Effect of Classification by Competitive Neural Network on Reconstruction of Reflectance Spectra Using Principal Component Analysis

Abbas Hajipour,[1] Ali Shams-Nateri[1,2]*

[1]Textile Engineering Department, University of Guilan, Rasht, Iran

[2]Center of Excellence for Color Science and Technology, Tehran, Iran

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*Abstract: The best way to describe a color is to study its reflectance spectrum, which provide the most useful information. Different methods were purposed for reflectance spectra reconstruction from CIE tristimulus values such as principal components analysis. In this study, the training samples were first divided into 3, 6, 9, and 12 subgroups by creating a competitive neural network. To do that, L*a*b*, L*C*h or L*a*b*C*h were introduced to neural network as input elements. In order to investigate the performance of reflectance spectra reconstruction, the color difference and RMS between actual and reconstructed data were obtained. The reconstruction of reflectance spectra were improved by using a six or nine-neuron layer with L*a*b* input elements*. © 2016 Wiley Periodicals, Inc. Col Res Appl, 42, 182–188, 2017; Published Online 5 April 2016 in Wiley Online Library (wileyonlinelibrary.com). DOI 10.1002/col.22050

Key words: reconstruction; reflectance spectra; classification; competitive neural network; principal component analysis

INTRODUCTION

The common way for representation of colors is using standard trichoromatic color coordinate system such as CIEXYZ or CIELAB. However, this representation is affected by several parameters such as the illuminant, observer and metameric issues and imaging sensors.[1–4] Therefore, the most informative and complete way to characterize a color is to give its reflectance spectrum, which is defined as the ratio of the reflected radiant flux to the incident flux under a specific condition.[1–3,5–7]

Spectral data is recognized as the "fingerprint" of an object, which is independent of the applied light source and the observer, and provides the most fundamental and useful information in many applications such as textile dyeing, printing, color constancy, archives, network museums, and specially in e-commerce.[2,3,8,9] Thus, color could be described in two different ways using colorimetric values or spectral information. A spectrum shows a physical quantity over some continuous ranges of wavelengths, usually in the visible range from 400 to 700 nm, which can be directly measured using spectrophotometers.[1,10]

The transformation from spectral reflectance to colorimetric coordinates is many-to-one and therefore colorimetric data for objects cannot be unambiguously transformed back to spectral reflectance.[11] Thus, different methods such as simulated annealing, simplex method, neural networks, application of subtractive and additive Gaussian primaries, linear methods, the Hawkyard method, the improved Hawkyard method, genetic algorithms, matrix R method, Principal Component Analysis (PCA), nonnegative matrix factorization, Independent Component Analysis, the lookup-table method, and local linear interpolation method have been developed to extraction the reflectance spectrum from their corresponding colorimetric data.[1,2,5,8,10,12–23]

Among these methods, PCA is simple, linear, and nonparametric method and has been widely used to estimation of spectra.[8,24–27] PCA is an important mathematical technique in color science, which has been used in data analysis, compression, and extraction of the data-based covariance matrix. The advantage of PCA technique is

*Correspondence to: A. Shams-Nateri (e-mail: a_shams@guilan.ac.ir)

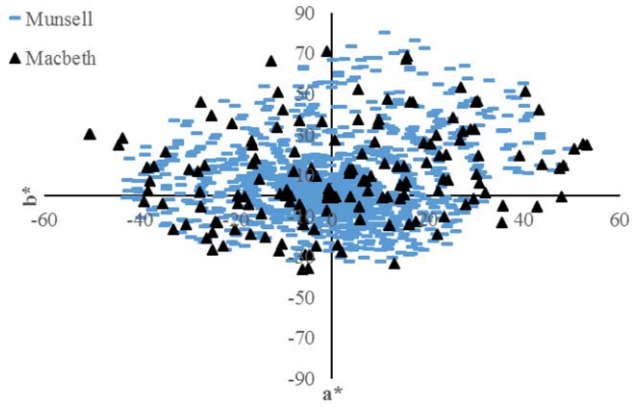

Fig. 1. Chromaticity distribution of training (Munsell) and testing (Macbeth) samples.

the possibility of reflectance spectra reconstruction by only using a small number of basis functions. The first basis vector represents the maximum variance in the reflectance spectra data and the later basis vectors maximally represent the remaining variance. Thus, more than 95% of the variance in a reflectance spectra set can be recovered by using only the first three basis functions.[25–30]

In recent years, some researchers used the PCA in reconstruction of reflectance spectra. As an example, Ansari *et al.*[14] improved recovery of reflectance spectra from CIE tristimulus values using a progressive database selection technique. Shams-Nateri[28] found that the recovery of reflectance spectra depends on an illumination–observer combination and number of principal components. Zhang and Xu[8] divided spectral space into near gray subgroup and 10 subgroups according to the 10 separate hue angles in Munsell space. Then, they calculated the principal components for individual subgroups. The obtained results show that their method is quite accurate. Shams-Nateri studied the effect of wavelength intervals on reflectance spectra recovery.[26] He found the performance of reflectance reconstruction increased with decreasing the wavelength interval.

Self-organization is one of the most attractive topics in the neural network field. These networks have a two-layer

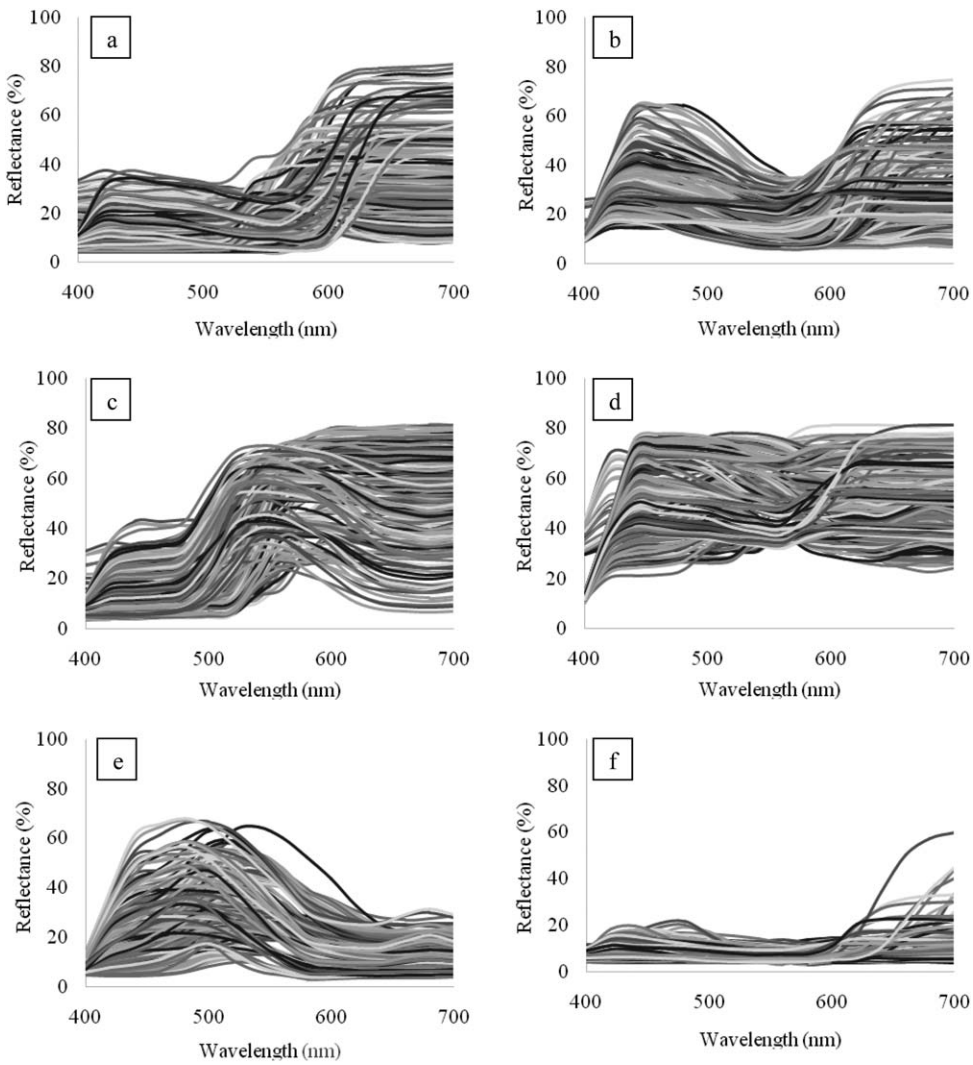

Fig. 2. The reflectance spectra of training samples in different subgroups as (a) 1, (b) 2, (c) 3, (d) 4, (e) 5, and (f) 6, using a 6-neuron layer with L*a*b* inputs elements.

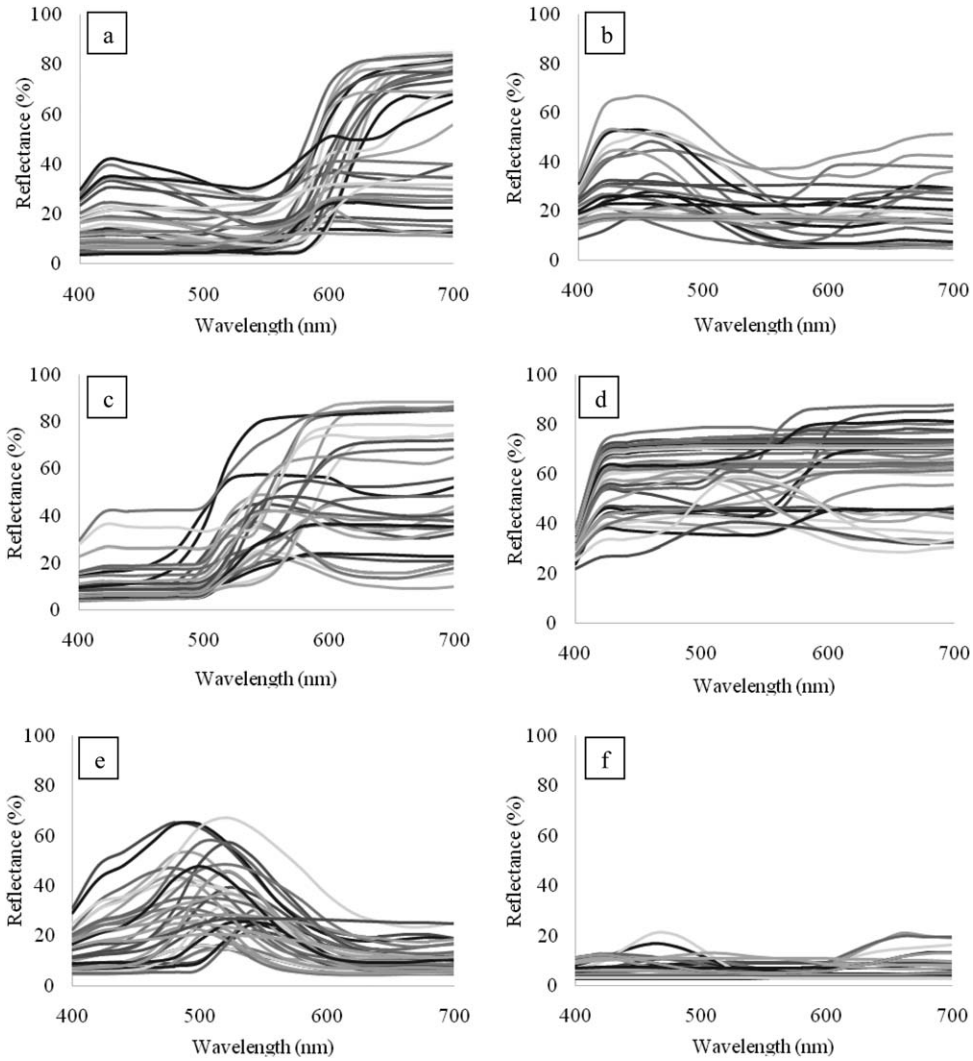

Fig. 3. The reflectance spectra of testing samples in different subgroups as (a) 1, (b) 2, (c) 3, (d) 4, (e) 5, and (f) 6, using a 6-neuron layer with L*a*b* inputs elements.

structure including of the input layer and the competitive layer. All nodes in the input and competitive layers connect fully with one another. Such networks can detect the correlations in their input and organize groups of similar input vectors. The classification of inputs by a competitive neural networks is dependent only on the distance between input vectors and there is no strict mechanism in a competitive layer design.[31,32]

In this research, a new method is proposed for reconstruction of reflectance spectra from CIEXYZ tristimulus values. First, the reflectance spectra of training data were divided according to CIELAB colorimetric coordinate into 3, 6, 9, and 12 subgroups by a competitive neural network. Then, the testing samples were classified by trained neural network. The PCs of subgroups were extracted and recovery of reflectance spectra was done. To investigate the accuracy of reconstruction, the color difference and RMS between actual and reconstructed data were obtained. The clustering method as K-means was also used to investigate the improvement of the proposed method.

MATERIALS AND METHODS

In this work, the reflectance spectra of 1296 Munsell color chips were used for reconstruction of 240 Macbeth Color Cheker cards reflectance spectra. The chromaticity distribution of the training and testing samples under a D65 illuminant source and 10° standard colorimetric observer is shown in Fig. 1. The wavelength intervals of spectrum were fixed at 20 nm within the visible spectrum from 400 nm to 700 nm.

The reflectance spectra reconstruction was carried out by following method:

- Calculating the CIE tristimulus values and CIELAB coordinates (L*, a*, b*, C*, h, where, L* describes lightness, a* is the redness-greenness axis, b* is the yellowness-blueness axis, C* is the saturation, and h is the hue angle) of 1296 Munsell color chips and 240 Macbeth ColorCheker cards under D65 illuminant and 10° standard colorimetric observer[7,33,34];
- Creating a competitive neural network by 1296 Munsell color chips as training data. First, a 3, 6, 9, or 12-neuron layer with three (L*, a*, b* or L*, C*, h) or five (L*, a*,

TABLE I. The cumulative variance obtained from PCs of difference methods of competitive neural network.

Input elements	Number of neuron	Mean	Median
Common method	–	98.16	–
L*a*b*	3	97.52	97.69
	6	97.08	97.48
	9	97.37	97.70
	12	97.30	98.00
L*C*h	3	98.77	98.94
	6	99.09	99.20
	9	99.12	99.43
	12	99.04	99.34
L*a*b*C*h	3	98.78	98.96
	6	99.08	99.20
	9	99.09	99.41
	12	99.12	99.38

b*, C*, and h) input elements was created and 1296 Munsell color chips were classified into 3, 6, 9, or 12 subgroups, respectively. As an example, the reflectance spectra of training samples in different subgroups using a 6-neuron layer with L*a*b* inputs elements are shown in Fig. 2;

- Calculating the mean reflectance spectra of subgroups;
- Calculating the tristimulus values of each mean reflectance;
- Classifying the reflectance spectra of 240 Macbeth ColorCheker cards by trained competitive neural network into 3, 6, 9, or 12 subgroups. For an example, the reflectance spectra of testing samples in different subgroups using a 6-neuron layer with L*a*b* inputs elements are shown in Fig. 3;
- Extracting the PCs of training reflectance spectra data sets;
- Calculating the tristimulus value ($X_{pc,i}$, $Y_{pc,i}$, $Z_{pc,i}$) of PCs (PC_i) by Eq. (1):

$$\begin{cases} X_{pc,i}=k\sum_{\lambda} E_\lambda \times PC_{\lambda,i}\times \overline{x_\lambda} \\ Y_{pc,i}=k\sum_{\lambda} E_\lambda \times PC_{\lambda,i}\times \overline{y_\lambda} \\ Z_{pc,i}=k\sum_{\lambda} E_\lambda \times PC_{\lambda,i}\times \overline{z_\lambda} \end{cases} \quad (1)$$

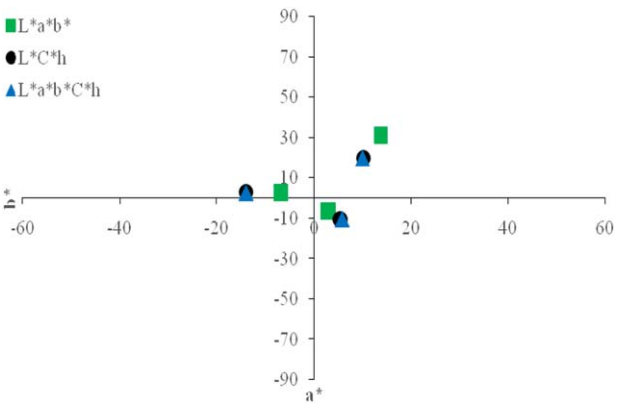

Fig. 4. Chromaticity distribution of the mean reflectance of three-neuron layer method.

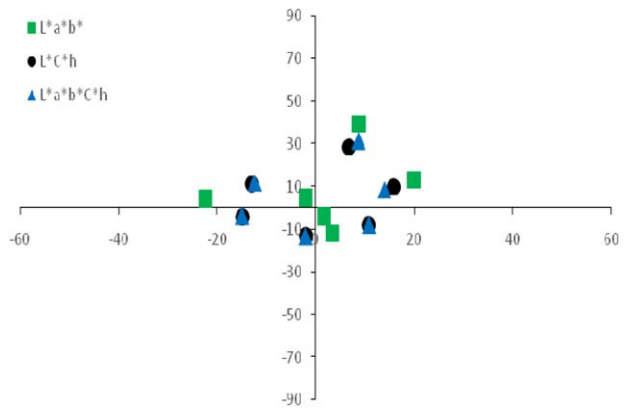

Fig. 5. Chromaticity distribution of the mean reflectance of six-neuron layer method.

where i is the number of PCs. $\overline{x}$, $\overline{y}$ and $\overline{z}$ are color matching functions, E is spectral power distribution of the light source, and k is the normalization constant:

$$k=\frac{100}{\sum_\lambda E_\lambda \times \overline{y_\lambda}} \quad (2)$$

- Calculating the transformation matrix (M) by Eq. (3):

$$M=(XYZ-XYZ_m)\times(XYZ_{pc})^{-1} \quad (3)$$

where XYZ are testing specimen's tristimulus values, XYZ_m is tristimulus values of mean reflectance (R_m) of training samples;

- Estimating the reflectance spectra of testing samples by Eq. (4)[7,28,33–35]:

$$R_\lambda = R_m + M\times \begin{pmatrix} PC_{\lambda,1} \\ PC_{\lambda,2} \\ \cdot \\ \cdot \\ PC_{\lambda,n} \end{pmatrix} \quad (4)$$

The K-means method was also used for clustering of the training and testing samples and compared with the common method.

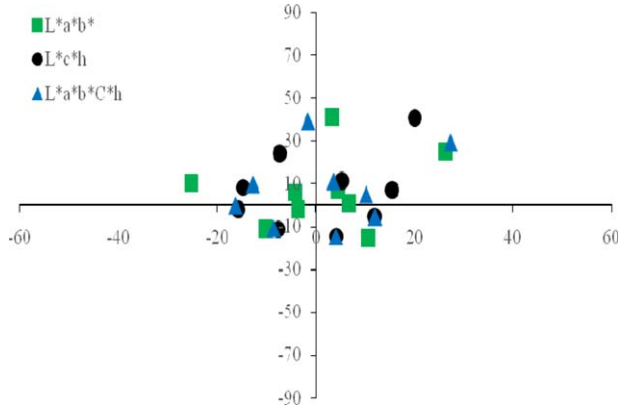

Fig. 6. Chromaticity distribution of the mean reflectance of nine-neuron layer method.

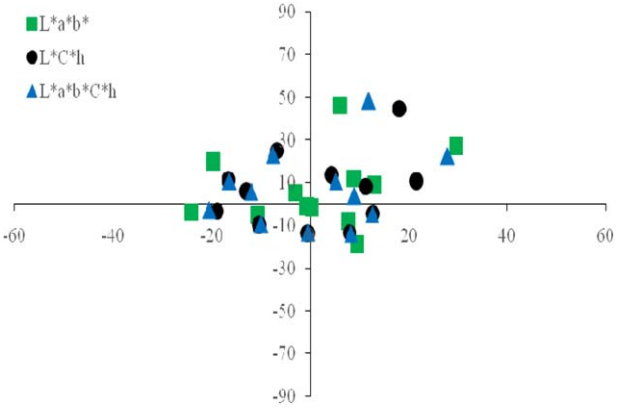

Fig. 7. Chromaticity distribution of the mean reflectance of 12-neuron layer method.

To investigate the accuracy of reconstruction, the color difference as an Euclidean distance between actual and reconstructed data under D75 and F11 illuminants and 10° standard colorimetric observer was obtained by Eq. (5):

$$\Delta E^*_{ab} = \sqrt{(\Delta L*)^2 + (\Delta a*)^2 + (\Delta b*)^2} \quad (5)$$

In addition, the spectrophotometric accuracy of reconstruction was calculated by the root mean square (RMS):

$$\mathrm{RMS} = \sqrt{\frac{\sum_\lambda (\Delta R_\lambda)^2}{16}} \quad (6)$$

Where ΔR is the difference between the actual and predicted reflectance spectra.

RESULT AND DISCUSSION

At the first step, the cumulative variance of the first three PCs of reflectance spectra for different subgroups was calculated as shown in Table I. From this table, it can be seen that more than 95% of the variance is accounted by the first three PCs. Consequently, the first three PCs could approximate the reflectance spectra, while the rest are negligible.

The mean reflectance spectra of subgroups in each method can indicate the spectrophotometric and colorimetric parameters of subgroups. Therefore, to investigate further the methods and subgroups, CIELAB coordinates of mean reflectance were calculated. The chromaticity distribution of the mean reflectance of L*a*b*, L*C*h, and L*a*b*C*h methods with 3, 6, 9, and 12 subgroups are shown in Figs. 4–7, respectively. In these figures, the horizontal axis is a* and vertical axis shows b*. As shown in these figures, the categories of L*C*h and L*a*b*C*h methods are very similar. These figures also show that the chromaticity distribution of the mean reflectance of major of categories is about the origin of colorimetric coordinate. The reason for this is that the chromaticity distribution of the most of training samples are about the origin of coordinate as shown in Fig. 1.

To investigate the accuracy of recovery, color difference, and RMS between actual and the reconstructed data were calculated. The color differences between the actual and the reconstructed data for 10° standard colorimetric observer and under D75 and F11 illuminants are shown in Tables II and III, respectively. It can be found from these tables, in some case the colorimetric accuracy were improved in comparison to common method and the colorimetric accuracy obtained by L*a*b* method is better than L*C*h and L*a*b*C*h methods. However, the best colorimetric accuracy was obtained by six-neuron and nine-neuron layers with L*a*b* input elements. The percentage of samples recoverd by these methods with color difference more than 0.5 CIELAB units under D75 illuminant and 3 CIELAB units under F11 illuminant is also lower than common method. Any general trend was not observed from these Tables.

To investigate further the reconstruction, spectrophotometric accuracy (RMS) of recovered reflectance spectra were measured and summarized in Table IV. According to this table, in some case the RMS was improved in comparison to common method. Similar to colorimetric accuracy, the best results were obtained by six and nine neurons with L*a*b* input elements and any general trend was not observed in results. As shown in Figs. 2 and 3, the classification of testing samples into subgroups

TABLE II. Color differences between the actual and the reconstructed data by competitive neural network under D75 illuminant and 10° standard colorimetric observer.

Input elements	Number of neuron	Mean	Median	Max	Min	SD	$\%\Delta E^*_{ab} > 0.5$
Common method	–	0.28	0.20	1.46	0.03	0.24	13.75
L*a*b*	3	0.24	0.15	1.69	0.01	0.24	13.75
	6	0.19	0.14	0.83	0.00	0.17	5.42
	9	0.21	0.18	1.19	0.01	0.16	5.42
	12	0.20	0.20	1.19	0.01	0.17	4.58
L*C*h	3	0.27	0.20	1.21	0.00	0.21	10.42
	6	0.28	0.26	1.07	0.03	0.18	10.00
	9	0.29	0.27	1.09	0.01	0.21	11.25
	12	0.31	0.26	2.40	0.02	0.30	16.25
L*a*b*C*h	3	0.27	0.20	1.22	0.00	0.21	10.42
	6	0.31	0.30	1.27	0.01	0.20	11.67
	9	0.27	0.19	1.37	0.00	0.22	11.67
	12	0.27	0.24	1.28	0.01	0.21	15.00

TABLE III. Color differences between the actual and the reconstructed data by competitive neural network under F11 illuminant and 10° standard colorimetric observer.

Input elements	Number of neuron	Mean	Median	Max	Min	SD	$\%\Delta E^*_{ab} > 3$
Common method	–	2.94	2.70	12.39	0.35	1.77	40.42
L*a*b*	3	2.62	2.27	12.02	0.16	1.60	28.75
	6	2.18	1.79	11.99	0.15	1.58	32.50
	9	2.30	1.73	11.30	0.25	1.65	30.83
	12	2.37	2.15	13.19	0.16	1.91	31.67
L*C*h	3	2.88	2.56	11.27	0.26	1.69	42.50
	6	2.82	2.25	11.12	0.30	1.83	38.75
	9	2.86	2.71	10.01	0.27	1.84	42.92
	12	3.26	2.55	27.09	0.07	3.10	43.75
L*a*b*C*h	3	2.86	2.53	11.35	0.25	1.68	42.92
	6	2.86	2.55	11.48	0.32	1.86	42.50
	9	2.68	2.61	10.61	0.32	1.64	40.83
	12	2.93	2.61	8.70	0.17	1.92	43.33

is almost correct. As shown in Fig. 1, the major source of large errors is maybe lack of needed samples in training set. However, the maximum error was decreased in some case. As an example, the reconstructed sample with RMS error of 0.1947 by common method, was recovered with RMS error of 0.1324 by a 6-neuron layer with L*a*b* input elements. In addition, it can be seen from Tables (II–IV), the results of three-neuron layer with L*C*h and L*a*b*C*h input elements are very similar as mean reflectance colorimetric distribution of them.

The improvement of the proposed method was also compared with the clustering method as K-means. The RMS of reconstructed reflectance spectra by K-means method is given in Table V. As shown in this table, the accuracy of k-means method even is less than common method.

In addition, comparison of performances among the suggested method and Zhang and Xu method[8] was made. In this method, the samples were first divided into 11 subgroups and then reflectance spectra reconstruction was performed. The mean, median, max, and SD of RMS of samples recovered by this method are 0.0352, 0.0246, 0.3436, and 0.0351, respectively. Therefore, the accuracy of suggested method in this study is better than Zhang and Xu method.

Therefore the best results for reconstruction of reflectance spectra by suggested methods, are observed using six and nine neurons with L*a*b* inputs elements.

TABLE IV. RMS between the actual and the predicted reflectance spectra by competitive neural network.

Input elements	Number of neuron	Mean	Median	Max	Min	SD
Common method	–	0.0386	0.0318	0.1947	0.0076	0.0281
L*a*b*	3	0.0395	0.0312	0.2098	0.0059	0.0284
	6	0.0345	0.0270	0.1324	0.0033	0.0249
	9	0.0328	0.0262	0.1659	0.0032	0.0260
	12	0.0380	0.0383	0.1367	0.0032	0.0245
L*C*h	3	0.0360	0.0224	0.2103	0.0049	0.0300
	6	0.0385	0.0272	0.1420	0.0044	0.0268
	9	0.0401	0.0291	0.2213	0.0057	0.0321
	12	0.0454	0.0273	0.4572	0.0048	0.0569
L*a*b*C*h	3	0.0360	0.0226	0.2106	0.0048	0.0302
	6	0.0414	0.0296	0.2240	0.0057	0.0312
	9	0.0381	0.0296	0.1846	0.0056	0.0302
	12	0.0393	0.0298	0.1762	0.0047	0.0308

TABLE V. RMS between the actual and the predicted reflectance spectra by K-means method.

Input elements	Number of cluster	Mean	Median	Max	Min	SD
L*a*b*	3	0.0453	0.0326	0.4607	0.0072	0.0464
	6	0.0883	0.0640	0.4148	0.0094	0.0651
	9	0.0740	0.0680	0.2992	0.0033	0.0545
	12	0.2039	0.0752	0.9890	0.0147	0.2265
L*C*h	3	0.0552	0.0362	0.3914	0.0064	0.0545
	6	0.0803	0.0439	0.5908	0.0092	0.0868
	9	0.1179	0.0687	1.1371	0.0075	0.1690
	12	0.1281	0.0629	1.0363	0.0039	0.1575
L*a*b*C*h	3	0.0735	0.0436	0.4254	0.0052	0.0799
	6	0.0636	0.0530	0.2609	0.0043	0.0547
	9	0.0763	0.0483	0.4894	0.0064	0.0923
	12	0.0991	0.0584	0.7031	0.0069	0.1107

CONCLUSION

This paper studies the effect of classification on reflectance spectra reconstruction by PCA techniques. The classification of reflectance spectra was done by using a competitive neural network with a 3, 6, 9, or 12-neuron layer by L*a*b*, L*C*h or L*a*b*C*h as input elements. This method is built upon the work of Zhang & Xu,[8] but the training of subgroups is self-organized, and the processing is simpler than existing methods. The chromaticity distribution of the mean reflectance of training samples in different methods was investigated. The result shows the colorimetric specification of the mean reflectance of training sample categories in L*C*h and L*a*b*C*h methods are very similar. The performance of reflectance spectra reconstruction was evaluated by measuring the color difference and RMS between actual and reconstructed data. The best estimation for reconstruction of reflectance spectra by suggested methods, is obtained using a six-neuron and nine-neuron layer with L*a*b* inputs elements. Therefore, by using the suggested method can improve the accuracy of reflectance spectra reconstruction.

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