Wavelength intervals effect on reflectance spectra reconstruction

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The principal component analysis is an important method in reflectance spectra reconstruction. This is a research into the effects of a wavelength interval on the performance of reflectance spectra estimation by the principal component analysis technique. The spectral reflectance is reconstructed by using 20, 10 and 5 nm intervals. The RMS accuracy of reflectance spectra fitting is 0.0079, 0.0074 and 0.0072, respectively for 20, 10 and 5 nm intervals with 6 principal components. As the obtained results indicated, the performance of reflectance estimation increased with decreasing the wavelength interval.

Keywords: reflectance spectra, reconstruction, wavelength interval, tristimulus, principal component analysis (PCA).

1. Introduction

The best method to compute tristimulus values is to use smaller intervals, so that the tristimulus values calculation based on the 5-nm color-matching and illuminant data are more accurate than 10 or 20 nm wavelength intervals. Although reflectance data exist in larger intervals, such as 10 or 20 nm, the 5 nm interval data can be used if interpolation process is applied to the reflectance spectra data [1, 2].

There are serious limitations concerning reflectance spectra estimation from the on cone excitations and tristimulus values. In mathematical theory there is an infinite number of combinations of surface-reflectance functions, illuminant power distributions and color matching functions that could generate known tristimulus values.

In several papers, it has been attempted to extract the reflectance spectra data from the three-dimensional color information, such as X, Y and Z, by using different mathematical strategies, namely the simplex method, simulated annealing method, the application of ideal subtractive or additive Gaussian primaries, the neural networks approach and linear methods. The popular method of reflectance spectra reconstruction is based on the principal component analysis technique. The principal component vectors and basis functions are themselves functions of wavelength which are similar to the reflectance spectra. But the basis functions component values are bipolar which

means that not all vector components are positive. Actually, however, it is not always needed to subtract the mean of reflectance spectra to use a linear model of reflectance. The linear model can be used to evaluate the reflectance spectra of samples by the linear summation of the basis functions weighted by coefficients. The reflectance spectra of all samples can be reconstructed perfectly by using all the n basis functions and the appropriate values of the weights $a_1, ..., a_n$

$$R(\lambda) = a_1 B_1(\lambda) + a_2 B_2(\lambda) + a_3 B_3(\lambda) + ... + a_n B_n(\lambda)$$

However, the advantage of principal component analysis (PCA) techniques is that it is possible to reconstruct reflectance spectra by only using a small number of basis functions. Because the first basis function represents the maximum variance in the reflectance spectra data, the later basis functions maximally represent the remaining variance. Therefore, more than 95% of the variance in a reflectance spectra set can be reconstructed only by using the first three basis functions. The acceptable recovery of spectral reflectance has been obtained by using 3 to 9 principal components. Also the recovery of reflectance spectra depends on an illumination–observer combination [2–10]. In pervious research, the effects of standard colorimetric observers and illuminant sources combination on reflectance spectra reconstruction were studied. The obtained results indicated that the accuracy of reconstruction depends on the illuminant sources combination, standard colorimetric observers and the number of principal components. The best spectral reflectance recovery is obtained by 1931 standard observers and six principal components [6]. Also, a recipe prediction was approved by the principal component analysis-based spectrophotometric match prediction method with different numbers of principal components. The accuracy of the principal component based technique was comparable with the normal single constant spectrophotometric color matching method [7]. In addition, the principal component analysis techniques were used to estimate CIE tristimulus values of Munsell chips under various illuminants from known tristimulus values under special illuminant [8].

ANSARI et al. gathered a large archive of surface colors, consisting of 1269 Munsell color samples, 2802 acrylic paints and 917 colored textiles for spectral reflectance recovery from their tristimulus values based on a hue database [9]. Instead of using one set of reflectance spectra to determine principal components, various data sets of reflectance spectra were preselected based on the color specifications of a given sample to extract the eigenvectors. AGAHIAN and AMIRSHAHI [10] suggested a new matching approach based on the matching of the first three principal components of the sample and the target in a 3-D eigenvector space. The first three basic functions of 1269 samples were extracted and considered as axes of eigenvector space. The principal components of two different collections of textile samples were determined in these spaces and considered as matching criteria. The results obtained indicated some improvements in comparison with previous algorithms in terms of spectral accuracy as well as colorimetric accuracy. The proposed approach leads to better results by increasing the number of selected eigenvectors [10].

2. Materials and methods

The reflectance spectra of 1269 Munsell color chips were obtained from the web site of the University of Joensuu (Finland) [11]. The CIE tristimulus values of Munsell color chips are calculated under A, EE (equal energy) and D65 illuminants and 10-degree standards colorimetric observer. The reflectance spectra database is randomly divided into two parts as a training and testing data set with 800 and 469 samples, respectively. The training data were used to estimate the principal component and others were used to estimate the accuracy of reflectance spectra reconstruction from the CIE tristimulus values.

Reflectance spectra reconstruction is done by the following method:
– Calculating the tristimulus values of 1269 Munsell color chips;
– Calculating the mean reflectance spectra of training data;
– Calculating the tristimulus values of mean reflectance;
– Extracting the principal components of training reflectance spectra data set;
– Calculating the tristimulus value of principal components;
– Calculating the transformation matrix (the principal component coordinates) by using the tristimulus values of training reflectance spectra and principal components;
– Calculating the reflectance spectra from principal components by means of transformation matrix and mean reflectance;
– Evaluating the performance of reflectance spectra recovery.

3. Results and discussion

The reflectance spectra with 5, 10 and 20 nm interval from 400 to 700 nm are used to evaluate the effects of wavelength intervals on the performance of reflectance spectra estimation from the CIE tristimulus values.

Initially, the eigenvector of reflectance spectra of training dataset were calculated by the mean-centered principal component analysis technique. The eigenvalues of principal components of reflectance spectra dataset with 20 nm interval (16 wavelengths)
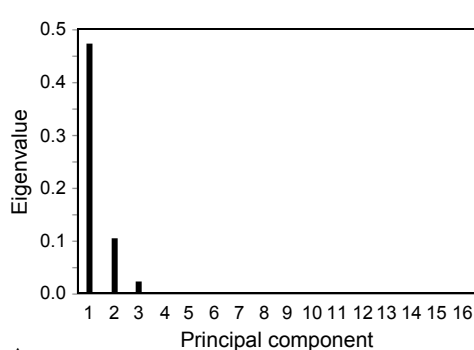
Fig. 1. Eigenvalue of principal components of reflectance spectra with 20 nm interval.
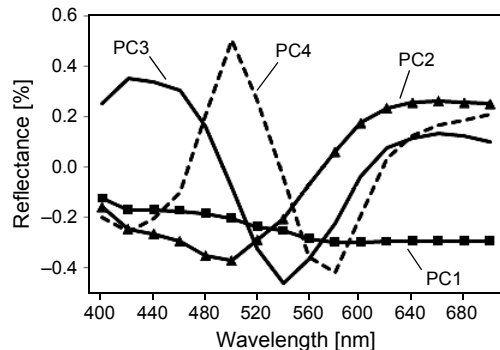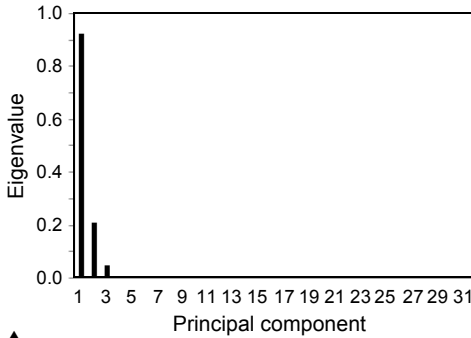
Fig. 2. The first four principal components of reflectance spectra with 20 nm interval.

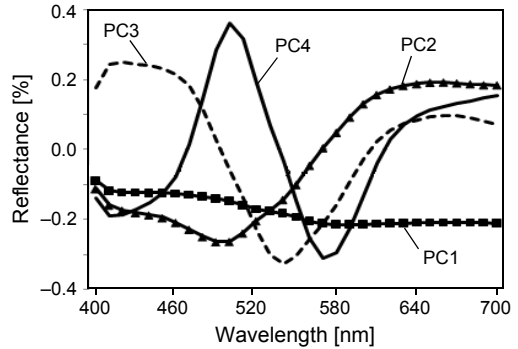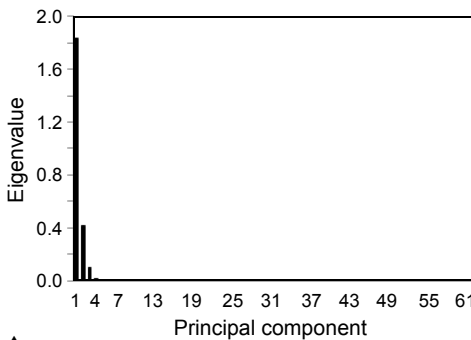Fig. 3. Eigenvalues of principal components of reflectance spectra with 10 nm interval.

Fig. 4. The first four principal components of reflectance spectra with 10 nm interval.

Fig. 5. Eigenvalues of principal components of reflectance spectra with 5 nm interval.
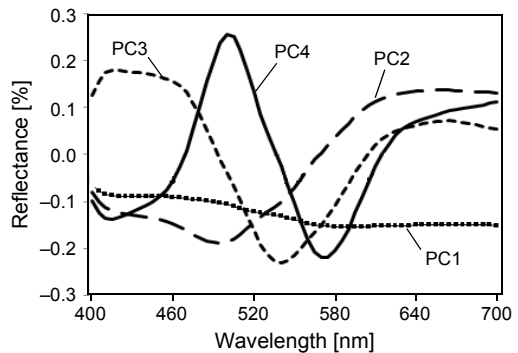
Fig. 6. The first four principal components of reflectance spectra with 5 nm interval.

are shown in Fig. 1. As shown in Fig. 1, the 99.53% of total variance is explained by first four principal components eigenvectors. Figure 2 shows the first four principal components eigenvectors. The eigenvalues of principal components of reflectance spectra dataset with 10 nm interval (31 wavelengths) are shown in Fig. 3. As shown in this figure, the 99.55% of total variance is explained by first four principal components eigenvectors. Figure 4 shows the first four principal components eigenvectors of this dataset. Figure 5 shows the eigenvalues of dataset with 5 nm interval (61 wavelengths). As shown in this figure, the 99.56% of total variance is explained by first four principal components eigenvectors. Figure 6 shows the first four principal components eigenvectors of this dataset.

Afterward, the reflectance spectra of testing samples were reconstructed by using 20, 10, 5 nm wavelength intervals. The results of reflectance spectra recovery were compared with RMS values of reflectance spectra fitting – see Tab. 1. As shown in this table, the spectrophotometry accuracy values of reflectance spectral recovery from

T a b l e 1. Spectrophotometry accuracy of reflectance spectra reconstruction (RMS).

Number of wavelength	Wavelength interval [nm]	Number of PC	Mean	Max.	Min.	STD
16	20	3	0.0191	0.1253	0.0025	0.0146
		4	0.0125	0.0898	0.0013	0.0107
		5	0.0085	0.0688	0.0013	0.0078
		6	0.0079	0.0687	0.0011	0.0079
31	10	3	0.0186	0.1202	0.0021	0.0143
		4	0.0122	0.0861	0.0013	0.0106
		5	0.0110	0.0922	0.0012	0.0113
		6	0.0074	0.0738	0.0011	0.0082
61	5	3	0.0184	0.1195	0.0017	0.0143
		4	0.0120	0.0843	0.0013	0.0105
		5	0.0107	0.0899	0.0012	0.0110
		6	0.0072	0.0712	0.0011	0.0078

their tristimulus values by 20 nm wavelength interval are 0.0191, 0.0125, 0.0085 and 0.0079, respectively, for 3, 4, 5 and 6 principal components (PCs). The spectrophotometry accuracy of reflectance spectral recovery by 10 nm wavelength intervals is 0.0186, 0.0122, 0.011 and 0.0074, respectively, for 3, 4, 5 and 6 principal components. The spectrophotometry accuracy values of reflectance spectral recovery from their tristimulus values by 5 nm wavelength interval are 0.0184, 0.0120, 0.0107 and 0.0072, respectively, for 3, 4, 5 and 6 principal components.

4. Conclusions

This paper studies the effect of wavelength intervals on reflectance reconstruction by principal component analysis techniques. The reflectance spectra recovery was done by using 20, 10 and 5 nm wavelength intervals. The spectrophotometry accuracy of reflectance spectra reconstruction with 6 principal components and 20, 10 and 5 nm wavelength intervals, respectively, are 0.0079, 0.0074 and 0.0072 RMS. The obtained results show that the performance of reflectance spectra estimation increased with decreasing the wavelength interval.

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