Perceptual Reflectance Weighting for Estimating Kubelka-Munk Coefficients

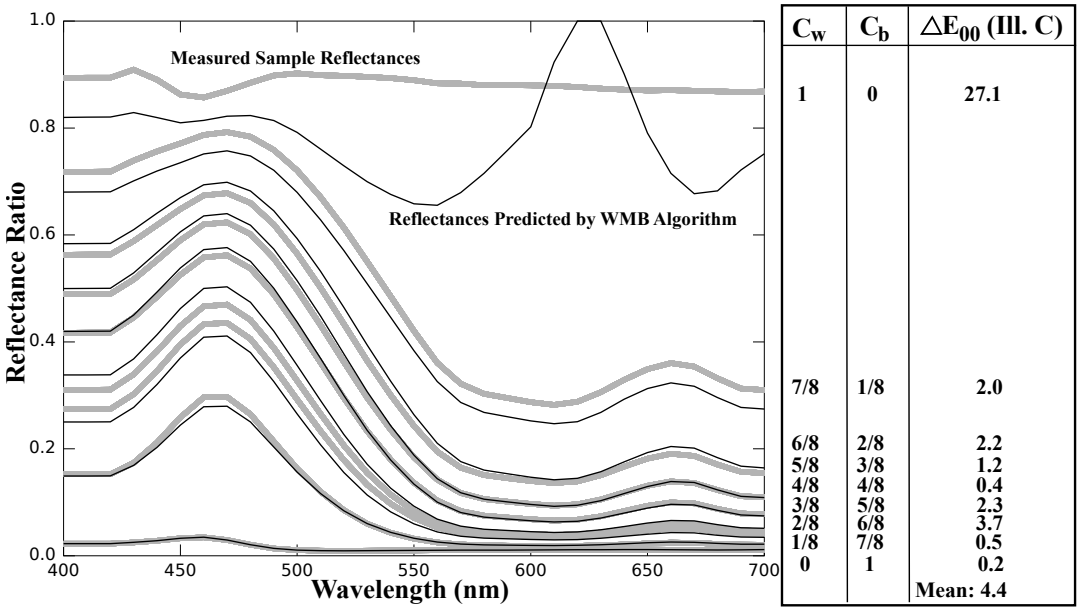
Paul Centore

Abstract

The Kubelka-Munk model relates the colours of mixtures to the absorption and scattering coefficients (K and S) of the constituent colorants. A 1987 least squares algorithm by Walowit, McCarthy, and Berns estimates K and S for a set of constituent colorants, from the reflectance spectra of mixtures of those colorants. Their algorithm implicitly weights all the least squares residuals equally. As a result of analyzing residuals and perceptual factors, the current paper recommends a new weighting, called perceptual reflectance weighting. The residuals are shown to follow a probability distribution that depends on S, reflectance level, and reflectance measurement errors. These errors are modeled as an unbiased normal distribution, with the same variance at all reflectance levels. In addition, CIE L describes how perceptual response depends on reflectance level. Perceptual reflectance weighting combines both these dependencies into one weight. The 1987 algorithm is easily modified, by multiplying each row (except the last) of its coefficients matrix by the appropriate weight, and by using the original estimates of S. An example, taken from practice, illustrates that the new weights can significantly change and improve the 1987 algorithm.*

1 Introduction

The Kubelka-Munk model[1] predicts the colour of a mixture of paints, provided one knows the absorption coefficient, K, and scattering coefficient, S, for each constituent paint, at each wavelength. An important practical problem is to determine K and S for the constituent colorants, by measuring the reflectance spectra of mixtures of the constituents at known concentrations. In 1987, Walowit, McCarthy, and Berns



C_w	C_b	$\triangle E_{00}$ (Ill. C)
1	0	27.1
7/8	1/8	2.0
6/8	2/8	2.2
5/8	3/8	1.2
4/8	4/8	0.4
3/8	5/8	2.3
2/8	6/8	3.7
1/8	7/8	0.5
0	1	0.2
		Mean: 4.4

Figure 1: Reflectance Spectra Predicted by 1987 WMB Algorithm

published a least-squares algorithm[2] (referred to here as the WMB algorithm) for this problem. The current paper proposes modifying this algorithm with a weighting function. In this weighted WMB algorithm, each row (except the last) of the matrix KSCOEFS in the WMB algorithm is multiplied by a factor which depends on the reflectance level of the measurement that generated that row. In addition, the unmodified WMB algorithm is run once to produce estimates of S, which are needed to calculate the weighting factors.

The new weighting was motivated by the performance of the original WMB algorithm, when analyzing some artist's acrylic paint samples. Figure 1 shows the reflectance spectra for a tint ladder of Phthalo Blue (Red Shade), manufactured by Golden Artist Colors. The tint ladder was produced by mixing the blue with Golden's Titanium White, in various proportions. A table gives the concentration by volume of white, C_w, and blue, C_b, in each mixture. The thick grey lines in the plot are the measured reflectance spectra of the mixed samples.

The WMB algorithm was used to estimate K_w, S_w, K_b, and S_b (the coefficients for the white and the blue), at each multiple of 10 nm in the visible spectrum. Using the estimated coefficients, the Kubelka-Munk model could predict the reflectance spectrum for each concentration; the thin black lines on the plot show these predictions. A prediction is considered accurate if the colour difference between the

measured and predicted spectra is small. Colour difference was evaluated with the CIE ΔE_{00} formula,[3] as modified by Sharma,[4] calculated with respect to Illuminant C.

The table beside the plot lists the ΔE_{00} values for the different mixtures. While most are not much more than 2 (a common threshold for acceptable matches), the prediction for white is very bad, at 27. The plot shows that the white prediction varies wildly around the white measurements. This large deviation drives the average ΔE_{00} to a high value of 4.4.

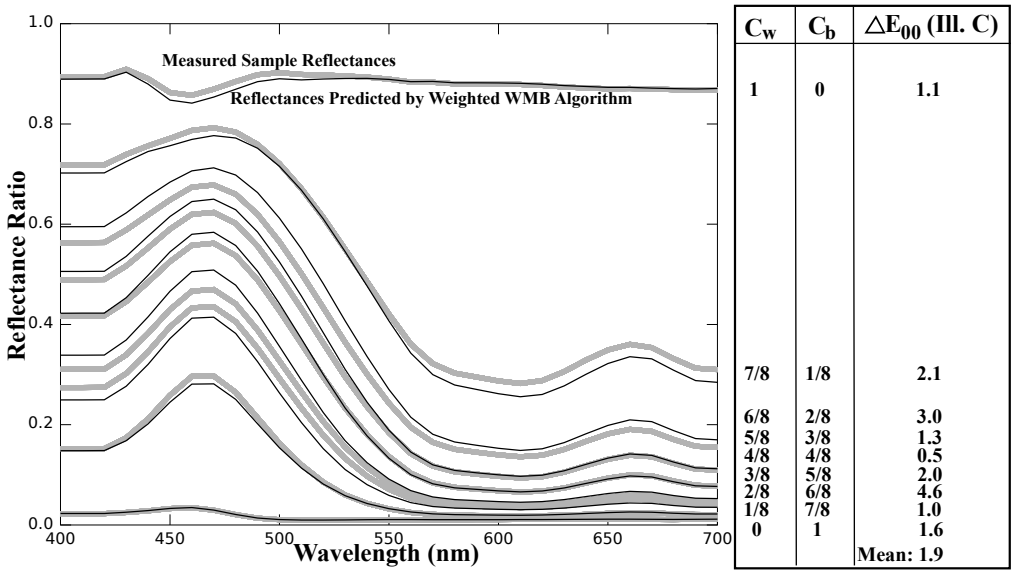
Additionally, the predicted reflectance spectra seem to become progressively less accurate as reflectance level increases. The current paper finds that sensitivity in Kubelka-Munk relationships explains the less accurate matches for lighter colours. A weighting function is derived to compensate for this sensitivity. (The possibility of a weighting function had been mentioned in a follow-up paper[5] by the algorithm's authors.)

The recommended weighting function is based on two relationships. First, as Nobbs[6] and Okumura[7] have already pointed out, the ratio K/S is sensitive to small changes in measured reflectances, at low reflectance levels. K/S is insensitive to changes at high reflectance levels. As a result, the large reflectance errors in Figure 1 are tolerated for light colours, but not for dark colours. The current paper shows how sensitivity gives undue importance to some least-squares residuals, thus degrading the algorithm's result. A central result is Equation (29), which expresses a residual as a probability distribution that depends on both S and the reflectance measurement error. A reflectance measurement error is modeled as an unbiased normal distribution, whose variance does not depend on reflectance level. Equation (29) allows the calculation of each residual's variance, from which an appropriate weight can be derived.

The second relationship, described by Munsell value or CIE lightness (L^*), is that humans respond more to reflectance changes at low reflectances than at high reflectances. The weighted WMB algorithm aims to predict reflectance spectra that are *perceptually* close to the mixtures' actual reflectance spectra. Thus a change in reflectance level is only as important as the corresponding change in L^*. Therefore the weight from Equation (29) has been multiplied by an additional, perceptual, factor, that depends on reflectance level. Viggiano[8] has already calculated this new factor, in the context of a metamerism index.

The weighted WMB algorithm uses *perceptual reflectance weighting*, which simultaneously encompasses *reflectance weighting* (from the first relationship) and *perceptual weighting* (from the second relationship).

Figure 2 shows the results of the weighted WMB algorithm, given the same



C_w	C_b	$\triangle E_{00}$ (Ill. C)
1	0	1.1
7/8	1/8	2.1
6/8	2/8	3.0
5/8	3/8	1.3
4/8	4/8	0.5
3/8	5/8	2.0
2/8	6/8	4.6
1/8	7/8	1.0
0	1	1.6
		Mean: 1.9

Figure 2: Reflectance Spectra Predicted by Weighted WMB Algorithm

mixtures that appeared in Figure 1. The measured reflectance spectra are identical in both figures, but the predicted spectra are more accurate in the second figure. The average ΔE_{00} has decreased from 4.4 to 1.9. The improvement is particularly obvious in the match for white. In the second figure, this match is practically identical in terms of reflectance, and its ΔE_{00} is only 1.1. The matches for the darker colours in the second figure, though not quite as good as in the first figure, are still well within acceptability. Overall, perceptual reflectance weighting does not favor either light or dark colours.

This paper is organized as follows. First, the least squares context, including weights and residuals, is discussed. Then, Kubelka-Munk relationships are used to relate residuals to reflectance measurement variability, yielding expressions for reflectance weighting. Third, perceptual relationships are analyzed, yielding expressions for perceptual weighting. The two are combined into perceptual reflectance weighting, and an algorithm is presented that is a simple modification of the 1987 WMB algorithm. A sensitivity analysis gives order-of-magnitude estimates of the relative sizes of the weights. Finally, the algorithm is applied to an example.

2 Weights for Kubelka-Munk Estimation

2.1 Least Squares, Residuals, and Weights

The linear least squares algorithm estimates the parameters of a linear model, from a set of measured data points.[9] A model is a function that uses varying inputs and fixed parameters, to calculate outputs. Some of the parameters are known, and others are unknown; the goal is to estimate the unknown parameters. Each data point consists of a set of model inputs, and measurements of the corresponding outputs. The inputs are assumed to contain no errors, but the output contains measurement errors, which are unbiased and normally distributed. The variances of the errors might be identical, in which case they will not affect the estimates of the parameters. If they are not identical, they will affect the estimates.

If one hypothesizes a set of values for the unknown parameters, then the model becomes a function that can be evaluated. The quality of a hypothesized function's fit is indicated by its *residuals*. A residual is the difference between a measured output, for a known input, and the output that the function predicts for that input. There is a residual for each data point, so there can be a large set of residuals. Rather than comparing residuals directly, one should compare residuals that have been *weighted* by the standard deviations (the square roots of the variances) of the outputs' measurement errors. If the variance of the i^{th} output is σ_i^2, and the value of the i^{th} residual is r_i, then the weighted residual $r_{\text{W}i}$ is given by

$$r_{\text{W}i} \;=\; \frac{r_i}{\sigma_i}. \tag{1}$$

The least squares algorithm finds the set of parameters which minimizes W, the weighted sum of squared residuals:

$$W \;=\; \sum_{i=1}^{N} \left(\frac{r_i}{\sigma_i} \right)^2. \tag{2}$$

Weighting accounts for the fact that a large residual difference might be caused by a large measurement error, rather than by poorly chosen parameters. It is more important for a fit to agree closely with a very accurate measurement, than to agree with a less accurate measurement. If each data point has the same variance σ^2 (even if that variance is unknown), then σ_i factors out of Equation (2), and is not needed for the least squares algorithm.. If σ_i does vary significantly from residual to residual, then it can greatly affect the outcome of the algorithm, even if the data itself remains unchanged.

A least squares implementation cannot avoid using weights, even if only implicitly. The 1987 algorithm tacitly assumes that the weights in a set of linear Kubelka-Munk relationships are identical. The current paper recommends a different set of weights, based on reflectance measurement errors and perceptual relationships. The recommended σ_i's can differ by several orders of magnitude, and thus significantly affect the algorithm's outcome.

2.2 The Least Squares Formulation for Kubelka-Munk

The WMB algorithm assembles a system of linear relationships, based on the Kubelka-Munk model. If there were no measurement or model error, the system could be solved exactly. Because of error, however, a least squares approach is used to find the best (though still not exact) set of Kubelka-Munk coefficients. The algorithm's original presentation[2] does not explicitly specify how weights are assigned.

A geometric least squares example will explain how the weights are introduced. Consider the problem of identifying the point (x, y) in the Cartesian plane, which satisfies a set of linear relations, which are only known to within some error. For example, suppose measurements indicate that (x, y) should lie on each of the following lines (shown in Figure 3):

$$\begin{aligned} -0.40x - 0.27y + 0.80 &= 0, && (3)\\ -0.60x + 0.40y + 0.60 &= 0, && (4)\\ 0.20x - 0.67y + 1.00 &= 0. && (5) \end{aligned}$$

Without measurement error, the three lines would intersect perfectly at (x, y), and satisfy the linear system

$$\begin{bmatrix} -0.40 & -0.27 \\ -0.60 & 0.40 \\ 0.20 & -0.67 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} -0.80 \\ -0.60 \\ -1.00 \end{bmatrix}. \quad (6)$$

Because of measurement error, the lines actually form a small triangle. It would be thus expected that (x, y) is *near* each line rather than exactly on it.

To be consistent with the WMB algorithm's original presentation,[2] the following notation will be used for the matrices and vectors in Equation (6):

$$\text{KSCOEFS} \times \text{KANDS} = \text{OBS}. \quad (7)$$

According to the least squares algorithm, the parameters KANDS that come closest to satisfying Equation (7) are given by

$$\text{KANDS} = (\text{KSCOEFS}^{\intercal}\text{KSCOEFS})^{-1}\,\text{KSCOEFS}^{\intercal}\text{OBS}, \quad (8)$$

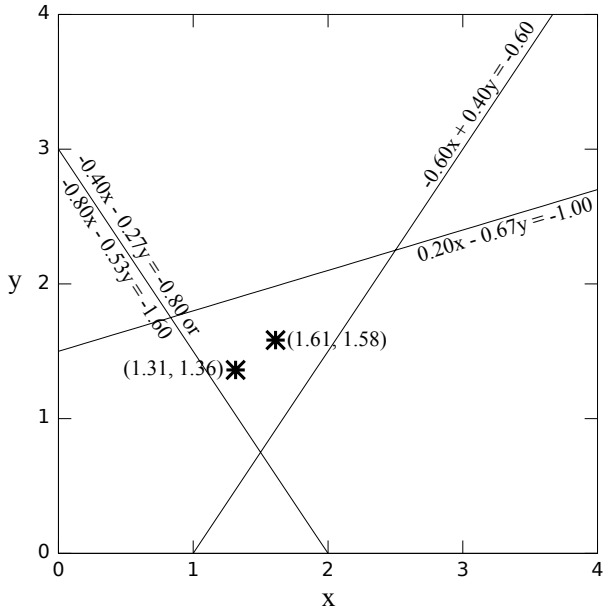


Figure 3: Example of Least Squares Formulation

where $^\intercal$ denotes matrix transposition. Applying Equation (8) to Equation (6) gives

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 1.61 \\ 1.58 \end{bmatrix}. \tag{9}$$

This point is also shown on the figure. It is approximately at the center of the triangle, and about equally near to each of the three lines.

This simple example contains an easily overlooked subtlety: the very form of the matrices and vectors introduces some implicit assumptions about weights. Apparently irrelevant changes can alter the least squares solution. For example, multiple Equation (3) by 2, getting

$$-0.80x - 0.53y + 1.60 = 0, \tag{10}$$

and adjust Equation (6) accordingly to get

$$\begin{bmatrix} -0.80 & -0.53 \\ -0.60 & 0.40 \\ 0.20 & -0.67 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} -1.60 \\ -0.60 \\ -1.00 \end{bmatrix}. \tag{11}$$

Applying Equation (8) to Equation (11) gives

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 1.31 \\ 1.36 \end{bmatrix}. \tag{12}$$

This point also appears in the figure. It is definitely different from the first point. Rather than being near the center of the triangle like the first point, it is closer to the first line than to the other two lines.

This result is surprising, because Equations (3) and (10) are identical. In fact, the points that satisfy the equations *exactly* do not change. The interpretation of points that satisfy the equations *approximately*, however, do change. The left hand side of Equation (11) can be thought of as a linear model with unknown parameters x and y. The value -1.60 in Equation (11) is analogous to a measured output. Equation (10) is the difference, i.e the residual, between the model output, assuming a given x and y, and the measured output, -1.60. Those x-y-pairs which are on the line have residual 0, whether the line is given by Equation (3), Equation (10), or any other constant multiple of Equation (3). The residuals of all other x-y-pairs, however, change when Equation (3) is multiplied by a constant factor. Using Equation (3), the residual for the first point is 0.33, while using Equation (10), the residual for the first point is 0.66, twice the value.

To minimize W, the least squares algorithm moves the original solution closer to the first line when the residual from the first line is increased. Similar adjustments would occur if the other linear relationships were multiplied by constant factors. Multiplying the i^{th} linear relationship by a constant has the same effect as Equation (2), which multiplies the i^{th} residual by $1/\sigma_i$. In both cases, some residuals are weighted more or less, relative to other residuals. The weight itself can be seen as $1/\sigma_i$, the inverse of the standard deviation for the i^{th} residual. If the standard deviations of the residuals are known, then they should be used to find a more accurate least squares solution.

Step 3 of the WMB algorithm calculates a series of linear relationships involving reflectance measurements and Kubelka-Munk coefficients. Each linear relationship has a left side (given by a row of KSCOEFS $\times$ KANDS) and a right side (given by an entry in OBS). The residuals are the differences between the left and right sides. Because no multiplicative factors are used, the residuals are, in effect, all weighted equally. Since the right side of all the linear relationships is an entry of 0 in OBS, a weight for the i^{th} residual would be implemented simply by multiplying the i^{th} row of KSCOEFS by the desired weight. Ideally, that weight would be $1/\sigma_i$. The next section of the current paper calculates the σ_i's. The weighted WMB algorithm incorporates these σ_i's into KSCOEFS, and then evaluates Equation (8).

3 The Weighted WMB Algorithm

3.1 Linear Kubelka-Munk Relationships

The Kubelka-Munk model[1] characterizes a paint by using an absorption coefficient, K, and a scattering coefficient, S. Both coefficients are functions of wavelength, and both vary between 0 and 1. If the paint is applied as a masstone, the bulk reflectance R (often denoted R_∞ for a masstone) can be related to the ratio of K and S:

$$\frac{K}{S} = \frac{(1-R)^2}{2R}. \tag{13}$$

For convenience, the right-hand side will be denoted as a function, $f(R)$. A set of n paints can be mixed together, in concentrations $C_1, C_2, ...C_n$, to produce a new paint, of a different colour. If the i^{th} paint has Kubelka-Munk coefficients K_i and S_i, then the Kubelka-Munk coefficients for the mixture are given by

$$K_{\text{mix}} = C_1K_1 + C_2K_2 + ... + C_nK_n, \tag{14}$$
$$S_{\text{mix}} = C_1S_1 + C_2S_2 + ... + C_nS_n. \tag{15}$$

Equations (14) and (15) can be substituted into Equation (13) to give relationships for the paint mixture as a whole:

$$\left(\frac{K}{S}\right)_{\text{mix}} = \frac{C_1K_1 + C_2K_2 + ... + C_nK_n}{C_1S_1 + C_2S_2 + ... + C_nS_n} = \frac{(1-R_{\text{mix}})^2}{2R_{\text{mix}}}. \tag{16}$$

For brevity, the last four equations omit any dependence on wavelength.

In practice, the reflectance spectra R for paints and their mixtures can be measured directly (leaving aside the Saunderson correction[1]). Likewise, the concentrations C_i are known. It is desired to determine K and S, at a given wavelength, for each of the n constituent paints, given reflectance data for a set of m mixtures of those paints, in known concentrations.

The WMB algorithm uses a least squares approach to determine K and S. For each mixture, Equation (16) is rearranged to give a linear relationship:

$$-C_1K_1 - C_2K_2 - ... - C_nK_n + \left(\frac{K}{S}\right)_{\text{mix}} (C_1S_1 + C_2S_2 + ... + C_nS_n) = 0, \tag{17}$$

where each C_i is understood to depend on the mixture. In vector form, Equation

(17) becomes:

$$\left[-C_1, -C_2, ..., -C_n, \left(\frac{K}{S}\right)_{\text{mix}} C_1, \left(\frac{K}{S}\right)_{\text{mix}} C_2, ..., \left(\frac{K}{S}\right)_{\text{mix}} C_n\right] \begin{bmatrix} K_1 \\ K_2 \\ ... \\ K_n \\ S_1 \\ S_2 \\ ... \\ S_n \end{bmatrix} = 0. \quad (18)$$

The vertical vector does not depend on the mixture, but the horizontal vector does. All the horizontal vectors, one for each mixture, can be stacked to form an $m \times n$ matrix, and the 0 on the right-hand side can be repeated vertically m times to give a vertical 0-vector. Thus, Equation (18) can generate a single matrix equation that contains information for all the mixtures. In order to avoid a physically unrealistic solution, in which every K and S is identically 0, a constraint row is added, consisting of all 1's, at the bottom of the $m \times n$ matrix; the augmented matrix is denoted KSCOEFS. Similarly, a single 1 is added to the bottom of the vertical 0-vector, producing a vector called OBS. When the vertical vector of K's and S's is denoted KANDS, Equation (18) becomes a matrix equation identical to Equation (7), which was presented in the original 1987 algorithm.

Apart from the constraint, this least squares formulation is similar to the example in Figure 3. Each row of the matrix KSCOEFS gives a linear relationship, which is analogous to a line in the plane. The vector KANDS corresponds to the x-y-pair, though of course it has a higher dimension. In the following subsections, a closer examination of $f(R)$ and human perceptual response will determine the probabilistic form of the residuals for these relationships, from which weights can be calculated for the rows of KSCOEFS.

3.2 Reflectance Weighting

Least squares algorithms use the inverse standard deviation of a residual as a weight. This section calculates how a standard deviation, σ_i, depends on reflectance, R. The dependence relationship will help motivate the weighted WMB algorithm. Typically, σ_i is the standard deviation of the measurement error. In the WMB algorithm, however, residuals are obtained by evaluating Equation (17), while the measurements are spectrophotometric reflectance measurements of paint mixtures. We will manipulate Equation (17) to express a residual as a function of spectrophotometer error. Both

the residual and the spectrophotometer error are probability distributions, rather than single values. σ_i is the standard deviation of the residual's distribution.

We will model a spectrophotometric measurement, R_m, of a true reflectance level, R_t, as unbiased and normally distributed:

$$R_m - R_t \sim N\left(0, \sigma_m^2\right). \tag{19}$$

A measurement is said to be unbiased if its expected value is the true value, so the mean error is 0. A measurement with normal error will be within $2\sigma_m$ of the true value 95% of the time, and within $3\sigma_m$ 99% of the time. We will posit, furthermore, that σ_m^2 is independent of reflectance level. As remarked earlier, it is not necessary to know the value of σ_m^2, provided that it is identical for all measurements.

Begin with Equation (17) for a particular mixture. Suppose that K and S are the true Kubelka-Munk coefficients for that mixture. We wish to find the probability distribution of the residual r for that mixture. Combine Equations (13) through (17) to get

$$\begin{aligned} r &= K_{\text{mix}} - f(R_{m,\text{mix}})S_{\text{mix}} && (20)\\ &= S \cdot \left(\frac{K}{S} - f(R_m)\right), && (21) \end{aligned}$$

where some subscripts have been dropped for conciseness. The function f inverts to R_t, the true reflectance:

$$f(R_{\text{t}}) = \left(\frac{K}{S}\right). \tag{22}$$

Substitute Equation (22) into Equation (21) to get

$$r = S \cdot \left(f(R_t) - f(R_m)\right). \tag{23}$$

Now use a Taylor expansion to approximate $f(R)$ as a linear function around R_m. This linear approximation is valid when R is not too far from R_m.

$$f(R) \doteq f(R_m) + f'(R_m)(R - R_m). \tag{24}$$

As long as the spectrophotometer is reasonably accurate, R_t should not be too far from R_m, so let R be R_t in Equation (24), and substitute into Equation (23):

$$\begin{aligned} r &= S \cdot \left(f(R_m) + f'(R_m)(R_t - R_m) - f(R_m)\right) && (25)\\ &= Sf'(R_m)(R_t - R_m) && (26)\\ &\sim Sf'(R_m)N(0, \sigma_m^2). && (27) \end{aligned}$$

Differentiate the right-hand side of Equation (13) to get

$$f'(R) = \frac{R^2 - 1}{2R^2}. \tag{28}$$

Evaluate Equation (28) at R_m, and substitute into Equation (27) to get

$$r \sim S\frac{(R_m^2 - 1)}{2R_m^2}N(0, \sigma_m^2). \tag{29}$$

Equation (29) is a central result of this paper. It gives the statistical distribution from which the residuals are drawn. The inverse weight, $1/\sigma_i$, of the i^{th} residual, r_i, is the standard deviation of r_i. From Equation (29), it follows that

$$\sigma_i = S_i\frac{1 - R_i^2}{2R_i^2}\sigma_m, \tag{30}$$

where R_i is the measured reflectance of the i^{th} mixture. The term σ_m might be unknown, but it is a common factor in all the weights, and so can be discarded. The reflectance term R_i is measured directly. The scattering coefficient S_i is not known exactly, but it can be estimated by running the original 1987 algorithm, without adding any weights, and using Equation (15). Later analysis, of the factors' orders of magnitude, will show that this approximation is adequate.

3.3 Perceptual Weighting

Reflectance weighting shifts the weight criterion from residuals to reflectance differences. Perceptually, however, value or lightness compression can make this new criterion misleading, because humans judge the same reflectance percentage difference to be more substantial at lower reflectance levels than at higher reflectance levels. The residuals of the least squares problem, then, should be adjusted to incorporate perceptual terms, and not just reflectance terms. CIELAB coordinates[10] relate the perceived lightness, L^*, to the photopic luminance, Y :

$$L^* = 116\,(Y/Y_n)^{1/3} - 16, \tag{31}$$

where Y_n is the tristimulus value of the reference white. While Y/Y_n is not identical with reflectance, the two are roughly equivalent. Therefore

$$L^*(R) \doteq 116R^{1/3} - 16. \tag{32}$$

Using a linear approximation to Equation (32), and evaluating at $R = R_t$, we get

$$L^*(R_t) \doteq L^*(R_m) + \frac{116}{3} R_m^{-2/3} (R_t - R_m) \tag{33}$$

$$L^*(R_t) - L^*(R_m) \sim \frac{116}{3} R_m^{-2/3} N(0, \sigma_m^2) \tag{34}$$

Apart from the normal distribution, Equation (34) has already been derived and used by Viggiano,[8] for a perceptual metric involving metamerism.

Equation (34) suggests that residuals should be weighted more heavily when reflectance levels are low, to account for lightness compression. When R_m is near 1, the right-hand side of Equation (34) is smaller than when R_m is near 0; the term $R_m^{-2/3}$ is always at least 1. An increased weight corresponds to a decreased σ_i, so we should divide the σ_i in Equation (30) by the coefficient in Equation (34) to get a new standard deviation:

$$\sigma_{Li} = \frac{3}{232} S_i R_i^{-4/3} \big(1 - R_i^2\big) \sigma_m. \tag{35}$$

Since the least squares solution will not be affected if we multiply every standard deviation by the same constant, we can obtain a simpler expression:

$$\sigma_{Li} = S_i R_i^{-4/3} \big(1 - R_i^2\big). \tag{36}$$

When the σ's in Equation (36) are used in the WMB algorithm, the resulting weights account for both reflectance measurement errors and human lightness compression. This perceptual reflectance weighting is the basis for the weighted WMB algorithm.

3.4 The Weighted WMB Algorithm

The following algorithm is recommended as a refinement to the 1987 algorithm of Walowit, McCarthy, and Berns:

1. Run the 1987 algorithm, for the sole purpose of estimating the Kubelka-Munk scattering coefficients $S_1, S_2, \ldots, S_n$, for each of the constituent colorants.
2. The i^{th} colorant mixture has known concentration coefficients, $C_{i,1}, C_{i,2}, \ldots, C_{i,n}$, which have been chosen to sum to 1. Estimate S_i by

$$S_i = C_{i,1} S_1 + C_{i,2} S_2 + \ldots + C_{i,n} S_n. \tag{37}$$

3. Calculate the standard deviation, σ_i, of the residual for the i^{th} colorant mixture by

$$\sigma_i = S_i R_i^{-4/3}\big(1 - R_i^2\big). \tag{38}$$

4. Construct the i^{th} row of the matrix KSCOEFS as in the 1987 algorithm. Divide this row by σ_i.
5. Assemble all the modified rows into a weighted KSCOEFS matrix, and add a row of 1's at the bottom.
6. Calculate OBS and KANDS in accordance with the 1987 algorithm, using the weighted KSCOEFS matrix from our Step 5. KANDS gives the desired Kubelka-Munk coefficients.

Nobbs[6] had previously suggested some sets of weights for Kubelka-Munk estimation, that differ from those in the weighted WMB algorithm. His Equations (6.82), (6.84), and (6.86), like our Equation (30), account for the sensitivity of K/S as a function of R. Rather than estimate S for each mixture as we have done, however, Nobbs suggests some simplifying assumptions, for example that K or S is constant, or that the expression $K(K+2S)$ is constant. Our Step 1 obviates these assumptions. Furthermore, Nobbs does not account for lightness compression, as we do. Nevertheless, Nobbs's weights should be a significant improvement over equal weights. The further refinements in the weighted WMB algorithm should similarly improve on Nobbs's weights.

3.5 Sensitivity Analysis

Sensitivity in the relationship between Kubelka-Munk coefficients and reflectance measurements is the reason that weights must be chosen carefully. Figure 4, a plot of the function $f(R)$ defined by Equation (13), illustrates this sensitivity. The two indicated points show that a difference of 1% in R, when going from $R = 0.02$ to $R = 0.03$, causes a difference of 7 in K/S. The same 1% difference in R, however, when going from $R = 0.85$ to $R = 0.86$, only causes a minuscule difference of 0.002 in K/S. At higher reflectance levels, then, a very small change in K/S can lead to a large change in R, orders of magnitude larger than the same small change in K/S at a lower reflectance level. By weighting all residuals equally, the weighted WMB algorithm is in effect looking at the differences in Kubelka-Munk terms (such as K/S), rather than reflectance terms. Thus the large reflectance changes in the upper curve of Figure 1 are discounted, because they do not affect K and S very much. To account for reflectance correctly, perceptual reflectance weighting assigns

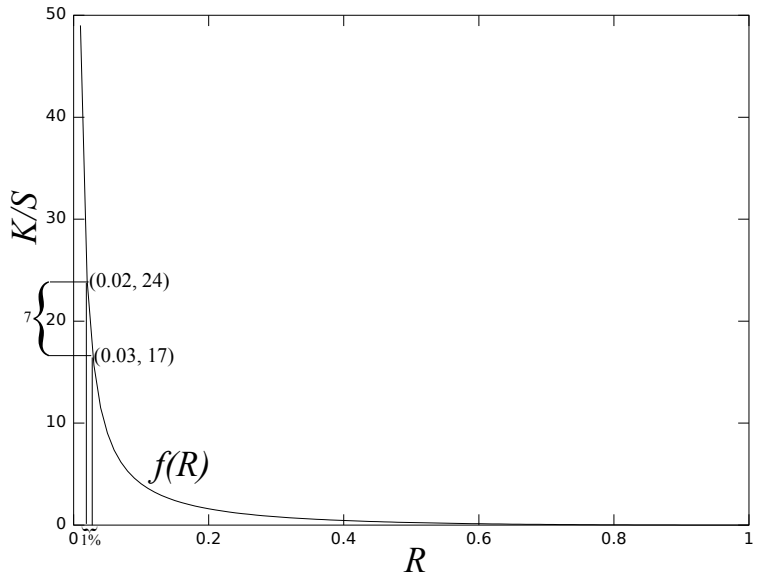


Figure 4: Sensitivity due to $f(R)$

unequal weights. This section will show that the nw weights can vary by several orders of magnitude.

The new weights are derived from Equation (36), which can be decomposed into three factors:

$$\sigma_{Li} = S \cdot \frac{(R^2 - 1)}{2R^2} \cdot R^{2/3}. \tag{39}$$

The first term is the scattering coefficient, the second term (by Equation (28)) is the derivative of the relationship between K/S and R, and the third term involves the derivative of lightness compression. This section investigates the weight disparity for the various residuals when perceptual reflectance weighting is used. Disparity in this context refers to the differences, or ratios, between the weights associated with a set of paint mixtures, at a particular wavelength. A convenient measure of disparity is the *condition number*, which is the ratio of the maximum weight to the minimum weight. Since weight is the inverse of σ, the condition number for weights and σ's is the same. Also, the condition number does not change when all the weights are multiplied by the same constant.

It will be seen that the largest weights can exceed the smallest weights by a few orders of magnitude. This disparity contrasts with the 1987 algorithm, where all the weights are equal. Most of the disparity results from the second term, $f'(R)$, which

can introduce differences of several orders of magnitude. The third term would cause at most just over one order of magnitude. The first term, the scattering coefficient, might cause at most two orders of magnitude.

These estimates were made for artist's paints, though they would apply in many other situations, too. It is rare for even the darkest artist's paints to attain a Munsell value much less than 1. A Munsell value of 1 corresponds to a reflectance (for an ideal grey) of 1.2%. For artist's paints, then, we can safely assume that R has a lower limit of about 1%. All three terms, even the scattering coefficient, are related to R. In addition, unless they are deliberately thinned with a glazing medium, artist's paints, even "transparent" paints, have some coverage capability, so will tend to transmit less light rather than more. These properties will help find bounds for the three terms.

First, the scattering coefficient, S. All the light that impinges on a thin internal layer of paint (in accordance with the Kubelka-Munk model) is either absorbed, scattered, or transmitted, so we can write

$$K + S + T = 1, \tag{40}$$

where T is the proportion of light that is transmitted. Rearrange Equation (40) to read $K = 1 - S - T$, substitute the new expression into $K/S = f(R)$, and rearrange further to get

$$S = \frac{1 - T}{f(R) + 1}. \tag{41}$$

The upper bound on S is, of course, 1. When R reaches its lower limit of 1%, then $f(R)$ is about 49, so the denominator is about 50. Even if the transmission coefficient T were as high as 50%, the value of S would still be no lower than 0.01. The largest condition number of S is therefore not much more than 100, and would often be less.

The second term is the derivative of $f(R)$, shown in Figure 5. The logarithmic plot shows that weights can differ by several orders of magnitude. At 3% reflectance, for example, the slope is -555, while at 75% reflectance, it is -0.389, a difference of more than three orders of magnitude.

The third term is $R^{2/3}$. This function is 1 when R is 100%, and decreases monotonically as R decreases. When R reaches its lower bound of 1%, the function attains its minimum value, which is only about 0.046, differing by a factor of about 22 from the maximum. The greatest condition number between two weights is therefore not much more than one order of magnitude.

The third term works in the opposite direction to the second term. At low reflectance levels, the eye responds more to small reflection differences. Thus more

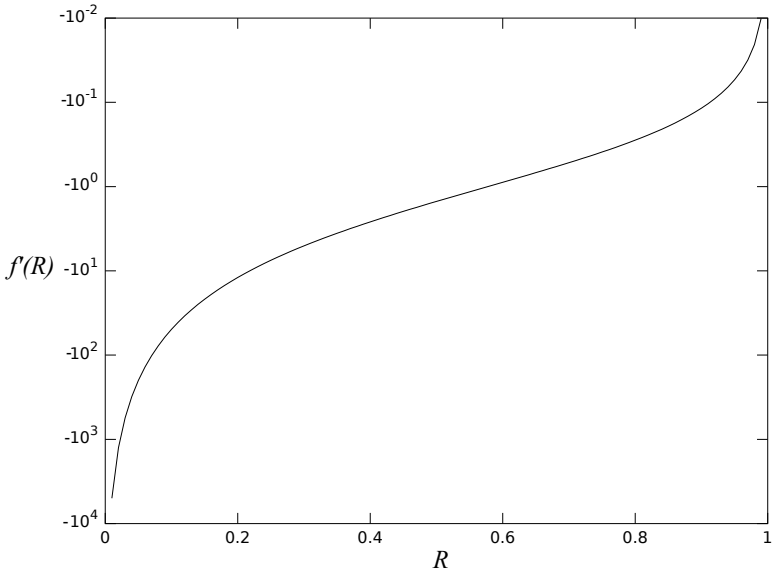


Figure 5: Derivative of $f(R)$

care is taken over dark colours than light colours. The second term, $f'(R)$, however, emphasizes matches for lighter colours, to avoid errors like the poor match for white in Figure 1. Since the condition number of $f'(R)$ can be multiple orders of magnitude, while the third term causes a condition number of at most 22, it is clear that $f'(R)$ dominates.

Similarly, $f'(R)$ dominates the scattering coefficient, whose condition number is at most two orders of magnitude. This dominance is also why the 1987 algorithm provides acceptable estimates for the scattering coefficients. Even if its estimates of S are in error by a large factor, such as 3, that error will be dwarfed by $f'(R)$, which likely exceeds S by some orders of magnitude.

4 Examples

An example, based on the tint ladder in Figure 1, will illustrate the weighted WMB algorithm. The thin black lines in Figure 1 are predicted reflectance spectra, that the Kubelka-Munk model generated from a set of estimated K and S values. Our example will posit that

1. There exist two paints with those exact K and S values,
2. The colours produced by mixing those two paints are in accordance with the

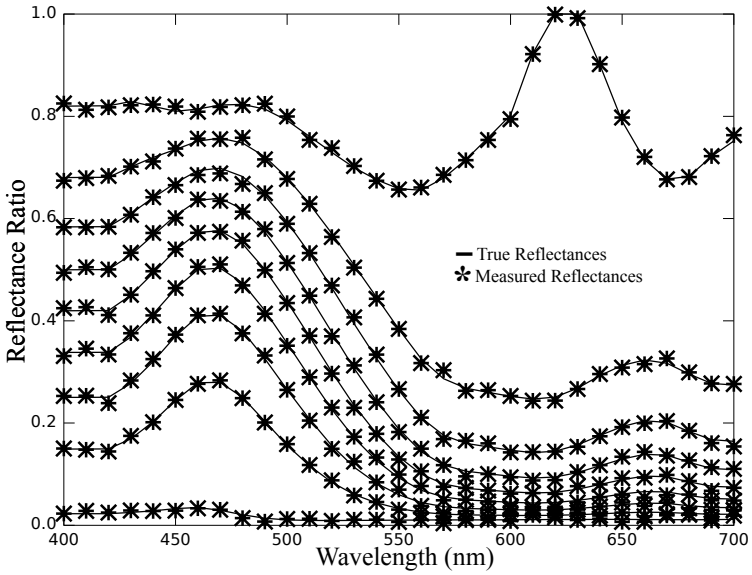


Figure 6: True (Kubelka-Munk) Reflectances and Measured Reflectances

Kubelka-Munk model, and

3. Our starting data is reflectance measurements of those paints at the concentrations shown in Figure 1. The measurements are subject to a random error, which follows a normal distribution with mean 0 and standard deviation 0.5 percentage points. Figure 6 shows the data as asterisks that are near, but usually not on, the thin black lines. (In practice, of course, only the asterisks would be available, and not the lines.)

Our goal is to reconstruct the thin black lines seen in Figure 1, using the reflectance data provided by the asterisks. The WMB algorithm will be compared with the weighted WMB algorithm.

This example is different from actual problems, in that it assumes that the Kubelka-Munk model is a complete and perfect description of paint mixing. Any needed adjustments, such as the Saunderson correction,[1] are assumed to have been implemented. These assumptions eliminate model error, and isolate measurement error, so that the algorithms are tested, rather than the Kubelka-Munk model itself.

Figure 7 shows the results of both the WMB and weighted WMB algorithms, when applied to the asterisk data. The WMB predictions are erratic, especially for lighter colours. The weighted WMB predictions, on the other hand, are smoother and more accurate, for both lighter and darker colours. This disparity is obvious in the right half, where the reflectance spectra are not evenly spaced. The 1987 algorithm,

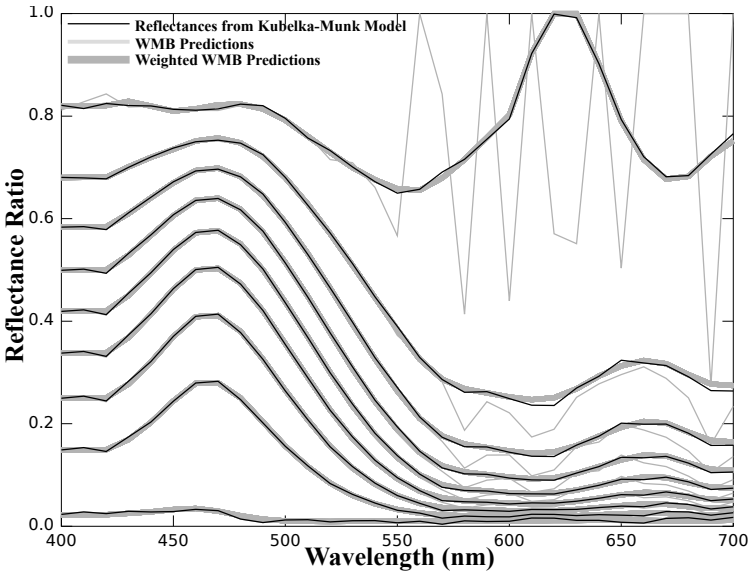


Figure 7: Comparison of WMB and Weighted WMB Algorithms

which weights all the mixtures equally, finds the large reflectance differences in the upper curve acceptable, because they only cause slight changes in the residuals from Equation (17). The weighted WMB algorithm, on the other hand, correctly weights the lighter colours more. Even small residuals for the lighter colours are assigned a heavy penalty, because they cause disproportionately large reflectance differences. Overall, the weighted WMB algorithm is more stable and accurate than the original 1987 algorithm.

As mentioned earlier, the data in this example were generated from the Kubelka-Munk model. In the real world, of course, that model might only be approximate. In Figures 1 and 2, the two algorithms were applied to such real-world data. Despite the fact that no Saunderson correction was used, the weighted WMB algorithm did a creditable job of prediction, and avoided some of the erratic outcomes of the 1987 algorithm.

Figure 8 shows the condition numbers for the weights used by the weighted WMB algorithm in Figure 2, and for the three contributing terms from Equation (39). As expected, the second term, $(R^2-1)/2R^2$, dominates: in the right half of the spectrum, the heaviest residual carries 25,000 times as much weight as the lightest residual. The first term, S, reaches a maximum ratio of just over 100, while the third term, $R^{2/3}$, reaches a maximum ratio of just over 10, in line with expectations. The individual terms combine to give an overall maximum ratio of about 250, in the right half of

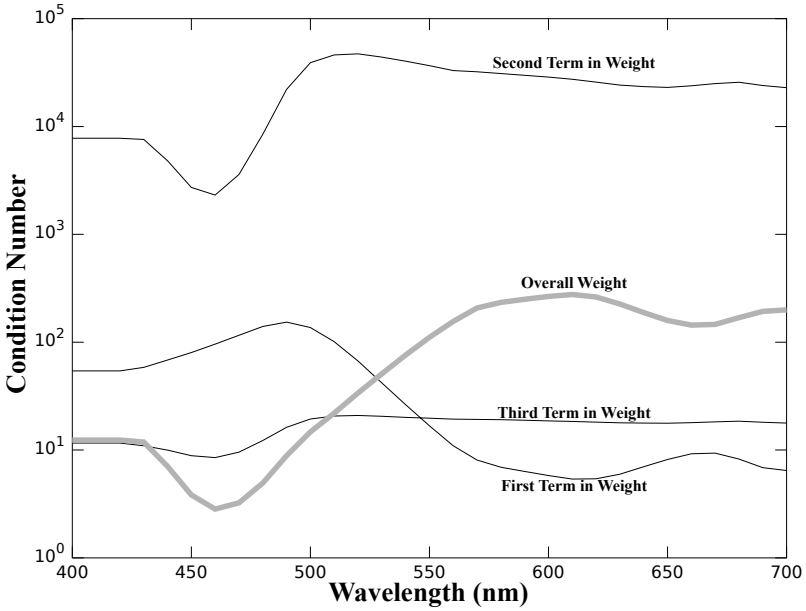


Figure 8: Condition Numbers in Weighted WMB Algorithm, for Figure 2

the spectrum. Even in the left half of the spectrum, the weighted algorithm gives some residuals five to ten times more importance than other residuals. The weights evenly cover a wide gamut, as seen by considering the weights for the nine curves at 620 nm. If the residual for the darkest curve is scaled to have a value of 1, then the other eight curves, from darkest to lightest, have respective weights of 16, 39, 57, 78, 130, 121, 211, and 263. These weights are a significant departure from the original 1987 algorithm which treats all residuals equally.

While the predicted reflectances vary dramatically, the Kubelka-Munk coefficients seem hardly to vary at all. Figure 9 shows the K and S coefficients, for the lightest and darkest colours in Figure 2, calculated by the unweighted and weighted WMB algorithms. Usually less than 1%, the differences in the figure appear inconsequential. For lighter colours, however, sensitivity magnifies such small differences in K and S into the large reflectance differences seen in Figure 2. The weighted WMB algorithm compensates for this sensitivity by weighting the residuals for lighter colours very heavily, in terms of their reflectance and perceptual consequences. The original WMB algorithm makes no such provision, and can thus produce large reflectance errors. The small percentage difference between the WMB and weighted WMB estimates of S is another justification for using the WMB estimate of S in the weighted WMB algorithm: a slight percentage error in S does not greatly affect the weights given by

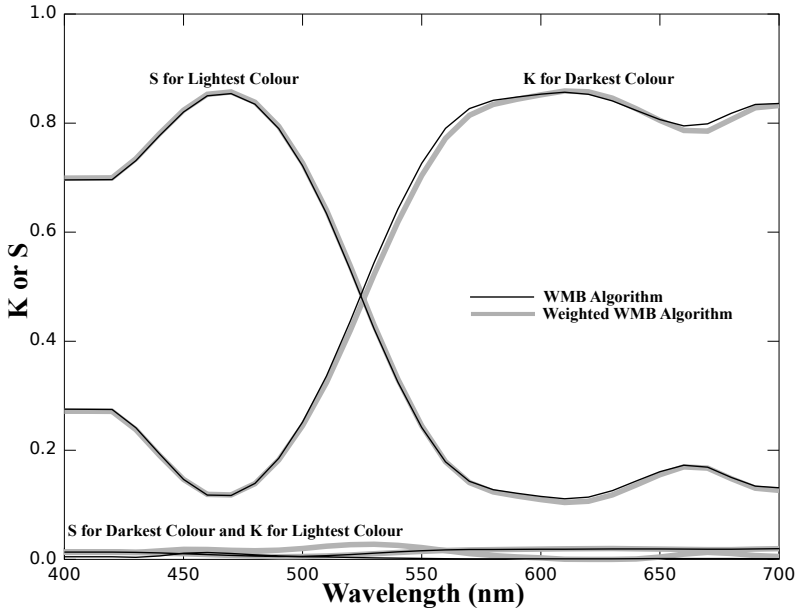


Figure 9: Kubelka-Munk Coefficients for Original and Weighted WMB Algorithms

Equation (38).

5 Summary

A practical and a theoretical example, along with a mathematical derivation, have shown that perceptual reflectance weighting of residuals can significantly improve the 1987 Kubelka-Munk estimation algorithm of Walowit, McCarthy, and Berns. The 1987 algorithm is easily modified, by multiplying each row of its coefficient matrix KSCOEFS by an appropriate weight factor. The multiplicative factors were derived analytically from two sources: the relationship between K/S and reflectance level, and the relationship between perceived lightness and reflectance level. It is hoped that real-world application will lead to further refinement and understanding of least squares Kubelka-Munk estimation algorithms.

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