Deriving a Suitable Vector Space Describing a Subtractive Color Mixing for Multi-Primary Printing Systems

Di-Yuan Tzeng and Roy S. Berns***

**Multi-Functional Printer, Imaging Team, Hewlett-Packard Company, Boise, Idaho, USA*

***Munsell Color Science Laboratory, Rochester Institute of Technology, USA*

Abstract

This paper will describe methodologies to derive color transformations from spectral reflectance factor to vector spaces that best approximate the subtractive color mixing behavior in working with principal component analysis (PCA). This research aims at finding an optimal spectral representation for digitizing reflective images with high spectral accuracy and lower digital storage. This paper will also discuss the limitation of Kubelka-Munk Turbid Theory for opaque material when applying principal component analysis for spectral reconstruction. Sample sets from three types of subtractive color mixing devices were tested to verify the colorimetric and spectral performance of the proposed transformations in working with PCA and compared to the PCA reconstructed accuracy performed in reflectance space and absorption-scattering space by Kubelka-Munk Theory.

Introduction

In the latest multi-spectral reproduction technologies, researchers frequently perform Principal Component Analysis (PCA) using reflectance factor of color samples requiring reproduction.[1-11] Often, the number of significant dimensions (basis vectors) exceeds the number of physical parameters, for example, a photographic system requires more than three dimensions for spectral reconstruction. This contradicts the knowledge that photographic materials are manufactured by three known dyes. The use of PCA to estimate the reflectance factor makes sense to the spectral-capturing applications since a snap-shot is to record the linear energy reflected from a colored surface.[12-14] Nevertheless, the color synthesis by PCA using reflectance factor as the representation for photographic materials is not optimal since it often requires five or more eigenvectors to obtain satisfactory reconstruction accuracy hence requires five or more channels of digital storage to store the reconstruction coefficients together with the five or more basis vector information of photographic images. However, the recording of spectral information of photographic material should be achievable using only three channels of digital values and three primary or basis vectors if the spectral metrics is other than spectral reflectance. Table I shows the spectral and colorimetric of the "three" eigenvector reconstruction for an IT8.7/2 reflection target of photographic print performed in both spectral reflectance and spectral absorption spaces (introduced by Kubelka-Munk theory discussed in the following sections), where the spectral accuracy was quantified by an index of metamerism that consists of both a parameric correction[15] for D50 and the use of CIE94[16] under illuminant A. The colorimetric accuracy is calculated using CIE94 under D50 for the 1931 observer.

Table I: The colorimetric and spectral performance of three eigenvector reconstruction in both reflectance and absorption spaces for an IT8.7/2 reflection target

	Reflectance		Absorption	
	ΔE^*_{94}	M. I.	ΔE^*_{94}	M. I.
Mean	1.8	0.6	0.5	0.1
STD	1.5	0.6	0.2	0.1
Maximum	8.5	3.6	1.0	0.4
Minimum	0.0	0.0	0.0	0.0
RMS	0.014		0.006	

From Table I, it is apparent that three eigenvector reconstruction in reflectance space is not as capable of retaining spectral information as that of in absorption space. Especially, the large magnitude of maximum error of metamerism index (M. I.), vector component root-mean-square (RMS) error, and the color different in units of ΔE*94 render low confidence of spectral information preservation. Unless more eigenvectors are used for spectral reconstruction in reflectance space, as a consequence, leading to the need of more digital storage. On the contrary, the error shown for three eigenvector reconstruction in absorption space preserves the spectral information with high confidence. Therefore, the image information of photographic material is better off stored with its spectral absorption characteristics from the perspective of digital storage.

Motivated by the observation above, transformations to account for the real physical dimensions of a set of measurements as well as agreeing with the process of an opaque coloration is the focus of this paper. The spectral density or spectral absorption units are the obvious choices of exploring the possibility of lower number of basis vector reconstruction of surface colored materials.

Kubelka-Munk Turbid Media Theory for Subtractive Color Mixing

The transformation between reflectance factor and the absorption coefficient K or the ratio, (K/S) of absorption coefficient K to scattering coefficient S is often based upon Kubelka-Munk turbid media theory.[17-18] For the simplicity, the rest of this paper will use Φ to representation K or K/S. Equations (1) and (2) are used for opaque materials such as acrylic or architectural coating paints and textiles, where the $R_{\lambda,\infty}$ is the spectral reflectance factor of an opaque material and λ represents the visible wavelength.

$$R_{\lambda,\infty} = 1 + \Phi_\lambda - \sqrt{\Phi_\lambda^{\ 2} + 2\Phi_\lambda}\ , \quad (1)$$

$$\Phi_\lambda = (1 - R_{\lambda,\infty})^2 / 2R_{\lambda,\infty}\ . \quad (2)$$

Equations 3 and 4 are used for transparent color layer in optical contact with an opaque support such as photographic paper, where $R_{\lambda,g}$ is the spectral reflectance factor of an opaque support and X is the thickness of the transparent colorant layer. Equation (4) is the inverse transformation of Eq. (3) by assuming that the thickness, X, is unity.

$$\lim_{S\to 0} R_\lambda = R_{\lambda,g} e^{-2\Phi_\lambda X}\ , \quad (3)$$

$$\lim_{S\to 0} \Phi_\lambda = -0.5\ln\left(\frac{R_\lambda}{R_{\lambda,g}}\right)\ . \quad (4)$$

Hence, the subtractive color synthesis takes the form of the linear combination of the Φ of the primary colorants modulated by their corresponding concentrations or by the linear combination of the eigenvectors, $e_{\lambda,\Phi}$ derived from Φ space modulated with suitable eigenvector coefficients, b, shown as Eq. (5),

$$\Phi_{\lambda,\text{mixture}} = \sum_{i=1}^{n} c_i \phi_{\lambda,i} \cong \sum_{i=1}^{n} b_i e_{\lambda,\Phi,i}\ , \quad (5)$$

where, $\Phi_{\lambda,\text{mixture}}$ is the spectral absorption or absorption-scattering coefficient ratio of the synthesized color mixture, n is the number of primary colorant used for synthesis, c is the primary colorant's concentration, and ϕ is the absorption or absorption-scattering coefficient ratio of a primary colorant normalized to its unit concentration. Notice that the n number of primary should be identical to the number of eigenvector used for synthesis. The justification of discarding mean vector term for eigenvector reconstruction in Eq. (5) can be seen at Tzeng and Berns' publication in 2005.[19]

Kubleka-Munk turbid media theory is based on a two-flux assumption, that is, the light in the colorant layer only become scattered upward or downward. No other directional scattering is assumed. Hence, the Kubleka-Munk transformation itself is an approximation of coloration processes.[20-21] Accuracy is quite reasonable for photographic materials' optical characteristics modeled by Eqs. (3) and (4). However, as this research progressed, it was discovered that the transformation for opaque materials does not always describe the optical properties of mixtures formed by the corresponding coloration. In retrospect, this leads to the violation of the two flux assumption. A real material most frequently scatters light in all directions which causes the failure of Eqs. (1) and (2). Furthermore, consider a spectrophotometer measuring the surface of a multicolor object. Its field of view may cover several color surfaces. In this case, the reading of the spectrophotometer is the result of spatial averaging more than two reflected color energies inside its field of view.[22] Hence, the additive color mixing has already happened in reflectance space. Since the Kubelka-Munk opaque transformation is highly nonlinear, the additivity of colorant vectors is, therefore, not well defined in Φ space.

In dealing with the failure of Kubelka-Munk turbid media theory, many more theories utilizing multi-flux methods in solving radiation transfer problem have been published by a number of authors for improving the predicting accuracy.[23-27] However, these complex models, despite their improved correlation with the true optics of colorant mixtures, usually required considerable parameter optimization in order to result in acceptable accuracy. Based on these reason, this research's intension is to derive a relatively simplified empirical transformation which is capable of approximating the opaque color mixing behavior.

Deriving a Simplified Empirical Transformation for Subtractive Color Mixing

The primary keys for the derivation of an empirical space are: obtaining a new colorant vector space with reduced dimensionality that corresponds to the physical dimensionality of a given sample set; and the vector addition and scalar multiplication in new vector space should approximately describe the process of subtractive opaque coloration. Consider the subtractive opaque colorant mixing, the more colorants that are added for coloration, the darker the resultant mixture is. A vector space formed by adding reflectance factors is not realizable for opaque colorations. The transformation from R space to the proposed subtractive color mixing space for an opaque coloration, denoted as Ψ, and its inverse transformation were determined and described by

$$\Psi_\lambda = \vec{a} - R_\lambda^{\frac{1}{w}}, \quad (6)$$

$$R_\lambda = (\vec{a} - \Psi_\lambda)^w, \quad (7)$$

where Ψ_λ represents the new linear vector of an opaque colorant, the $\vec{a}$ which resembles to a flat spectrum of $\vec{1}$ vector is empirically determined from a set of subtractive samples requiring reproduction. The power term, w, is experientially suggested to be $2 \le w \le 3$ to avoid highly nonlinear inverse transformation back to R from Ψ space. The large degree of nonlinear inverse transformation amplifies the spectral components near zero absorbsivity of slight mismatch leading to the unrealizable reflectivity needing special treatment to clip the overly amplified reflective vector components back to unity for colorimetric and spectral performance metrical evaluation. This is found to be the limitation of utilizing Kubelka-Munk theory for opaque media together with eigenvector reconstruction.[28] Figure 1 shows the example of the enhanced spectral error in the resultant R space of Kubelka-Munk transformation of slight mismatch in low absorbsivity spectral region.

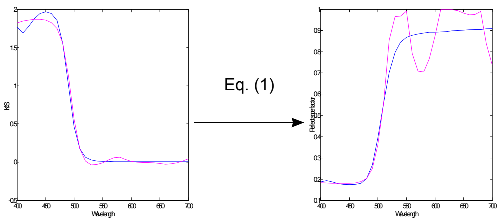

Figure 1. An example of enhanced R space spectral error reconstructed in Φ space by the Kubelka-Munk transformation of Eq. (1)

The derivation of $\vec{a}$ is to optimize the $\vec{a}$ such that the intended number of eigenvectors, say six, generated for the resultant Ψ corresponding to the optimized $\vec{a}$ reaches the maximum spectral reconstruction accuracy by using exactly six eigenvectors.

The forward and backward transformations for the transparent or translucent colorant in optical contact with an opaque substrate are show in Eqs. (8) and (9), respectively,

$$\Psi_\lambda = R_{\lambda,substrate}^{\frac{1}{w}} - R_\lambda^{\frac{1}{w}}, \quad (8)$$

$$R_\lambda = (R_{\lambda,substrate}^{\frac{1}{w}} - \Psi_\lambda)^w, \quad (9)$$

where the $R_{\lambda,substrate}$ is the spectral reflectance factor of a paper or substrate and $2 \le w \le \infty$. The

use of $R_{\lambda,substrate}^{\frac{1}{w}}$ as the offset vector has a significant meaning. Consider that transforming a spectrum, which is exactly $R_{\lambda,substrate}$, to the linear color mixing space, the result is a zero vector. This corresponds to the fact that there is not any primary colorant presented in the linear space. Equation (8) transforms the spectral reflectance factor to the representation for a subtractive color mixing process. Hence, the synthesis, quantitatively described by Eq. (10), of color mixtures is again the linear combinations of the primary colorants modulated by their corresponding concentrations or by the linear combination of the eigenvectors, $e_{\lambda,\Psi}$ derived from Ψ space modulated with suitable eigenvector coefficients, b, shown previously similar to Eq. (5).

$$\Psi_{\lambda,mixture} \sum_{i=1}^{n} c_i \psi_{\lambda,i} \cong \sum_{i=1}^{n} b_i e_{\lambda,\Psi,i}, \quad (10)$$

where ψ_λ is the linear representation of a primary colorant normalized to its unit concentration, c is the corresponding concentration, and n is the number of the primary colorants.

Experimental and Results

Three data sets of were used to test the performance of the proposed transformation.

Six-Primary Opaque Color Mixtures

The first set of 105 opaque paint mixtures from six linearly independent colorants of yellow, cyan, magenta, green, blue, and black (two Sakura poster colors and four Pentel poster colors) was generated by hand mixing and measured with Macbeth Color-Eye® 7000 integrating sphere spectrophotometer with specular component included. Equation (6) was utilized to perform the transformation to the linear color mixing space since the data were generated from opaque paints. PCA was performed in the reflectance, R, the proposed, Ψ, and Kubelka-Munk, Φ, spaces to evaluate the colorimetric and spectral performance. The w term in Eq. (6) was chosen to be 2 and the corresponding $\vec{a}$, plotted at Figure 2, was found through the optimization using Matlab fmincon function.

Table II shows the color and spectral accuracy of six eigenvector reconstruction for the three spaces, in addition, the accuracy of seven eigenvector reconstruction in R space is also shown for comparison. It can be seen that the proposed Ψ space offers the highest reconstruction accuracy among the three. Its RMS error is almost a half of the other two. The accuracy rendered by that of R space implies that the number of eigenvectors needs to increase to seven to achieve the similar accuracy to that of the proposed.

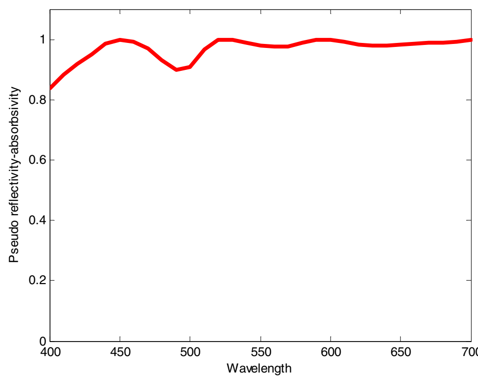

Figure 2. The optimized offset vector in Eqs. (6) and (7) for the 105 poster color mixtures

Table II: The colorimetric and spectral performance of six eigenvector reconstruction in R, Ψ, and Φ spaces for the 105 poster colors.

	ΔE^*_{94}		M. I.		
Space	Mean	Max	Mean	Max	RMS
R with 6 eig	1.0	2.8	0.3	0.7	0.012
R with 7 eig	0.3	1.1	0.1	0.2	0.006
Ψ with 6 eig	0.5	1.2	0.2	0.4	0.007
Φ with 6 eig	0.5	1.9	0.1	0.5	0.012

Four-Primary Electro-Photographic (EP) Color Mixtures

The second set of 1099 colors uniformly sampling at the HP 9500 color MFP's (Multi-functional-printer) printer gamut were used for testing the proposed transformations of Eqs. (8) and (9) since the 1099 samples are transparent-translucent colorants (EP toners are often highly scattering) in optical contact with a paper substrate by its nature of electro-photographic (EP) process. The EP colors were printed with primaries of cyan, magenta, yellow, black, and AMFM screened halftone pattern. The power term w was empirically chosen to be 3.5. The colorimetric and spectral performance by four eigenvector reconstruction for the R and the proposed Ψ space are shown in Table III. The proposed Ψ space for this case again provides a better performance with four eigenvector reconstruction as oppose to that performed in R space. The accuracy of five eigenvector reconstruction is also shown to match the equivalent spectral performance to that of Ψ reconstructed with only four bases. The number of the spectra reconstructed using four basis with color error of ΔE^*_{94} larger than 1 in Ψ is 23 and in R space is 129 out of 1099. The number is reduced to 31 with five eigenvector reconstruction in R space. This again implies that relatively lack of sufficient dimensions in R space to account for large spectral variance by only four basis reconstruction.

Table III: The colorimetric and spectral performance of four eigenvector reconstruction in R, and Ψ spaces for the 1099 electro-photographic colors.

	ΔE^*_{94}		M. I.		
Space	Mean	Max	Mean	Max	RMS
R with 4 eig	0.6	2.9	0.1	0.8	0.009
R with 5 eig	0.4	2.0	0.1	0.3	0.007
Ψ with 4 eig	0.5	1.8	0.1	0.5	0.006

Six-Primary Digital Commercial Press Color Mixtures

The last set of 2457 colors uniformly sampling at the HP Indigo commercial digital press' color gamut spanned by printing primaries of cyan, magenta, yellow, green, orange, and black were used for testing the proposed transformations of Eqs. (8) and (9). The colorant of Indigo press is known to be more transparent and the color formation of its printing process is more linear. The Indigo colors were printed with conventional ordered dithered halftone pattern with rotated screen angles, where the two extra printer primaries of orange and green, are designated to use the same screen angles of cyan and magenta, respectively, since they are mutually complimentary color to each other. The power term w was again empirically chosen to be 3.5. The colorimetric and spectral performance by six eigenvector reconstruction for the R and the proposed Ψ space are shown in Table IV. The proposed Ψ space for this set of data equips with an excellent spectral performance, thus, excellent colorimetric accuracy, with six eigenvector reconstruction. Even though the same number basis reconstruction in R space offers satisfactory spectral and colorimetric accuracy, there are still spectra reconstructed with high degree of spectral error. The accuracy of eight eigenvector reconstruction is also shown to match the equivalent spectral performance to that of Ψ reconstructed with only six bases. The number of the spectra reconstructed using six bases with color error of ΔE^*_{94} larger than 1 in R space is 70 out of 2457 and in Ψ is none. The number is reduced to none by eight eigenvector reconstruction in R space.

Table IV: The colorimetric and spectral performance of six eigenvector reconstruction in R, and Ψ spaces for the 2457 Indigo Digital Press colors.

	ΔE^*_{94}		M. I.		
Space	Mean	Max	Mean	Max	RMS
R with 6 eig	0.4	2.8	0.1	0.5	0.007
R with 8 eig	0.1	0.5	0.1	0.3	0.004
Ψ with 6 eig	0.1	0.7	0.1	0.5	0.004

Conclusion

This research proposes new mathematical transformations to linear spaces approximating subtractive color mixing. Three types of subtractive colorations were used to evaluate the model performance from perspective of digital storage in conjunction with the required spectral and colorimetric accuracy. The proposed absorption or density like color mixing space, Ψ, tops the reconstruction accuracy performed in reflectance space with saving of one to two basis vectors, thus, one to two less channels of image storage. This saving is significant when an image size is utterly large.

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