Mathematical notation for FIDUCEO publications

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version 1.b

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Contents

1 Introduction

FIDUCEO publications include research articles, reports, presentations and "cookbooks" for Earth observation metrology. There are many variables, arising at different satellite data processing levels, and a large variety of uncertainty, error covariance and error correlation matrices that can be specified in relation to satellite data. To facilitate

- coherence of nomenclature across publications for the benefit of readers
- ease of sharing equations and text across members of the consortium
- ease of re-packaging and re-presenting selections of FIDUCEO "recipes" across a variety of media prepared by different project team members

it is necessary to define and use a standardised mathematical notation across the project and all its forms of publication.

It is recognised that where FIDUCEO notation conflicts with the requirements of particular journals, deviations in externally published articles may be inevitable.

1.1 Scope

This document defines

- conventions for type-faces of variables of different classes (single-valued, indices, vectors, matrices), so that a reader knows immediately what class of variable each term in an equation is
- conventions for the symbols to use for the data and data transformations associated with each satellite data processing level from L0 to L3
- conventional symbols for common indices required in FIDUCEO "recipes"
- conventions for super- and sub-scripting key variables that have many potential variants, particularly error correlation and error covariance matrices
- standard presentations of commonly used equations

1.2 Version Control

Version	Reason / changes	Reviewer	Date of Issue
1.a	Initial release	R Quast, M Taylor, P Harris, G Holl, T Popp	17/11/17
1.b	• Use q for polynomial index subscript. • Use m for measurement index. • Introduction notation for common/harmonisation effect, and associated comments in text • Three alternative forms of expressing measurement function parameters	N/A	21/2/18

1.3 Applicable documents

ISO 80000-2:2008, Quantities and units -- Part 2: Mathematical signs and symbols to be used in the natural sciences and technology, https://www.iso.org/standard/31887.html

2 Use of typeface to identify classes of quantities/terms

2.1 Purpose

Purpose of standardisation: to enable readers to identify at a glance the nature of terms in equations in FIDUCEO publications, distinguishing

- constants
- single-valued variables
- vector variables
- matrix variables

The conventions reflect the standard ISO 80000-2:2009.

2.2 Conventions

Class of quantity/terms		Convention	Examples
Constant		Upright, non-bold	$\mathrm{\pi}, \mathrm{e} \cong 2.71, \mathrm{k}, \mathrm{h}, \mathrm{c}$
Variable quantities:		Italic	$\boldsymbol{R}, L, y, \boldsymbol{x}$
	Single-valued	Lower-case[1], non-bold	y, i, c, ϵ
	Vector[2]	Lower-case, bold	$\boldsymbol{z}, \boldsymbol{\gamma}, \boldsymbol{y}$
	Matrix	Upper-case, bold	$\boldsymbol{R}, \boldsymbol{\Gamma}, \boldsymbol{J}$
Labels, including matrix transpose		Upright[3], non-bold	$\boldsymbol{R}^{\mathrm{T}}$
Indices		Italic, non-bold	i, j, k, c, s, l, e, p

Table 1. Conventions for use of typeface to distinguish classes of quantity/terms

Note 1. The following single-value variables are conventionally upper case, and are permitted as exceptions

- L for radiance
- T for temperature or brightness temperature
- R for reflectance (but not for radiance)
- C for sensor counts

Note 1. These exceptions form a coherent set, in that all are quantities representing sensor measured values. Note2. The generic variable for calibrated sensor measured values (covering radiance, brightness temperature and reflectance) is lower case, namely, y. Note 3. A multi-channel or multi-pixel list of any of the measured sensor values is always $\boldsymbol{y}$, and never (for example) $\boldsymbol{L}$, which would conflict with the use of upper-case bold to designate matrices. Note 4: upper case may also exceptionally be used for a specific value of an index variable, for example, $i = I$.

Note 2. Vectors are by default column vectors. Inline definition of a column vector can be presented, for example, as $\boldsymbol{b}^{\mathrm{T}} = [b_1, b_2, \dots, b_n]$.

Note 3. However, a variable or index used to label a symbol is still presented in italic, e.g., $\boldsymbol{R}_c$.

3 Indices

3.1 Purpose

Purpose of standardisation: to avoid mis-interpretation of the co-ordinates in imagery or of the nature of indexed summations, which are common in FIDUCEO. This is achieved by choosing indices that are

- only used to indicate a specific indexing variable, such that indexing with respect to i, for example, has a unique meaning, and does not merely represent a generic "counter"
- as far as possible, not also variables or common constants (complete consistency here seems not to be achievable, however)
- intuitive with respect to what they represent, as far as possible

Moreover, conventions about the interpretation of indices are defined to make equations as legible as possible.

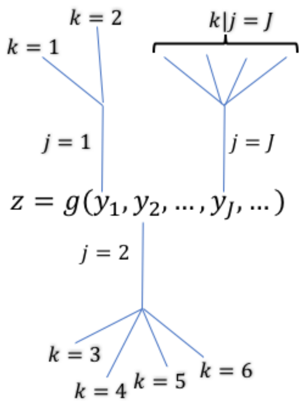
3.2 Conventional symbols for indices

Description of index	Conventional symbols
Terms (parameters, not including constants) in a measurement function	$j = 1, n_j$
Effects (sources of error of all types)	$k = 1, n_k$
Independent effects (sources of independent random errors)	$i = 1, n_i$
Structured effects (sources of structured random and systematic errors)	$s = 1, n_s$
Common effects (sources of large-scale bias-like errors, mainly harmonisation)	$h = 1, n_h$
Channels (bands of different wavelengths)	$c = 1, n_c$
Line number (co-ordinate within an image, along-track or scan-line index)	$l = 1, n_l$
Element number (co-ordinate within an image, across-track or scan-pixel index)	$e = 1, n_e$
Pixel (index of an arbitrary list of selected image pixels)	$p = 1, n_p$
Polynomial index (wherever sets of polynomial indices are used)	$q = 1, n_q$
Calibration count (index of the multiple counts obtained while viewing a target)	$b = 1, n_b$
Measurement index (multiple measured values, e.g., target PRT values, grid averages)	$m = 1, n_m$
Sensor index (multiple sensors, e.g., several PRT in a target, sensors on series of satellites)	$n = 1, n_n$

Table 2. Conventional symbols for indices with specific meaning, including how the range of indices is conventionally notated: index x runs from 1 to n_x.

Note 1. **Effects** are associated with precisely 1 **term** each (by construction/definition; the term may be a vector term, e.g., the case of a set of coefficients jointly obtained). A single effect may represent more than one physical origin of errors where these errors have identical spatio-temporal AND spectral correlations properties (and may only be jointly quantifiable).

The indexing therefore is linked to the uncertainty analysis tree diagrams:



Note 2. A single **term** is associated with 1 or many **effects**. Therefore, a summation over or listing of all effects, k, is implicitly a summation over or listing encompassing all terms, j, as well.

Note 3. Three specific subsets of the set of effects are identified by their indices:

- **Independent effects** are indexed with $i = 1, n_i$
- **Structured effects** are indexed with $s = 1, n_s$
- **Common effects** are indexed with $h = 1, n_h$.

Index h stands for harmonisation, since the uncertainty in harmonised calibration coefficients is expected to be the main (or only) effect addressed in this category (and this is assumed in the construction of the easy FCDR products). Typically, common/harmonisation effects will be treated differently and separately from the independent and structured effects, and are not included in the list k.

The mapping between the indices can be visualised (for an imaginary case) thus (treating common effects separately):

j=	1					2			3											…
k=	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	…
i=	1						2						3			4	5			…
s=		1	2	3	4	5		6	7	8	9	10		11	12			13	14	…

In this example, the valid values of $k|j$ (effects given term, i.e., the effects that operate on a particular term) would for $k|j = 2$ be the values {6, 7, 8}.

Since all effects in k are either independent (independent random errors) or structured (structured random errors and systematic errors), it follows that

$$\sum_{k=1}^{n_k} a_k = \sum_{i=1}^{n_i} a_i + \sum_{s=1}^{n_s} a_s$$

Note 4. An arbitrary selection of **image pixels** is indexed by $p = 1, n_p$, such that each value of p signifies a unique line-element pair (l, e). Various reasons for the selection of a set of p may arise that include:

- p corresponding to all the elements in a line, an index that could also be written $e|l$, i.e., all elements given a selected line
- p corresponding to all the lines for a given element, an index that could also be written $l|e$
- p corresponding to all the image pixels whose latitude and longitude fall within a defined area of Earth's surface (such as the cell of a regular grid)

- p corresponding to all the image pixels whose latitude and longitude fall within a defined area of Earth's surface that meet some classification criterion, such as "not near a coast-line" or "no cloud"

3.3 Usage conventions for indices

Non-specific references. In the absence of any further context (such as appearing within a summation or the index explicitly set equal to a non-index value or number, as in $p = P$), indexed variables refer to "any instance of the variable with respect to the index", i.e., a_k in isolation means "a for any of the effects, k".

Implicit range of summation. To keep notation as legible as possible, the limits of summation are implicitly from 1 to the maximum of the index if not explicitly stated otherwise, so

$$\sum_k a_k = \sum_{k=1}^{n_k} a_k$$

Conditional indexing. For a sum over all the effects for a specific measurement function term, $j = J$, write this as "effects given term":

$$\sum_{k|j=J} a_k$$

If we have a quantity a_j that depends only on the term index and a quantity that depends on the effect index b_k, and we want to sum their product, then using these conventions we can write this neatly as the left-hand side of this expression:

$$\sum_j \sum_{k|j} a_j b_k = \sum_j \left(a_j \sum_{k|j} b_k \right)$$

noting that the connection of a given b_k to a particular term is left implicit (b is not indexed with respect to j explicitly).

Paired indexing. Where two instances of a particular dimension (line, element, pixel or channel) are referenced in one expression (for example when considering correlations between errors in pairs of measured values across a dimension), index the second of the pair using a prime; thus, c, and c'.

4 Measurement functions and levels of satellite data

4.1 Purpose

In FIDUCEO, we undertake measurement-function centred analysis of uncertainty involved in a number of transformations between satellite processing levels. To minimise confusion, conventions mapping symbols to processing levels and measurement functions will be useful. Somewhat idealised, the situation is as in Figure 1.

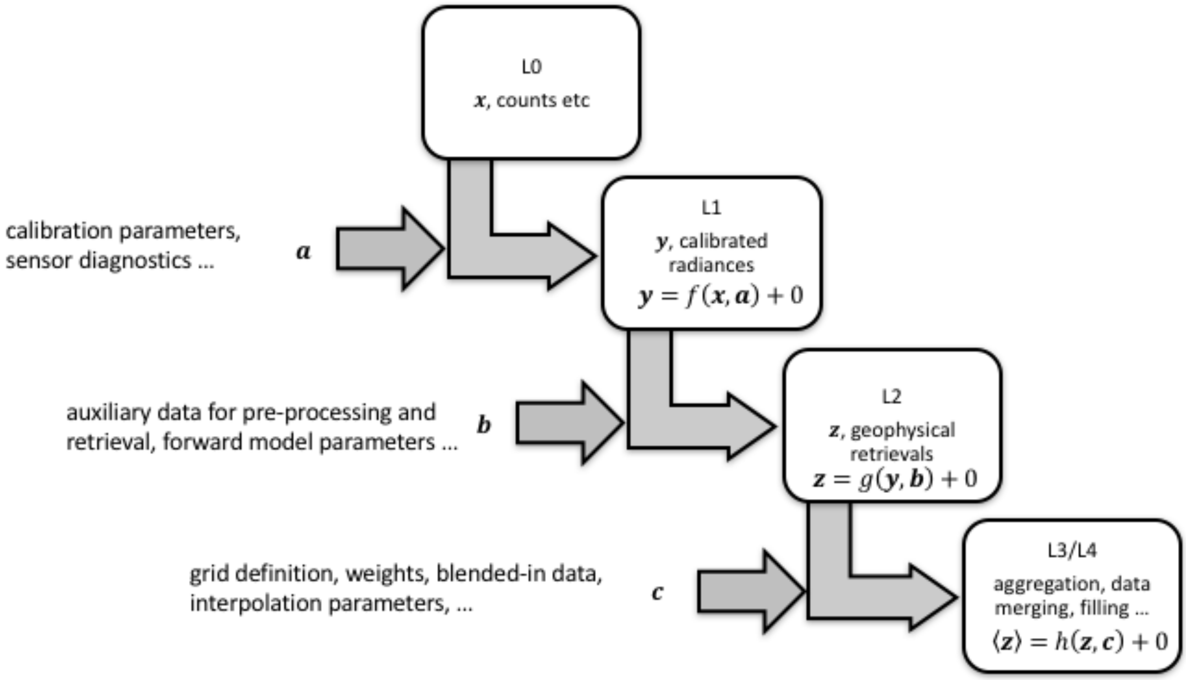


Figure 1. Idealised representation of satellite data processing levels, and the variables and measurement functions involved at each level and in transformations between levels.

Figure 1 is a simplification: for example, counts data may in reality be available in level 1a (L1a) products (and indeed, it would be our recommendation that agencies make L1a products with counts, calibration data and sensor diagnostics readily accessible in every case). Nonetheless, the figure usefully illustrates the concept of the data and symbols in the sequence of transformations constituting a processing chain from L0 (or L1a) to L3 (or higher).

4.2 Conventional symbols for levels of satellite data and measurement functions

Conceptual data level / quantity	Symbol	Obtained from measurement function	Example auxiliary data used in measurement function	Symbol
Level 0 / Counts	$\boldsymbol{x}$ (or C)	N/A	N/A	N/A
Level 1 / Radiance	$\boldsymbol{y}$ (or L, T, R)	$\boldsymbol{y} = f(\boldsymbol{x}, \boldsymbol{a}) + 0$ or $y = f\left(x_1, \ldots, x_{n_j}\right) + 0$ or $y = f\left(x_1, \ldots, x_{n_j}, \boldsymbol{a}\right) + 0$	Calibration parameters, sensor diagnostics, predictors for errors from systematic effects.	$\boldsymbol{a}$
Level 2 / Geophysical	$\boldsymbol{z}$	$\boldsymbol{z} = g(\boldsymbol{y}, \boldsymbol{b}) + 0$ or $z = g\left(y_1, \ldots, y_{n_c}\right) + 0$ or $z = g\left(y_1, \ldots, y_{n_c}, \boldsymbol{b}\right) + 0$	Auxiliary data for pre-processing, prior data, forward model parameters.	$\boldsymbol{b}$
Level 3 / Gridded	$\langle \boldsymbol{z} \rangle$	$\langle \boldsymbol{z} \rangle = h(\boldsymbol{z}, \boldsymbol{c}) + 0$	Grid definition, weights	$\boldsymbol{c}$

Note 1. For general presentation of a measurement function and its uncertainty analysis in non-specific circumstances (not referring to a particular stage of satellite data processing), use the notation most similar to the standard metrology notation, namely, $y = f\left(x_1, \ldots, x_{n_j}\right) + 0$.

Note 2. The distinction between measurement function "data" $(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z})$ and "auxiliary data" $(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c})$ is not always useful (nor always entirely clear). Particularly when the index across measurement function terms, j, is explicitly in use, it may be more convenient for all the quantities in, for example, $\boldsymbol{x}$ and $\boldsymbol{a}$, to be written on an equal basis as terms, x_j, in the measurement function (as in Note 1 above). In other cases, it is useful to maintain a distinction: for example the form $y = f\left(x_1, \ldots, x_{n_j}, \boldsymbol{a}\right) + 0$ is useful if treating uncertainty from calibration coefficients (listed in $\boldsymbol{a}$) separately to the uncertainty in all the other measurement function terms.

Note 3. In EO, the observation vector (radiances) is, as above, $\boldsymbol{y}$, whereas the state vector (geophysical retrieval) is usually $\boldsymbol{x}$, in contradiction to the above. In FIDUCEO cookbooks, etc., this mis-match will be tolerated because of the extra clarity that unique symbols for different levels of processing brings. This would also apply to external publications where counts, radiance and retrieval are all discussed. However, in external publications (papers) where only radiance and retrieved quantity are discussed, the more usual EO convention may be adopted if thought to be beneficial, or required by the journal.

Note 4. $\boldsymbol{c}$ is a letter also used for channel index, but as a channel index it is never bold and is usually a subscript or superscript. $\boldsymbol{c}$ in bold is also used for a column vector of sensitivity coefficients in certain presentations of analytic propagation of uncertainty. In the case where propagation of uncertainty through $\langle \boldsymbol{z} \rangle = h(\boldsymbol{z}, \boldsymbol{c}) + 0$ is discussed, double use of $\boldsymbol{c}$ as sensitivity coefficient is avoided by writing the column vector of sensitivity coefficients as $\partial h / \partial \boldsymbol{z}$.

5 List of standard symbols

r	**error correlation coefficient**; $r(a,b)$ is explicitly the correlation of errors in a with errors in b
ρ	**correlation coefficient**; $\rho(a,b)$ is explicitly the correlation of variability of (values of) a with (values of) b -- i.e., includes natural variability
u	**(standard) uncertainty** (in a single measurand/quantity); $u(a)$ is explicitly the uncertainty in a Note: following metrological practice, we also define $u(x,x')$ in the context of the "Law of the GUM" as the covariance of the error in x and x', such that $u(x,x) = u(x)^2$. However, this usage is not promoted in other contexts.
x	**parameter/term** in a measurement function for radiance (radiance used generically here to encompass band radiance, spectral radiance, brightness temperature, reflectance, etc); indexed by j, i.e., the j^{th} term is x_j ; these terms include level 0 data such as counts
y	**radiance** (or band radiance, spectral radiance, brightness temperature, reflectance – i.e., level 1 data) ; in the context of measurement function analysis, y is always preferred, and fits with usage in retrieval theory of $\boldsymbol{y}$ as observation vector (but also see next entry); in the context of analysis of retrieval uncertainty, y_j may refer to the j^{th} term in the function, irrespective of whether that term represents a radiance or other auxiliary data used in the retrieval, where this is convenient for writing expressions that apply to all terms compactly ; however, y_c would always refer to a radiance in channel c
L, T, R	**alternative for radiance/BT/reflectance** in other contexts: traditional symbols may be use instead of y: L for channel radiance, T for brightness temperature, or R for reflectance; L_λ for spectral radiance per unit wavelength etc. in line with BS EN ISO 80000-7:2008
z	**retrieved variable**, i.e., a geophysical state variable, level 2 data
$c_j = \frac{\partial f}{\partial x_j}$	**sensitivity coefficient** of measurand with respect to measurement function parameter x_j. . The symbol may be used both for the derivative evaluated in a particular circumstance, and for the function (this latter usage is not conventional in metrology). The same symbol is used for sensitivity coefficients at other processing levels, e.g., $c_j = \frac{\partial g}{\partial y_j}$, although see also Note 4 in section 4.2. This is so that the matrix equations of propagation of uncertainty use the same core symbols irrespective of which level of measurement function they refer to.
$\boldsymbol{R} = \begin{bmatrix} r_{1,1} & r_{1,2} & \cdots \\ r_{2,1} & r_{2,2} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}$	**error correlation matrix** : matrix of correlations of errors in a vector variable ; if indexed with respect to k this refers to the error correlation matrix for a particular effect, e.g., $\boldsymbol{R}_k$. The diagonal elements are equal to 1.
$\boldsymbol{U} = \begin{bmatrix} u_1 & 0 & \cdots \\ 0 & u_2 & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}$	**uncertainty matrix** : diagonal matrix of standard uncertainties relevant to a multi-variate measurand; if indexed with respect to k this refers to the uncertainty matrix for a particular effect, e.g., $\boldsymbol{U_k}$ having diagonal elements $u_{k\,1}$ etc.; note that because diagonal by definition, only a single

	index for row (column) is needed on each element.
$\boldsymbol{C}$	**sensitivity matrix** : matrix of sensitivity coefficients; in some contexts (one-effect-at-a-time equations) this is square and diagonal; in other contexts (using matrices to sum multiple effects), non-square and filled.
$\boldsymbol{S}$	**(measurand) error covariance matrix** : measurand covariance matrix ; e.g., $\boldsymbol{S}(\boldsymbol{y})$ is explicitly the covariance matrix of errors in the vector variable $\boldsymbol{y}$
$\boldsymbol{V}$	**parameter error covariance matrix** : covariance matrix of errors in a vector of parameters
$\boldsymbol{I}$	**identity matrix** (1s on diagonal only, 0s on off-diagonals)
$\boldsymbol{J}$	**all-ones matrix** (all elements are 1)
t	**time**
(ϕ, λ)	**latitude, longitude** the usual convention for geodetic co-ordinates
$\phi(\lambda)$	**(normalised) spectral response function** as a function of **wavelength**
$\delta_{v,w}$	**delta function** which equals 1 when the indices are equal ($v = w$), 0 otherwise

6 Conventions for labelling covariance and correlation matrices

6.1 Purpose

There are a very large number of different error correlation and error covariance matrices that can be defined and will be used. Often these may have some common elements, but apply across different dimensions (cross-element, cross-line, cross-pixel, cross-channel, cross-effect). It seems impossible to define or remember a set of different letters for all these possible matrices, and therefore the approach is to use superscripts and subscripts to distinguish the dimensions which error correlation and error covariance matrices apply. The conventions are a little complex. But hopefully they are also as simple as possible to be unique and clear, without being "simpler than possible".

The conventions are not designed to apply to other types of matrices, although if they happen to fit, they may be used.

6.2 Meaning of matrix labels by position

The same indices may appear as labels in different positions around the matrix symbol, and have different meanings according to their position, as follows:

$$M^{[\text{index 1}][,\text{index 2}]\ldots}_{\text{matrix dimension}[,\text{effects class}]}$$

where the meaning and possible values for each position are

Modifier	Possible values	Meaning / comments
matrix dimension	c	Cross-channel error covariance or correlation matrix
	p	Cross-pixel error covariance or correlation matrix (arbitrary pixel set)
	l	Cross-line error covariance or correlation matrix (lines in sequence)
	e	Cross-element error covariance or correlation matrix (elements in sequence
		This is always present to indicate whether a matrix describes inter-relationships of errors in different channels or in different pixels of an image. Note 1: The cross-line and cross-element cases are, of course, special cases of cross-pixel in general. This means any equation representing cross-pixel can be trivially applied to cross-line and cross-element by substituting $p \to l$ or e. To avoid multiplying equations that mean essentially the same thing, therefore, p should be used except in cases where distinguishing cross-line and cross-element matrices is required. Note 2: in any non-general statement (such as the uncertainty propagation equation presented in general), the matrix dimension is required, as indicated by not being placed in square brackets above. The other labels that are in square brackets may or may not be required according to meaning, as explained below.

Modifier	Possible values	Meaning / comments
effects class	i s h	Independent effects Structured effects Common effects Note that this label is optional. If no index is given in this position, all types of effects k are by convention included (which is why k is not a possible value, being then redundant). This notation is introduced to notate the distinction in the FIDUCEO easy-FCDR format between independent and structured uncertainty information.
index 1, etc	$p, l, e,$ k, i, s, j	Indices across which the matrix **does not average or sum**, i.e., the matrix applies to **any instance** or (in the context of a summation, for example) a **particular instance** of any index or indices given. Note 1: The index that is likely to be aggregated first in a sequence of operations is effects (or measurement function terms). We put this term (k, i, s, j) rightmost if more than one index is used. Note 2: The channel index is not permitted in an index position. There are two reasons. First, it does not make sense to sum or average covariance/correlation matrices across channels, so it is not necessary always explicitly to note that c is not being averaged or summed. Second, there would be loss of legibility if the channel index was always required whenever writing the spatio-temporal covariance/correlation matrix of a multi-channel image.

6.3 Examples

- The cross-channel error correlation matrix for one identified effect $k = K$ evaluated at a particular image pixel $p = P$

$$\boldsymbol{R}_c^{p=P,k=K}$$

- The cross-channel error correlation matrix for one identified effect $k = K$ evaluated at any of the image pixels p

$$\boldsymbol{R}_c^{p,k=K}$$

- The cross-channel error correlation matrix evaluated for any of the effects k at any of the image pixels p

$$\boldsymbol{R}_c^{p,k}$$

- The cross-channel error covariance matrix evaluated for any one of the effects k and representative for all image pixels (e.g., because averaged across an adequate sample of single-pixel evaluations)

$$\boldsymbol{S}_c^k$$

- The total cross-channel error covariance matrix combining all independent effects evaluated at any of the image pixels p

$$\boldsymbol{S}_{c,i}^p$$

- The cross-pixel error covariance matrix from all structured effects in any of the channels c arising from any one measurement function term j and evaluated at any of the image pixels p

$$\boldsymbol{S}_{p,s}^{p,j}$$

- The cross-element (or across track) error correlation matrix combined across all effects and representative for all image pixels

$$\boldsymbol{R}_e$$

This is quite complicated, but since there are so many potential error covariance and correlation matrices that can be calculated for a multi-channel image, we need a unique system to discriminate them.

6.4 Referring to elements within a matrix

The element (v, w) (row, column) of a matrix $\boldsymbol{M}$ is written $[M]_{v,w}$, such that (with reference to the definition of the error correlation matrix):

$$r_{v,w} = [R]_{v,w}$$

7 Standard presentations of some common equations

Equation	Context	Standard form
Law of the GUM	Single-variable measurand, total uncertainty estimated for each term in measurement function, errors in terms not necessarily independent	$$u(y)^2 = \sum_{j=1}^{n_j} c_j^2 u(x_j)^2 + 2\sum_{j=1}^{n_j-1}\sum_{j'=j+1}^{n_j} c_j c_{j'} u(x_j, x_{j'})$$ or $$u^2 = \boldsymbol{c}^{\mathrm{T}}\boldsymbol{S}\boldsymbol{c}$$ with $\boldsymbol{c}^{\mathrm{T}} = [c_1, c_2, ..]$ and $\boldsymbol{S} = \begin{bmatrix} u(x_1)^2 & u(x_1, x_2) & \cdots \\ u(x_2, x_1) & u(x_2)^2 & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}$
	Vector measurand, uncertainty matrix, sensitivity matrix and error correlation matrix available for each effect, errors from effects being by construction independent	$$\boldsymbol{S} = \sum_j \sum_{k\|j} \boldsymbol{C}_j \boldsymbol{U}_k \boldsymbol{R}_k \boldsymbol{U}_k^{\mathrm{T}} \boldsymbol{C}_j^{\mathrm{T}}$$
Optimal estimation	Retrieving a geophysical variable from a radiance vector using *a priori* information	$$\hat{\boldsymbol{z}} = \boldsymbol{z}_{\mathrm{a}} + \boldsymbol{S}_{\mathrm{a}}\boldsymbol{K}^{\mathrm{T}}\left(\boldsymbol{K}\boldsymbol{S}_{\mathrm{a}}\boldsymbol{K}^{\mathrm{T}} + \boldsymbol{S}_c + \boldsymbol{S}_F\right)^{-1}\left(\boldsymbol{y} - \boldsymbol{F}(\boldsymbol{z}_{\mathrm{a}})\right)$$ where $\boldsymbol{S}_F$ is the forward model error covariance (including representativity if appropriate) and $\boldsymbol{F}$ is the forward model function; in a paper where it is unambiguous, the more conventional $\boldsymbol{x}_{\mathrm{a}}$ etc may be used, but for all FIDUCEO cookbooks etc stick with $\boldsymbol{z}_{\mathrm{a}}$