Reconstruction of surface reflectance spectra by means of tristimulus values

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Abstract

Reflectance spectra of 3160 specimens from the Munsell and the NCS atlases have been used as a model group in PCA and we have verified that a basis of six eigenvectors, without mean vector, is sufficient for a good spectra reconstruction. The use of the PCA provides good reconstructions but has the drawback of not allowing the reconstruction of spectra of specimens from other sample sets different from the model group. If the results are to be applied to spectra of samples other than those used previously, it is necessary to calculate the corresponding principal components in a different way. The use of six tristimulus values from each spectrum measured, obtained using the CIE D65 and A illuminants, in the calculation of the principal components, M_i, permits the reconstruction of any spectrum, while providing, in addition, a high degree of metamerism between the measured and the reconstructed spectra.

Introduction

Numerous studies have investigated the possibility of reconstructing reflectance spectra for colored surfaces with a limited number of eigenvectors, using *Principal Components Analysis (PCA)*. Hardeberg [1]included 15 or so articles on this subject in the bibliography accompanying his article on spectral dimensionality of color objects. The articles published by Tzeng & Berns [2] and Ayala et al. [3] provide a good update on the topic and include a wide bibliography.

We have verified that a basis of six eigenvectors, without mean vector, is sufficient for a good spectra reconstruction [4].

The use of the PCA provides good reconstructions but has the drawback of not allowing the reconstruction of spectra of specimens from other sample sets different from the model group. If the results are to be applied to spectra of samples other than those used previously, it is necessary to calculate the corresponding principal components in a different way.

In our case, the way to calculate the principal components M_i, as a function of the tristimulus values, is as in Ayala et al. [3]. In a similar way to that employed in this study [3], in order to test the model, we will use the color differences between the coordinates obtained from the experimental spectrum and those of the reconstructed one, calculated using the CIE64 observer and F11 illuminant, so as to be able to evaluate better the goodness of fit. With the illuminants A and D65, the measured and reconstructed spectra correspond, by construction, to metameric colors, and to almost metameric colors if the illuminants D50 and D75 are used.

Materials and methods

A. Principal Component Analysis and Tristimulus Values

Response data ρ_λ (reflectance spectrum between 400 to 700 nm, at $\Delta\lambda$ = 10 nm) are available for r (31) levels of the variable λ (wavelength) and can be plotted as a response curve. The result of PCA is that the components of the generic vectors (i.e., the reflectance spectra) can be expressed as:

$$\rho_\lambda = M_1 V_{1\lambda} + M_2 V_{2\lambda} + \cdots + M_p V_{p\lambda} \qquad p \le r \tag{1}$$

where $V_{i\lambda}$ represents the components of the i-th eigenvector and M_i the specific coefficients, called principal components, of each reconstructed vector.

A way to calculate the principal components M_i as a function of the tristimulus values is as follows [3]:

The CIE expressions for the tristimulus values are

$$X = k\sum_\lambda \rho_\lambda S_\lambda \bar{x}_\lambda \Delta\lambda, \quad Y = k\sum_\lambda \rho_\lambda S_\lambda \bar{y}_\lambda \Delta\lambda$$
$$Z = k\sum_\lambda \rho_\lambda S_\lambda \bar{z}_\lambda \Delta\lambda$$

where ρ_λ is the spectral reflectance, S_λ the relative spectral power distribution of the selected standard illuminant, $\bar{x}_\lambda$, $\bar{y}_\lambda$, $\bar{z}_\lambda$ are the color-matching functions of the selected standard observer, and $\Delta\lambda$ the wavelength interval of the measurements.

Expression (1) for ρ_λ can be substituted into expressions for any of the tristimulus values, and, as an example, X has the following expression:

$$X = k\sum_\lambda \left(M_1 V_{1\lambda} + M_2 V_{2\lambda} + \ldots + M_p V_{p\lambda}\right) S_\lambda \bar{x}_\lambda \Delta\lambda$$

which can be written as

$$X = M_1 k\sum_\lambda V_{1\lambda} S_\lambda \bar{x}_\lambda \Delta\lambda + \ldots + M_p k\sum_\lambda V_{p\lambda} S_\lambda \bar{x}_\lambda \Delta\lambda \tag{2}$$

because the M_i coefficients are independent of the wavelength for any single reconstituted curve.

Letting

$$X_i = k\sum_\lambda V_{i\lambda} S_\lambda \bar{x}_\lambda \Delta\lambda$$

one can write Eq. (2) as

$$X = M_1 X_1 + M_2 X_2 + \ldots + M_p X_p$$

where X_i could be considered the theoretical tristimulus values of each eigenvector. Analogous expressions are obtained for the Y and Z tristimulus values:

$$Y = M_1 Y_1 + M_2 Y_2 + \ldots + M_p Y_p$$
$$Z = M_1 Z_1 + M_2 Z_2 + \ldots + M_p Z_p$$

As we have pointed out in the introduction, our aim is to reconstruct the reflectance spectra with a basis of six eigenvectors. In order to know the six M_i coefficients, we will need six equations and six tristimulus values obtained from each spectrum in order to provide a solution to a system like the one below:

$$X_D = M_1 X_{1D} + M_2 X_{2D} + \cdots + M_6 X_{6D}$$
$$Y_D = M_1 Y_{1D} + M_2 Y_{2D} + \cdots + M_6 Y_{6D}$$
$$Z_D = M_1 Z_{1D} + M_2 Z_{2D} + \cdots + M_6 Z_{6D}$$
$$X_A = M_1 X_{1A} + M_2 X_{2A} + \cdots + M_6 X_{6A}$$
$$Y_A = M_1 Y_{1A} + M_2 Y_{2A} + \cdots + M_6 Y_{6A}$$
$$Z_A = M_1 Z_{1A} + M_2 Z_{2A} + \cdots + M_6 Z_{6A}$$

where, X_{iD}, Y_{iD}, Z_{iD} y X_{iA}, Y_{iA}, Z_{iA} are the tristimulus values for the characteristic vector i, while X_D, Y_D, Z_D y X_A, Y_A, Z_A are the tristimulus values of the specimen, all calculated using Observer CIE64 and Illuminants D65 and A, respectively. The M_i coefficients are then a function of these tristimulus values of the specimen:

$$M_1 = f_1(X_D, Y_D, Z_D, X_A, Y_A, Z_A)$$
$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (3)$$
$$M_6 = f_6(X_D, Y_D, Z_D, X_A, Y_A, Z_A)$$

The first six eigenvectors obtained from the model group, together with the corresponding M_i coordinates, permit the reconstruction of the reflectance spectra by applying the following equation:

$$\rho_\lambda = M_1 V_{1\lambda} + M_2 V_{2\lambda} + \ldots + M_6 V_{6\lambda} \quad (4)$$

B. Samples

We measured the spectra of 1485 chips from the Munsell Book of Color, Matte Finish Collection [5] and 1675 chips from the NCS Atlas [6] with a HunterLab UltraScan spectrocolorimeter, range 400–700 nm at 10 nm intervals, d/0 geometry and specular reflectance included.

Principal components analysis was applied to the group of 3160 spectra from the Munsell and NCS atlases, the "model group". Also, in the works of model validation, the 1269 spectra of Munsell specimens measured by Parkkinen and colleagues [7] and the reflectances of 170 miscellaneous items measured by Vrhel, Gershon, and Iwan [8] have been used under the same conditions as our measurements: 400–700 nm at $\Delta\lambda$ = 10 nm. These 1269 Munsell spectra and the 170 spectra measured by Vrhel were used separately as "validation groups". In this way, spectra measured with a different device were introduced into the data set, thus broadening the variability of the sampling method used.

Tristimulus values and the color coordinates L^*, a^*, b^*, C_{ab}^* and h_{ab} were calculated from the measured and the reconstructed spectra using the CIE64 Observer and the CIE Illuminants A, D50, D65, D75, and F11, in accordance with the CIE method [9].

The six tristimulus values obtained from measured spectra, calculated using the CIE64 Observer and the CIE Illuminants A and D65 respectively, have been used as data for calculating the principal components, *Mi*, of each spectrum.

The color differences, in CIELAB units, have been calculated using the expression

$$\Delta E_{ab}^* = \left[\left(L_1^* - L_2^*\right)^2 + \left(a_1^* - a_2^*\right)^2 + \left(b_1^* - b_2^*\right)^2 \right]^{\frac{1}{2}} \quad (5)$$

The calculations of the tristimulus values and the CIELAB coordinates, as well as PCA and subsequent spectra reconstruction from tristimulus values, were performed with our own software. The package SPSS 11.0 was used for statistical data processing.

Reconstruction of spectra

The sum of the first six eigenvalues obtained from the zero-centered covariance matrix is 0.9994, equivalent to 99,94 % accumulated variance explained in the variance-covariance matrix. The minimum value suggested by Hardeberg [1] for considering the accuracy as being good when reconstructing reflectance spectra is 99%. The corresponding 6 eigenvectors can be found at [10]. Table I shows statistics of the color differences between the original spectra and those reconstructed from PCA.

Table I.- Statistics of color differences (in CIELAB units) between colors obtained from experimental and reconstructed spectra, from PCA, for each specimen of the Munsell and the NCS atlases (N=3160 specimens). Color coordinates calculated with CIE64 Observer and CIE D65, A, D75 and F11 Illuminants.

Illuminant	D65	A	D75	F11
Munsell+NCS (N=3160)				
Mean	0.45	0.38	0.46	1.14
Min.	0.00	0.00	0.00	0.03
Max.	3.91	2.73	4.07	20.28
Std. Dev.	0.46	0.35	0.48	1.31

Below we present the expressions found for calculating the principal components from the tristimulus values of each measured spectrum, obtained with the Illuminants D65 and A and the CIE 64 Observer.

$$M_1 = -1.0969X_D - 0.9342Y_D + 0.3125Z_D + 0.1856X_A + 1.5836Y_A - 0.2742Z_A$$
$$M_2 = 1.2599X_D + 1.3694Y_D - 0.2324Z_D - 0.1287X_A - 2.1471Y_A - 0.0454Z_A$$
$$M_3 = -0.5978X_D - 0.4320Y_D + 0.2391Z_D + 0.1500X_A + 0.7025Y_A - 0.3542Z_A$$
$$M_4 = 1.3110X_D + 1.1339Y_D - 0.2214Z_D - 0.1847X_A - 1.8994Y_A - 0.0952Z_A$$
$$M_5 = -1.2072X_D - 1.2774Y_D + 0.4163Z_D + 0.0572X_A + 2.0945Y_A - 0.5190Z_A$$
$$M_6 = 0.9518X_D + 1.4812Y_D + 0.0371Z_D + 0.0945X_A - 2.2219Y_A - 0.8673Z_A$$

In order to study the reliability of the method, the color coordinates L^*, a^*, b^*, C_{ab}^* , and h_{ab} were calculated from the measured and the reconstructed spectra using the CIE64 Observer and the CIE Illuminants A, D50, D65, D75, and F11.

Because of the method used to calculate the principal components *Mi*, the experimental and the reconstructed spectra have, practically, the same tristimulus values and correspond to two metameric colors for the illuminants D65 and A and the CIE64 Observer (Fig. 1). These spectra have almost metameric spectra under D50 and D75 Illuminants. Color differences are higher under F11 Illuminant (Fig. 2).

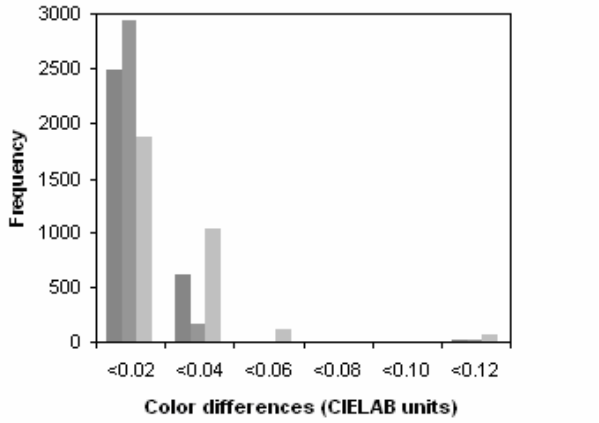

Fig. 1. Histogram of color differences between color coordinates from measured and reconstructed spectra, from tristimulus values, of 3160 samples of model group under illuminants D65 ■, A ■ and D75 ■.

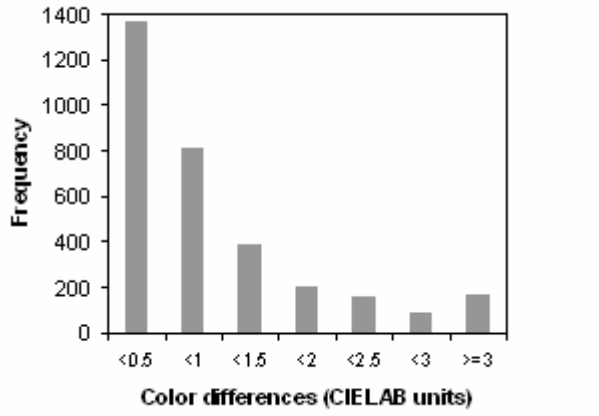

Fig. 2. Histogram of color differences between color coordinates from measured and reconstructed spectra, from tristimulus values, of 3160 samples of model group under illuminant F11.

In Table II we show the statistics of color differences with the illuminants D65, A, D75 and F11 obtained when the spectra of model group and test groups are reconstructed using these principal components obtained from tristimulus values.

Table II.- Statistics of color differences (in CIELAB units) between colors obtained from experimental and reconstituted spectra, from tristimulus values, for each specimen of the Munsell and the NCS atlases (N=3160 specimens), Munsell measured by Parkinnen et al. (N=1269 specimens) and miscellaneous objects measured by Vrhel (N=179 specimens). Color coordinates calculated with CIE64 Observer and CIE D65, A, D75 and F11 Illuminants.

Illuminant	D65	A	D75	F11
Munsell+NCS (N=3160)				
Mean	0.01	0.01	0.02	0.96
Min.	0.00	0.00	0.00	0.01
Max.	0.10	0.10	0.13	9.32
Std. Dev.	0.01	0.01	0.02	1.01
Munsell (N=1269)				
Mean	0.01	0.01	0.02	1.00
Min.	0.00	0.00	0.00	0.01
Max.	0.10	0.10	0.11	7.99
Std. Dev.	0.01	0.01	0.02	1.07
Miscellaneous (N=170)				
Mean	0.01	0.01	0.02	0.94
Min.	0.00	0.00	0.00	0.02
Max.	0.10	0.10	0.20	8.39
Std. Dev.	0.01	0.02	0.03	1.10

A number of examples of measured spectra and their corresponding reconstructions are shown in Fig. 3 and Fig. 4.

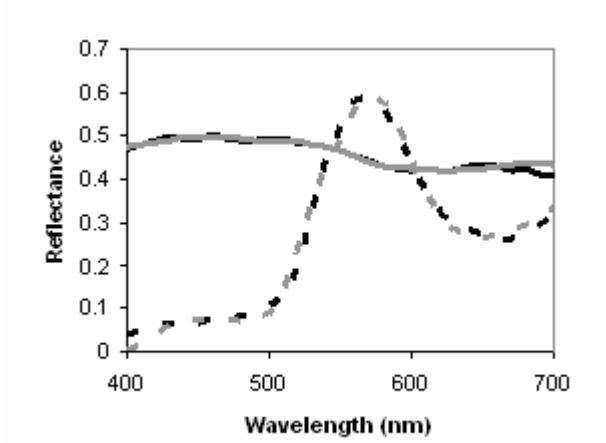

Fig. 3. Examples of reconstruction for a Munsell sample, 10B72 ━ and 10B72r ─ (ΔE=0.06 for F11 illuminant) and a NCS sample, 2070G80 ▬ and 2070G80r ┄ (ΔE*=2.67 for F11 illuminant).*

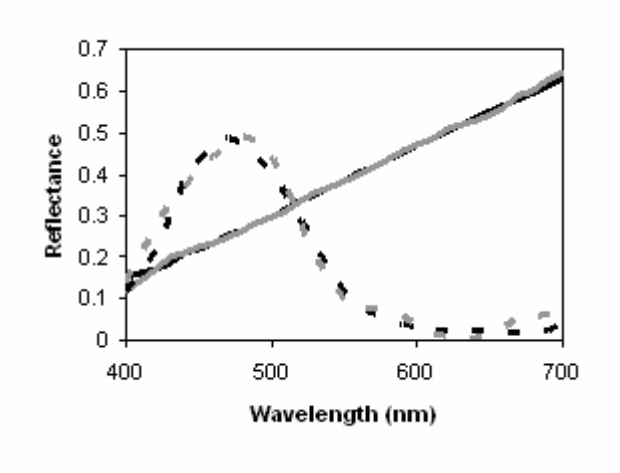

Fig. 4. Examples of reconstruction for two Vrhel samples: 50 -- and 50r -- (ΔE=2.74 for F11 illuminant) and 66 ─ and 66r ─ (ΔE*=0.08 for F11 illuminant).*

Conclusions

A basis of six eigenvectors is sufficient to obtain a good reconstruction of reflectance spectra. The use of the tristimulus values of the colors used in this work, obtained with the illuminants D65 and A, and the CIE64 observer, allows us to calculate the corresponding principal components and to improve the results in comparison with the reconstruction by PCA. The spectra reconstructed in this way reveal a high level of metamerism under the illuminants A, D50, D65 and D75. For illuminant F11 the metamerism is a little less although it is still very high.

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