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TECHNICAL REPORT

Determination of Measurement Uncertainties in Photometry

Supplement 2: Spectral measurements and derivative quantities

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Descriptor: Photometry
Spectrophotometry
Calibration

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The International Commission on Illumination (CIE) is an organization devoted to international co-operation and exchange of information among its member countries on all matters relating to the art and science of lighting. Its membership consists of the National Committees in about 40 countries.

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3. To provide guidance in the application of principles and procedures in the development of international and national standards in the fields of light and lighting.
4. To prepare and publish standards, reports and other publications concerned with all matters relating to the science, technology and art in the fields of light and lighting.
5. To maintain liaison and technical interaction with other international organizations concerned with matters related to the science, technology, standardization and art in the fields of light and lighting.

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3. De donner des directives pour l'application des principes et des méthodes d'élaboration de normes internationales et nationales dans les domaines de la lumière et de l'éclairage.
4. De préparer et publier des normes, rapports et autres textes, concernant toutes matières relatives à la science, la technologie et l'art dans les domaines de la lumière et de l'éclairage.
5. De maintenir une liaison et une collaboration technique avec les autres organisations internationales concernées par des sujets relatifs à la science, la technologie, la normalisation et l'art dans les domaines de la lumière et de l'éclairage.

Les travaux de la CIE sont effectués par Comités Techniques, organisés en six Divisions. Les sujets d'études s'étendent des questions fondamentales, à tous les types d'applications de l'éclairage. Les normes et les rapports techniques élaborés par ces Divisions Internationales de la CIE sont reconnus dans le monde entier.

Tous les quatre ans, une Session plénière passe en revue le travail des Divisions et des Comités Techniques, en fait rapport et établit les projets de travaux pour l'avenir. La CIE est reconnue comme la plus haute autorité en ce qui concerne tous les aspects de la lumière et de l'éclairage. Elle occupe comme telle une position importante parmi les organisations internationales.

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Die Internationale Beleuchtungskommission (CIE) ist eine Organisation, die sich der internationalen Zusammenarbeit und dem Austausch von Informationen zwischen ihren Mitgliedsländern bezüglich der Kunst und Wissenschaft der Lichttechnik widmet. Die Mitgliedschaft besteht aus den Nationalen Komitees in rund 40 Ländern.

Die Ziele der CIE sind:

1. Ein internationales Forum für Diskussionen aller Fragen auf dem Gebiet der Wissenschaft, Technik und Kunst der Lichttechnik und für den Informationsaustausch auf diesen Gebieten zwischen den einzelnen Ländern zu sein.
2. Grundnormen und Verfahren der Messtechnik auf dem Gebiet der Lichttechnik zu entwickeln.
3. Richtlinien für die Anwendung von Prinzipien und Vorgängen in der Entwicklung internationaler und nationaler Normen auf dem Gebiet der Lichttechnik zu erstellen.
4. Normen, Berichte und andere Publikationen zu erstellen und zu veröffentlichen, die alle Fragen auf dem Gebiet der Wissenschaft, Technik und Kunst der Lichttechnik betreffen.
5. Liaison und technische Zusammenarbeit mit anderen internationalen Organisationen zu unterhalten, die mit Fragen der Wissenschaft, Technik, Normung und Kunst auf dem Gebiet der Lichttechnik zu tun haben.

Die Arbeit der CIE wird durch Technische Komitees geleistet, die in sechs Divisionen organisiert sind. Diese Arbeit betrifft Gebiete mit grundlegendem Inhalt bis zu allen Arten der Lichtenwendung. Die Normen und Technischen Berichte, die von diesen international zusammengesetzten Divisionen ausgearbeitet werden, sind auf der ganzen Welt anerkannt.

Alle vier Jahre findet eine Session statt, in der die Arbeiten der Divisionen berichtet und überprüft werden, sowie neue Pläne für die Zukunft ausgearbeitet werden. Die CIE wird als höchste Autorität für alle Aspekte des Lichtes und der Beleuchtung angesehen. Auf diese Weise unterhält sie eine bedeutende Stellung unter den internationalen Organisationen.

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This Technical Report has been prepared by CIE Technical Committee 2-72 of Division 2 "Physical Measurement of Light and Radiation" and has been approved by the Board of Administration as well as by Division 2 of the Commission Internationale de l'Eclairage. The document reports on current knowledge and experience within the specific field of light and lighting described, and is intended to be used by the CIE membership and other interested parties. It should be noted, however, that the status of this document is advisory and not mandatory.

Ce rapport technique a été élaboré par le Comité Technique CIE 2-72 de la Division 2 "Mesures Physiques de la Lumière et des Radiations" et a été approuvé par le Bureau et Division 2 de la Commission Internationale de l'Eclairage. Le document expose les connaissances et l'expérience actuelles dans le domaine particulier de la lumière et de l'éclairage décrit ici. Il est destiné à être utilisé par les membres de la CIE et par tous les intéressés. Il faut cependant noter que ce document est indicatif et non obligatoire.

Dieser Technische Bericht ist vom Technischen Komitee CIE 2-72 der Division 2 "Physikalische Messungen von Licht und Strahlung" ausgearbeitet und vom Vorstand sowie Division 2 der Commission Internationale de l'Eclairage gebilligt worden. Das Dokument berichtet über den derzeitigen Stand des Wissens und Erfahrung in dem behandelten Gebiet von Licht und Beleuchtung; es ist zur Verwendung durch CIE-Mitglieder und durch andere Interessierte bestimmt. Es sollte jedoch beachtet werden, dass das Dokument eine Empfehlung und keine Vorschrift ist.

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DETERMINATION OF MEASUREMENT UNCERTAINTIES IN PHOTOMETRY SUPPLEMENT 2: SPECTRAL MEASUREMENTS AND DERIVATIVE QUANTITIES

Summary

This report is a second supplement to CIE 198:2011 *Determination of Measurement Uncertainties in Photometry* for the determination of measurement uncertainties associated with the values of selected quantities in photometry. It deals with spectral measurements and combinations of measured spectral distributions, in particular with the effect of correlations between the measured spectral values that arise from the measurement and calibration processes.

Guidelines are given for identifying sources of correlation in spectral measurements. Calibration is treated as a transfer from a reference to the object of interest. Various processes of interpolation and correction may be applied to measured spectral values before they are combined. Examples of treating correlations introduced by such processes are included. Uncertainties in a number of important radiometric and photometric quantities determined from spectral measurements are provided, including the use of Monte-Carlo methods.

Photometer examples covered are photometric response, photometer $V(\lambda)$ mismatch index and spectral mismatch factor. Dominant wavelength, correlated colour temperature and blue-light hazard measurements are covered, with particular emphasis on LED sources.

DÉTERMINATION DES INCERTITUDES DE MESURE EN PHOTOMÉTRIE SUPPLÉMENT 2: MESURES SPECTRALES ET QUANTITÉS DÉRIVÉES

Résumé

Ce rapport est un deuxième supplément à la publication CIE 198: 2011 Détermination des incertitudes de mesure en photométrie pour la détermination des incertitudes de mesure associées aux valeurs des grandeurs sélectionnées en photométrie. Il traite des mesures spectrales et des combinaisons de distributions spectrales mesurées, en particulier de l'effet des corrélations entre les valeurs spectrales mesurées issues des processus de mesure et d'étalonnage.

Des directives sont données pour identifier les sources de corrélation dans les mesures spectrales. L'étalonnage est traité comme un transfert d'une référence à l'objet d'intérêt. Différents procédures d'interpolation et de correction peuvent être appliquées aux valeurs spectrales mesurées avant leur combinaison. Des exemples de traitement des corrélations introduites par de tels processus sont inclus. Des incertitudes sur un certain nombre de grandeurs radiométriques et photométriques importantes déterminées à partir de mesures spectrales sont fournies, y compris l'utilisation des méthodes de Monte-Carlo.

Les exemples liés aux photomètres sont la réponse photométrique, l'indice générale d'adaptation à $V(\lambda)$ et le facteur de correction d'adaptation spectrale. Les mesures de longueur d'onde dominante, de température de couleur proximale et de danger de lumière bleue sont couvertes, avec un accent particulier sur les sources LED.

BESTIMMUNG VON MESSUNSICHERHEITEN IN DER PHOTOMETRIE SUPPLEMENT 2: SPEKTORADIOMETRIE UND ABGELEITETE GRÖßEN

Zusammenfassung

Dieser Bericht ist ein zweites Supplement zur Publikation CIE 198:2011 *Bestimmung von Messunsicherheiten in der Photometrie* zur Bestimmung von Messunsicherheiten im Zusammenhang mit den Werten ausgewählter Messgrößen in der Photometrie. Es behandelt Spektralmessungen und Kombinationen von gemessenen spektraler Verteilungen, insbesondere den Korrelationseffekt zwischen gemessenen spektralen Werten, die durch die Mess- und Kalibrierprozesse entstehen.

Es werden Richtlinien zur Identifizierung von Korrelationsquellen bei spektralen Messungen gegeben. Kalibrierung wird als eine Übertragung von einer Referenz zum Objekt betrachtet. Verschiedene Interpolations- und Korrekturprozesse können auf gemessene spektrale Werte angewendet werden, bevor sie zusammengesetzt werden. Beispiele für die Behandlung von Korrelationen, die durch solche Prozesse entstehen, sind inbegriffen. Unsicherheiten in einer Vielzahl wichtiger radiometrischer und photometrischer Größen, die aus spektralen Messungen bestimmt werden, werden erläutert, inklusive der Nutzung von Monte-Carlo-Methoden.

Beispiele zu Photometern beinhalten die photometrische Antwort, den $V(\lambda)$ -Fehlanpassungsindex und den spektralen Fehlanpassungsfaktor. Bunttongleiche Wellenlänge, ähnlichste Farbtemperatur sowie Blaulichtgefährdungs-Messungen werden betrachtet, mit speziellem Schwerpunkt auf LED-Quellen.

1 Introduction

This second supplement to CIE 198:2011 *Determination of Measurement Uncertainties in Photometry* (CIE 2011a) is intended as a practical help and guidance and collects modules and examples. It is planned that CIE Division 2 will develop more modules and examples for current and newly created quantities in existing and future technical reports, respectively, which will be added as additional supplements.

Supplement 1, Parts 1 to 4, were previously published. These included:

- Part 1: Modules for the Construction of Measurement Equations (CIE 2011b);
- Part 2: Examples for Models with Individual Inputs (CIE 2011c);
- Part 3: Examples for the Solving of Systems of Equations (CIE 2011d);
- Part 4: Examples for Models with Distributions. (CIE 2011e)

Supplement 2 deals with spectral measurements and quantities that are calculated from them.

Many quantities of interest in radiometry, photometry and colorimetry are obtained by measuring values at a series of wavelengths, then combining those in a particular way to form the desired outcome. Most commonly these are weighted sums of the measured values. The uncertainty of each measured value is determined by the variability of the influence components of the measurement. Because the measured values are of the same quantity at different wavelength settings, some of the influence components will affect all the values in a common manner. Hence the measured values contain correlations that affect the uncertainty of any result formed by combining them.

Measured values are often used to calculate values at different wavelengths than those of the measurement, by interpolation or fitting. These new values are found by combining the original measured values and thus introduce or modify correlations among the set of values that are used for subsequent combinations. Correlations introduced by mathematical operations – logical correlations in contrast to measurement correlations – can be relatively complex.

Reference spectral standards are often reported as a table of spectral values and their total uncertainties. Calibration of the spectral values of test artefacts introduces more correlations in the measurement as well as propagating those present in the reference data through to the spectral values of the test item. Properly accounting for uncertainties of quantities calculated by combining the calibrated spectral values requires that correlations within the reference values should be provided, as well as the total uncertainties.

2 Scope

The primary concern of this document is the origin and treatment of correlations in measured spectral values and their propagation through the various operations commonly applied to obtain various quantities of interest. Examples for a number of such quantities and their uncertainties are given, including the propagation of correlations through calibration against a reference artefact. Examples are also given for uncertainty propagation through Monte-Carlo simulation, including the treatment of correlations in the input values.

While specific examples are given to illustrate the importance of correlations, a full uncertainty treatment of all the influence components for each example is not given. Representative values for uncertainties of a medium quality measurement are applied to all examples, where the influence components are treated by generic type, but results are presented in such a way that they can be scaled by influence components for a particular system and application.

3 Symbols used in this document

$u(x)$	standard uncertainty of quantity x
$u^2(x)$	variance of quantity x : $u(x) = +\sqrt{u^2(x)}$
$u(x, y)$	covariance of quantities x and y
$r(x, y)$	correlation coefficient between x and y : $r(x, y) = \frac{u(x, y)}{u(x)u(y)}$
S_i	spectral value at the i^{th} wavelength
$u_{\text{rel}}(x)$	relative standard uncertainty of quantity x : $u_{\text{rel}}(x) = \frac{u(x)}{x}$
$u_{\text{rel}}^2(x)$	relative variance of quantity x : $u_{\text{rel}}^2(x) = \frac{u^2(x)}{x^2}$
$u_{\text{rel}}(x, y)$	relative covariance of quantities x and y : $u_{\text{rel}}(x, y) = \frac{u(x, y)}{xy}$
$u_k(S_i)$	uncertainty of S_i contributed by the k^{th} independent measurement component
	NOTE For clarity, the symbols $u_{u,k}(S_i)$ and $u_{c,k}(S_i)$ may be used to denote measurement components that are uncorrelated (subscript u) or correlated (subscript c) at different wavelengths, respectively.
$u_k^*(S_i)$	signed uncertainty of S_i contributed by the k^{th} independent measurement component; used where the sign of the sensitivity coefficient for the effect of that component may vary
U_S	uncertainty matrix (variance-covariance matrix) for a spectrum of values S_i
c, c_k	sensitivity coefficients – linear dependence of the uncertainty of a quantity on a particular component
$C_{a,b}$	matrix (or vector) of sensitivity coefficients for the dependence of output variable(s) a on input variable(s) b

4 Uncertainties associated with spectroradiometric values

The methods to establish uncertainty of a single quantity to be measured (JCGM 2008a) are now well known. The measurement depends on various influence quantities that might include amplifier gain, background levels, temperature, etc. The measurement equation or equations showing the dependence of the measurand on these factors then allows the determination of sensitivity coefficients, or multipliers of the contribution of the uncertainty of the influence factors to the uncertainty of the desired measurand. For example, the measured value of irradiance from a point source of known luminous intensity depends on the square of the distance from the source, so the contribution of relative uncertainty in that distance is doubled in its contribution to relative irradiance. Many, if not most, quantities influencing a measurement are independent and can be treated separately and summed in quadrature to determine the total uncertainty of the measurand.

Sometimes the factors contributing to a single measurand may not be independent, but related. This correlation between the influence quantities must be considered when estimating the uncertainty of the measurand. The typical example quoted is that of a quantity which depends on temperature and pressure, but pressure also depends on temperature. Variation of the temperature within its uncertainty range produces a correlated variation in the pressure.

Another example is a mass calibration, where various weights are added to balance the mass of the required object. Each of the added masses will trace back to a common reference; the uncertainty of that reference then contributes a number of times to the required measurement; these correlations must be included in the uncertainty of the measurement. Treating the uncertainties of the contributing masses as uncorrelated (random) will under-estimate the uncertainty of the combination.

When a series of similar measurements is made, common factors in the measurement process may be present for each member. Radiometric measurements of spectral power distributions (SPD) or “spectra” (singular “spectrum”) are examples where correlations are common, arising from a common influence component affecting the measured values at each wavelength. Note that correlations are only important when measurements are combined, as in the examples of the mass calibration. However, combining spectral values is common in radiometry, photometry and colorimetry, and an understanding of correlations and the propagation of uncertainty of combinations of correlated quantities is important to properly estimate uncertainties.

NOTE Measured spectral data are a convolution of the true spectrum with the line-spread function of the measurement system. This convolution means that values at adjacent wavelengths are also related through the bandwidth of the measurement, which is particularly evident around non-linear gradients such as spectral lines and cut-on/cut-off filters. This is not a process in which the measured value departs from the true value due to the precision of the measurement system, but one which is determined by the resolution and wavelength spacing of the measurement. Only uncertainty of the measurement process is covered in this document.

4.1 Correlation of measured spectral values

At an individual wavelength of a spectral radiometric measurement, the various factors that contribute to measurement uncertainty are generally independent. Examples might be wavelength error, amplifier noise, amplifier gain, stray light or amplifier offset to be subtracted. Uncertainties for each can be measured from repeat measurements, estimation from previous experience, etc. Because the effects are independent, the total uncertainty at a given wavelength can be found by summing the component uncertainties in quadrature.

However, each component effect influencing the measured value at a given wavelength can now be separated into those that are uncorrelated and those that are correlated at different wavelengths. When spectral measurements are combined, the uncertainty contribution of effects that are uncorrelated at the different wavelengths is reduced, effectively averaged to an extent depending on the relative weighting of the values, but that of correlated components is not.

Correlated components of a spectrum of measurements S_i ($i = 1, \dots, n$), where i denotes measurement at the i^{th} of n wavelengths, are fully correlated at different wavelengths. For example, amplifier offsets, or amplifier gain are the same across the spectrum (in the absence of drift with time or gain changes during the measurement sequence); if the value assigned to the gain has a particular offset within its uncertainty range, that same offset is applied to the measurement at all wavelengths. Stray light levels are closely related at adjacent wavelengths, generally described by some functional relation with wavelength and related to the total light levels; changing the parameters of the function within their uncertainty ranges will affect the values assigned to the stray light at all wavelengths.

For each independent measurement variable x_k having a component uncertainty $u(x_k)$ which is correlated at the different wavelengths, the corresponding variance in the spectral quantity is propagated through the measurement equation (examples are given below):

$$S_i = f(\lambda_i, x_k) = f_{i,k} \quad (1)$$

where λ_i denotes the i^{th} wavelength.

The variance of the spectral quantity for this correlated component is

$$u_k^2(S_i) = c_{i,k}^2 u^2(x_k) \quad (2)$$

where $c_{i,k} = \frac{\partial f_{i,k}}{\partial x_k}$ is the sensitivity coefficient¹ for the dependence of the spectral value on the corresponding measurement variable. The corresponding uncertainty for the spectral value is then

$$u_k(S_i) = +\sqrt{u_k^2(S_i)} = |c_{i,k}| u(x_k) . \quad (3)$$

The covariance between spectral values S_i and S_j for this uncertainty component is

$$u_k(S_i, S_j) = c_{i,k} u(x_k) c_{j,k} u(x_k) . \quad (4)$$

This can be rewritten to separate the sign of the sensitivity coefficient from its amplitude as

$$u_k(S_i, S_j) = \text{sgn}(c_{i,k}) |c_{i,k}| u(x_k) \text{sgn}(c_{j,k}) |c_{j,k}| u(x_k) = \text{sgn}(c_{i,k}) \text{sgn}(c_{j,k}) u_k(S_i) u_k(S_j) . \quad (5)$$

The correlation coefficient corresponding to this covariance is given by

$$r_k(S_i, S_j) = \frac{u_k(S_i, S_j)}{\sqrt{u_k^2(S_i) u_k^2(S_j)}} = \pm 1 , \quad (6)$$

showing that for correlated uncertainty components, the corresponding spectral values themselves are also fully correlated, but that the sign of the correlation can be positive or negative. For most component effects spectral values are positively correlated; one important exception is correlations due to wavelength uncertainty, as shown below.

Where the sign of the sensitivity coefficient for a given correlated effect may change across the spectrum, we can treat the uncertainty of the spectral value due to that effect as “signed”:

$$u_k^*(S_i) = c_{i,k} u(x_k) . \quad (7)$$

NOTE The use of sensitivity coefficients to propagate uncertainty and correlations assumes that the output quantities have a linear dependence on the input quantities over the uncertainty range about their measured values.

4.2 Uncertainty components of spectral measurements

Many effects can influence the uncertainty of each measured spectral value. The uncertainty of each influence component is determined either by statistical analysis of repeated measurements (Type A) or by estimation (Type B). Some influence components contribute to uncertainty in a random (uncorrelated) manner at different wavelengths, characterized by what is clearly “noise” superimposed upon an otherwise smooth spectrum. Others affect the measured spectral values in a related manner at all wavelengths, that is, the effect is correlated across the spectrum.

While influence components must be assessed for each measurement system, they can generally be divided into three classes; scaling, offset and wavelength related. Each class contains components for which the spectral values are uncorrelated and correlated at the different wavelengths.

Component effects at a given wavelength in a spectral measurement are generally independent and each can be treated with a simple measurement equation relating the required spectral value S_i to the measured signals.

¹ Sensitivity coefficients may be calculated by direct differentiation or numerically by the effect on the output quantity of a small perturbation about the mean value of the input quantity.

At the i^{th} wavelength, the measurement equation is

$$S_i = g_i (V_{S,i} - V_{0,i}) - b_i \quad (8)$$

where

- g_i is the amplifier gain;
- $V_{S,i}, V_{0,i}$ are signals (voltage or current) recorded with source radiation present and absent, respectively;
- b_i refers to offsets that remain after gain correction.

4.2.1 Scaling components

Scaling components can include geometric quantities such as lamp position and uniformity, amplifier gains or wavelength-independent source noise or drift. Amplifier gains are typically independent of wavelength, i.e. $g_i = g_f$ where g_f is a constant, but can vary through the measurement. Source variations will generally be wavelength dependent.

Assuming that a fixed gain is used to measure the source and background voltages, uncertainty and covariance contributions to the spectral value are

$$u(S_i) = (V_{S,i} - V_{0,i}) u(g_f)$$

For $i \neq j$:

$$u(S_i, S_j) = 0 \quad \text{uncorrelated components}$$

$$u(S_i, S_j) = u_c(S_i) u_c(S_j) \quad \text{correlated components}$$
(9)

where the spectral values are to be combined linearly, such as in weighted sums, and the scaling factor is constant across the measurement, correlations introduced by scaling can be avoided by applying the scaling after forming the sum.

If the scaling factor is varying in time (e.g. amplifier gain is changing slowly – “drifting” – during the measurement sequence) or changed for particular wavelength ranges (gain changes in regions of weak signal) then correlations between the gain terms need to be included:

$$u(S_i) = (V_{S,i} - V_{0,i}) u(g_i)$$

For $i \neq j$:

$$u(S_i, S_j) = 0 \quad \text{uncorrelated components}$$

$$u(S_i, S_j) = u_c(S_i) u_c(S_j) \quad \text{correlated components}$$
(10)

Fortunately, amplifier gains are typically stable and accurately known and the contribution to uncertainty of the spectral values is often negligible (see 5.9 for a counter example).

Source noise or drift is treated as a change in signal voltage:

$$u(S_i) = g_i u(V_i)$$

For $i \neq j$:

$$u(S_i, S_j) = 0 \quad \text{uncorrelated components}$$

$$u(S_i, S_j) = u_c(S_i) u_c(S_j) \quad \text{correlated components}$$
(11)

NOTE Sensitivity coefficients for these effects are always positive, as are correlations, and signed uncertainties are not required.

4.2.2 Offset components

Offsets such as amplifier offsets or stray light reaching the detector without wavelength selection, such as light scattered directly to the detector from physical components of the spectrometer are subject to the gain of the amplifier and form part of the signal $V_{0,i}$; for these,

$$u(S_i) = g_i u(V_{0,i})$$

For $i \neq j$:

$$u(S_i, S_j) = 0 \quad \text{uncorrelated components}$$

$$u(S_i, S_j) = u_c(S_i) u_c(S_j) \quad \text{correlated components}$$
(12)

Stray light that arises from dispersed light scattered to the detector and appearing at a different wavelength setting to the primary response is subject to the same process as the required true spectrum. Accurately determining the level of such stray light (the signal b_i) in regions where the source is weak is one of the most difficult aspects of spectral measurement. For this component,

$$u(S_i) = u(b_i)$$

For $i \neq j$:

$$u(S_i, S_j) = 0 \quad \text{uncorrelated components}$$

$$u(S_i, S_j) = u_c(b_i) u_c(b_j) \quad \text{correlated components}$$
(13)

NOTE Sensitivity coefficients for these effects are negative, hence correlations are always positive and signed uncertainties are not required.

4.2.3 Wavelength components

The sensitivity coefficient for the dependence of the spectral value S_i upon wavelength is simply its derivative with respect to wavelength. This is evaluated numerically from values at nearby wavelengths, and it can be either positive or negative. Hence it is important to use signed uncertainties:

$$u^*(S_i) = \frac{\partial S_i}{\partial \lambda} u(\lambda)$$

For $i \neq j$:

$$u(S_i, S_j) = 0 \quad \text{uncorrelated components}$$

$$u(S_i, S_j) = u_c^*(S_i) u_c^*(S_j) \quad \text{correlated components}$$
(14)

For components correlated at different wavelengths, the correlation coefficient is either +1 or -1 as demonstrated in Figure 1. The two curves demonstrate the correlation between values for correlated wavelength shift within the uncertainty band. If the assigned wavelength is higher than the true value, measured values A and B are lower and measured values C and D are higher, respectively, than the true spectral values at the assigned wavelength. Pairs A,B and C,D are positively correlated. All other combinations (e.g. A,C) have one member higher and one member lower – these combinations are negatively correlated.

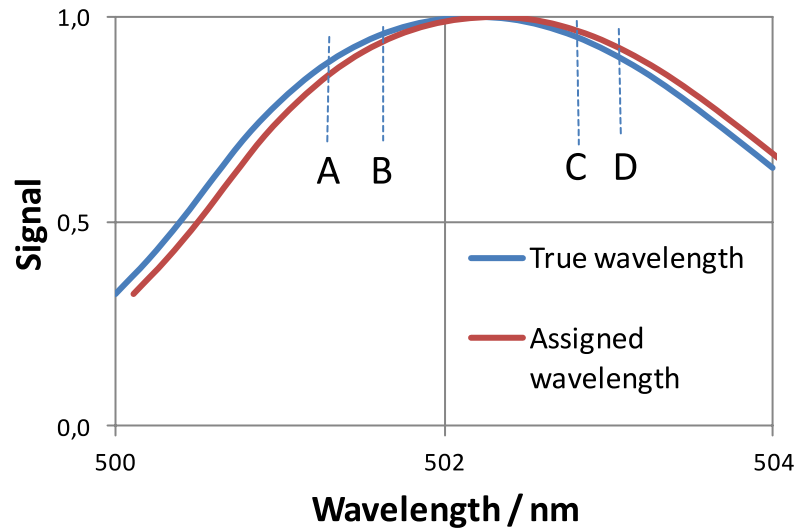


Figure 1 —Systematic shift in wavelength can generate positive and negative correlations

4.2.4 Estimating systematic uncertainties in spectral measurements

Consider a background spectrum recorded with the source blocked such as that shown in Figure 2, recorded at 5 nm intervals. The fine structure is clearly random noise. The mean value of the spectrum is 0,15. If we assume that this represents a constant value b to be subtracted from a spectrum recorded with the source enabled, the standard deviation of 0,06 for the $n = 41$ values represents the uncertainty $u(b)$ of the random (uncorrelated) background at each wavelength. The mean value also has uncertainty; the standard deviation of the mean, $u(b)/\sqrt{n} = 0,0015$, is then the correlated uncertainty component of the background, fully correlated between wavelength pairs. The red lines on the figure indicate a range of ± 1 standard deviation of the mean about the mean. Repeated measurements of the background spectrum should confirm the standard deviation of the mean. These uncertainties apply for a single source spectrum under the same conditions; if the background noise and the uncertainty of the mean for a single source spectrum are significant, they can be reduced by bracketing repeat measurements of both background and source spectra.

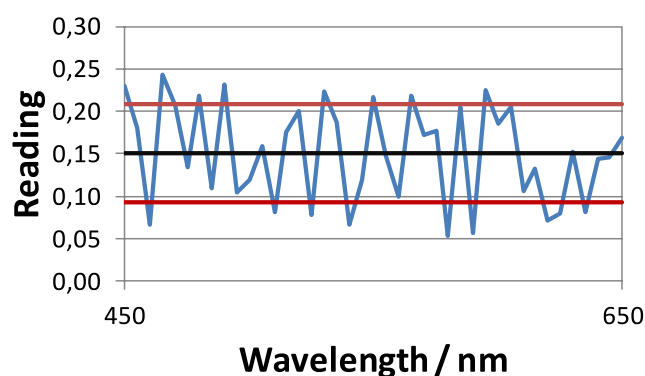


Figure 2 — Example of a random background spectrum

Stray light is light that reaches the detector through a path other than that which is intended. Stray light adds to the true spectrum and so constitutes an offset which cannot be removed by averaging repeated measurements. It can be internal or external and homochromic or heterochromic as follows:

- Internal stray light is stray light that arises from within the spectrometer itself, such as scattering from imperfections in the grating or reflections of the zeroth order off the walls of the chamber or other components in the spectrometer.
- External stray light has its origin outside the spectrometer, such as reflections of the source from other surfaces in the room or from other light sources such as instrument indicator lights.
- Homochromic stray light is stray light of the same wavelength as that being measured, such as from multiple reflections within optical components or from external stray light.
- Heterochromic stray light is stray light from wavelengths other than that being measured such as most internal stray light.

Offsets due to stray light can be estimated using filters (Shaw and Goodman 2008) . In array spectrometers, particularly in physically smaller or poorly-designed models, internal stray light can be a dominant source of uncertainty. Methods of characterizing and correcting for internal stray light within the measurement range of the spectrometer are available (Zong et al. 2006, Nevas et al. 2012). For scanning spectrometers the internal stray light is usually negligible and external stray light needs to be evaluated and minimized, particularly if absolute spectral measurements are being performed.

Wavelength uncertainty components are derived from calibration using narrow-band spectral sources such as isolated atomic line emissions (CIE 2014a) or absorption features in rare earth glasses. The line positions are typically obtained from an encoder, step counts from a stepper motor or pixel position along a detector array. For the line positions x_i , residuals, e_i , are calculated as the difference between the predicted wavelength $f(x_i)$ and the calibration wavelength λ_i :

$$e_i = f(x_i) - \lambda_i . \quad (15)$$

The prediction function is commonly linear for a scanning spectrometer with a sine-bar scanning mechanism, or a low-order polynomial, or may be a more complicated function such as an offset-cosine for a directly-rotated grating spectrometer. Figure 3 shows a plot of residuals for an array spectrometer where the prediction function is a cubic polynomial. The variance of the residuals, χ^2 , is given by

$$\chi^2 = \frac{1}{N-n} \sum_{i=1}^N e_i^2 \quad (16)$$

where

- N is the number of calibration wavelengths;
- n is the number of fitted parameters.

Provided the calibration lines are isolated and properly identified, their uncertainty is negligible. The uncertainty in position is determined mainly from the precision with which the line centre is able to be determined. This in turn depends on the resolution of the spectrometer, the scanning interval within the resolution (fixed as the pixel spacing for an array) and any interpolation or fitting methods employed. Deconvolution can be a useful technique to determine line centres (Gardner 2014). The precision of fitting the line centres is used to determine the uncorrelated (random) uncertainty in position, propagated in turn through the prediction function to determine the uncertainty in the predicted wavelength. Least-squares fitting means that all the parameters a of the prediction function depend on all the combined input positions and hence, even for the random uncertainty of the position, the fit parameters are correlated, usually at a high level. Fitting processes (regression) typically provide the matrix of correlation coefficients for the parameters U_a , assuming an uncorrelated uncertainty of the input points. With this matrix, the wavelength uncertainty (variances and covariances) propagated from the position uncertainty can be determined at any wavelength using

$$U_{\lambda} = C_{\lambda,a} U_a C_{\lambda,a}^T \quad (17)$$

where $C_{\lambda,a}$ is the sensitivity matrix for the dependence of the wavelength at given position on the parameters, i.e. the derivatives of the fitting function with respect to the parameters, at each of the required wavelengths. The superscript ^{T} indicates the transpose (used with the same meaning throughout this document). This is the uncertainty prediction band. At any wavelength there is also an uncorrelated component, whose variance is that of the residuals, e_i . Adding the variance of the residuals to the predicted variances (the diagonal elements of U_{λ}) leads to the confidence band of uncertainties. Figure 4 shows the prediction and confidence bands (68 % confidence interval) for the cubic fit of Figure 3, assuming that the line centres can be determined to 0,1 pixel. Corresponding correlation coefficients between pairs of wavelengths are shown in Figure 5. The variance of the residuals dominates that predicted variance and thus forms the major contribution to the correlations. Fitting is covered in more detail in Clause 8.

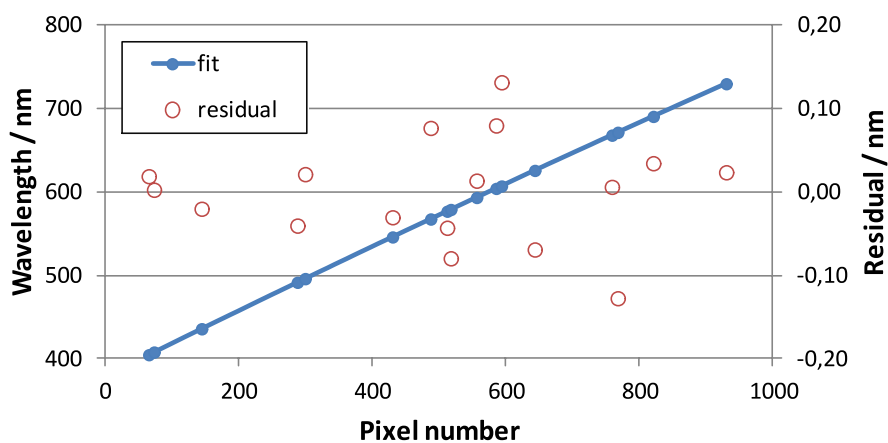


Figure 3 — Cubic fit and residuals for the wavelength scale of an array spectrometer

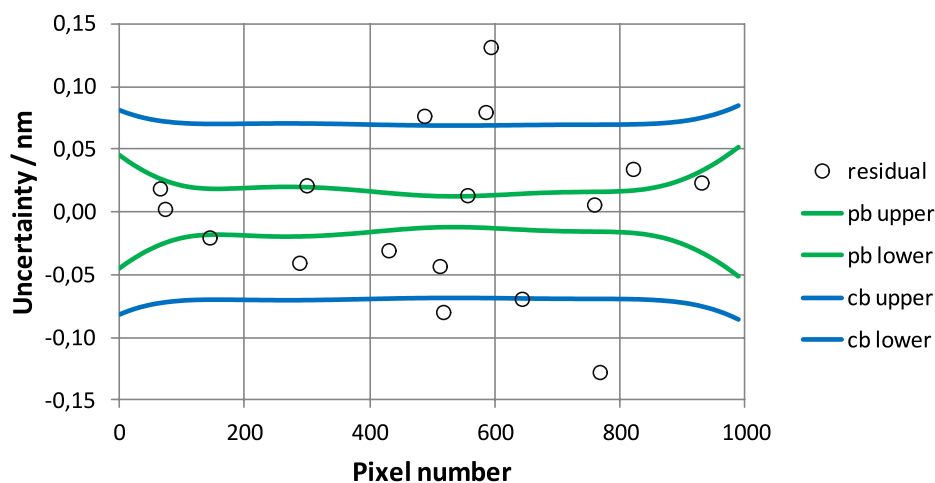


Figure 4 — Uncertainty prediction bands (pb) and confidence bands (cb) for the wavelength calibration of an array spectrometer compared to the residuals

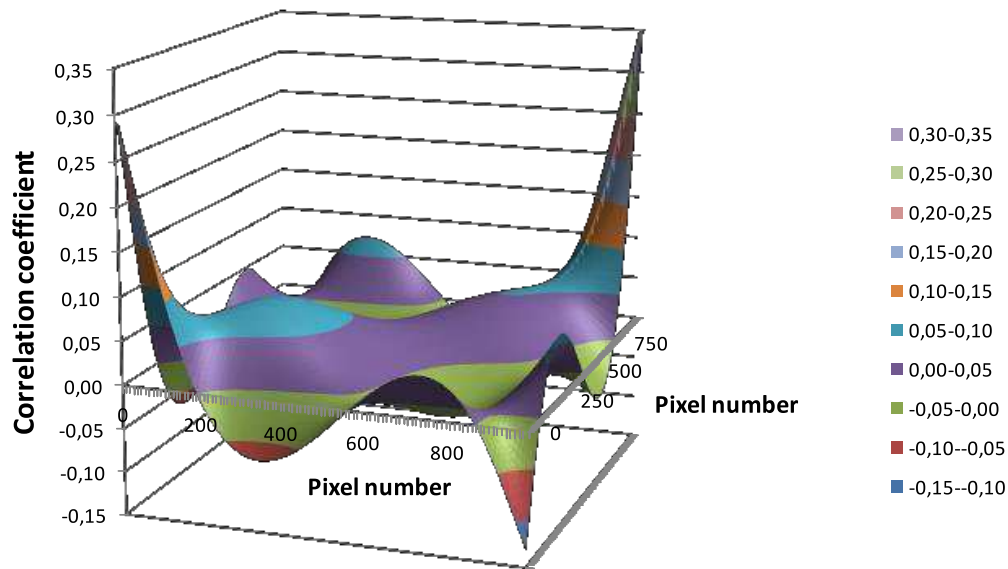


Figure 5 — Correlation coefficients vs. Pixel number for the wavelength uncertainty of the array spectrometer

Scanning spectrometers generally have a wavelength scale that is approximately linear. Calibration is performed by measuring the scale readings for line sources of known wavelength then minimizing residuals between predicted and measured positions. For scanning spectrometers where the resolution can be varied, the wavelength calibration function can be determined at high resolution. Hyper-scanning at the broader resolution (recording at many steps within the resolution) is a useful means of accurately determining line centres at the broader resolution, enhanced if Richardson-Lucy deconvolution is also applied (Gardner 2014). Figure 6 shows the prediction and confidence bands for a spectrometer with a linear scale if the residuals of Figure 3 applied and the line centres were determined with 0,1 nm uncertainty. Note that this is lower accuracy than 0,1 pixel (approx. 0,04 nm) for the array spectrometer, hence the confidence uncertainties are less dominated by the variance of the residuals and the correlations are higher than for the array calibration.

In both cases, the prediction band uncertainties rise sharply in the regions where the wavelength scale is extrapolated beyond the range of the calibration.

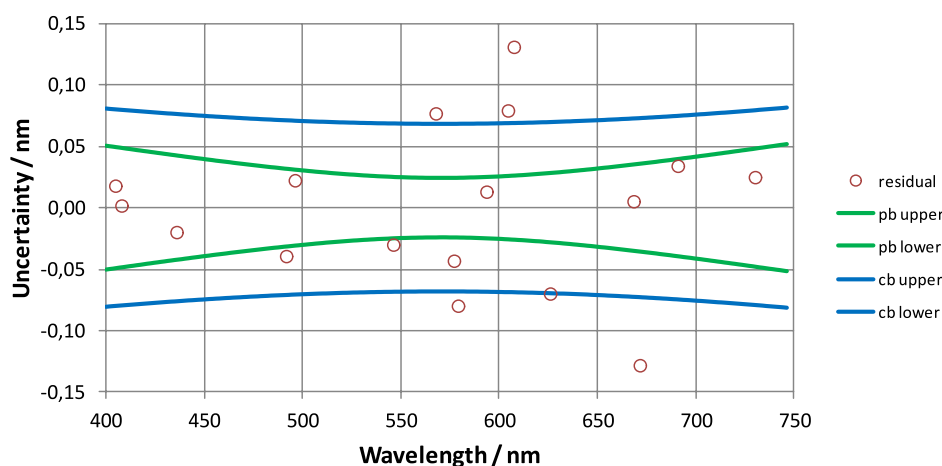


Figure 6 — Uncertainty prediction bands (pb) and confidence bands (cb) for the wavelength calibration of a scanning spectrometer compared to the residuals

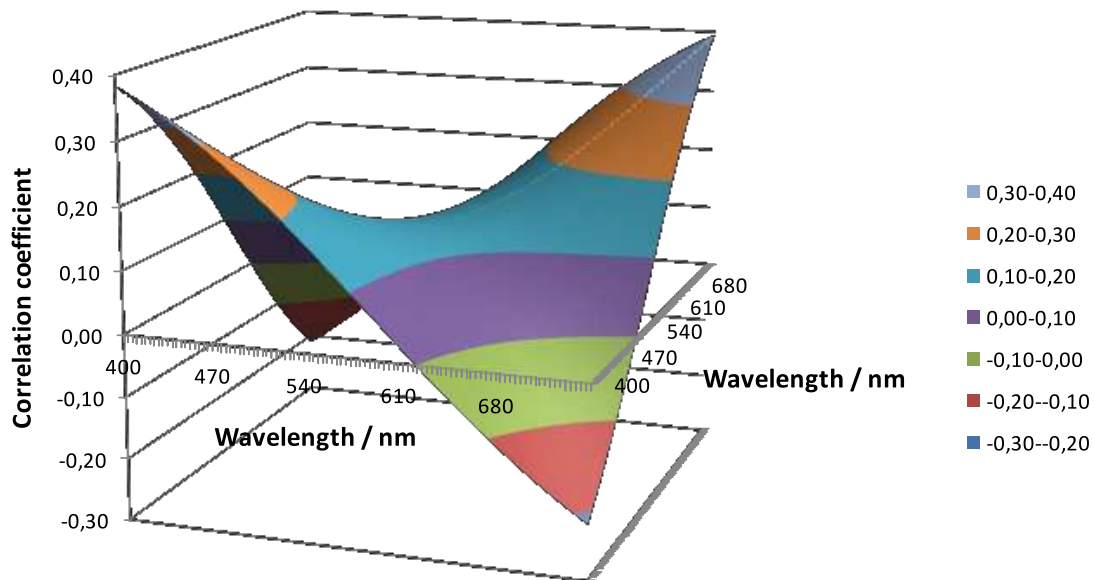


Figure 7 — Correlation coefficients vs. wavelength (nm) for the wavelength uncertainty of a scanning spectrometer

For a scanning spectrometer, the wavelength scale should be calibrated with a narrow bandwidth (small slits) to determine the relative offsets from the scale reading. A supplementary calibration at a single line (e.g. zero order) or possibly a number of lines, but not a full determination of the scanning function, is then used to determine the wavelength offset at a resolution used for a spectral measurement, generally lower than that used to determine the scanning function. Determining the line centre for the wider bandwidth may be shifted relative to that determined with narrow slits, and in general will be less precise thus adding to the correlated wavelength error. Hyper-scanning followed by Richardson-Lucy deconvolution is also effective to reduce this added correlated component and relative scale offsets themselves, plus determine positions for otherwise unresolved lines.

The procedures above are relatively complicated and are only necessary where wavelength accuracy is important to a result that combines the spectral values. A simple method that may be effective in many cases is analogous to that of the background components: take the variance of the residuals as that representing uncorrelated wavelength uncertainty and the uncertainty of mean residual as that representing correlated wavelength uncertainty. If wavelength uncertainty is then a minor contributor to the desired outcome, it is not necessary to use the full treatment of the fitting. For both examples above this would yield a total wavelength uncertainty of 0,07 nm and a constant correlation coefficient of 0,06. While the estimate of the uncertainty agrees reasonably with Figure 4 and Figure 6, the estimate of the correlations is low compared to those shown in Figure 5 and Figure 7.

If the deviation from linearity is small, the uncertainty of the fit may be described as a rectangular distribution applied to the maximum deviation from linearity (Kessel et al. 2016), fully correlated at all wavelengths.

4.2.5 Drift vs noise

Random variation of an influence factor on a time scale short compared to the time to record a spectrum appears as noise. If the variation is slow compared to the measurement time, it appears as “drift” and affects all values in a coordinated manner. If repeat spectra are recorded, the values at different wavelengths appear as correlated. A practical example is shown in 5.9.

5 Uncertainty of combinations of spectral values

Consider now the propagation of uncertainties from individual spectral values to some combination of those values, typically a weighted sum, but also applicable to interpolation, fitting, bandwidth correction and other manipulations of the directly measured spectral values for which we have been able to determine uncertainties, including covariances, from an understanding of the measurement process itself. Denoting the spectral value at the i^{th} wavelength as S_i and the combination as some function of those:

$$F = f(S_i); \quad i = 1, \dots, n, \quad (18)$$

the contribution to the variance of F from the k^{th} independent uncertainty component is given by

$$u_k^2(F) = \sum_{i=1}^n \left(c_i u_k(S_i) \right)^2 + 2 \sum_{i=1}^n \sum_{j \neq i=1}^n c_i c_j r_k(S_i, S_j) u_k(S_i) u_k(S_j) \quad (19)$$

where $c_i = \frac{\partial F}{\partial S_i}$ is the sensitivity coefficient for the dependence of F on S_i .

For uncorrelated components, the second term is zero:

$$u_{R,k}^2(F) = \sum_{i=1}^n \left(c_i u_k(S_i) \right)^2. \quad (20)$$

For correlated components, $r_k = \pm 1$ for each pair, and Equation (19) reduces to

$$u_{c,k}^2(F) = \sum_{i=1}^n \left(c_i u_{c,k}(S_i) \right)^2 + 2 \sum_{i=1}^n \sum_{j \neq i=1}^n c_i c_j u_{c,k}^*(S_i) u_{c,k}^*(S_j) = \left(\sum_{i=1}^n c_i u_{c,k}^*(S_i) \right)^2. \quad (21)$$

This shows that spectrum uncertainty components that are correlated across wavelengths contribute linearly when the spectral values are combined. Signed uncertainties must be used when correlations for a given effect can be positive or negative through the spectral range.

If uncertainties for combinations of spectral values are propagated using the partially correlated uncertainties arising from summing over the correlated and uncorrelated components, the full expression of Equation (19) must be used. In some cases it can be useful to propagate the uncertainties through the spectral combination separately for each component, as described in the next clause.

5.1 Propagation through spectral combinations by uncertainty component

Weighted sums of spectral values are common in photometry (photometric response) and colorimetry (tristimulus values) in particular. They have the form

$$F = \sum_{i=1}^n w_i S_i \quad (22)$$

where the S_i values are partly correlated due to a mix of uncorrelated and correlated uncertainty components. The weights, w_i , a product of tabulated values carrying no uncertainty and a wavelength interval carrying negligible uncertainty, are the sensitivity coefficients required to propagate uncertainty from the spectral values to F . The variance of F due to the k^{th} uncertainty component of the measurement can be calculated separately depending on whether that component is correlated or not at different wavelengths:

$$\begin{aligned}
 \text{Uncorrelated: } u_{u,k}^2(F) &= \sum_{i=1}^n w_i^2 u_{u,k}^2(S_i) \\
 \text{Correlated: } u_{c,k}^2(F) &= \left(\sum_{i=1}^n w_i u_{c,k}^*(S_i) \right)^2
 \end{aligned} \tag{23}$$

The k components are independent. The total variance of F is found by summing the variances due to the individual component effects and the uncertainty of F given as the (positive) square-root of the variance.

For such simple combinations, propagating uncertainties by individual components of the spectral measurement avoids the need to calculate correlation coefficients for each pair of spectral values. This is illustrated in Figure 8. While individual effects may be correlated or uncorrelated across the spectrum, they are independent. The contribution of a given effect to the uncertainty of the combined spectral values is calculated using the applicable part of Equation (23) but these latter values can be combined in quadrature. The uncertainties of individual spectral values include a mix of uncorrelated and correlated component effects and can't be simply combined in quadrature to form the total uncertainty of the combined spectral values.

NOTE Summing variances by effect assumes that each effect is linear over a small range about the mean value. While this is generally true for measured spectral values, it may not be true for values calculated from the spectral values; the general $V(\lambda)$ mismatch index f_1' (see 13.1) is an example.

Spectrum	Effect 1	Effect 2	...	Effect k	Combined →
S_1	$u_1(S_1)$	$u_2(S_1)$	...	$u_k(S_1)$	$u(S_1)$
S_2	$u_1(S_2)$	$u_2(S_2)$	...	$u_k(S_2)$	$u(S_2)$
$\vdots$	$\vdots$	$\vdots$		$\vdots$	$\vdots$
S_n	$u_1(S_n)$	$u_2(S_n)$		$u_k(S_n)$	$u(S_n)$
Combined ↓	$u_1(F)$	$u_2(F)$	...	$u_k(F)$	$u^2(F) = \sum_k u_k^2(F)$

NOTE Greyed values are partly correlated.

Figure 8 — Propagating mixed correlated and uncorrelated measurement uncertainties when spectral values are combined

5.2 Partial correlations

Just as the total variance of spectral values is found by adding the variances due to the component effects at each wavelength, the total covariance between two values at different wavelengths is found by adding the covariances for the component effects. For random effects, the covariance between values at different wavelengths is zero. It follows that when variances and covariances are summed over a mix of correlated and uncorrelated component effects, the magnitude of the corresponding correlation coefficient is less than 1, that is, the spectral values are *partly correlated*. The uncertainty values in the rightmost column of Figure 8 are partly correlated and can't be summed as squares with the appropriate sensitivity coefficients to form the variance of the spectral combination.

5.3 Forming the covariance matrix from the measurement uncertainty components

If the uncertainty contributions for the individual influence components are available for each spectral value, the variance-covariance matrix of the spectrum can be built by summing the variance-covariance matrices U_k for each effect k of Figure 8.

For uncorrelated influence component, the covariance terms are zero and the variance-covariance terms for element i, j of U_k for effect k are

$$\begin{aligned} u_{u,k}(S_i, S_j) &= u_{u,k}^2(S_i) & \text{for } i = j \\ u_{u,k}(S_i, S_j) &= 0 & \text{for } i \neq j \end{aligned} \quad (24)$$

For a correlated component, element i, j of U_k is given by

$$u_{c,k}(S_i, S_j) = u_{c,k}^*(S_i) u_{c,k}^*(S_j) \quad (25)$$

where all the signed uncertainties are positive or all negative (in practice this means if the spectrum is monotonic in wavelength), the sign superscript can be dropped as all correlation terms will be positive. If the spectrum contains peaks or valleys, a correlated wavelength uncertainty component may reduce uncertainty in a combination of the spectral values in that region (see 4.2.3).

Some reports now include separate values for the quadrature sum of the independent correlated and uncorrelated components at each wavelength (Goodman et al. 2015)]. These values can be used to generate a variance-covariance matrix for the spectral values as in Equations (24) and (25), but will not include any reductions in covariance for correlated wavelength effects. Such separation will also not properly account for the relatively complex correlations introduced by fitting functions such as those described in 8.4.

5.4 Partial correlation where the correlation coefficient is constant

Consider a spectrum where the measured² values at different wavelengths are partly correlated through a combination of uncorrelated and correlated components, but the ratio between correlated and total uncertainty at each wavelength is constant. For a pair of spectral values S_i, S_j , variances are given as the sum of the variances of the systematic and random parts:

$$\begin{aligned} u^2(S_i) &= u_c^2(S_i) + u_u^2(S_i) \\ u^2(S_j) &= u_c^2(S_j) + u_u^2(S_j) \end{aligned} \quad (26)$$

The systematic component correlates the two spectral values, with the correlation coefficient given by

$$r(S_i, S_j) = \frac{u_c(S_i) u_c(S_j)}{u(S_i) u(S_j)} = r^2 \quad (27)$$

where r is the ratio of correlated to total uncertainty. From Equations (26) and (27), the ratio of correlated to uncorrelated uncertainties can be found; this is shown in Figure 9. It can be seen that highly correlated data, typically the case for primary standards, remains highly correlated through stages of transfer that add random uncertainty. For example, the correlation coefficient for a spectrum where the ratio of correlated to uncorrelated uncertainty is constant

² This subclause applies to measured values only. Spectrum values given by interpolation or fitting have complex correlations that cannot be separated as systematic and random parts at each wavelength.

at 4:1 is 0,970. Doubling the uncorrelated uncertainty component reduces the correlation coefficient to only 0,885.

NOTE The correlated and uncorrelated components at each measured spectral value may be specified in different ways, such as separate values, total uncertainty value plus total uncorrelated or correlated uncertainty, or their variance equivalents. These are all inter-related through Equation (26), from which the ratio of correlated to uncorrelated effects can be calculated at each wavelength.

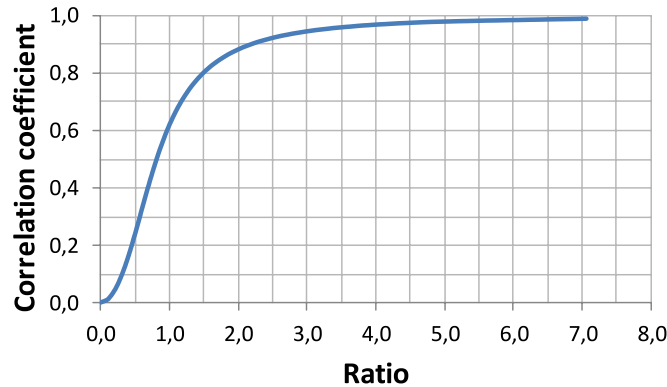


Figure 9 — Correlation coefficient for fixed correlated to uncorrelated uncertainty ratio

5.5 Correlation of multiple combinations of the same spectral values

Consider a second function that is also a combination of the same spectral values as F :

$$G = g(S_i); \quad i = 1, \dots, n . \quad (28)$$

The variance and hence uncertainty of G is found in the same manner as described above for F . But now each value of S_i is common to both F and G , and contributes a term to the covariance of F and G . For each individual effect k , independent of whether the effect is correlated or uncorrelated at different wavelengths, the covariance is given by

$$u_k(F, G) = \sum_{i=1}^n c_{F,i} c_{G,i} u_k^2(S_i) . \quad (29)$$

Note that for systematic effects, this reduces to

$$u_k(F, G) = \sum_{i=1}^n c_{F,i} u_{c,k}^*(S_i) \sum_{i=1}^n c_{G,i} u_{c,k}^*(S_i) = u_{c,k}^*(F) u_{c,k}^*(G) , \quad (30)$$

showing that for fully correlated effects, different combinations of the same spectral values are also fully correlated.

As an example, consider the variances and covariances of tristimulus values calculated from spectral measurements:

Tristimulus values are weighted sums across the visible spectrum representing the response of the eye to incident light. The weighting functions are the tabulated colour-matching functions $\bar{x}(\lambda)$, $\bar{y}(\lambda)$, $\bar{z}(\lambda)$, and the integrated response to each of these are the X , Y , Z tristimulus values, which are the basic quantities used to describe three-dimensional colour coordinates. The tristimulus values are given by

$$X = \sum_{i=1}^n \bar{x}_i w_i S_i; \quad Y = \sum_{i=1}^n \bar{y}_i w_i S_i; \quad Z = \sum_{i=1}^n \bar{z}_i w_i S_i \quad (31)$$