Nonlinear Principal Component Analysis for Compression of Spectral Data

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ABSTRACT

Abstract— In this study, the principal component analysis (PCA) technique and its nonlinear version (NLPCA) are employed for the compression and reconstruction of spectral data. The reflectance spectra of 1269 matt Munsell color chips are used as original dataset in 400 to 700 nm with 10 nm intervals. The hidden patterns of spectral data are determined by employing the classical PCA as well as its nonlinear version. Different numbers of feature vectors are used in both methods and the results compared by using the root mean square error (RMS), the goodness fit coefficients (GFC) as well as the color difference values under D65 illuminant and 1964 standard observer. Results show the priority of NLPCA over the PCA in low-dimensional spaces i.e. up to 4 basic functions, while different results are observed in higher-dimensional spaces.

1 INTRODUCTION

While the spectral data, like reflectance spectra of surfaces, provide full information about the visual properties of objects in different viewing conditions, they suffer from the sizes of information that would be transferred. In fact, opposed to colorimetric tristimulus values the spectral data are composed of several channels, e.g. 31 points in visible spectrum from 400 to 700 nm with 10 nm interval. To clarify the differences between the spectral and colorimetric data, it should be emphasized that the spectral data is unique for each object and is known as the "fingerprint" of sample while different objects with different spectral properties could provide identical color in a given set of viewing condition. This issue is known as metamerism and is evident in most color reproducing systems.

In the recent decades, some methods have been presented to reduce the sizes of spectral data while the main features of data have been kept. In fact, it was shown that the three dimensional colorimetric data are not fairly enough to convey the adequate information about the objects in different viewing conditions and the 31 dimensional behavior of the reflectance spectra would prepare surplus information and lead to some problems in data transformation. Hence, some mathematical techniques have been employed to extract the basic functions of spectral information to present them in the lower dimensional spaces with the minimum loss of information. One of the most applicable techniques which have been used in the field of spectral data reducing method is the principal component analysis technique abbreviated by PCA.

PCA has been widely used in compression and reconstruction of reflectance spectra of surface colors [1-6]. Fairman and Brill [2] explained the application of classical PCA method for the compression of spectral reflectance as well as the reconstruction of spectra from the corresponding CIEXYX tristimulus values. Different methods were also introduced to increase the efficiency of compression as well as the reconstruction techniques by choosing the suitable sets in the learning step and/or weighing the samples prior to extraction of principal directions [5].

Recently, the application of nonlinear version of PCA (denotes by NLPCA) has been reported [7]. Opposed to the classical method, the extracted features by NLPCA are not limited to the orthonormal vectors.

In this study, the classical and nonlinear versions of PCA are employed to reduce the spectral reflectances of 1269 samples of Munsell color chips. Compression process is performed by using different number of principle components i.e. 1 to 10 bases, and the effects of selected sizes on the reconstructed spectra have been reported. Results of employing of NLPCA and PCA methods in different employed sizes are evaluated by the values of root mean square errors (RMS) and the Goodness Fit Coefficient (GFC) between the original and the reconstructed spectra. The color difference values, i.e. ΔE, between the actual and synthesized spectra are also reported under D65 illuminant and 1964 standard observer.

2 Theoretical background

2.1 Principal Component Analysis

The main aim of PCA is to reduce the dimensions of the data set. To fulfill this goal, the hidden patterns of data becomes uncover and a small set of underlying basic functions are extracted and used as the projection space for the original data. By this way, samples are redefined in the new reduced space. The size of the reduced space depends on the nature of the data and the expected accuracy in reconstruction process. Since the mean centered data is

usually used in the classical PCA method, the mean vector should be added for the reconstruction of data from compressed information. Equation (1) mathematically shows this procedure for the spectral compression-reconstruction purpose.

$$\hat{R} \approx V_0 + \sum_{j=1}^{k} C_j V_j \qquad (1)$$

Where $\hat{R}$ is the reconstructed spectral reflectance, V_0 is the mean vector of spectral reflectance of dataset, C_j shows the specification of sample for the j[th] principle component, while V_j illustrates the j[th] eigenvector. k is the size of selected reduced space i.e. the numbers of chosen principle directions which are used for compression purpose.

The column vector *C* that weights the columns of *V* can be derived from Equation (2).

$$C = V^T (R - V_0) \qquad (2)$$

Where *V* is the selected eigenvectors, V_0 is the mean vector of spectral reflectance, and R is the spectral reflectance of dataset.

2.2 Non Linear Principle Component Analysis

Similar to classical PCA, the nonlinear principle component analysis recognizes and removes correlation among variables for dimensionally reduction while opposed to PCA it is not limited to linear correlation among the variables.

Let R is an m×n matrix where m and n represent the number of observations and the number of variables respectively. By using a nonlinear vector function, the nonlinear principle components are achieved as illustrated in Equation 3.

$$T = G(R) \qquad (3)$$

Where G is nonlinear vector function composed of f nonlinear functions G = {G1, G2,…, Gf } and T is the nonlinear principle components.

For reconstruction process, the second nonlinear vector function is employed and data could be reconstructed as showed in Equation 4.

$$\hat{R} = H(T) \qquad (4)$$

Where H is nonlinear vector function composed of m nonlinear functions H= {H1, H2,…, Hm} and $\hat{R}$ is the reconstructed spectral reflectance. By using an artificial neural network (ANN) the functions G and H are selected in a manner to minimize the $\left\| R - \hat{R} \right\|$.

It was already shown that the functions which is shown in Equation (5) could fit any nonlinear functions *v=f(u)* to an arbitrary degree of accuracy.

$$u_k = \sum_{j=1}^{N_2} w_{jk2} \sigma \left(\sum_{i=1}^{N_1} w_{ij1} u_i + \theta_j \right) \qquad (5)$$

Where $\sigma(x)$ is any continuous and monotonically increasing function with $\sigma(x) \to 1$ as $x \to +\infty$ and $\sigma(x) \to 0$ as $x \to -\infty$. As shown in Equation (6), a sigmoidal function is a suitable one.

$$\sigma(x) = \frac{1}{1 + e^{-x}} \qquad (6)$$

Clearly, Equations 5-6 are the describing equations for a feedforward artificial neural network (ANN). The nets consisted of N1 inputs, a hidden layer of N2 nodes as well as a linear output node for each nod. The weight for the connection of node i in layer k to node j in layer k + 1 is shown by w_{ijk} in Equation 5. Nodes of same layers are fully interconnected while the intralayer links are not allowed. The nodal biases that are adjustable parameters like the weights introduced by θ [8].

3 EXPERIMENTS

In this study, we borrowed an ensemble of 1269 reflectance spectra of the chips in the Munsell Book of Color–Matt Finish Collection [9]. The spectral reflectances of samples were measured with Perkin Elmer Lambda 9 spectrophotometer and the wavelength range was from 380 to 800 nm with 1 nm interval. In this research, the reflectance data were fixed between 400 to 700 nm at 10 nm intervals.

4 RESULTS

To compare the PCA and NLPCA techniques, the reflectance spectra of 1269 color chips of Munsell Color System were used and compressed and compressed in reduced spaces by using the classical PCA as well as the NLPCA techniques. Different numbers of principle components from 1 to 10 were used for both methods.

To quantitatively compare the results of different methods, the RMS, GFC and CIELAB color difference (ΔE) values were calculated between the reconstructed and the original spectra. Equation 6 was used to calculate the GFC value and the results were evaluated as unacceptable (GFC<0.9990), acceptable (GFC≥0.9990), good (GFC≥0.9995) and excellent (GFC≥0.9999).

$$GFC = \frac{\sum R(\lambda)\hat{R}(\lambda)}{\sqrt{\sum [R(\lambda)]^2}\sqrt{\sum [\hat{R}(\lambda)]^2}} \qquad (6)$$

Where $R(\lambda)$ is the actual reflectance value of sample in the λ^{th} wavelength and $\hat{R}(\lambda)$ shows the reflectance value of the reconstructed spectra in the same wavelength.

To show the effect of the sizes of compressed spaces, the fluctuations of the mean value of RMSs against the number of principle components was plotted for both PCA and NLPCA methods and illustrated in Figure1.

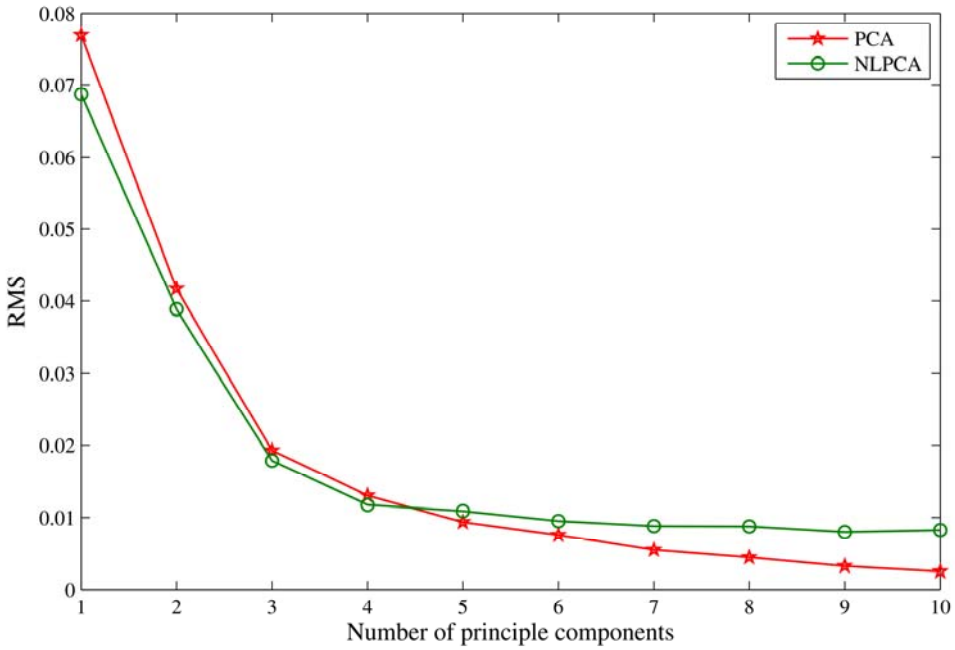

Figure 1- The fluctuations of the mean value of RMSs against the number of chosen basic functions.

Table 1 shows the mean of RMS values, the frequencies of different grades of GFC and the mean of color difference values for different numbers of basic functions obtained by employing of PCA and NLPCA techniques.

Table 1- The values of mean of RMS and ΔE as well as the frequencies of different grades of GFC obtained by PCA and NLPCA compression and reconstruction techniques using different numbers of principal components.

	PCA						NLPCA					
No. PC	RMS	GFC			ΔE		RMS	GFC			ΔE	
		Acceptable	Good	Excellent	mean	max.		Acceptable	Good	Excellent	mean	max.
1	0.0769	124	7	0	22.05	69.35	0.0687	189	20	0	19.68	65.44
2	0.0417	445	91	0	15.05	75.42	0.0389	520	112	0	13.80	55.95
3	0.0192	942	342	5	3.41	27.32	0.0178	977	412	5	3.65	39.03
4	0.0130	1123	702	41	1.39	11.66	0.0117	1164	721	29	2.02	15.59
5	0.0094	1216	887	81	0.82	5.17	0.0109	1216	753	61	1.98	24.38
6	0.0076	1236	1011	123	0.80	5.21	0.0095	1232	905	94	1.51	20.38
7	0.0055	1264	1116	417	0.18	2.93	0.0088	1228	922	143	1.25	13.57
8	0.0045	1267	1148	589	0.14	1.52	0.0088	1235	960	133	0.94	6.06
9	0.0032	1268	1248	810	0.14	1.24	0.0080	1246	994	193	1.22	17.07
10	0.0025	1269	1261	972	0.09	1.13	0.0083	1232	948	180	1.21	19.13

As Table 1 and Figure 3 show, the mean of RMS values for both PCA and NLPCA totally decrease by increasing the number of employed basic functions. However, the decreasing continues for classic PCA while the rate rapidly decreases for NLPCA method. As the results show, the NLPCA exhibits better performance in the lower dimensions, let say up to 4, while the classic PCA leads to superior results when higher dimensions were employed. The achievements are totally reconfirmed by the GFC and ΔE values. As the results show while the errors converge to zero in the PCA, they do not totally meet the lower values for NLPCA and remain constant in higher dimensional spaces.

5 CONCLUSION

In this paper, the NLPCA method was employed for the compression and reconstruction of spectral data and its performance was compared with classical PCA routine. The spectral reflectances of 1269 samples of Munsell colored chips were used for compression and reconstruction purposes. The compression and reconstruction were conducted with different number of principle components, i.e. 1 to 10. To make comparison between the PCA and NLPCA performances, the mean of RMS, the GFC and ΔE values between the original and the reconstructed spectra were utilized. Results showed that, the NLPCA performed better than PCA while less than or equal to 4 bases were employed. By contrast, when more than 4 principle components were used, the PCA showed better performances than NLPCA.

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