On the propagation of uncertainty in complex-valued quantities

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Abstract

This paper explores a recent suggestion to use a bivariate form of the Gaussian 'error propagation law' to propagate uncertainty in the measurement of complex-valued quantities (Ridler N. M. and Salter M. J., *Metrologia*, 2002, **39**, 295-302). Several alterative formulations of the law are discussed, in which the contributions from individual input terms are more explicit. The calculation of complex-valued sensitivity coefficients is discussed and a matrix generalization of the notion of a 'component of uncertainty' in a measurement result is introduced. A form of 'chain rule' is given for the propagation of uncertainty when several intermediate equations are involved.

1 Introduction

The recommendations of the 'Guide to the Expression of Uncertainty in Measurement' (*Guide*) in the evaluation and reporting of measurement uncertainty have been widely adopted [1]. However, the *Guide* deals essentially with measurement uncertainty in scalar-valued quantities. The measurement of complex-valued quantities is an important area that is not addressed in the *Guide*.[1]

Recently, Ridler and Salter described a method for handling complex quantities that arise in radio frequency and microwave measurements [3]. The approach used a *region of uncertainty* in the complex plane to describe the uncertainty in a complex-valued quantity. This elliptically shaped region is determined by a variance-covariance (covariance) matrix associated with the measurement result as well as the level of confidence required. A bivariate form of the Gaussian 'error propagation law' [4] was used to obtain the covariance matrix. This law propagates input quantity uncertainties through the measurement equation and is an extension of the scalar procedure described in the *Guide* [1].

This paper further investigates the bivariate law with a view to facilitating its use and interpretation. In ref. 3, the law is presented succinctly and elegantly in a matrix equation. However, the relationship of terms to the corresponding complex input quantities is somewhat difficult to see in this form. The paper draws attention to the role played by (2×2) sub-matrix elements in these calculations. These can be related directly to the input quantities and have analogs in the scalar form of the propagation law, like sensitivity coefficients, components of uncertainty and correlation coefficients.

The paper also looks at the relationship between complex derivatives and the bivariate

[1]There is an on-going effort to revise and expand the scope of the *Guide*, coordinated by the Joint Committee for Guides in Metrology [2].

form for sensitivity coefficients and gives a simple mapping to transform from one to the other. A 'chain rule' for the propagation of uncertainty is presented, which can be used to manage complexity in measurement scenarios where a sequence of intermediate steps combine to produce a single result.

1.1 Notation

Bivariate and complex quantities are written in bold italic type (e.g., $\boldsymbol{x}, \boldsymbol{S}$) and scalar quantities are indicated in plain italic type (e.g., x). When referring to the scalar components of a bivariate or complex quantity, subscripts '1' and '2' are used; when the quantity is complex, '1' labels the real component and '2' the imaginary (e.g., $\boldsymbol{x} = x_1 + \mathrm{j}\, x_2$ with $\mathrm{j} \equiv \sqrt{-1}$.).

Vectors and matrices are written in bold Roman capitals (e.g., $\mathbf{M}$) and a prime is used to indicate the matrix transpose (e.g., $\mathbf{M}'$). When identifying the scalar components of a bivariate or complex vector, the bivariate subscripts ('1' and '2') are concatenated in front of the subscript for the particular vector element. For example, the elements of a column vector of m complex elements can be identified as

$$[\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_m]' \Leftrightarrow [x_{11}, x_{21}, x_{12}, x_{22}, \cdots, x_{1m}, x_{2m}]' \ . \tag{1}$$

This unconventional labelling style has also been used with some matrices in an effort to highlight the relationship of a particular matrix element to the scalar quantities that contribute to its value.

2 Propagation of uncertainty

This section reviews the method of propagating covariance outlined in Section 8 of [3]. Here, single, rather than multiple, output quantities are considered and a slightly different notation is used, otherwise the approach is the same. The section finishes with a few comments that motivate the remainder of the paper.

An arbitrary measurement function

$$\boldsymbol{y} = \boldsymbol{f}(\mathbf{X}) = \boldsymbol{f}(\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_m) \ , \tag{2}$$

describes a relation between a complex-valued quantity of interest, the *measurand* $\boldsymbol{y}$, and m influence quantities on which its value depends. The function $\boldsymbol{f}$ is comprised of two scalar functions, f_1 and f_2, that evaluate the real and imaginary components respectively (i.e., $\boldsymbol{y} = f_1(\mathbf{X}) + \mathrm{j}\, f_2(\mathbf{X})$).

The uncertainty in the values assigned to input quantities is represented by a $2m \times 2m$ covariance matrix,

$$\mathbf{V}(\mathbf{X}) = \begin{bmatrix} u^2(x_{11}) & u(x_{11}, x_{21}) & \cdots & u(x_{11}, x_{1m}) & u(x_{11}, x_{2m}) \\ u(x_{21}, x_{11}) & u^2(x_{21}) & \cdots & u(x_{21}, x_{1m}) & u(x_{21}, x_{2m}) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ u(x_{1m}, x_{11}) & u(x_{1m}, x_{21}) & \cdots & u^2(x_{1m}) & u(x_{1m}, x_{2m}) \\ u(x_{2m}, x_{11}) & u(x_{2m}, x_{21}) & \cdots & u(x_{2m}, x_{1m}) & u^2(x_{2m}) \end{bmatrix} , \tag{3}$$

where the diagonal terms $u^2(x_{ij})$ represent the standard variance of the associated inputs x_{ij} and the terms $u(x_{ij}, x_{kl})$ off the diagonal represent the covariance between x_{ij} and x_{kl}.

The uncertainty in $\boldsymbol{y}$ is expressed in a (2×2) covariance matrix, obtained using a bivariate form of the Gaussian 'error propagation law'. The law prescribes how uncertainty in values assigned to the inputs propagates to an estimate of the uncertainty in a measurement result. The covariance is

$$\mathbf{V}(\boldsymbol{y}) = \mathbf{J}(\boldsymbol{y})\, \mathbf{V}(\mathbf{X})\, \mathbf{J}(\boldsymbol{y})' \,, \tag{4}$$

where $\mathbf{J}(\boldsymbol{y})$ is the $2 \times 2n$ Jacobian matrix of the partial derivatives of the scalar components of $\boldsymbol{f}$ with respect to the scalar elements of $\mathbf{X}$,

$$\mathbf{J}(\boldsymbol{y}) = \begin{bmatrix} \frac{\partial f_1}{\partial x_{11}} & \frac{\partial f_1}{\partial x_{21}} & \frac{\partial f_1}{\partial x_{12}} & \frac{\partial f_1}{\partial x_{22}} & \cdots & \frac{\partial f_1}{\partial x_{1m}} & \frac{\partial f_1}{\partial x_{2m}} \\ \frac{\partial f_2}{\partial x_{11}} & \frac{\partial f_2}{\partial x_{21}} & \frac{\partial f_2}{\partial x_{12}} & \frac{\partial f_2}{\partial x_{22}} & \cdots & \frac{\partial f_2}{\partial x_{1m}} & \frac{\partial f_2}{\partial x_{2m}} \end{bmatrix} . \tag{5}$$

2.1 Comments

The propagation law (4) is formulated for bivariate quantities. Nevertheless, when a problem is expressed in terms of complex quantities, it makes sense to retain a complex representation in subsequent analysis, if possible. For instance, the $4m$ distinct scalar partial derivatives in the matrix $\mathbf{J}(\boldsymbol{y})$ are difficult to relate to the complex quantities in the problem. The calculation would be made more transparent if complex differentiation could be used to obtain $\mathbf{J}(\boldsymbol{y})$.

The covariance matrices $\mathbf{V}(\mathbf{X})$ and $\mathbf{V}(\boldsymbol{y})$ are a rather terse expression of uncertainty and it is difficult to see how elements in these matrices relate back to the measurement domain. In scalar measurements, metrologists usually supplement information about the combined uncertainty in a result by calculating 'sensitivity coefficients'[2] or the related notion of 'components of uncertainty'[3] – values indicating the relative importance that small changes in an input quantity will have on a result.

3 A closer look at the propagation law

This section looks at the propagation law (4) in relation to the individual inputs and the output of a measurement equation and presents alternative expressions that reflect the underlying measurement context.

Subsection 3.1 looks at the relationship of the Jacobian matrix $\mathbf{J}(\boldsymbol{y})$ to the input terms and shows that there is a convenient (2×2) block structure related to the notion of a sensitivity coefficient. These Jacobian matrix blocks can be associated with complex partial derivatives of the measurement equation.

Subsection 3.2 presents alternative expressions of the propagation law. Several of these iterate over (2×2) sub-matrix components, which can be related to the input terms and resemble familiar elements in the scalar case.

[2] the partial derivative of the measurement equation with respect to a particular input

[3] the product of a sensitivity coefficient and the standard uncertainty of the input quantity – it has the same units as the measurand

Subsection 3.3 presents chain rules for the propagation of uncertainty. These can be used when the expression of a measurement equation involves a hierarchy of intermediate equations.

Subsection 3.4 discusses the possibility of using scalar values to summarize the more detailed information contained in (2×2) uncertainty matrices.

3.1 Complex numbers and the Jacobian matrix

The Jacobian matrix $\mathbf{J}(\boldsymbol{y})$ has a (2×2) block structure that can be associated with the derivatives of $\boldsymbol{f}$ with respect to individual bivariate inputs:

$$\mathbf{J}(\boldsymbol{y}) = \left[\begin{array}{cccc} \mathbf{J}_1(\boldsymbol{y}) & \mathbf{J}_2(\boldsymbol{y}) & \cdots & \mathbf{J}_m(\boldsymbol{y}) \end{array} \right] , \tag{6}$$

where

$$\mathbf{J}_j(\boldsymbol{y}) = \left[\begin{array}{cc} \frac{\partial f_1}{\partial x_{1j}} & \frac{\partial f_1}{\partial x_{2j}} \\ \frac{\partial f_2}{\partial x_{1j}} & \frac{\partial f_2}{\partial x_{2j}} \end{array} \right] . \tag{7}$$

These blocks represent the bivariate sensitivity coefficients of the problem. They can be related directly to the complex partial derivatives of $\boldsymbol{f}$ by a simple and elegant matrix representation for complex numbers. For any complex $\boldsymbol{z} \equiv a + \mathrm{j}\, b$ the mapping

$$\mathbf{M}(\boldsymbol{z}) \equiv \left[\begin{array}{cc} a & -b \\ b & a \end{array} \right] \tag{8}$$

generates a 2×2 matrix representation for $\boldsymbol{z}$. Such matrices behave as complex numbers under the usual matrix operations for arithmetic: division corresponds to multiplication by the matrix inverse, and taking the matrix transpose corresponds to the complex conjugate operation. Furthermore, if a complex function $\boldsymbol{f}(\boldsymbol{z})$ is analytic in the region of interest, the Cauchy-Riemann relations will apply to its partial derivatives [6], so

$$\frac{\partial f_1}{\partial a} = \frac{\partial f_2}{\partial b} \, , \; \frac{\partial f_1}{\partial b} = -\frac{\partial f_2}{\partial a} \, . \tag{9}$$

Equations (8) and (9) show that the full Jacobian matrix could be written as

$$\mathbf{J}(\boldsymbol{y}) = \left[\begin{array}{cccc} \mathbf{M}\left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}_1}\right) & \mathbf{M}\left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}_2}\right) & \cdots & \mathbf{M}\left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}_m}\right) \end{array} \right] . \tag{10}$$

3.1.1 Example

The following equation sometimes arises in relation to the measurement of radio frequency (RF) power

$$\boldsymbol{\Gamma}_{\mathrm{g}} = \boldsymbol{S}_{22} - \frac{\boldsymbol{S}_{12}\boldsymbol{S}_{23}}{\boldsymbol{S}_{13}} \, . \tag{11}$$

It describes the equivalent voltage reflection coefficient $\boldsymbol{\Gamma}_{\mathrm{g}}$ of an RF signal generator in terms of the complex scattering parameters, $\boldsymbol{S}_{ij}$, of a 3-port coupler connecting the generator to a power meter.

Associating the terms $\boldsymbol{S}_{22}, \boldsymbol{S}_{12}, \boldsymbol{S}_{23}, \boldsymbol{S}_{13}$ with inputs 1, 2, 3, and 4 respectively, the

(2×8) Jacobian matrix for the reflection coefficient is easily obtained as[4]

$$\mathbf{J}(\mathbf{\Gamma}_{\mathrm{g}}) = \left[\begin{array}{cccc} \mathbf{M}\,(1) & \mathbf{M}\left(-\frac{\boldsymbol{S}_{23}}{\boldsymbol{S}_{13}}\right) & \mathbf{M}\left(-\frac{\boldsymbol{S}_{12}}{\boldsymbol{S}_{13}}\right) & \mathbf{M}\left(\frac{\boldsymbol{S}_{12}\boldsymbol{S}_{23}}{\boldsymbol{S}_{13}^2}\right) \end{array} \right] . \tag{12}$$

3.2 Alternative expressions of the propagation law

3.2.1 Propagation and the correlation coefficients

A covariance matrix is symmetric and positive definite. It can always be factored into a matrix of correlation coefficients and a matrix of standard deviations [5]

$$\mathbf{V}(\mathbf{X}) = \mathbf{S}(\mathbf{X})\,\mathbf{R}(\mathbf{X})\,\mathbf{S}(\mathbf{X})' , \tag{13}$$

where the matrix of correlation coefficients is

$$\mathbf{R}(\mathbf{X}) = \left[\begin{array}{ccccc} 1 & r(x_{11}, x_{21}) & \cdots & r(x_{11}, x_{1m}) & r(x_{11}, x_{2m}) \\ r(x_{21}, x_{11}) & 1 & \cdots & r(x_{21}, x_{1m}) & r(x_{21}, x_{2m}) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ r(x_{1m}, x_{11}) & r(x_{1m}, x_{21}) & \cdots & 1 & r(x_{1m}, x_{2m}) \\ r(x_{2m}, x_{11}) & r(x_{2m}, x_{21}) & \cdots & r(x_{2m}, x_{1m}) & 1 \end{array} \right] \tag{14}$$

and $\mathbf{S}(\mathbf{X})$ is a diagonal matrix of the standard uncertainties of the individual input components (i.e., the square root of the diagonal elements of $\mathbf{V}(\mathbf{X})$).

The propagation law can be expressed in terms of $\mathbf{R}(\mathbf{X})$ by substituting (13) in (4) and then letting

$$\mathbf{U}(\boldsymbol{y}) = \mathbf{J}(\boldsymbol{y})\,\mathbf{S}(\mathbf{X}) . \tag{15}$$

This gives the alternative form of the law

$$\mathbf{V}(\boldsymbol{y}) = \mathbf{U}(\boldsymbol{y})\,\mathbf{R}(\mathbf{X})\,\mathbf{U}(\boldsymbol{y})' . \tag{16}$$

Now, the $(2 \times 2m)$ matrix

$$\mathbf{U}(\boldsymbol{y}) \;=\; \left[\begin{array}{ccccccc} u_{1\cdot 11} & u_{1\cdot 21} & u_{1\cdot 12} & u_{1\cdot 22} & \cdots & u_{1\cdot 1m} & u_{1\cdot 2m} \\ u_{2\cdot 11} & u_{2\cdot 21} & u_{2\cdot 12} & u_{2\cdot 22} & \cdots & u_{2\cdot 1m} & u_{2\cdot 2m} \end{array} \right] \tag{17}$$

consists of the scalar components of uncertainty in $\boldsymbol{y}$ due to uncertainty in the scalar components of the input quantities. All elements have the same units as the measurand. It is instructive to see how these elements combine in the covariance matrix of the result. In the simplest scenario, all inputs can be assumed independent, so $\mathbf{R}(\mathbf{X})$ is the identity matrix, and the covariance matrix becomes

$$\mathbf{V}(\boldsymbol{y}) = \left[\begin{array}{cc} \sum_{j=1}^{m} \sum_{i=1}^{2} u_{1\cdot ij}^2 & \sum_{j=1}^{m} \sum_{i=1}^{2} u_{1\cdot ij} u_{2\cdot ij} \\ \sum_{j=1}^{m} \sum_{i=1}^{2} u_{1\cdot ij} u_{2\cdot ij} & \sum_{j=1}^{m} \sum_{i=1}^{2} u_{2\cdot ij}^2 \end{array} \right] . \tag{18}$$

A more realistic scenario would consider that the real and imaginary components of individual inputs could be correlated. The first and second diagonal elements of $\mathbf{V}(\boldsymbol{y})$

[4] A full bivariate treatment of the same problem can be found in [8].

then become, respectively,

$$\sum_{j=1}^{n}\left[\left(\sum_{i=1}^{2}u_{1\cdot ij}^{2}\right)+2\,r(x_{1j},x_{2j})\,u_{1\cdot 1j}u_{1\cdot 2j}\right] \tag{19}$$

$$\sum_{j=1}^{n}\left[\left(\sum_{i=1}^{2}u_{2\cdot ij}^{2}\right)+2\,r(x_{1j},x_{2j})\,u_{2\cdot 1j}u_{2\cdot 2j}\right] \tag{20}$$

and the off-diagonal elements are equal to

$$\sum_{j=1}^{n}\left[\sum_{i=1}^{2}u_{1\cdot ij}u_{2\cdot ij}+r(x_{1j},x_{2j})\,(u_{1\cdot 2j}u_{2\cdot 1j}+u_{1\cdot 1j}u_{2\cdot 2j})\right]\ . \tag{21}$$

3.2.2 Propagation in terms of sub-matrix components

Propagation laws (4) and (16) can be expressed in summation form by explicitly recognizing the (2×2) internal structure of the matrices $\mathbf{U}(\boldsymbol{y})$, $\mathbf{V}(\mathbf{X})$ and $\mathbf{R}(\mathbf{X})$. In $\mathbf{U}(\boldsymbol{y})$, there are m submatrices associated with the input quantities. Each

$$\mathbf{U}_j(\boldsymbol{y})=\begin{bmatrix}u_{1\cdot 1j} & u_{1\cdot 2j}\\ u_{2\cdot 1j} & u_{2\cdot 2j}\end{bmatrix} \tag{22}$$

is the product of a bivariate sensitivity coefficient, $\mathbf{J}_j(\boldsymbol{y})$, and a sub-matrix of standard uncertainties from the diagonal of $\mathbf{S}(\mathbf{X})$, corresponding to input j,

$$\mathbf{U}_j(\boldsymbol{y})=\begin{bmatrix}\frac{\partial f_1}{\partial x_{1j}} & \frac{\partial f_1}{\partial x_{2j}}\\ \frac{\partial f_2}{\partial x_{1j}} & \frac{\partial f_2}{\partial x_{2j}}\end{bmatrix}\begin{bmatrix}u(x_{1j}) & 0\\ 0 & u(x_{2j})\end{bmatrix}\ . \tag{23}$$

The $\mathbf{U}_j(\boldsymbol{y})$ are a bivariate analog of the scalar 'component of uncertainty'.[5] They are in the same units as the measurand and convey information about the relative importance of an input in the uncertainty of the result.

There is also a 2×2 block structure apparent in $\mathbf{V}(\mathbf{X})$, grouping the covariance of pairs of inputs,

$$\mathbf{V}_{ij}(\mathbf{X})=\begin{bmatrix}u(x_{1i},x_{1j}) & u(x_{1i},x_{2j})\\ u(x_{2i},x_{1j}) & u(x_{2i},x_{2j})\end{bmatrix}\ . \tag{24}$$

Along the diagonal of $\mathbf{V}(\mathbf{X})$, these blocks are bivariate covariance matrices associated with individual inputs. Off the diagonal, they contain the covariance elements for pairs of different inputs. For example, in the lower left (and upper right) of $\mathbf{V}(\mathbf{X})$ there is a (2×2) sub-matrix of the four possible covariance terms between the elements of $\boldsymbol{x}_1$ and $\boldsymbol{x}_m$. Similarly, blocks within $\mathbf{R}(\mathbf{X})$ represent the correlations between pairs of complex inputs

$$\mathbf{R}_{ij}(\mathbf{X})=\begin{bmatrix}r(x_{1i},x_{1j}) & r(x_{1i},x_{2j})\\ r(x_{2i},x_{1j}) & r(x_{2i},x_{2j})\end{bmatrix}\ . \tag{25}$$

[5] Strictly, the *Guide* uses the term 'component of combined standard uncertainty generated by the standard uncertainty of input estimate j' [1, p.93] and also ignores the sign of the partial derivative.

With this notation, equation (4) can be expressed as

$$\mathbf{V}(\boldsymbol{y}) = \sum_{i=1}^{m}\sum_{j=1}^{m} \mathbf{J}_i\left(\boldsymbol{y}\right)\, \mathbf{V}_{ij}(\mathbf{X})\, \mathbf{J}_j\left(\boldsymbol{y}\right)' \tag{26}$$

and equation (16) can be expressed as

$$\mathbf{V}(\boldsymbol{y}) = \sum_{i=1}^{m}\sum_{j=1}^{m} \mathbf{U}_i(\boldsymbol{y})\, \mathbf{R}_{ij}(\mathbf{X})\, \mathbf{U}_j(\boldsymbol{y})' \; . \tag{27}$$

The complex mapping (8) can be used for $\mathbf{J}_j\left(\boldsymbol{y}\right)$ if appropriate.

These equations resemble the summation expressions for the scalar law in the *Guide*. They may be easier to apply in certain circumstances, than the full matrix forms of equations (4) and (16). For instance, the terms in (18) – (21) are perhaps more easily obtained using equation (27).

3.3 A chain rule for complex uncertainty calculations

It is not unusual for a measurement equation to be conveniently expressed as a series of intermediate equations, reflecting distinct aspects of the calculation or procedure. In such cases, it is more difficult to formulate the uncertainty calculations and care must be taken not to overlook correlations between intermediate results. This section presents a form of chain rule that uses component matrices similar to the $\mathbf{U}_j(\boldsymbol{y})$ introduced in Section 3.2.2.

Suppose that the measurement function

$$\boldsymbol{y} = \boldsymbol{f}(\mathbf{X}) = \boldsymbol{f}(\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_m) \tag{28}$$

can be decomposed into a series of $N - m$ steps, each described by a function

$$\boldsymbol{x}_i = \boldsymbol{f}_i(\Lambda_i) \; ; \; i = m+1, \cdots, N \; . \tag{29}$$

The symbol Λ_i represents the set of input arguments to $\boldsymbol{f}_i$, which may include any of $\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_{i-1}$.

To obtain a value for $\boldsymbol{y} \equiv \boldsymbol{x}_N$, these functions are evaluated in the appropriate order with intermediate results from earlier steps providing inputs to subsequent calculations,

$$\boldsymbol{x}_i = \boldsymbol{f}_i(\Lambda_i) \; , \text{ for } i = m+1 \text{ to } N \; . \tag{30}$$

The partial derivatives of $\boldsymbol{f}$ can be obtained in a similar fashion, using either the chain rule for complex differentiation,

$$\frac{\partial \boldsymbol{f}_i}{\partial \boldsymbol{x}_j} = \sum_{\boldsymbol{x}_k \in \Lambda_i} \frac{\partial \boldsymbol{f}_i}{\partial \boldsymbol{x}_k} \frac{\partial \boldsymbol{f}_k}{\partial \boldsymbol{x}_j} \; , \text{ for } i = m+1 \text{ to } N \; , \tag{31}$$

or the corresponding chain rule for Jacobian matrices [7]

$$\mathbf{J}_j(\boldsymbol{f}_i) = \sum_{\boldsymbol{x}_k \in \Lambda_i} \mathbf{J}_k(\boldsymbol{f}_i)\mathbf{J}_j(\boldsymbol{f}_k) \; , \text{ for } i = m+1 \text{ to } N \; . \tag{32}$$

Now the uncertainty component matrices $\mathbf{U}_j(\boldsymbol{y})$ can be obtained by the right-multiplying $\mathbf{J}_j(\boldsymbol{f}_i)$ with the appropriate diagonal block from $\mathbf{S}(\mathbf{X})$, as in (23).

Alternatively, components of uncertainty can be propagated directly. Right-multiply both sides of equation (32) with the appropriate block from $\mathbf{S}(\mathbf{X})$ and let

$$\mathbf{U}_j(\boldsymbol{x}_i) = \begin{bmatrix} \frac{\partial f_{1i}}{\partial x_{1j}} & \frac{\partial f_{1i}}{\partial x_{2j}} \\ \frac{\partial f_{2i}}{\partial x_{1j}} & \frac{\partial f_{2i}}{\partial x_{2j}} \end{bmatrix} \begin{bmatrix} u(x_{1j}) & 0 \\ 0 & u(x_{2j}) \end{bmatrix} \tag{33}$$

to obtain

$$\mathbf{U}_j(\boldsymbol{x}_i) = \sum_{\boldsymbol{x}_k \in \Lambda_i} \mathbf{J}_k(\boldsymbol{f}_i)\mathbf{U}_j(\boldsymbol{x}_k) \text{ , for } i = m+1 \text{ to } N \text{ .} \tag{34}$$

This shows that uncertainty component matrices propagate at each intermediate step, weighted by the sensitivity of the step function. Equation (34) can be used to obtain the submatrices $\mathbf{U}_j(\boldsymbol{y})$ that comprise $\mathbf{U}(\boldsymbol{y})$. The algorithmic structure of this chain rule is amenable to programming on a computer [9].

Complex derivatives may be used by applying mapping (8)

$$\mathbf{U}_j(\boldsymbol{x}_i) = \sum_{\boldsymbol{x}_k \in \Lambda_i} \mathbf{M}\left(\frac{\partial \boldsymbol{f}_i}{\partial \boldsymbol{x}_k}\right) \mathbf{U}_j(\boldsymbol{x}_k) \text{ , for } i = m+1 \text{ to } N \text{ .} \tag{35}$$

However, if the uncertainty at intermediate steps is not required, it may be easier to use (31) and defer the transformation into component of uncertainty matrices until the final step of the calculation.

3.3.1 Example

The utility of a chain rule can be illustrated in a simple radio frequency (RF) power measurement scenario. When a power meter is connected directly to an RF generator the measured power, P, is given by

$$P = |\boldsymbol{b}_\mathrm{g}|^2 \frac{1 - |\boldsymbol{\Gamma}_\mathrm{g}|^2}{|1 - \boldsymbol{\Gamma}_\mathrm{g}\boldsymbol{\Gamma}_\mathrm{s}|^2} \text{ ,} \tag{36}$$

where the generator emits a signal of amplitude $\boldsymbol{b}_\mathrm{g}$ and the complex voltage reflection coefficients of the power meter and generator are $\boldsymbol{\Gamma}_\mathrm{s}$ and $\boldsymbol{\Gamma}_\mathrm{g}$, respectively.

If an arbitrary network is inserted between the meter and the generator, expression (36) remains valid, provided the quantities $\boldsymbol{\Gamma}_\mathrm{g}$ and $\boldsymbol{b}_\mathrm{g}$ are corrected for the effects of the network. The new reflection coefficient is

$$\boldsymbol{\Gamma}'_\mathrm{g} = \boldsymbol{S}_{22} + \frac{\boldsymbol{S}_{21}\boldsymbol{S}_{12}\boldsymbol{\Gamma}_\mathrm{g}}{1 - \boldsymbol{S}_{11}\boldsymbol{\Gamma}_\mathrm{g}} \text{ ,} \tag{37}$$

where the $\boldsymbol{S}_{ij}$ are complex scattering parameters characterizing the network. The new generator term is

$$\boldsymbol{b}'_\mathrm{g} = \boldsymbol{b}_\mathrm{g} \frac{\boldsymbol{S}_{21}}{1 - \boldsymbol{S}_{11}\boldsymbol{\Gamma}_\mathrm{g}} \text{ .} \tag{38}$$

There are now two intermediate steps involved prior to evaluating (36). Moreover, in practice, $\boldsymbol{\Gamma}_\mathrm{s}$ in (36) and the $\boldsymbol{S}$-parameters in (37) and (38) are likely to be measured

with a vector network analyzer, which further increases the complexity of the problem. A chain rule mitigates the difficulty of handling a problem like this by allowing it to be treated in steps.

3.4 Scalar summary values for uncertainty matrices

In some cases, a summary of the information contained in the covariance matrix for a complex result or the component-of-uncertainty matrices $\mathbf{U}_j(\boldsymbol{y})$ may desirable. This section will consider possible summary values for these matrices.

3.4.1 Covariance matrix

The term 'total variance' is used in multivariate statistics to describe the sum of the diagonal elements (the trace) of a covariance matrix [5]. It has an elegant geometrical interpretation. The eigenvectors of a bivariate covariance matrix lie along the major and minor axes of the elliptical 'region of uncertainty', described in ref. 3, and the sum of the associated eigenvalues is equal to the total variance [5]. This indicates that the orientation of the ellipse has no bearing on the total variance (total variance ignores correlations). It also suggests that the total variance effectively sums two mutually 'independent' contributions to variance in a measurement. (When the axes of the elliptical region are at an angle to the coordinate axes, correlation exists between the quantities associated with that choice of axes. The eigenvectors represent directions for a linear combination of quantities that are mutually independent.)

Good candidates for a summary variable for the covariance matrix are therefore either the total variance or the square root of the total variance, which has the same units as the measurand.

3.4.2 Component of uncertainty matrix

The component of uncertainty matrices $\mathbf{U}_j(\boldsymbol{y})$ are not covariance matrices and the geometric interpretation in the previous section does not apply to them.

The scalar elements of the $\mathbf{U}_j(\boldsymbol{y})$ have the same units as the measurand and contribute directly to the terms in the covariance matrix, as shown in equations (18) – (21). A likely summary variable for these matrices is the root-sum-square of *all* elements. This retains the units of the measurand and, from equation (18), the total variance could be obtained as the sum over all components in a measurement, of these summary values squared.

4 Conclusion

The bivariate form of the Gaussian law for propagation of variance is a useful extension of well-established procedures for scalar uncertainty propagation to complex-valued and multivariate measurements. Several alternative expressions of the law have been given here, which should help practitioners to apply it.

The main points are listed here.

- Succinct matrix expressions of the law can be based on (2×2) sub-matrices components, which represent bivariate analogs of familiar scalar concepts: sensitivity coefficients, equations (6); components of uncertainty, equation (22); covariance, equation (24) and correlation, equation (25).
- In many cases, complex partial derivatives can be transformed into (2×2) matrices using equation (8), to construct the Jacobian matrices required.
- Chain rules can be used to ease the problem of complexity in calculations.

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