PROGRESS IN COLOR, COLORANTS AND COATINGS

available online @ www.pccc.icrc.ac.ir

Progress in Color Colorants Coating 17 (2024), 53-60

Ministry of Science, Research and Technology
Institute for Color Science & Technology

Synthesis of Reflectance Spectra Using Non-Context-Based Features

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ARTICLE INFO

Article history:
Received: 24 Apr 2023
Final Revised: 02 Aug 2023
Accepted: 08 Aug 2023
Available online: 16 Oct 2023

Keywords:
Synthetic reflectance
Non-context-based primaries
Sigmoidal primaries
Gaussian primaries

ABSTRACT

The non-context-based approach is used for the synthesis of spectral reflectance curves of objects with known CIEXYZ tristimulus values. The method introduces two sets of features, i.e., the standard color-matching functions normalised by their sum in each wavelength and a group of two sigmoidal and one Gaussian bases that approximately fit the first set. The assigned spectra for the desired tristimulus colorimetric values are calculated using an additive color-mixing approach. Results of different methodologies are numerically compared in terms of root mean squared error (RMSE), goodness fit coefficient (GFC), and CIELAB color difference values between the actual and synthesised spectra. It is found that the synthesised spectra by the suggested primaries better resemble the actual behaviours of spectral reflectances of natural and synthetic objects in comparison to using three Gaussian primaries. Compared to other context and non-context-based approaches to spectral reconstruction, the suggested method is faster and does not require iterative optimisation. Prog. Color Colorants Coat. 17 (2024), 53-60© Institute for Color Science and Technology.

1. Introduction

In the visible spectrum, the reflection spectra of objects are known as inherent optical properties of materials and have very important applications, such as object identification and color-matching trails. Today, various easily accessible devices with three filters, like colorimeters and CCD digital cameras, have become popular, while measuring objects' reflectance spectra still requires more professional equipment like spectrophotometers. Hence, the estimation of the spectral reflectances of objects from the reduced spectral data, such as tristimulus color values, is of great attraction. This subject has been the object of many scientific studies over the decades, and numerous methods have been developed to accomplish this goal [1-8]. Efforts could be categorised into two groups, i.e., context-based approach and fixed non-context dependent primaries.

Although the methods based on the principal component analysis would probably be the most interesting context-based approach, other methods, such as nonnegative matrix factorisation, are also introduced in this category [9-11]. In a study by Rezaei and her coworkers, a comparison was conducted between two kernel-based approaches, namely support vector regression and kernel ridge regression, alongside PCA. The primary objective was to evaluate and compare the efficacy of these methods in reconstructing the reflectance spectra of colored surfaces based on their corresponding CIE XYZ tristimulus values [12]. On the other side, when the prefixed primaries are used, the Hawkyard iterative methodology [2, 3] and Sun et al.

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and Berns' Gaussian primaries [4,8] would be the most successful approaches.

Color is usually characterised by tristimulus values in well-defined spaces, such as CIEXYZ or RGB color systems. This type of object characterisation depends on the effects of other parameters generally, the relative spectral power distribution of the employed light source and the color matching functions of the standard observer or spectral sensitivities of the camera's RGB channels. The integration of the multiplication of these variables over the visible wavelength provides the color of objects that could be identical to the objects with different spectral behaviours, the phenomenon known as metamerism. Mathematically, the reverse calculation and estimation of reflectance spectra of objects from their tristimulus values are not as easy as a direct approach if additional information is unavailable. In fact, from the mathematical point of view, the estimation of spectral reflectances of objects from their tristimulus values is typically regarded as a one-to-many problem. The problem is similar to estimating the lengths of a rectangle from its perimeter and means that many rectangles with different side lengths could have the same perimeter. Therefore, accurately estimating the reflectance spectra from the colorimetric values is still an open and attractive research topic, and solving this inverse problem requires sophisticated optimisation algorithms. However, various methods with different degrees of success, complexity and accuracy have been developed for this purpose. Some inherent spectral properties of natural and synthetic materials, such as the smoothness of the reflectance spectra of objects over the visible band, provide some constraints that help to solve the problem more efficiently [1, 2].

As mentioned earlier, the principal component analysis method [5, 13] is the most common solution for this underdetermined mathematical problem. This method extracts the features of the entire spectral dataset and uses them as statistical primaries for further reflectance reconstruction. The success of the proposed method and those commonly used by other context-based systems fully depends on the selected dataset and the similarity between the context set and the target.

In the non-context approach to spectral reconstruction, based on the general behaviour of spectral reflectances of objects, it is tried to find a limited set of primaries, i.e., three, that provides the best spectral match for the samples with known tristimulus values. To this end, depending on the types of color mixing systems, different bases have been suggested and used as subtractive or additive primaries. While Hawkyard did not name the employed primaries as red, green and blue lights, the method was based on optimising the amount of them through an iterative methodology [2, 3]. Wang and his colleagues [14] mathematically analysed the convergence of the Hawkyard method and suggested a minor modification to ensure improvement in the iterative scheme. They investigated the iterative improvement sequence as a core principle of the Hawkyard method and discussed in detail the convergence property of the algorithm. Later, Berns [15] criticised the Hawkyard approach and assigned synthetic reflectances to objects with known tristimulus values by calculating the amounts of three red, green and blue Gaussian primaries through an additive color mixing approach that provides a well-defined system of equations without any necessity to refine the results through an iterative improvement procedure. Based on Berns' algorithm, Sun and his coworkers [4] and Attarchi and Amirshahi [6] introduced Gaussian primaries with adaptable half width at maximum values and a sigmoidal red to improve the quality of synthesised spectral reflectances.

This research tries to find more efficient non-context primaries to estimate the reflectance spectra of objects from their corresponding colorimetric data by taking advantage of former methods. Like most previous research, the number of primaries was restricted to three. Consequently, 3 non-context-based primaries were created based on the normalised standard color matching functions. Then, the weights of the primaries were calculated through an additive color matching approach, and the weighted sum of spectral behaviours of primaries was considered as the synthesised reflectance curve for the proposed colorimetric tristimulus values. Since the spectral patterns of proposed primaries somehow resembled the sigmoidal and Gaussian shapes, they are introduced as pseudo-sigmoidal and pseudo-Gaussian functions of wavelength. Finally, two sigmoidal and one Gaussian curves were fitted to the previous set of primaries and used as a new set for spectral reconstruction purposes. Results obtained from these approaches are compared to those obtained by the classical non-context methods that were introduced previously [2, 3, 8, 15].

Hawkyard [2, 3] developed an algorithm that assigns a synthetic reflectance curve for each set of

CIEXYZ tristimulus values. The method optimises the amount of three selected primaries through an iterative color-matching procedure and provides artificial reflectance spectra for a proposed object with known colorimetric specifications. The approach is a non-context-based model and uses a set of prefixed primaries.

The method was based on three practical criteria, i.e., the reflectance spectra are a smooth function of wavelength, the spectral power distributions (SPD) of a CRT color are also smooth if it is normalised by the SPD of the CRT peaks for white, and the CIEXYZ color space is inherently an additive color medium. Based on these annotations, Hawkyard suggested the following equation to estimate the spectral reflectances of objects from the corresponding XYZ colorimetric values (Eq. 1).

$$R_s(\lambda) = \frac{P_R(\lambda)X/X_W + P_G(\lambda)Y/Y_W + P_B(\lambda)Z/Z_W}{P_R(\lambda) + P_G(\lambda) + P_B(\lambda)} \quad (1)$$

Where, P_R, P_G and P_B are the spectral power distribution functions of primaries in the visible spectrum's red, green, and blue regions. These primaries were supposed to be the spectral color-matching functions of standard observers normalised by the sum of them. Accordingly X_W, Y_W and Z_W are the tristimulus value of the employed illuminant, and as Equation 1 shows, the SPD of the employed light source appears in the denominator of this equation. He estimated primaries' weights (amounts) and improved them through an iterative procedure to match the sample colorimetrically, and used them to synthesise the proposed object's spectral reflectance.

Soon after Hawkyard's article [2] was published, Berns criticised the proposed iterative method and suggested a set of Gaussian primaries to assign a synthetic reflectance to a set of XYZ tristimulus values. As Eq. 2 shows, the method simply calculates the amount of each primary based on an additive color mixing system.

$$\begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} X^1_{max} & X^2_{max} & X^3_{max} \\ Y^1_{max} & Y^2_{max} & Y^3_{max} \\ Z^1_{max} & Z^2_{max} & Z^3_{max} \end{bmatrix}^{-1} \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} \quad (2)$$

Where c_is are the weights of primaries X^i_{max} Y^i_{max} and Y^i_{max} X Y show the corresponding CIEXYZ tristimulus values of primaries and desired sample, finally, the assigned spectral reflectance, i.e. $R(\lambda)_{mix}$, could be simply calculated by Eq. 3.

$$R(\lambda)_{mix} = c_1 R(\lambda)^1_{max} + c_2 R(\lambda)^2_{max} + c_3 R(\lambda)^3_{max} \quad (3)$$

Where $R(\lambda)^i_{max}$ show the spectral behaviours of employed Gaussian primaries. Although the Berns method does not require an iterative improvement loop and seems very simple compared to the Hawkyard approach, the synthesised reflectances by the latter method are smoother and provide a better approximation for the actual reflectance spectra.

In the present paper, by considering the points used in the Hawkyard primaries and integrating them with the Berns additive mixing methodology, it has been tried to eliminate the iteration step in the Hawkyard approach. In addition, other sets of non-context primaries, including two sigmoidal and one Gaussian function, are introduced and employed for spectral estimation from colorimetric values.

2. Experimental

2.1. Gaussian (bell-shaped) functions

Gaussian functions are one of the most important mathematical functions, especially in statistics and modelling issues. They are commonly used in scientific and engineering applications and can model many physical phenomena. Gaussian functions are exponential functions used to express a wide range of features. The general form of Gaussian functions is shown in Eq. 4:

$$f(x) = a \cdot \exp\left(-\frac{(x-b)^2}{2c^2}\right) \quad (4)$$

Values a and b are real numbers, and c is a non-zero integer.

2.2. Probability density functions (PDFs)

In probability and statistics theory, the Gaussian function is represented as a probability density function for normal distribution (called PDF) and is shown by Equation 5 [17].

$$f(\lambda) = \frac{1}{\sqrt{2\pi}\sigma} e^{\left[-\frac{(\lambda-\mu)^2}{2\sigma^2}\right]} \quad (5)$$

Where, μ and σ show the mean and the variance of the Gaussian PDF, respectively.

2.3. Cumulative distribution functions (CDFs)

For a real-valued random variable X, X's cumulative distribution function (CDF) is the probability that X yields a value less than or equal to x. For continuous random variables, CDF can be defined as Eq. 6. Assume that f is the probability density function of X, then the cumulative distribution functions F for normal distribution could be shown by:

$$F(\lambda) = P(\Lambda \le \lambda) = \int_{-\infty}^{\lambda} f(\lambda) d\lambda \quad (6)$$

As Equation 6 shows, the CDF function is calculated from the integral of the PDF function. Conversely, a Gaussian function is obtained by a derivative of a sigmoid function. According to Figure 1, the CDF function is a representation of a sigmoid function, and the PDF function is a representation of a Gaussian function.

2.4. Sigmoid functions

The sigmoid or S-shaped function (the standard logistic function) is introduced as non-linear transfer functions at different physical, biological and evolutionary levels [16]. The mathematical form of the sigmoid function is shown in Eq. 7.

$$S(\lambda) = \frac{1}{1+e^{-\lambda}} \quad (7)$$

By adding constants C_1 and C_2 to the common form, the equation can be shown as (Eq. 8):

$$S(\lambda) = \frac{1}{1+e^{-C1(\lambda+C2)}} \quad (8)$$

As shown in the next section, it is notable that the first derivative of a sigmoid function is a bell-shaped function. Conversely, the integral of any bell-shaped function, as long as they are continuous and nonnegative, also results in a sigmoid function.

The data studied in this work was the reflectance spectra of 1269 Munsell matte chips [18]. The reflectance spectra were fixed within the 400 to 700 nm range at 10 nm intervals. The CIEXYZ tristimulus values of samples were calculated under D65 standard illuminant and 1964 standard observer and used as observations in the synthesised spectral reflectance assignment. Eq. 9 shows that the first set of primaries was the CIE 10-degree standard observer color matching functions normalised by their sum.

$$R(\lambda)^R = \frac{\bar{x}_\lambda}{\bar{x}_\lambda + \bar{y}_\lambda + \bar{z}_\lambda}$$
$$R(\lambda)^G = \frac{\bar{y}_\lambda}{\bar{x}_\lambda + \bar{y}_\lambda + \bar{z}_\lambda} \quad (9)$$
$$R(\lambda)^B = \frac{\bar{z}_\lambda}{\bar{x}_\lambda + \bar{y}_\lambda + \bar{z}_\lambda}$$

Where, $R(\lambda)^R$, $R(\lambda)^G$ and $R(\lambda)^B$ refer to the reflectance spectra of primaries $\bar{x}_\lambda$, $\bar{y}_\lambda$ and $\bar{z}_\lambda$ show the color matching functions of 1964 standard observer.

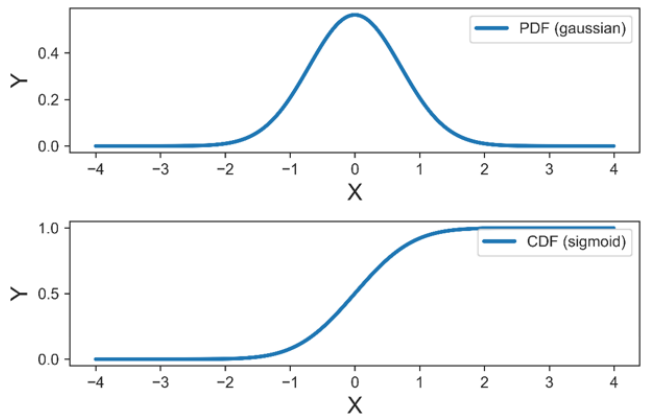

Figure 1: PDF and CDF functions.

The functions were normalised to their maximum to fix them between 0 to 1 and used as non-context primaries to assign a spectral reflectance to each colorimetric value. Figure 2 shows the spectral behaviours of extracted bases that resemble a pseudo-Gaussian curve for the green region of the visible spectrum and two pseudo-sigmoidal curves for the blue and red regions.

The desired primaries were then used to match the CIEXYZ values of samples colorimetrically, and the value of each primary was calculated and used, as shown in Eq. 10, to synthesise the proposed spectral reflectances.

$$R(\lambda)^{mix} = c_1 R(\lambda)^{R} + c_2 R(\lambda)^{G} + c_3 R(\lambda)^{B} \qquad (10)$$

The other set of primaries, including two classical sigmoidal and classical Gaussian curves, were those that fitted the first set, i.e., pseudo-Gaussian and pseudo-sigmoidal data, and were similarly used in synthetic reflectance effort. The new set is shown by Eq. 11, where R_λ^R and R_λ^B are sigmoidal red and blue and R_λ^G demonstrates the Gaussian green primaries. Figure 3 shows the spectral behaviours of designed primaries.

$$R(\lambda)^{R} = \frac{1}{1+\exp(-0.03904\lambda + 21.61005)}$$
$$R(\lambda)^{G} = \exp\left(-2.6 \times \frac{(\lambda - 520)^2}{2 \times 50^2}\right) \qquad (11)$$
$$R(\lambda)^{B} = \frac{1}{1+\exp(0.10871\lambda + -53.94465)}$$

The reconstruction procedures were performed using classical Gaussian and the following primaries:

- One pseudo-Gaussian and two pseudo-sigmoidal functions of wavelength are shown by Eq. 9, and
- One Gaussian and two sigmoidal functions of wavelength are demonstrated by Eq. 11.

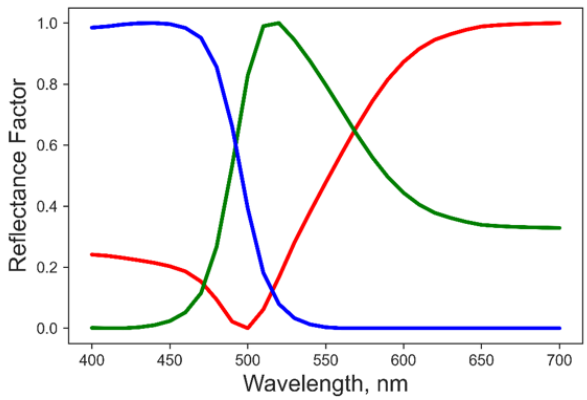

Figure 2: The extracted primaries from normalized CIE 10-degree standard color matching functions.

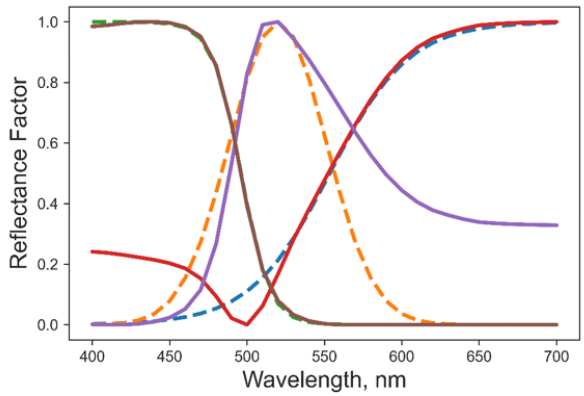

Figure 3: Classical sigmoidal and Gaussian curves are shown by broken line and the pseudo sigmoidal and Gaussian curves are demonstrated by solid line.

Results obtained from each method were spectrally and colorimetrically compared to actual reflectances. The root mean square (RMS) error between the actual and synthesised reflectances and the goodness fit coefficient (GFC), the cosine of the angle between the actual and created spectra, were calculated. Since the known values were the tristimulus values of samples under D65 illuminant and 1664 standard observer, in color domain, the CIELAB color differences under A and F11 light sources and 1964 standard observer were the measures that were used to evaluate the performance of each set of primaries.

3. Result and Discussions

Table 1 shows the results of the reconstruction of the reflectance spectra of Munsell samples with different methodologies in terms of RMS and GFC, as well as ΔE^*_{ab} color difference values under A and F11 illuminants and 1964 standard observer.

As Table 1 shows, Berns' Gaussian method provides the worst results among the employed models. On the other hand, Hawkyard, pseud Gaussian-sigmoid and classical Gaussian-sigmoid methods yield approximately identical performances. The results of the suggested methods, i.e., the pseud Gaussian-sigmoidal and the Hawkyard method, are precisely the same, while the classical Gaussian-sigmoidal are very close to them. Derivation of the same results for both pseudo and classical Gaussian-sigmoidal primaries and the Hawkyard method shows the possibility that the iterative calculation could be avoided without inquiring a cost in accuracy. Notably, the iterative loops can lead to a significant computing time in more complicated samples, such as the extraction of spectra of images. However, based on the additive color mixing law, the improvement caused by each iteration does not necessarily, and our experience showed that, in this case, the computing time for 1269 Munsell samples decreases from 1.88553 seconds to 0.0004 seconds if a computer with the Intel Core i7-8550U with 1.80 GHz frequency and 8 GB of ram is used. Again, it is emphasised that the negligible computing time is due to the nature of employed samples that were Munsell specimens in 10 nm spectral intervals.

To compare the results of different methods, the reflectance spectra of 18 randomly selected samples of the Munsell set are shown in Figure 4, along with the spectra that are assigned by employed methodologies.

As the plots of Figure 4 show, the differences between the actual and the synthesised spectra obtained from Gaussian primaries are evident. The subject is more apparent in the long wavelength region of the visible spectrum [8]. The problem originates from the inherent characteristic of the red Gaussian primary that is in descending manner after its maximum at 610 nm. That contradicts the inherent spectral characteristic of most natural and synthetic objects that show ascending reflectance behaviour in this particular visible spectrum region. In addition to this apparent paradox, the normal behaviours of employed Gaussian primaries with three distinguished peaks concentrated at 440, 540, and 603 nm provided a type of sawtooth effect that is not evident in the reflectance spectra of real objects.

Results from suggested sets of primaries are almost identical and are smoother than those obtained by the Berns method. This means that the proposed primaries can assign the reflectance spectra to a set of colorimetric data through a non-iterative approach.

Table 1: The RMS, GFC and color difference values under A and F11 illuminants and 1964 standard observer between the actual and reconstructed spectra with different methods for 1269 Munsell samples .

Method	RMS			GFC								
							A			F11		
	mean	max	Std	mean	min	Std	mean	max	Std	mean	max	Std
Gaussina	0.08	0.24	0.05	0.96	0.58	0.03	2.57	13.08	2.07	2.14	13.00	2.11
Hawkyard	0.03	0.19	0.03	0.99	0.71	0.01	1.72	13.10	2.00	2.61	14.87	2.63
Pseud Gaussian Sigmoidal	0.03	0.19	0.03	0.99	0.71	0.01	1.72	13.10	2.00	2.61	14.87	2.63
Classical Gaussian Sigmoidal	0.04	0.19	0.03	0.98	0.72	0.01	1.95	11.25	1.80	2.28	15.29	2.29

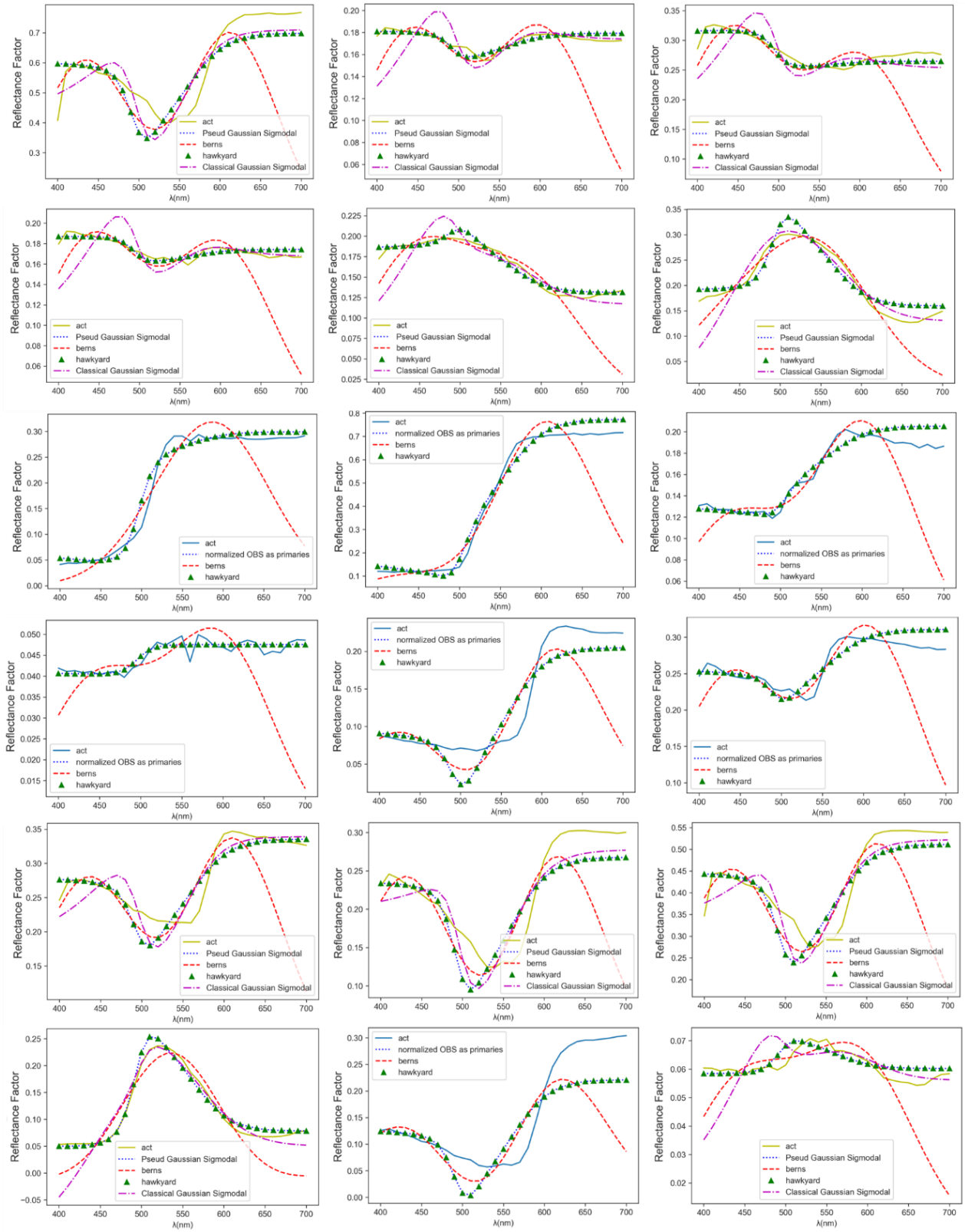

Figure 4: The Actual and synthesized spectra with different methods for 18 randomly selected samples.

4. Conclusion

Using additive colour mixing model, two sets of non-context-based primaries were introduced to assign synthetic reflectances to corresponding colorimetric tristimulus values. The performances of the extracted primaries in spectral reconstruction were compared to some other non-contest-based sets of spectra suggested previously. The employed bases were a set of one Gaussian and two sigmoidal functions of wavelength. The synthesising process was a fast non-iterative approach based on additive color mixing principles. Results showed that the assigned spectral reflectances are smoother than those obtained by the Gaussian method and yield almost identical results to the Hawkyard approach. In contrast, the suggested method does not require iteration to recalculate reflectance spectra.

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How to cite this article:
Rezaei I, Mahbadi AA, Amirshahi SH. Synthesis of Reflectance Spectra Using Non-Context-Based Features. Prog Color Colorants Coat. 2024;17(1):53-60. Doi: 10.30509/pccc.2023.167131.1214