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Evaluation of uncertainties for CIELAB color coordinates

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Abstract

CIELAB color coordinates are characteristics of visible object's spectra widely used in color science, and a reliable evaluation of the uncertainty associated with measured color coordinates is desirable. The calculation of CIELAB color coordinates requires the application of a nonlinear transformation. We consider two ways to calculate the uncertainty of CIELAB color coordinates that originates from the uncertainty of the observed spectrum. The first approach is based on a linearization of the nonlinear transformation and a propagation of variances and covariances. The second approach is a Monte Carlo procedure that completely accounts for the nonlinearity of the transformation. While the approach based on linearization results in analytical formulas, the adequacy of linearization ought to be checked and the proposed Monte Carlo method can serve as a reference method for this purpose. We illustrate such proceeding in a large range of scenarios and explore those cases for which the method based on linearization may safely be applied.

KEYWORDS
CIELAB color coordinates, measurement uncertainty, Monte Carlo method

1 | INTRODUCTION

The chromatic content of a visible object's spectrum is often summarized in terms of CIELAB color coordinates.[1–4] CIELAB color coordinates provide a device-independent representation and intend to transform a spectrum into a color space that reflects the nonlinear response of the human eye. The calculation of CIELAB color coordinates is carried out in two steps. First, tristimulus values are determined by a linear transformation of the spectrum. Then, a nonlinear transformation is applied to the tristimulus values yielding the CIELAB color coordinates. According to their definition, estimates for the CIELAB color coordinates are expected to be correlated.

An adequate evaluation of the uncertainty associated with the obtained CIELAB color coordinates is important, for example, to compare results of different measurements, to establish industrial tolerances or to decide on significant differences.[5] It is common practice in visual experiments to characterize visual differences in terms of calculated color coordinates without considering their associated uncertainties. However, for large uncertainties the difference in the color coordinates may turn out to be unreliable. Moreover, it is not unusual to find color tolerance specifications for products that cannot be met just due to the large measurement uncertainty of the colorimeter used. Since tristimulus values are often correlated, an uncertainty evaluation should include the calculation of correlations between the CIELAB color coordinates.[4–7] Basically, an uncertainty characterization can be carried out by propagating variances and covariances of the observed spectrum in terms of the CIELAB color coordinates.[8] This poses a challenging task and because of that the evaluation of covariances is sometimes omitted or simplified numerical approaches are applied.[9]

Metrology is concerned with measurements at the lowest level of uncertainty, and a reliable quantification of the uncertainty reached is therefore key in this field. For this reason, general guidelines for uncertainty evaluation have been developed in metrology[10,11] and successfully applied in many applications. The treatment of uncertainty in this article is based on these guidelines.

The tristimulus values depend linearly on the spectrum, and the propagation of variances and covariances associated with the observed spectrum to the tristimulus values can safely be carried out analytically. This does no longer hold for the propagation of resulting variances and covariances of the tristimulus values to the CIELAB color coordinates due to the nonlinearity of that relationship. One may linearize the nonlinear model and subsequently carry out an analytical propagation of variances and covariances. However, such a linearization may, or may not, prove sufficient.

In this article, we concentrate on the propagation of variances and covariances through the nonlinear relationship between the tristimulus values and the CIELAB color coordinates. Analytical formulas are derived based on a linearization. In addition, a Monte Carlo procedure is proposed that can be used to check the validity of the linearization. Both procedures are applied to a large range of scenarios to explore those cases where the simple analytical approach proves sufficient.

This article is organized as follows. In the next section, we provide the basic model and its Jacobian. This is followed by a brief introduction to uncertainty evaluation in metrology, where also the two proposed procedures are presented. In the results section examples with varying degrees of relevance of the nonlinearity in the model are discussed. Finally, some recommendations are given.

2 | CIELAB COLOR COORDINATES

CIELAB color coordinates are given by[1–3]

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

$$a^*=500\,(f(X/X_n)-f(Y/Y_n)) \tag{2}$$

$$b^*=200\,(f(Y/Y_n)-f(Z/Z_n)), \tag{3}$$

where

$$f(t)=\begin{cases} t^{1/3} & t>\left(\dfrac{6}{29}\right)^3 \\ \dfrac{1}{3}\left(\dfrac{29}{6}\right)^2 t+\dfrac{4}{29} & \text{otherwise} \end{cases}. \tag{4}$$

The tristimulus values X, Y, and Z are obtained by a weighted integral over the observed spectrum.[2] The quantities X_n, Y_n, and Z_n refer to CIE XYZ tristimulus values of the reference white point and are supposed to be known exactly. For the numerical results presented in this work we consider the CIE Standard Illuminant D65 with $X_n=95.047$, $Y_n=100.000$, and $Z_n=108.883$. The CIELAB color coordinates are considered to be determined from reflectance measurements and L^* has a maximum value of 100.

The function $f(t)$ shows a linear behavior for small values of its argument. For larger arguments the function depends nonlinearly on its argument. At $t=(6/29)^3\approx 0.0089$ the two regimes meet. Since typical tristimulus values range from 0 to 100, the linear model applies only to a rather small part of the possible tristimulus values. Note that the function is continuously differentiable also at $t=(6/29)^3$, cf. Equation 6 below.

The Jacobian matrix J of the model given by Equations 1–4 follows as

$$J=\begin{pmatrix} \dfrac{\partial L^*}{\partial X} & \dfrac{\partial L^*}{\partial Y} & \dfrac{\partial L^*}{\partial Z} \\ \dfrac{\partial a^*}{\partial X} & \dfrac{\partial a^*}{\partial Y} & \dfrac{\partial a^*}{\partial Z} \\ \dfrac{\partial b^*}{\partial X} & \dfrac{\partial b^*}{\partial Y} & \dfrac{\partial b^*}{\partial Z} \end{pmatrix}$$

$$=\begin{pmatrix} 0 & \dfrac{116}{Y_n}f'(Y/Y_n) & 0 \\ \dfrac{500}{X_n}f'(X/X_n) & -\dfrac{500}{Y_n}f'(Y/Y_n) & 0 \\ 0 & \dfrac{200}{Y_n}f'(Y/Y_n) & -\dfrac{200}{Z_n}f'(Z/Z_n) \end{pmatrix}, \tag{5}$$

where

$$f'(t)=\begin{cases} \dfrac{1}{3}t^{-2/3} & t>\left(\dfrac{6}{29}\right)^3 \\ \dfrac{1}{3}\left(\dfrac{29}{6}\right)^2 & \text{otherwise} \end{cases}. \tag{6}$$

Note that the derivative $f'(t)$ is continuous at $t=(6/29)^3$.

3 | UNCERTAINTY EVALUATION

In the following, a brief introduction is given on uncertainty evaluation in metrology according to the guidelines.[10,11] Then, the evaluation procedures based on a linearized model and the Monte Carlo approach are presented. While for the brief introduction a generic notation is used, the two evaluation procedures are then described in terms of the particular model.

An uncertainty exercise in metrology typically starts with setting up a mathematical model

$$\eta=g(\theta) \tag{7}$$

which relates the measurand or quantity of interest, η, to a number of N influencing quantities $\theta=(\theta_1,\ldots,\theta_N)^T$. The superscript T stands for the vector or matrix transpose. The measurand may be univariate or multivariate. In our case, the measurand consists of the three CIELAB color coordinates $(L^*,a^*,b^*)^T$ and is thus multivariate and the corresponding mathematical model (i.e. Equation 7) is given by the nonlinear transformation in Equations 1–4. Typically, there are several input quantities, that is, $N>1$, which are here conveniently summarized by the vector θ.

An uncertainty calculation then proceeds as follows. Information about the input quantities is gathered, for example, from measurements or other sources of information. This knowledge about the input quantities may then be summarized in terms of an estimate $\hat{\theta}$, together with a covariance matrix V_θ. The diagonal elements of V_θ are the variances associated with the single input quantities, and the off-diagonal elements are corresponding covariances. Covariances, variances and correlation coefficients are related through the equation $\mathrm{Corr}(\theta_1, \theta_2) = \mathrm{Cov}(\theta_1, \theta_2) / \sqrt{\mathrm{Var}(\theta_1)\,\mathrm{Var}(\theta_2)}$. So-called standard uncertainties are defined as the square root of variances. Then, the estimate and the variances are propagated through (a linearization of) the model given by Equation 7, yielding the estimate

$$\hat{\eta} = g(\hat{\theta}), \tag{8}$$

together with the covariance matrix

$$V_\eta = J\, V_\theta\, J^T, \tag{9}$$

where J denotes the Jacobian matrix for the model (Equation 7) with $J_{\alpha,\beta} = \partial g_\alpha / \partial \theta_\beta$. The Jacobian matrix resulting for the CIELAB color coordinates is given in Equations 5 and 6.

Under the assumption that a multivariate Gaussian distribution with mean $\hat{\eta}$ and covariance matrix V_η adequately represents one's state of knowledge about the measurand, so-called coverage regions can be calculated on the basis of Equations 8 and 9, i.e. regions over which this distribution assigns a prescribed probability. A 95% coverage interval for η_1, for example, would then be obtained as

$$I_{\eta_1} = [\hat{\eta}_1 - 1.96\ u(\eta_1),\ \hat{\eta}_1 + 1.96\ u(\eta_1)], \tag{10}$$

where $u(\eta_1) = \sqrt{(V_\eta)_{11}}$ denotes the standard uncertainty of η_1.

In cases where a linearization of the model given by Equation 7 is no longer adequate or when the normality assumption about the measurand is no longer justified, the guidelines in metrology suggest the application of a Monte Carlo procedure instead. The Monte Carlo procedure draws samples for the measurand from a distribution that is constructed as follows. First, a (joint) distribution is assigned to θ. Once this distribution for the input quantities is formed, the distribution for the measurand is determined by probability calculus using Equation 7. The joint distribution for θ may be a multivariate Gaussian distribution or any other distribution that appropriately encodes one's state of knowledge about the input quantities. Details of the Monte Carlo procedure are given below in the context of CIELAB color coordinates.

3.1 | Uncertainty evaluation using a propagation of uncertainties

In the following we assume that estimates $\hat{X}$, $\hat{Y}$, and $\hat{Z}$, along with a 3×3 covariance matrix $V_{(X,Y,Z)}$ for the tristimulus values X, Y, and Z, have been derived from the measurement of the corresponding spectrum. Applying the scheme of propagation of estimates and variances and covariances through the linearized model as described above then yields the following expressions for the resulting estimates $\hat{L}^*$, $\hat{a}^*$, $\hat{b}^*$

$$\hat{L}^* = 116 f(\hat{Y}/Y_n) - 16 \tag{11}$$

$$\hat{a}^* = 500\left(f(\hat{X}/X_n) - f(\hat{Y}/Y_n)\right) \tag{12}$$

$$\hat{b}^* = 200\left(f(\bar{Y}/Y_n) - f(\hat{Z}/Z_n)\right), \tag{13}$$

together with the associated covariance matrix $V_{(L^*,a^*,b^*)}$

$$V_{(L^*,a^*,b^*)} = J V_{(X,Y,Z)} J^T, \tag{14}$$

where the Jacobian matrix J is calculated according to Equation 5 at $(X,Y,Z)^T = (\hat{X},\hat{Y},\hat{Z})^T$. The standard uncertainties associated with the estimates of the color coordinates are then given by

$$u(L^*) = \sqrt{(V_{(L^*,a^*,b^*)})_{11}} \tag{15}$$

$$u(a^*) = \sqrt{(V_{(L^*,a^*,b^*)})_{22}} \tag{16}$$

$$u(b^*) = \sqrt{(V_{(L^*,a^*,b^*)})_{33}}. \tag{17}$$

Under the additional assumption of a Gaussian distribution, 95% coverage intervals for the color coordinates are obtained as

$$I_{L^*} = [\hat{L}^* - 1.96\ u(L^*),\ \hat{L}^* + 1.96\ u(L^*)], \tag{18}$$

$$I_{a^*} = [\hat{a}^* - 1.96\ u(a^*),\ \hat{a}^* + 1.96\ u(a^*)], \tag{19}$$

$$I_{b^*} = [\hat{b}^* - 1.96\ u(b^*),\ \hat{b}^* + 1.96\ u(b^*)]. \tag{20}$$

3.2 | Uncertainty evaluation using a Monte Carlo procedure

In the following we assume that a Gaussian distribution with mean $(\hat{X},\hat{Y},\hat{Z})^T$ and covariance matrix $V_{(X,Y,Z)}$ adequately models one's state of knowledge about the tristimulus values X, Y, and Z, gained from the measurement of the corresponding spectrum. Note that both $(\hat{X},\hat{Y},\hat{Z})^T$ and covariance matrix $V_{(X,Y,Z)}$ are known parameters of this distribution.

The distribution for the tristimulus values, together with the transformation given by Equations 1–4, uniquely determine the distribution for the CIELAB color coordinates. This distribution then encodes one's state of knowledge about the CIELAB color coordinates. However, the distribution cannot be calculated analytically and needs to be determined numerically. The Monte Carlo method below allows to draw samples from this distribution, which in turn can be used to infer that distribution or any functional derived from it such as, for example, its mean or its covariance matrix.

The Monte Carlo procedure is based on Ref. 11 and works as follows. Repeatedly, samples from the distribution for the tristimulus values X, Y, and Z are drawn and inserted into the transformation given by Equations 1–4, thereby resulting in a sample of the CIELAB coordinates from their target distribution. In repeating this step many times, a large sample from the sought distribution for the CIELAB coordinates is obtained. From this sample, the distribution for the CIELAB coordinates can be approximated, and estimates along with the associated standard uncertainties can be obtained. Likewise, correlation coefficients and 95% coverage intervals can be calculated. More precisely, the procedure works as follows:

1. Define the number M of Monte Carlo samples to be drawn. M should be large enough so that the results have sufficiently stabilized. We recommend to use $M=10^7$ and to repeat the whole process several times to ensure that the results have stabilized. We refer to Ref. 12 for more advanced, sequential schemes to determine the number of Monte Carlo samples.
2. For $k=1,2,\ldots,M$ repeat:
   a Draw a random sample X_k,Y_k,Z_k from the multivariate Gaussian distribution $N((\hat{X},\hat{Y},\hat{Z})^T, V_{(X,Y,Z)})$ for the tristimulus values.
   b Apply the transformation given by Equations 1–4 to obtain the sample $(L_k^*, a_k^*, b_k^*)^T$ from the sought distribution for the CIELAB color coordinates.
3. Calculate an estimate for the CIELAB color coordinates according to

$$(\hat{L}^*,\hat{a}^*,\hat{b}^*)^T=\frac{1}{M}\sum_{k=1}^{M}(L_k^*,a_k^*,b_k^*)^T, \tag{21}$$

   along with the associated covariance matrix

$$V_{(L^*,a^*,b^*)}=\frac{1}{M-1}\sum_{k=1}^{M}\left((\hat{L}^*,\hat{a}^*,\hat{b}^*)^T-(L_k^*,a_k^*,b_k^*)^T\right)^T \left((\hat{L}^*,\hat{a}^*,\hat{b}^*)^T-(L_k^*,a_k^*,b_k^*)^T\right).$$

4. Calculate a 95% coverage interval

$$I_{L^*}=[L^*_{(\alpha M)},L^*_{((\alpha+0.95)M)}]=[L^*_{low},L^*_{high}] \tag{23}$$

   for L^* and similarly for a^* and b^*. In Equation 23, $L^*_{(1)} \le L^*_{(2)} \le \ldots \le L^*_{(M)}$ denotes the sequence of ordered random samples obtained for L^*, where α is chosen from the interval [0, 0.05]. There exists no unique 95% coverage interval and any value from [0, 0.05] can be taken for α. An additional specification is needed to define a particular value for α (and hence a particular coverage interval). An example of such a specification is the choice of a probabilistically symmetric coverage interval using $\alpha=0.025$ for a 95% coverage interval. Alternatively, also shortest coverage intervals can be calculated.

The results of the Monte Carlo procedure may conveniently also be visualized graphically, for example by histograms for samples of single components of the CIELAB color coordinates, or by a two-dimensional scatter plot of samples for two CIELAB color coordinates. A MATLAB®[13] implementation of the Monte Carlo procedure for CIELAB color coordinates is available from the authors on request.

4 | RESULTS

Table 1 lists seven different sets of tristimulus values that were used for the numerical calculations. In addition, Table 1 shows the corresponding CIELAB color coordinate values obtained by applying Equations 1–4 to the tristimulus values. Each row corresponds to a different color. The entries in this table were taken as the estimates $\hat{X},\hat{Y},\hat{Z}$. The associated covariance matrix was formed as

$$V_{(X,Y,Z)}=u_r^2\begin{pmatrix}\hat{X}^2 & \rho|\hat{X}\hat{Y}| & \rho|\hat{X}\hat{Z}| \\ \rho|\hat{X}\hat{Y}| & \hat{Y}^2 & \rho|\hat{Y}\hat{Z}| \\ \rho|\hat{X}\hat{Z}| & \rho|\hat{Y}\hat{Z}| & \hat{Z}^2\end{pmatrix}, \tag{24}$$

where u_r denotes the relative uncertainty and ρ the (same) correlation coefficient for the tristimulus values. Two different values were taken for the relative uncertainty, namely $u_r=0.01$ and $u_r=0.05$. For the correlation coefficient ρ the cases $\rho=0$ (no correlation), $\rho=0$ (moderate correlation) and $\rho=0.9$ (strong correlation) were considered, so that altogether $7\times2\times3=42$ different scenarios resulted.

For each scenario, both uncertainty evaluation procedures were applied. To illustrate the results and to focus on possible differences between the linearized GUM approach and the Monte Carlo procedure, the relative deviation of the estimates was determined as

$$\Delta L^*=\frac{\hat{L}^*_{\mathrm{GUM}}-\hat{L}^*_{\mathrm{MC}}}{l_{\mathrm{MC}}(L^*)}, \tag{25}$$

where the subscripts GUM and MC refer to the results by the GUM approach and by the Monte Carlo approach. The deviation is expressed in terms of the length of the (probabilistically symmetric) 95% coverage interval resulting for the Monte Carlo procedure (see Equation 23)

$$l_{\mathrm{MC}}(L^*)=L^*_{\mathrm{high}}-L^*_{\mathrm{low}}. \tag{26}$$

Likewise, relative deviations Δa^* and Δb^* were formed for the estimates of a^* and b^*, respectively. In addition, the relative deviation $\Delta l(L^*)$ (and similarly $\Delta l(a^*)$ and $\Delta l(b^*)$) of the lengths of the corresponding 95% coverage intervals was evaluated via

TABLE 1 Tristimulus values and corresponding CIELAB color coordinates considered for uncertainty evaluation

		Tristimulus estimates			CIELAB color coordinates		
Case	Color	$\hat{X}$	$\hat{Y}$	$\hat{Z}$	$\hat{L}^*$	$\hat{a}^*$	$\hat{b}^*$
1	White	81.50	86.10	90.70	94.36	−0.65	2.08
2	Middle gray	21.70	23.10	24.60	55.18	−1.20	0.90
3	Black	0.91	0.98	1.06	8.82	−0.83	0.09
4	Yellow	56.40	58.68	6.75	81.12	1.56	88.29
5	Green	12.40	18.80	12.50	50.45	−32.84	17.37
6	Red	14.10	7.68	1.19	33.31	52.15	40.63
7	Blue	1.78	1.11	6.75	9.88	21.24	−33.83

$$\Delta l(L^*) = \frac{l_{\mathrm{GUM}}(L^*) - l_{\mathrm{MC}}(L^*)}{l_{\mathrm{MC}}(L^*)}, \tag{27}$$

where, according to Equation 18, $l_{\mathrm{GUM}}(L^*)$ is given by $l_{\mathrm{GUM}}(L^*) = 2 \times 1.96\ u(L^*)$.

Figures 1–3 show the relative deviations resulting for the estimates (upper graphs) and coverage interval lengths (lower graphs) for the CIELAB color coordinates in all scenarios. As can be seen, throughout all considered scenarios the relative deviation for both the estimate and the coverage interval length is found to be less than 0.5% even when considering an uncertainty of $u_r = 0.05$ for the tristimulus values. Hence, both approaches yield nearly identical results for all considered scenarios. We note, however, that for larger uncertainties differences between the results can become significant.

Figure 4 illustrates an example for the joint distribution of a^* and b^* obtained by the Monte Carlo method for case 1 from Table 1 when considering $u_r = 0.05$ and $\rho = 0$. In this case, the histograms for a^* and b^* appear to be of Gaussian shape and the corresponding scatter plot indicates a marked

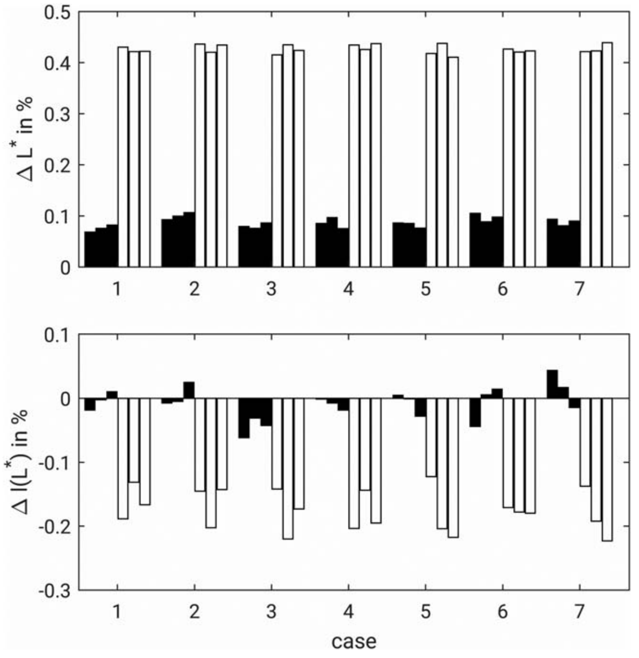

FIGURE 1 Relative deviations of the estimates ΔL^* (Equation 25, upper) and coverage interval length $\Delta l(L^*)$ (Equation 27, lower) obtained when comparing the analytical approach and the Monte Carlo method. For each case given Table 1 the scenarios are ordered as follows: the first three scenarios (black) correspond to $u_r = 0.01$ using $\rho = 0$, $\rho = 0.2$ and $\rho = 0.9$, the second three scenarios (white) show the corresponding relative deviations for $u_r = 0.05$

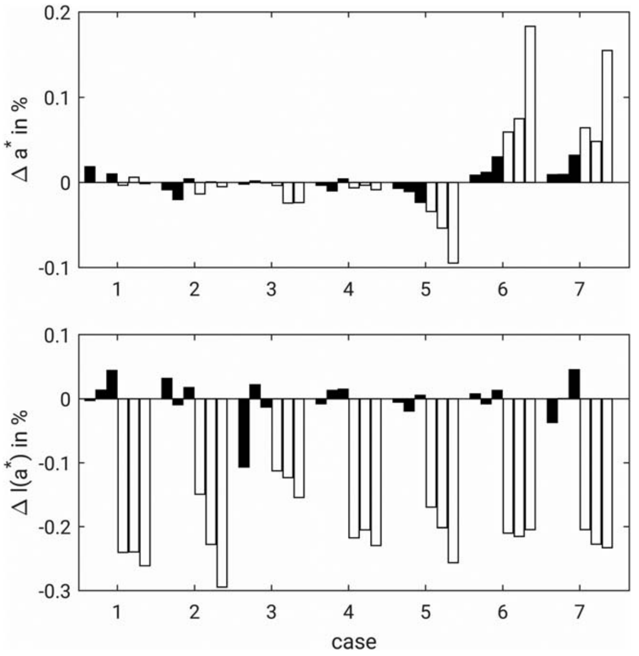

FIGURE 2 Relative deviations of the estimates Δa^* (Equation 25, upper) and coverage interval length $\Delta l(a^*)$ (Equation 27, lower) obtained when comparing the analytical approach and the Monte Carlo method. The scenarios are ordered in the same way as utilized for Figure 1

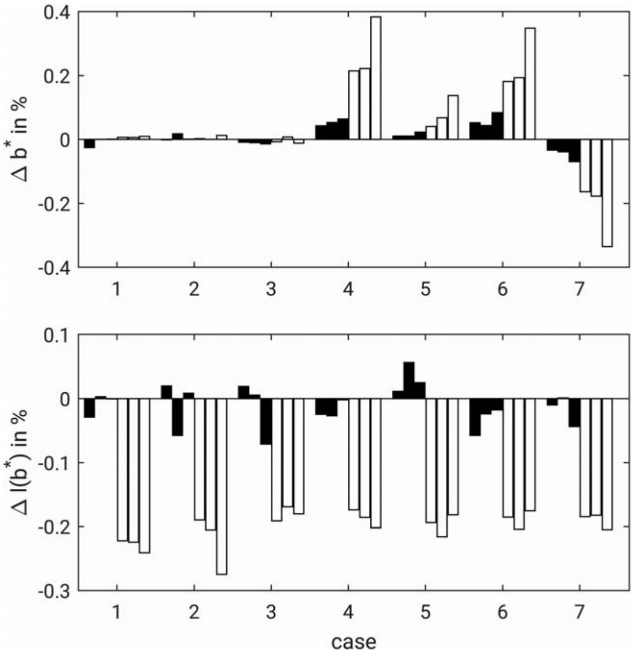

FIGURE 3 Relative deviations of the estimates Δb^* (Equation 25, upper) and coverage interval length $\Delta l(b^*)$ (Equation 27, lower) obtained when comparing the analytical approach and the Monte Carlo method. The scenarios are ordered in the same way as utilized for Figure 1

correlation between a^* and b^*. As discussed above, this scenario is well covered by the linearized GUM approach yielding nearly the same estimates and coverage intervals.

Figure 5 shows a histogram of the color differences ΔE_k $(k=1,\ldots,M)$ resulting for the Monte Carlo evaluation of

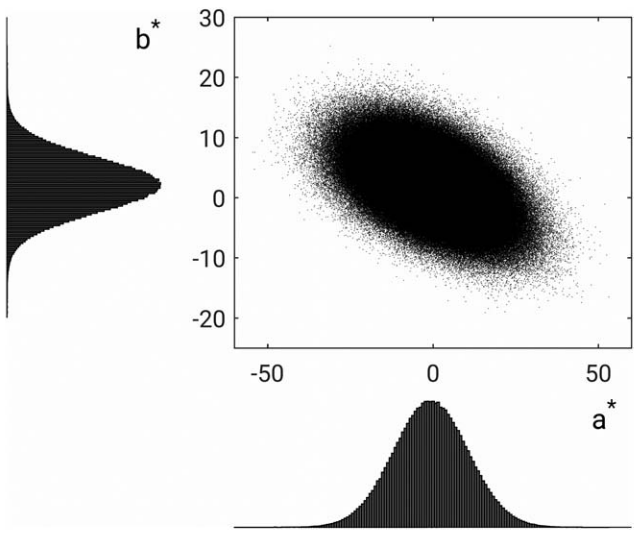

FIGURE 4 Illustration of the 2-dimensional joint distributions of CIELAB color coordinates (a^*, b^*) obtained by the Monte Carlo procedure for case 1 in Table 1 with $u_r=0.05$ and $\rho=0$. The histograms depict the corresponding marginal distributions for a^* and b^*

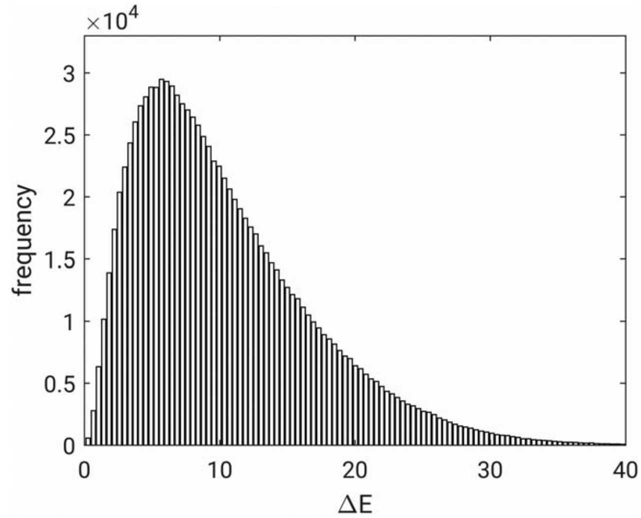

FIGURE 5 Histogram of the ΔE values obtained by Equation 28 for the Monte Carlo results for case 1 in Table 1 with $u_r=0.05$ and $\rho=0$

case 1 from Table 1 when considering $u_r=0.05$ and $\rho=0$. The ΔE_k values were calculated by

$$\Delta E_k=\sqrt{\left(L_k^*-\hat{L}^*\right)^2+\left(a_k^*-\hat{a}^*\right)^2+\left(b_k^*-\hat{b}^*\right)^2}, \qquad (28)$$

where the estimates $\hat{L}^*$, $\hat{a}^*$, and $\hat{b}^*$ were obtained by Equation 21. The ΔE_k values calculated in this way from the Monte Carlo evaluation can be utilized, for example, to assess whether the uncertainties of the CIELAB color coordinates are relevant with respect to perceptible color differences.

We also applied the Monte Carlo method to a situation where a rather large relative uncertainty of $u_r=0.2$ is assumed for case 1 using again $\rho=0$. When applying the linearized GUM approach and the Monte Carlo approach to this scenario relative deviations of $\Delta L^* \approx 1.7\,\%$ and $\Delta l(L^*) \approx 3\,\%$ with respect to the Monte Carlo results emerge which might possibly no longer be considered as being tolerable.

5 | SUMMARY AND CONCLUSIONS

CIELAB color coordinates are frequently applied to characterize the chromaticity of visible a object's spectrum and a reliable quantification of the uncertainty associated with these coordinates is important. CIELAB color coordinates depend nonlinearly on the tristimulus values, and the propagation of the uncertainty associated with measured tristimulus values to the color coordinates is challenging. Based on current guidelines for uncertainty evaluation in metrology we have provided two approaches for this purpose, one approach based on linearization and one on a Monte Carlo method. While the approach based on linearization results in analytical formulas, the adequacy of linearization ought to be checked. The proposed Monte Carlo method can be used as a reference method to check the validity of a linearization. We applied both methods to a large range of scenarios representing different underlying spectra, varying size of uncertainties and degree of correlation. In most cases, the simple procedure based on linearization yields almost the same results as the Monte Carlo method and, in viewing the latter approach as a reference, may safely be recommended. However, for large uncertainties of the tristimulus values, significant different results can be reached. In those cases, we recommend the use of the Monte Carlo approach.

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