Spectral Reconstruction on the Basis of Several Samples and Principal Components Analysis

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Abstract: One important problem of colorimetry is that how to determine the spectral characteristics of colour samples with the help of some known parameters. If we take the spectral reflection features of a big amount of sample sets and use a linear algebraic-statistical method, the principal component analysis, we can determine that handful of parameters whose linear combination helps to reconstruct the spectral distribution of the elements of the original sample sets. The average vector given by this method and the first couple of eigenvectors can reproduce the elements of the samples with a good approximation, therefore, in case of a large set of colour samples, it is enough to weigh the first few base vectors to reconstruct the samples.

Keywords: spectral reconstruction, principal component analysis, eigenvector

1. Introduction

When we want to determine the spectrum and the reflectance function of colour samples, we need a spectrophotometre in the first case. However, it is sometimes not possible to purchase a spectrophotometre, and even if we have one, it is difficult to use it. It is especially difficult when it is not easy or even impossible to get closer to the samples. So the question arises as to how we can replace it with an everyday, easy-to-use device. In nearly all cases, there is a digital camera from which it is easy to extract three values that comply with an additive colour mixing model and determine a colour stimulus. It is shown, as follows, how the reflectance function of the coulour stimulus that is given with three values can be determined with the help of several samples and the principal component analysis.

2. Elements

2.1. The concept of colour

Colour can be defined as a perception in our brain. We need optical radiation (what we commonly refer to as light) which, after entering our eyes and being absorbed by our retina, induces nervous signs. In case of monochromatic radiation, the perceived colour depends on the wavelength of the radiation; in case of complex radiation, the perceived colour is determined by the amount of energy the radiation transfers in different wavelength ranges.

Colour can be defined as a property of an object and this property shows in what ration the object absorb or reflect the different-wavelength components of the light that shines it. However, this refers to a property of surfaces.

2.2. Spectrum, reflectance function

The spectrum of a light source, the reflectance function of a colour sample*($\varphi(\lambda)$)* can be defined as the amount of energy transferred on a given wavelength or rather how big its radiated power is. Spectra may be continuous (Figure 1.), when all the values appear between two wavelengths. For instance, incandescent metals, solids in general and liquids emit such spectra, whose model was given by Planck. Spectra may be linear (Figure 2.), where only few lines appear in a narrow interval. Such spectrum is provided by incandescent gases that are made up of atoms or simple molecules. In case of secondary lights, namely surfaces that are exposed to light and reflect it somehow, we talk about reflectance function. (Figure 3.)

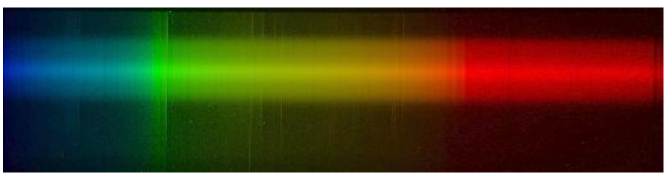

Figure 1. Continuous spectrum

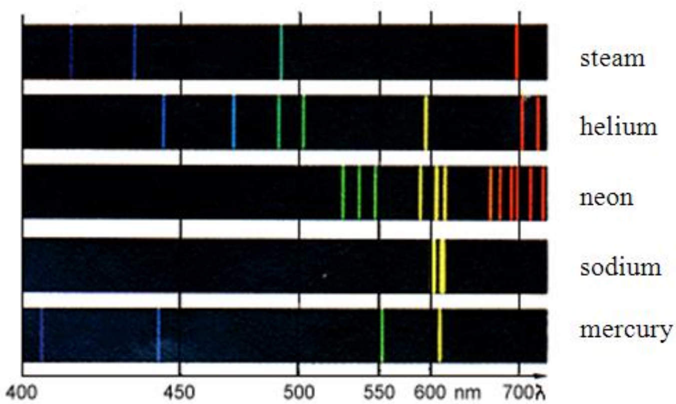

Figure 2. Linear spectra

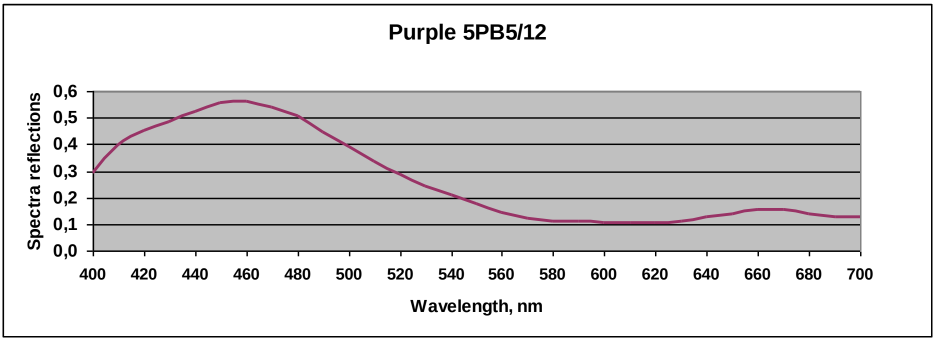

Figure 3. The reflectance function of the 5PB5/12 Munsell sample

Any spectrum as a colour stimuli can be described with three values (X, Y, Z) because of the types of receptors in the human eye. These values are the so called colour-stimuli components, which are calculated with the use of colour matching functions ($\bar{x}$ (λ), $\bar{y}$ (λ), $\bar{z}$ (λ)) that are considered as weighting functions (Figure 4.).

$$X = k \int_{380nm}^{780nm} \varphi(\lambda)\bar{x}(\lambda)d\lambda \,,\; Y = k \int_{380nm}^{780nm} \varphi(\lambda)\bar{y}(\lambda)d\lambda \,,\; Z = k \int_{380nm}^{780nm} \varphi(\lambda)\bar{z}(\lambda)d\lambda \quad (1)$$

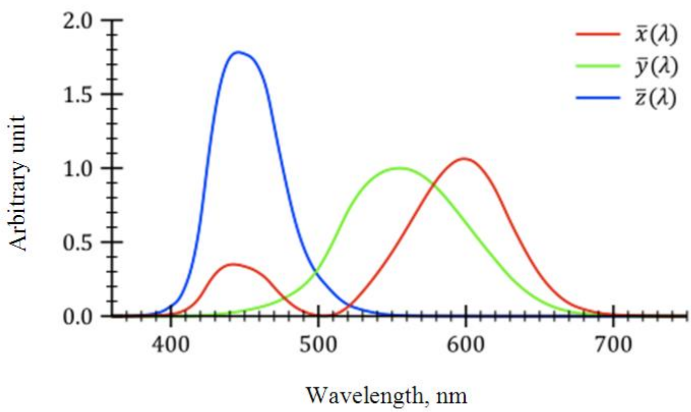

Figure 4. $\bar{x}$, $\bar{y}$ és $\bar{z}$ colour-matching functions of CIE

2.3 Metamerism

Although the metamer colours are perceived in the same way, their spectral power distribution is different. The sameness may be true for more colours. If colour A is identical with colour B, and colour B is identical with colour C, then colour A is identical with colour C as well. Therefore, it means that the colour determined with values X, Y, Z can be provided with several *φ(λ)* spectra.

3. Mathematical method

The following description is based on László Koltay mathematician's lecture notes [1].

Let $\xi:\Omega \to R^p$ be a vector probability variable. The expected value of vector ξ as a probability variable is denoted by $E(\xi)= m \in R^p$, and its covariance matrix is denoted by $\mathrm{cov}(\xi,\xi)=V \in R^{p \times p}$. Let the centralised ξ be $\xi^*=\xi-m$. Let us denote the eigenvalues arranged in decreasing order of the covariance matrix V by $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_p$. It follows from the properties of the covariance matrix that all its eigenvalues are non-zero.

The orthogonal and normalised system of the eigenvectors relating to the eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_p \geq 0$ is denoted by $v_1, v_2, \ldots, v_p \in R^p$. The summary above implies that the scalar probability variables are called the *principal components* of the vector ξ probability variables.

$$\tau_i = v_i^T \cdot \xi^*,\ i=1,2,\ldots,p \quad (2)$$

It is an extremely important property of the principle components that the original probability variable can be given by the linear combination of them in the following way.

$$\xi = \sum_{i=1}^{p} \tau_i \cdot v_i + m \quad (3)$$

This property was applied in the study about day-time radiance distribution [2] as well, moreover, the minimal number of eigenvectors was determined with this method to produce real samples [3]. We can read about how to produce the original samples from characteristic vectors in publication [4], and about the role of the mean vector in publication [5].

4. The examination of Munsell-colour samples

The Munsell colour range is a widely-accepted system of colorimetry, which describes the colours with three features (hue, value, saturation). The colour range was worked out by Albert Henry Munsell, American painter and professor in order to make the names of colours mean the same for everybody (Figure 5.). This system is based on the human colour perception, each colour is denoted by a combination of lettres and numbers.

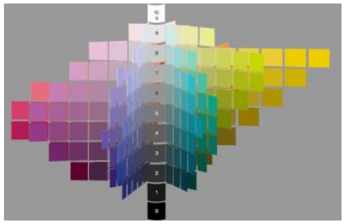

Figure 5. The Munsell colour system

373 colour samples of the system was examined. The known spectral reflectance factors of the samples are the probability vectors. The reflectance factors are given at 10-nm equidistant intervals between 400 nm and 700 nm, therefore, the vectorspace is 31-dimensional.

The values X, Y, Z belonging to given samples may be determined with the help of colour matching functions (Table 1.).

Table 1: Values X, Y, Z belonging to the 5PB5/12 sample

	Original
X =	2.0266
Y =	2.0470
Z =	5.4070

The eigenvalues of the eigenvectors relating to the covariance matrix of 373 colour samples are determined with the use of Matlab software (Table 2.).

Table 2: A fragment of the components of the mean vector and the first five eigenvectors

Mean vector	0.1804	0.2355	0.2572	0.2635	0.2677	0.2716	0.2765	0.2822
v_1	0.0894	0.1344	0.1544	0.1589	0.1605	0.1613	0.1622	0.1628
v_2	-0.0921	-0.1464	-0.1765	-0.1897	-0.1994	-0.2093	-0.2200	-0.2306
v_3	0.1410	0.2077	0.2326	0.2315	0.2219	0.2047	0.1777	0.1364
v_4	-0.1214	-0.1632	-0.1653	-0.1492	-0.1345	-0.1157	-0.0853	-0.0344
v_5	-0.0603	-0.1508	-0.1929	-0.1832	-0.1391	-0.0731	0.0150	0.1277

Each eigenvector may also have negative values, except the one belonging to the highest eigenvalue. It is shown that the eigenvector of the nth eigenvalue as an abstract spectrum has (n-1) zero values. We can use the *Solver* function of Excel to determine the weights that are needed in the linear combination of the eigenvectors. The constraints are chosen on the basis that whether we know or not the reflectance function of the sample. In case of a known reflectance funcion, we minimalise the squared sum of the deviations between the known and reconstructed function values and use it as a constraint. It is proved that the samples can be generated approximately well with the mean vector and the first five eigenvectors (Figure 6).

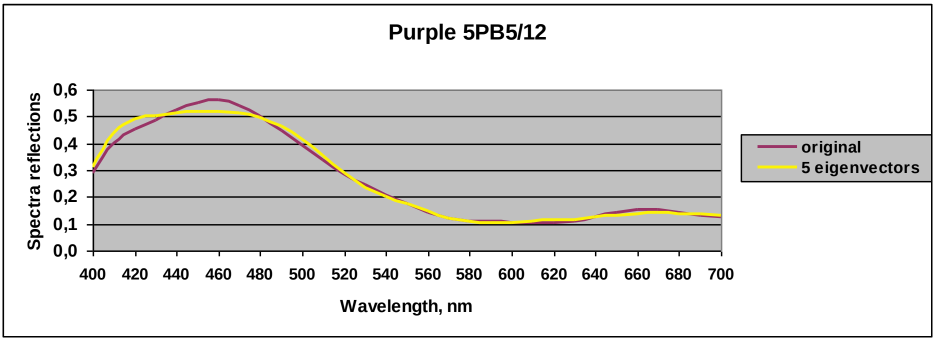

Figure 6. The original and calculated reflectance function

In case of unknown reflectance function, we set the constraint that the derivative of the squared sum of the deviations between the original and the reconstructed values X, Y, Z must be minimal (Table 3.). We use the mean vector and the first five eigenvectors in this case, too (Figure 7.).

Table 3: The original and reconstructed X, Y, Z values

	Original	Reconstructed
X =	2.0266	2.0266
Y =	2.0470	2.0470
Z =	5.4070	5.4070

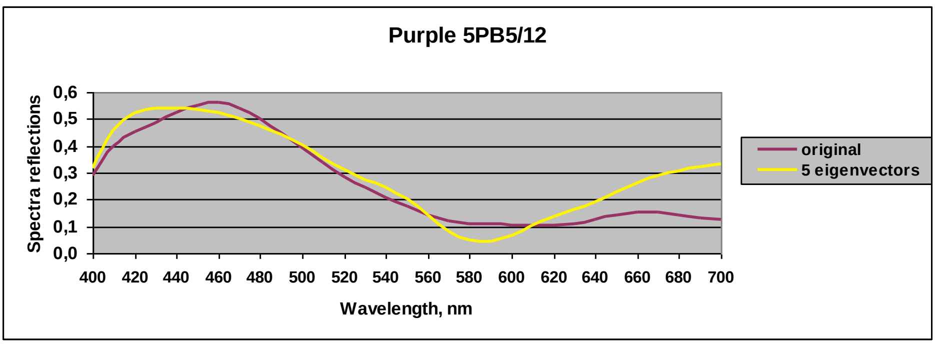

Figure 7. The original and calculated reflectance function

We give a constraint for the first derivative in order to reach a better interpollation between the original and the reconstructed function. To reduce the number of local minima and maxima, the second derivative is limited. A further condition is made, the reconstructed function cannot have negative values. *Solver* is used to set the constraints (Figure 8.).

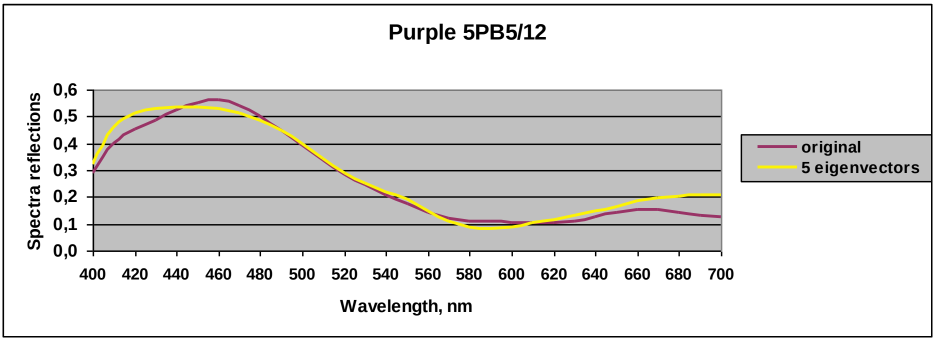

Figure 8. The adjusted reflectance function

5. Summary

We can conclude that it is not necessary to apply all the 31 eigenvectors to generate 373 samples within measuring accuracy, it is enough to apply the mean vector and the first five eigenvectors. Using this method, any colour sample given by values X, Y, Z can be related to a metamer after a short time of calculation. This method works in case of spectra that are different from the spectra belonging to the training samples.

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