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An As-Short-as-Possible Mathematical Assessment of Spectrophotometric Color Matching

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Abstract: Color match prediction is one of the most important aspects to be considered by industries dealing with colorants. Several generally applicable theoretical models have been proposed so far for helping the colorists in achieving an exact color match. Such approaches, often based on extensive experimental tests and provided of exhaustive results, are differentiated by a specific range of application (textiles, study, paintings, etc.). Therefore, the results are subjected to restrictions or constraints (number of colorants, reliability of the prediction, etc.). The present paper describes, into a mathematical form, three widely known techniques adopted in the scientific literature for evaluating the spectrophotometric color match prediction of a target shade: Kubelka-Munk, Stearns-Noechel and Artificial Neural Networks. The proposed method starts from such wide known methodologies and by means of mathematical assessment provides some useful equations to be straightforwardly used for color matching. Moreover an Artificial Neural Network based formulation is provided. The results of the work shows that the expected color distance between the predicted the real color of a shade is less than 0.8, in terms of CIE L*a*b* distance.

Key words: Reflectance, color formulation, color matching transfer function, color distance, absorptivity and the scattering

INTRODUCTION

One of the main efforts of the industries dealing with colorants is to find the correct proportion of the colorants required to achieve an exact color match. This process, called color match prediction consists in generating, usually by means of trial and error techniques, a recipe to match a desired or target shade and is often performed by a trained colorist. Computer Color Matching (CCM) is a widely known technology for the color match prediction (Zhang and Li, 2008). This method overcomes the lacks of the experimental color matching approach thus resulting more convenient, accurate and time saving (Agahian, 2008). Spectrophotometric and colorimetric color matching are two methods that are conventionally used. Colorimetric algorithms aim to minimize the color differences (usually expressed in tristimulus values) between a target and a color sample. Spectrophotometric color matching is a technique able to achieve a sample with spectrophotometric curve similar to target reflectance curve. Referring to spectrophotometric approaches, the most commonly adopted are based on the Kubelka-Munk theory (Kubelka, 1954) that is widely used for describing the colour properties of a fabric.

The Kubelka-Munk (K-M) theory is generally used for the analysis of diffuse reflectance spectra obtained from weakly absorbing samples. It provides a correlation between reflectance and concentration.

As widely known (Burlone, 1990), K-M establishes that internal reflectance of a colorant composing a shade, $p(\lambda, \alpha_1)$, depends on absorption, K_λ and scattering, S_λ according to the following equation:

$$\left(\frac{K}{S}\right)_\lambda = \frac{(1 - p(\lambda))^2}{2p(\lambda)} \quad (1)$$

where, λ is the wavelength in the visible range (300-700 nm). $p(\lambda)$ is the spectral response (reflectance) of a generic colorant composing the reference shade. $(K/S)_\lambda$ is the ratio between the absorption and the scattering coefficients for a given wavelength.

Equation 1 is valid for a single wavelength (or monochromatic light). The values of K_λ and S_λ need to be computed from measurements of the reflectance of the mixture composing the shade. More in detail the (K/S) ratio of a mixture is an additive combination of each colorant's unit absorptivity, K_λ and unit scattering S_λ ,

scaled by effective concentration, c , plus the absorption and scattering of the substrate (notated by subscript t) as described in the following Equation:

$$\left(\frac{K}{S}\right)_{\lambda, \text{mix}} = \frac{k_{\lambda, t} + \alpha_1 k_{\lambda, 1} + \alpha_2 k_{\lambda, 2} + \dots + \alpha_i k_{\lambda, i} + \dots + \alpha_n k_{\lambda, n}}{s_{\lambda, t} + \alpha_1 s_{\lambda, 1} + \alpha_2 s_{\lambda, 2} + \dots + \alpha_i s_{\lambda, i} + \dots + \alpha_n s_{\lambda, n}} \quad (2)$$

where, $(K/S)_{\lambda, \text{mix}}$ is the (K/S) ratio of a mixture, α_i is the proportion of the i th component composing the mixture. $K_{\lambda, i}$ and $S_{\lambda, i}$ are, respectively, the absorptivity and the scattering coefficient of the i th component composing the mixture.

For each component in the mixture, both the absorption and scattering properties need to be known. For opaque materials, where the colorants do not scatter in comparison to the substrate, the mixing equation may be simplified as follows (Westland *et al.*, 2000):

$$\left(\frac{K}{S}\right)_{\lambda, \text{mix}} = \left(\frac{k_{\lambda, t}}{s_{\lambda, t}}\right) + \alpha_1 \left(\frac{k_{\lambda, 1}}{s_{\lambda, 1}}\right) + \dots + \alpha_n \left(\frac{k_{\lambda, n}}{s_{\lambda, n}}\right) \quad (3)$$

Stearns and Noechel worked with fine wool fibers blended in the form of slubbing with the help of a draw frame. In their approach, called S-N approach, they assumed that the reflectance value of the blend lies between the reflectance values of the constitutive fibers and is different from the mean of the primary reflectances weighted by the relative mass percentages. Several studies, related to the tristimulus-matching algorithm based on the approach firstly proposed by Stearns and Noechel (1944) and its implementations (Thompson and Hammersley, 1978; Kazmi *et al.*, 1996), allows a reliable prediction of the formula for matching a given colour standard. The S-N based approach estimates the spectrum of a blend (i.e., the term $f(R(\lambda))$ in Eq. 4) obtained by mixing differently colored once known the empiric constant b , according to the following relationship:

$$f[R(\lambda)] = \frac{1 - R(\lambda)}{b \cdot [R(\lambda) - 0.01] + 0.01} \quad (4)$$

where, $R(\lambda)$ is the reflectance and b is a dimensionless constant that can be determined by means of several experimental tests (Banyard *et al.*, 2006; Rong and Feng, 2006). $F(R(\lambda))$ represents the mixture function (Westland *et al.*, 2002).

Artificial Neural Networks (ANNs) are able to provide alternative mappings between colorant concentrations and spectral reflectances (Furferi and Carfagni, 2010; Bishop *et al.*, 1991) and more generally, determine non-linear transforms between colour spaces.

The FFBP ANNs are known to be suitable for applications in the pattern classification field, especially where the limits of classification are not exactly defined (Furferi and Governi, 2008). A properly trained FFBP ANN is capable of generalizing the shape of a spectrophotometric response on the basis of the information acquired during the training phase. In order to properly teach the network to respect the classification made by the picker, a proper target set is required.

In all the previously mentioned cases, computer recipe prediction systems require a mathematical model able to obtain an accurate color matching. In other words such a model, called color recipe mapping, is required to process colorant concentrations and spectral responses, in input, so as to provide, as output, the spectral response of a desired shade obtained by mixing the colorants.

Starting from well known relationships acknowledged at the state of the art, the main objective of the work is to provide three different formulations for the assessment of the color recipe mapping. These formulations, based respectively on K-M, Stearns Noechel and ANN techniques, may be adopted by researchers and practitioners in order to assess the exact color matching once they know the concentrations and the spectral response of the colorants composing a particular recipe.

MATERIALS AND METHODS

Definitions: Let $p_i(\lambda)$ be the spectral response in the visible wavelength of the i th of the n colorants composing the desired shade (called reference): $i = 1, 2, \dots, n$. The colour spectrum $R(\lambda, \alpha_i)$ obtained by a linear combination of the spectra of each component, called Weighted Average Spectrum (WAS), can be stated as follows:

$$R(\lambda, \alpha_i) = \sum_{i=1}^n \alpha_i p_i(\lambda) \quad (5)$$

As λ indicates the wavelength, in the range (400-700 nm), the size of vectors $p_i(\lambda)$ and $R(\lambda, \alpha_i)$ is 1×31 .

Of course, the following equation must be satisfied:

$$\sum_{i=1}^n \alpha_i = 1 \quad (6)$$

The WAS may be related to the real spectral response of the reference $R_s(\lambda)$ measured by means of a spectrophotometer.

In other words, the color recipe mapping is defined by a transfer function F that state the functional connection between $R(\lambda, \alpha_i)$ and $R_s(\lambda)$:

$$R_s(\lambda) = F(R(\lambda, \alpha_i)) \quad (7)$$

Once known the transfer function $\Phi(\lambda, \alpha_i)$, it is possible to give a reliable estimation of the reference spectral response starting from the spectral response and the proportion of each colorant i.e., it is possible to assess the exact color matching.

As previously mentioned, the present work aims to state three different formulations for mathematically defining the mapping function F:

- K-M based formulation
- Stearns-Noechel based formulation
- ANN based formulation

These formulations are based on the assumption that a function $\Phi(\lambda, \alpha_i)$ exists such that:

$$F(R(\lambda, \alpha_i)) = \Phi(\lambda, \alpha_i) \cdot R(\lambda, \alpha_i) \quad (8)$$

In other words if $R_{sj}(\lambda)$ is the j th element of $R_s(\lambda)$, $R_j(\lambda, \alpha_i)$ the j th element of $R(\lambda, \alpha_i)$ and $\phi_j(\lambda, \alpha_i)$ is the j th element of $\Phi(\lambda, \alpha_i)$, with $j = 1, 2, \dots, 31$, Eq. 8 can be written, element by element, as follows:

$$R_{sj}(\lambda) = \phi_j(\lambda, \alpha_i) \cdot R_j(\lambda, \alpha_i) \quad (9)$$

This transfer function can be considered applicable for any variation of the parameters α_i as long as the Eq. 2 is respected:

K-M based formulation: A first mathematical definition of the transfer function $\phi_j(\lambda, \alpha_i)$ may be afforded by means of the K-M formulation. Combining Eq. 1 with Eq. 9 it is possible to write:

$$\left(\frac{K}{S}\right)_{\lambda, mix} = \frac{(1 - \phi_j(\lambda, \alpha_i) \cdot R_j(\lambda, \alpha_i))^2}{2\phi_j(\lambda, \alpha_i) \cdot R_j(\lambda, \alpha_i)} \quad (10)$$

Thus obtaining:

$$\phi_j^2(\lambda, \alpha_i) \cdot R_j^2(\lambda, \alpha_i) - 2\phi_j(\lambda, \alpha_i) \cdot R_j(\lambda, \alpha_i) \cdot \left[\left(\frac{K}{S}\right)_{\lambda, mix} + 1\right] + 1 = 0 \quad (11)$$

Finally, solving for $\phi_j(\lambda, \alpha_i)$:

$$\phi_j(\lambda, \alpha_i) = \frac{1}{R_j(\lambda, \alpha_i)} \left(1 + \left(\frac{K}{S}\right)_{\lambda, mix} - \sqrt{\left(\frac{K}{S}\right)_{\lambda, mix}^2 + 2\left(\frac{K}{S}\right)_{\lambda, mix}} \right) \quad (12)$$

This equation reassumes the studies conducted by Allen (1966) and cited by McDonald (1997) and Berns (2000).

Stearns-noechel based formulation: According to Allen (1966), if the degree of metamerism between the target and the prediction is not too great it can be written the following equation (Philips-Invernizzi *et al.*, 2002):

$$R_{sj}(\lambda) - R_j(\lambda, \alpha_i) = \frac{dR(\lambda)}{df(R(\lambda))} \cdot [f(R_{sj}(\lambda)) - f(R_j(\lambda, \alpha_i))] \quad (13)$$

By combining Eq. 13 and 9 it can be demonstrated that:

$$R_{sj}(\lambda) - R_j(\lambda, \alpha_i) = R_j(\lambda, \alpha_i) \cdot [\phi_j(\lambda, \alpha_i) - 1] \quad (14)$$

According to Eq. 4 the term $\frac{dR(\lambda)}{df(R(\lambda))}$ in Eq. 13 can be rewritten as follows:

$$\frac{dR(\lambda)}{df(R(\lambda))} = -\frac{(0.01 + 0.99b)}{[b \cdot f(R(\lambda)) + 1]^2} \quad (15)$$

Finally, combining Eq. 15 with Eq. 14 it is possible to state that:

$$\phi_j(\lambda, \alpha_i) = 1 - \frac{(0.01 + 0.99b)}{[b \cdot f(R(\lambda)) + 1]^2} \cdot \frac{f(R_{sj}(\lambda)) - f(R_j(\lambda, \alpha_i))}{R_j(\lambda, \alpha_i)} \quad (16)$$

ANN based formulation: Let suppose that:

- An ANN has been structured as follows (Furferi and Carfagni, 2010):
 - Three layers: input, hidden and output layer
 - Hidden layer made of logistic neurons followed by an output layer of logistic neurons again
 - 31 input, h hidden and 31 output units
- The ANN has been trained using, as input, the spectral responses of the colorants composing the shade and, as output, the spectral factors of the reference
- The training was performed using a back-propagation algorithm (Allen, 1980) until the MSE reach a value equal to, at least, 0.01

Accordingly it is possible to define the following terms (Ghwanmeh *et al.*, 2006):

- W_1 (size $n \times 2n$) and W_2 (size $2n \times 1$), respectively, the weight matrices of the hidden and of the output layer of the trained ANN

- b_1 (size $1 \times 2n$) and b_2 (size 1×1), respectively, the bias vector of the hidden layer and the scalar bias value of the output layer of the trained ANN
- H , vector containing the $2 \times n$ hidden neurons of the hidden layer of the ANN
- F and G , transfer functions between, respectively, input and hidden layer and hidden and output layer (Bouzenada *et al.*, 2007)
- O (size 1×31), the output vector of the ANN
- ε (size 1×31), the output error vector of the net

As a result, for each wavelength in the range 400-700 nm it is possible to write the following equations:

$$\begin{cases} H(\lambda) = F(R(\lambda, \alpha_i) \circ W_1 + b_1) \\ R_s(\lambda) = O + \varepsilon \\ O = G(W_2 \circ H(\lambda) + b_2) \end{cases} \quad (17)$$

Finally it is possible to evaluate the spectral response $R_s(\lambda)$ given the n reflectance factors $R(\lambda, \alpha_i)$ and the proportions α_i :

$$R_s(\lambda) = G\left((W_2 \circ F(R(\lambda, \alpha_i) \circ W_1 + b_1) + b_2)\right) + \varepsilon \quad (18)$$

From Eq. 17 it is possible to derive the expression for the transfer function $\phi_j(\lambda, \alpha_i)$:

$$\phi_j(\lambda, \alpha_i) = \frac{1}{R(\lambda, \alpha_i)} \left\{ G\left((W_2 \circ F(R(\lambda, \alpha_i) \circ W_1 + b_1) + b_2)\right) + \varepsilon \right\} \quad (19)$$

Equation 18 demonstrates that the color recipe mapping depends upon the transfer functions F and G . If, for instance, both function may be considered linear and the term ε is neglected (being the network error, in a proper training this term tends to zero) it can be written:

$$\phi_j(\lambda, \alpha_i) = W_2 \cdot W_1 + \left(\frac{b_1 W_2 + b_2}{R(\lambda, \alpha_i)} \right) \quad (20)$$

If G is linear and F is a log-sigmoid function (these functions are, typically, adopted for mapping functions with ANNs) and the term ε is neglected, Eq. 18 becomes:

$$\phi_j(\lambda, \alpha_i) = \frac{1}{R(\lambda, \alpha_i)} \left\{ W_2 \circ \tanh(R(\lambda, \alpha_i) \circ W_1 + b_1) + b_2 \right\} \quad (21)$$

RESULTS

The three formulations expressed by Eq. 12, 16 and 20 provide a mathematical assessment of the color recipe

mapping on the basis of three different, well recognized, methods. On the basis of the results provided in scientific literature, each of the three formulas may be adopted under specific restriction and in a different field of application. In order to understand the differences between the proposed approaches, thus analyzing their performances an experimental test may be assessed.

In detail, 80 differently colored fabrics were collected during an extensive experimental campaign conducted in 2009 by the colourists working in the company New Mill S.p.A. of Prato, Italy. Each blend is composed by a certain number of raw materials each one characterized by a different color (e.g., by a different spectrophotometric response). In Table 1 three examples of the 30 fabrics chosen for validating the approach are listed.

The validation was carried out according to the following tasks:

- Spectrophotometric measurement of the colorants.
- Evaluation of the transfer function by using equations 12, 16 and 20 respectively
- Prediction of the transformed spectral reflectance factors of the blend
- Measurement of CIE $L^*a^*b^*$ colour distance (DE CIEL $^*a^*b^*$) between the predicted spectrophotometric response and the measured one (Mridula *et al.*, 2008)

The results of the whole validation, depicted in the last row of Table 2, shows that the color prediction, in terms of CIE $L^*a^*b^*$ colour distance, is less than 0.8 for all the three approaches. The K-M and the S-N based formulations prediction error, in terms of color distance, increase when the number of colorants is greater than 8. This can be easily viewed in Table 2: the mean values of

Table 1: Three examples of the 30 fabrics chosen for validating the approach

Fabric ID.	No. of components	Material	Colorant proportions	%
W-P1	4	Wool	α_1	30.0
		Wool	α_2	45.0
		Polyester	α_3	10.0
		Polyester	α_4	15.0
C-W-P1	6	Cotton	α_1	29.6
		Cotton	α_2	11.8
		Cotton	α_3	8.6
		Viscose	α_4	18.5
		Viscose	α_5	15.5
		Polyester	α_6	16.0
W-P-M1	8	Wool	α_1	20.5
		Wool	α_2	18.6
		Wool	α_3	11.1
		Wool	α_4	15.6
		Polyamide	α_5	12.3
		Polyamide	α_6	5.6
		Polyamide	α_7	3.1
		Mohair	α_8	13.2

Table 2: Results of the validation test. For each Fabric Id. The CIE L*a*b* colorimetric distance between the predicted values and the measured one is provided

Fabric ID.	No. of colorants	K-M approach	S-N approach	ANN approach
		DECIEL*a*b*	DECIEL*a*b*	DECIEL*a*b*
W-P1	4	0.34	0.36	0.42
W-P2	4	0.41	0.43	0.38
W-P3	4	0.38	0.41	0.37
W-P4	4	0.42	0.37	0.45
W-P5	4	0.28	0.32	0.42
W-P6	4	0.19	0.23	0.19
W-P7	4	0.52	0.43	0.28
W-P8	4	0.51	0.46	0.32
W-P9	4	0.47	0.42	0.19
W-P10	4	0.38	0.41	0.45
Mean value for W-P ID.		0.39	0.38	0.35
C-W-P1	6	0.43	0.39	0.38
C-W-P2	6	0.42	0.43	0.48
C-W-P3	6	0.53	0.52	0.38
C-W-P4	6	0.38	0.44	0.43
C-W-P5	6	0.29	0.31	0.28
C-W-P6	6	0.57	0.52	0.45
C-W-P7	6	0.58	0.53	0.48
C-W-P8	6	0.43	0.58	0.59
C-W-P9	6	0.39	0.42	0.39
C-W-P10	6	0.52	0.29	0.28
Mean value for C-W-P ID.		0.45	0.44	0.42
W-P-M1	8	0.73	0.78	0.53
W-P-M2	8	0.75	0.79	0.56
W-P-M3	8	0.73	0.72	0.58
W-P-M4	8	0.82	0.69	0.62
W-P-M5	8	0.63	0.76	0.69
W-P-M6	8	0.65	0.71	0.59
W-P-M7	8	0.78	0.65	0.52
W-P-M8	8	0.69	0.67	0.52
W-P-M9	8	0.84	0.78	0.49
W-P-M10	8	0.86	0.82	0.62
Mean value for W-P-M ID.		0.75	0.74	0.57
Mean value for the whole validation set		0.53	0.52	0.44

the three approaches are quite similar for fabrics with Id. W-P and C-W-P, whose shade is composed by 4 or 6 colorants.

In detail the K-M approach provides a prediction with a color distance averagely equal to 0.39 for 4 colorants and of 0.45 for 6 colorants. The S-N approach, considering a constant b equal to 0.15, provides a colour distance equal to 0.38 and to 0.44 for, respectively, 4 and 6 colorants. For fabrics composed by 8 materials (i.e., 8 colorants, having every material a different color) the color distances evaluated for the K-M and the S-N approaches are higher than the ANN based one. In detail the K-M and S-N based approaches provides value, respectively, of 0.75 and 0.74 while the ANN based approach give an average distance equal to 0.57. On the basis of this validation task, it is evident that the K-M and the S-N based approaches, proposed in the present work,

may be adopted when the number of colorants is less than 6. Otherwise, the ANN based formulation may be considered more affordable.

DISCUSSION

Starting from the literature, the present paper provided in as-a-short-as-possible manner, three different mathematical formulations for performing the color matching. The provided equations, useful for establishing a functional mapping between colorant concentrations and spectrophotometric response of the reference shade, are, in particular, based on three widely known techniques: K-M, S-N and ANNs. On the basis of validation task and of literature analysis it may be affirmed that the K-M based equation (Eq. 12) is suitable for assessing the color recipe mapping of textiles, papers, wood, paints, inks and plastics once the absorption and scattering coefficients are evaluated. Accordingly, it requires a database to compute both K_λ and S_λ . Moreover, for materials such as textiles (where the colorants do not scatter in comparison to the substrate) the mixing equation is simplified (Eq. 3). The performance of this method is well established in literature since 1980 as demonstrated by Allen (1980), Nobbs (1997), Berns (2000) and Zhao and Berns (2009). Such researchers showed that the color prediction, in terms of CIE L*a*b* colour distance, is less than 0.8 and the maximum allowable number of colorants composing the desired shade is 6. This is in accordance with the validation task proposed in the present study.

The S-N based Eq. 16 provides good results for color recipe prediction of textile and woven fabrics. This mathematical formulation requires the determination of constant b (Yang and Miklaveic, 2005). Once properly defined such a constant, the S-N based equation provides results, in terms of CIE L*a*b* colour distance less than 0.8 with a maximum number of colorants equal to 5-6. The method has been developed for a higher number of components by Rong and Feng (2006) with good results: the maximum color difference was 4.48 CIE L*a*b* units and the average color difference was 1.02 CIE L*a*b* units for four-components fiber blends under D65 illuminant.

These results are in accordance with the one proposed in the present study. Anyway for different materials composing a fabric (e.g., a carded cloth) the constant value is hard to be computed; as a consequence this method is useful especially for textiles composed by a single, differently colored, material.

The ANN based approach (Eq. 19) that authors propose in this work may be, probably, suitable for

assessing the color recipe mapping of papers, wood, paints, inks and plastics whose shade is composed by any number of colorants, accordingly to Darko *et al.* (2008). Moreover the approach is suitable also for shades composed by different materials (e.g., textiles composed by a mixture of wool, cotton, polyester etc.). Although, this approach does not need the assessment of constants or coefficients, it requires a training phase by means of a database of spectral responses. Once properly trained the ANN-based approach allows results, in terms of CIE $L^*a^*b^*$ colour distance, less than 0.8. Finally, while the training phase may be computationally expensive, the simulation phase, i.e., the determination of the transfer function, may be performed in few seconds. The authors aimed to provide such techniques into a mathematical form in order to help researchers and practitioners (colorists), to easily evaluate the color of a shade given the spectral factors of the colorants. Therefore, the authors want to encourage other researchers working in the field of colorimetry and spectrophotometry to provide a large number of results of their experimentations using the provided equations.

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