery errors ($T_\lambda - \hat{T}_\lambda$) vs wavelengths for matrix R method.

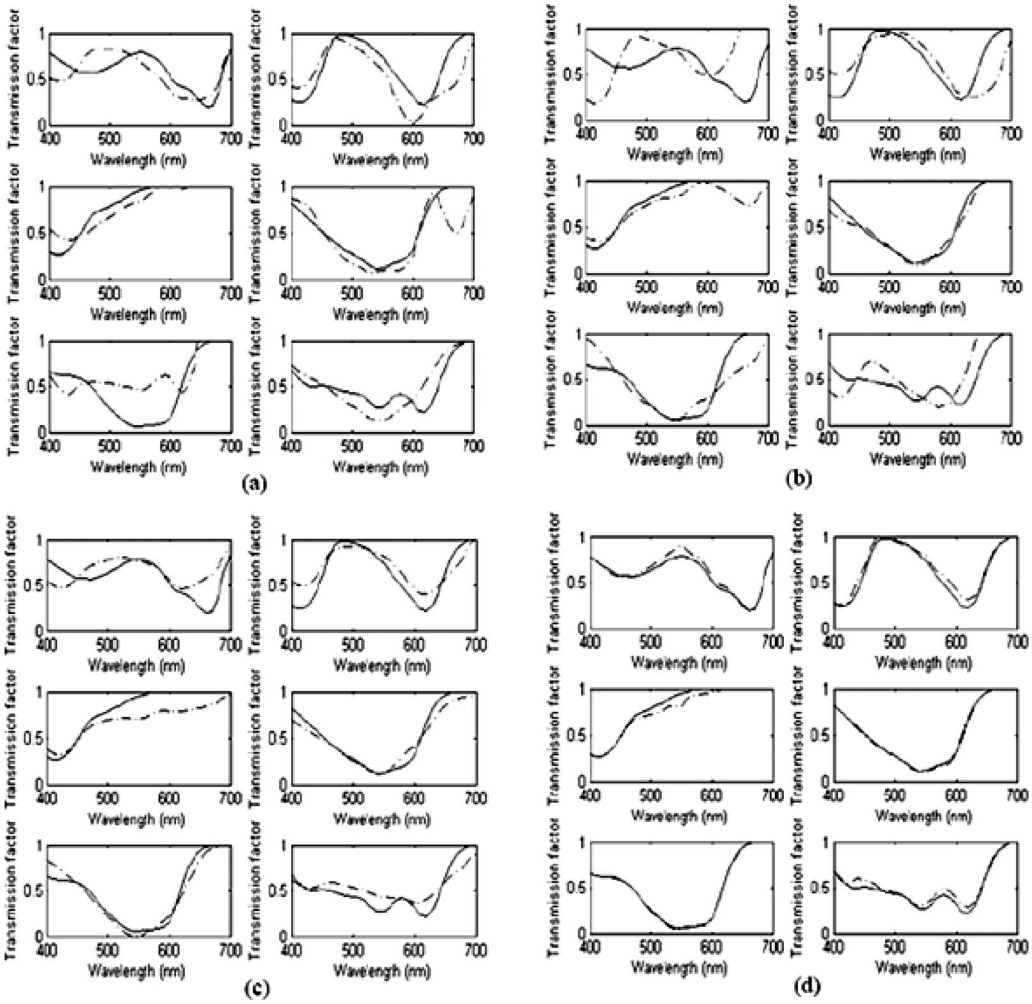

Figure 11. Spectral recovery of eight randomly selected samples by different methods. (a) PCA with three eigenvectors, (b) PCA with six eigenvectors, (c) pseudoinverse, and (d) matrix *R*.

values and then converted to CIEXYZ data. As suggested by Zhao and Berns, the metameric black from spectral transmission factors predicted by the pseudoinverse method was fused with the fundamental stimuli from tristimulus values estimated by colorimetric characterization to get the spectral transmission factors. Table IV summarizes the results of the performances of the pseudoinverse and matrix *R* methods. As the results show, the performance of pseudoinverse method for the reconstruction of spectral behavior of transparent samples is better than PCA, using three eigenvectors. On the other hand, this method led to the worst colorimetric error. As Figure 9 shows, the residuals between the actual and reconstructed transmission spectra at the two ends of the spectra decrease in comparison with PCA methods.

Finally, the matrix *R* method was also examined in the reconstruction process; it led to the minimum spectral error. As Figure 10 shows, the residuals between the actual and reconstructed transmission spectra are significantly smaller in comparison to other methods, and satisfactory recoveries have been achieved by this technique.

As Table IV shows, the colorimetric errors of PCA method by using six eigenvectors are the least among the employed methods under both D65 and A illuminants, while the spectral error of this method is greater than obtained with the matrix *R* method. On the other hand, as Fig. 9 shows, the maximum residual differences between the actual and reconstructed spectra have been concentrated in the two ends of the visible spectrum, where color matching functions are smallest. As the figures show, the minimum error in spectral reconstruction by PCA methods, opposite to matrix *R* method, are approximately located around 450, 550, and 610 nm, where the color matching functions benefit from their highest values. Clearly, this could lead to the minimum color difference values achieved by the PCA method.

The results of spectral recovery of eight randomly selected samples with the different reconstruction methods are shown in Figure 11. The superior performance of the matrix *R* method over the PCA and matrix pseudoinverse technique is clearly evident in this figure. On the other hand, using the PCA method and three eigenvectors leads to the worst results among the employed methods.

CONCLUSION

A variety of transparent colored solutions and a capturing box, which was equipped with a conventional digital camera and two sets of commercial light sources, were prepared to examine different methods of spectral transmission recovery techniques from the corresponding RGB data. Several methods including PCA, pseudoinverse, and matrix *R* techniques were employed in the recovery process, while some types of modifications were applied to improve their performance with transparent samples. Results of reconstructions were evaluated by mean, maximum, and standard deviation of color difference values under D65 and A illuminants and 1964 observer, for which the CIEDE2000 color difference formula was used. Besides, root mean square errors between the actual and reconstructed spectra were computed. The results showed that the pseudoinverse and PCA methods lead to unacceptable recovery outcomes. However, results of the PCA method improved on increasing the number of eigenvectors employed. Finally, the matrix *R* method led to the most acceptable accuracies overall in both spectral and colorimetric terms among the methods applied.

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