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Correlation coefficients for tristimulus response value uncertainties

J. L. Gardner and R. B. Frenkel

Abstract. Tristimulus response functions are either calculated from spectral-irradiance data or measured directly and used to calculate parameters representing colour. The tristimulus responses are correlated because they depend on the same spectral information. In this paper we derive and confirm the correlation coefficients between the tristimulus response functions. These coefficients are important in the estimation of uncertainty for colour coordinates.

1. Introduction

Consistent estimation of uncertainty according to the methods described in the ISO *Guide to the Expression of Uncertainty in Measurement* [1] is a major concern of modern metrology. This applies not only to the direct measurement of International System of Units quantities, but also to measurements derived from them. One such measurement is colour. Colour is described as a physical measurement using the tristimulus spectral response functions $x(\lambda)$, $y(\lambda)$ and $z(\lambda)$ shown in Figure 1, each as a function of the wavelength λ. These are convolved with the spectral irradiance of the source to calculate the tristimulus response values X, Y and Z. The 1931 chromaticity coordinates (x, y) of the Commission Internationale de l'Éclairage (CIE) [2] are then defined as

$$x = X/(X+Y+Z) \qquad (1)$$
$$y = Y/(X+Y+Z).$$

CIE Uniform Colour Space 1960 chromaticity coordinates (u, v) or 1976 (u', v'), if required, are calculated as transforms of x and y [2]. Tristimulus response values may also be transformed to colour descriptions for surfaces, typically CIE 1976 L*a*b* (CIELAB) [2].

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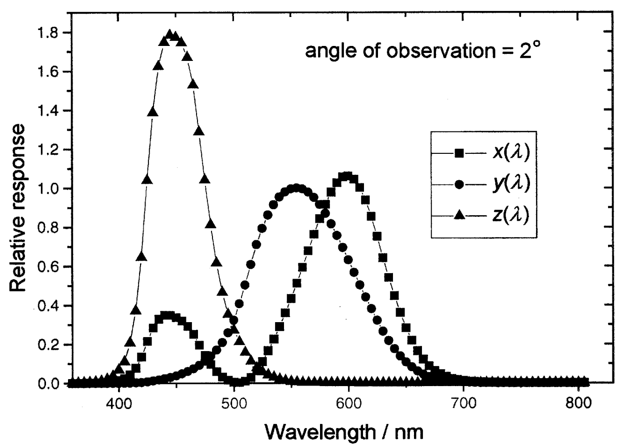

Figure 1. Tristimulus spectral response functions used to calculate colour coordinates.

The convolution of the spectral irradiance of the source with the $x(\lambda)$, $y(\lambda)$ and $z(\lambda)$ tristimulus functions is usually written in sum form:

$$X = \Sigma_i E_i X_i \qquad (2)$$
$$Y = \Sigma_i E_i Y_i$$
$$Z = \Sigma_i E_i Z_i,$$

where X_i, Y_i and Z_i are tabulated values of the tristimulus response functions, available in 1 nm or 5 nm wavelength intervals [2], and E_i is the (relative) spectral irradiance at wavelength i. Many modern instruments measure the spectral irradiance directly and then calculate chromaticity coordinates, with or without first calculating the tristimulus response values.

Tristimulus colorimeters have filtered detectors that perform the convolution optically.

Because the functions $x(\lambda)$, $y(\lambda)$ and $z(\lambda)$ overlap, their responses to a change in spectral irradiance are correlated and an uncertainty analysis of chromaticity coordinates in terms of uncertainties in X, Y and Z must take this correlation into account. This is particularly so in the case of the tristimulus colorimeter where the spectral-irradiance values are not available. Uncertainties in tristimulus values and subsequent chromaticity coordinates calculated from independent spectral-irradiance readings may be estimated directly in terms of the uncertainties of those readings. However, in some cases it is convenient to perform the uncertainty analysis in terms of uncertainties in X, Y and Z and here also the correlation coefficients are required.

In the following sections we show how the correlation coefficients may be derived, and confirm this by comparison of alternative ways of deriving uncertainties in (x, y) chromaticity coordinates from spectral measurements. It should be stressed that the application below considers only those uncertainty components in colour measurement which arise from variations in the source spectral distribution. Application of the correlations to deriving analytical expressions for uncertainties in (x, y) and other chromaticity coordinates for various light sources is described elsewhere [3].

2. Derivation of correlation coefficients between X, Y and Z

The correlation coefficient r_{XY} between X and Y is given by

$$r_{XY} = \mathrm{cov}(X, Y)/u(X)u(Y), \tag{3}$$

where $u(X)$, $u(Y)$ are the standard uncertainties in X and Y, respectively, and $\mathrm{cov}(X, Y)$ is the covariance between X and Y. Similar expressions hold for r_{XZ} and r_{YZ}.

The covariance in (3) is given by

$$\mathrm{cov}(X, Y) = \mathtt{E}\{[X - \mathtt{E}(X)][Y - \mathtt{E}(Y)]\} \tag{4}$$
$$= \mathtt{E}(XY) - \mathtt{E}(X)\mathtt{E}(Y), \tag{5}$$

where $\mathtt{E}$ denotes the expectation function [4]. Now

$$\mathtt{E}\{XY\} = \mathtt{E}\{\Sigma_i \Sigma_j X_i Y_j E_i E_j\} \tag{6}$$
$$= \Sigma_i \Sigma_j X_i Y_j \mathtt{E}\{E_i E_j\}, \tag{7}$$

as X_i, Y_j are fixed

$$= \Sigma_i X_i Y_i \mathtt{E}(E_i^2) + \Sigma_i \Sigma_{j \neq i} X_i Y_j \mathtt{E}(E_i)\mathtt{E}(E_j) \tag{8}$$

and

$$\mathtt{E}(X)\mathtt{E}(Y) = \Sigma_i X_i Y_i \{\mathtt{E}(E_i)\}^2 + \Sigma_i \Sigma_{j \neq i} X_i Y_j \mathtt{E}(E_i)\mathtt{E}(E_j). \tag{9}$$

On substitution of (8) and (9) into (5), the terms involving $j \neq i$ cancel and $\mathtt{E}(E_i^2) - \{\mathtt{E}(E_i)\}^2$ is the variance of E_i. Thus

$$\mathrm{cov}(X, Y) = \Sigma X_i Y_i u^2(E_i). \tag{10}$$

This expression is equivalent to that used by Robertson [5] in analysing errors in spectrophotometry.
Further,

$$u^2(X) = u^2(\Sigma X_i E_i) \tag{11}$$
$$= \Sigma u^2(E_i) X_i^2, \tag{12}$$

as the E_i values are independent.

The uncertainty in each value of E_i is usually of the form

$$u(E_i) = \alpha_0 + \alpha_i E_i, \tag{13}$$

where α_0 arises from background subtraction in spectral regions where the spectral irradiance is weak. Where signals are relatively strong, the background term can be ignored and, in many instances, the relative uncertainty of the spectral-irradiance values is constant so that α_i can be replaced by α. It then follows that

$$u^2(X) = \alpha^2 \Sigma E_i^2 X_i^2, \tag{14}$$

and similarly

$$u^2(Y) = \alpha^2 \Sigma E_i^2 Y_i^2. \tag{15}$$

Hence,

$$r_{XY} = \Sigma E_i^2 X_i Y_i / (\Sigma E_i^2 X_i^2 \Sigma E_i^2 Y_i^2)^{1/2}, \tag{16}$$

with similar expressions for r_{XZ} and r_{YZ}.

Where the detailed spectrum is known, the correlation can be accurately calculated. This may apply, for example, in the analysis of a comparison that includes values recorded by tristimulus colorimeters where the spectrum may be known to the coordinating laboratory. However, to provide a general analysis for a relatively broadband source, we can reasonably estimate the correlation coefficients by replacing the spectral terms E_i with the average spectral irradiance (this is strictly true only at the white point $x = y = 0.33$). The irradiance terms can then be taken outside and the summations reduce to

$$r_{XY} = \Sigma X_i Y_i / (\Sigma X_i^2 \Sigma Y_i^2)^{1/2}, \tag{17}$$

with similar expressions for r_{XZ} and r_{YZ}. Using the values tabulated for X_i, Y_i and Z_i from 360 nm to 830 nm at 5 nm intervals, we find $r_{XY} = 0.760$, $r_{XZ} = 0.255$ and $r_{YZ} = 0.082$. The correlation coefficients are all positive since X_i, Y_i and Z_i are everywhere positive.

3. Uncertainty in (x, y) chromaticity coordinates

The square of the standard uncertainty in x is given by [1]

$$u^2(x) = \left(\frac{\partial x}{\partial X}\right)^2 u^2(X) + \left(\frac{\partial x}{\partial Y}\right)^2 u^2(Y) + \left(\frac{\partial x}{\partial Z}\right)^2 u^2(Z) + 2r_{XY}\frac{\partial x}{\partial X}\frac{\partial x}{\partial Y}u(X)u(Y) + 2r_{XZ}\frac{\partial x}{\partial X}\frac{\partial x}{\partial Z}u(X)u(Z) + 2r_{YZ}\frac{\partial x}{\partial Y}\frac{\partial x}{\partial Z}u(Y)u(Z), \qquad (18)$$

where the first three terms represent the usual "sum of squares" for uncorrelated quantities. Robertson [5] used the equivalent expression with covariances, rather than correlation coefficients. Substituting for the derivatives we find

$$u^2(x) = \{u^2(X) - 2x\left[u^2(X) + r_{XY}u(X)u(Y) + r_{XZ}u(X)u(Z)\right] + x^2\left[u^2(X) + u^2(Y) + u^2(Z) + 2(r_{XY}u(X)u(Y) + r_{XZ}u(X)u(Z) + r_{YZ}u(Y)u(Z))\right]\}/(X+Y+Z)^2. \qquad (19)$$

Using (14), (15) and a similar expression for $u^2(Z)$, and the correlation coefficients resulting from the assumption that E_i can be replaced by its average value, this reduces to

$$u(x) = \alpha(0.0035 - 0.0150x + 0.0229x^2)^{1/2}. \qquad (20)$$

Similarly,

$$u(y) = \alpha(0.0038 - 0.0139y + 0.0229y^2)^{1/2}. \qquad (21)$$

This means that if the spectral-irradiance values are recorded with a relative uncertainty of 0.01, the corresponding uncertainty in (x, y) chromaticity values near the white point is (0.0003, 0.0004).

4. Uncertainty estimated directly from the spectrum

As a confirmation of the above correlation coefficients, we now consider the derivation of uncertainty in x and y directly from uncertainties in the spectral data. It is convenient to define

$$T_i = X_i + Y_i + Z_i \qquad (22)$$

so that

$$x = \Sigma E_i X_i / \Sigma E_i T_i. \qquad (23)$$

From the propagation law for uncertainty, the square of the standard uncertainty $u^2(x)$ in x is given by

$$u^2(x) = \sum \left(\frac{\partial x}{\partial E_i}\right)^2 u^2(E_i). \qquad (24)$$

Now

$$\frac{\partial x}{\partial E_i} = \frac{X_i - xT_i}{\Sigma E_i T_i}, \qquad (25)$$

and hence

$$u^2(x) = \frac{\Sigma(X_i - xT_i)^2 u^2(E_i)}{(\Sigma E_i T_i)^2}. \qquad (26)$$

Similarly

$$u^2(y) = \frac{\Sigma(Y_i - yT_i)^2 u^2(E_i)}{(\Sigma E_i T_i)^2}. \qquad (27)$$

Applying (13) and its subsequent simplification, and replacing the spectral irradiance with its average value as above, these reduce to

$$u(x) = \alpha(\Sigma X_i^2 - 2x\Sigma X_i T_i + x^2\Sigma T_i^2)^{1/2}/\Sigma T_i. \qquad (28)$$

$$u(y) = \alpha(\Sigma Y_i^2 - 2y\Sigma Y_i T_i + y^2\Sigma T_i^2)^{1/2}/\Sigma T_i. \qquad (29)$$

Using the tabulated values leads to exactly the same coefficients as (20) and (21), which is expected from the underlying assumptions.

5. Conclusion

Correlation coefficients for application in calculation of uncertainty estimates in colour measurement have been derived, and shown to be consistent with an alternative derivation of uncertainty for (x, y) chromaticity coordinates. Expressions of general applicability can be used to derive analytical expressions for uncertainty in colour measurements of a broadband source. The correlation coefficients may be more accurately estimated if the spectral-irradiance distribution is known.

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