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On covariance propagation of eigenparameters of symmetric n-D tensors

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SUMMARY

Symmetric tensors are typically encountered during investigations associated with stress and strain analysis and, thus, they are of particular interest to geophysicists and geodesists. Furthermore, symmetric tensors are studied using eigentheory analysis which provides the decomposition of the tensor on its principal components (n independent eigenvalues and the corresponding eigenvectors). In this paper, an analytical expression of the covariance matrix of the eigenvalues and eigenvectors of an n-D symmetric tensor is derived based on the principles of linear algebra and differential calculus. Through numerical tests, the proposed formulation is proven to give realistic uncertainty estimates of the determined eigenparameters. The methodology also reveals the significant impact on uncertainty assessments when the parameter dependencies between principal components are neglected.

Key words: covariance propagation, eigenvalues, eigenvectors, symmetric tensor.

1 INTRODUCTION

Symmetric tensor analysis typically results in the determination of eigenvalues and corresponding eigenvectors representing the associated principal values and orientations, respectively. This technique has been applied in different fields where eigenparameter analyses are involved. Particularly, in geophysics, this technique plays an important role in deformation (strain and stress) analysis and anisotropic magnetic susceptibility problems. Examples can be found in Wyss *et al.* (1992), Owens (2000a), Owens (2000b), Bressan *et al.* (2003), and Grafarend & Voosoghi (2003). In geomatics, the same concept is applied to find the size and orientation of an error ellipse (or ellipsoid) from a least-squares adjustment (Scheffé 1959, pp. 406–411), or to determine the principal scales and orientations in an affine transformation. Consequently, the accuracy assessments of these eigenparameters are essential to the reliability of the results' interpretation. According to Kagan (2000), the first attempt to estimate the errors of the eigenparameters of second-rank symmetric tensors should be credited to Hext (1963). In the classical error propagation approach, Jacobian matrices, which require the total differentiation of all random variables present in the model, are typically invoked. Several authors (see e.g. Angelier *et al.* 1982 and Wyss *et al.* 1992) utilized this approach, although, they restricted their investigation to determine the estimates of the eigenvalues. In addition, Soler & van Gelder (1991) extended the formulation to compute the covariance matrices of the eigenvalues and their principal directions. This theory was discovered not to be fully general, and an extension was incorporated into an erratum published in Soler & van Gelder (2006). Independently, Xu & Grafarend (1996a, b) also gave an analytical expression for the covariance matrices of the eigenvalues and principal rotation angles of a symmetric tensor with a second-order approximation. Recently, the statistical inference of the eigenspace components of a 2-D and 3-D symmetric rank-two random tensor has been further investigated by Cai (2004) and Cai *et al.* (2005).

One of the key points in propagating the covariance matrix of the principal components from symmetric tensors is that the parameters which determine principal orientations (i.e. eigenvectors) are mutually dependent. Propagating errors from dependent variables will result in an underestimated covariance matrix (Hamilton 1964, pp. 149–150). Hence, resolving the dependencies between the principal orientations is an essential step to achieve realistic uncertainty estimates in a principal component analysis problem and the main emphasis of this presentation. As the results of a practical application shown here indicate the final error estimates are more realistic when the dependencies between the variables are properly taken into consideration. Therefore, the current geophysical interpretation of accuracies of eigenvalues and eigenvectors of second-rank symmetric tensors may be affected if the theory described in this paper is not implemented.

2 MATHEMATICAL DERIVATIONS

2.1 A symmetric n-D tensor and its principal components

Any $n \times n$ symmetric matrix $\mathbf{E}$ can be written as a product of a diagonal matrix $\mathbf{\Lambda} = \mathrm{Diag}\,[\lambda_1, \lambda_2, \ldots, \lambda_n]$ and an orthogonal matrix $\mathbf{S}$ (see e.g. Bodewig 1959, pp. 54–57):

$$\mathbf{E} = \mathbf{S}^T \mathbf{\Lambda} \mathbf{S}. \tag{2.1.1}$$

Here, the diagonal matrix $\mathbf{\Lambda}$ consists of the n real eigenvalues of $\mathbf{E}$. The matrix $\mathbf{S}$ is a $n \times n$ rotation operator whose rows are formed by the n eigenvectors of $\mathbf{E}$. Those eigenvectors define the orientation of the principal axes. Note that, the number of independent parameters in matrix $\mathbf{E}$ is $m = n \times (n+1)/2 = C_2^{n+1}$, and $\mathbf{S}$ can be represented as the product of $(m-n) = n \times (n-1)/2 = C_2^n$ successive rotation matrices (see Schaffrin 1984).

2.2 Propagations of the covariance matrices

To propagate the covariance matrix, we start with applying total differentiation (Bodewig, 1959, p. 12) to (2.1.1) and obtain:

$$d\mathbf{E} = (d\mathbf{S}^T)\mathbf{\Lambda}\mathbf{S} + \mathbf{S}^T(d\mathbf{\Lambda})\mathbf{S} + \mathbf{S}^T\mathbf{\Lambda}(d\mathbf{S}). \tag{2.2.1}$$

Following the idea originating from Roth (1934) for a linear matrix equation, it has been shown by several authors (see e.g. Magnus & Neudecker 1988, pp. 27–62; Soler & van Gelder 1991; Grafarend & Schaffrin 1993) that:

$$\mathrm{vec}(\mathbf{ABC}) = (\mathbf{C}^T \otimes \mathbf{A})\mathrm{vec}(\mathbf{B}), \tag{2.2.2}$$

where $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ are three matrices such that the matrix product $\mathbf{ABC}$ is defined, vec represents the Vec Operator that stacks one column of a matrix underneath the previous one, and $\otimes$ denotes the Kronecker Product, defined by $\mathbf{A} \otimes \mathbf{B} = [\mathbf{a_{ij}B}]$ if $\mathbf{A} = [\mathbf{a_{ij}}]$.

By the definition of the vec of a matrix (Graham 1981, p. 18), it can easily be shown that:

$$\mathrm{vec}\,(\mathbf{A} + \mathbf{B} + \mathbf{C}) = \mathrm{vec}\,(\mathbf{A}) + \mathrm{vec}\,(\mathbf{B}) + \mathrm{vec}\,(\mathbf{C})\,. \tag{2.2.3}$$

Applying (2.2.2) and (2.2.3) to (2.2.1), one obtains:

$$\mathrm{vec}(d\mathbf{E}) = ((\mathbf{\Lambda}\mathbf{S})^T \otimes \mathbf{I})\mathrm{vec}(d\mathbf{S}^T) + (\mathbf{S}^T \otimes \mathbf{S}^T)\mathrm{vec}(d\mathbf{\Lambda}) \;\; + (\mathbf{I} \otimes (\mathbf{S}^T\mathbf{\Lambda}))\mathrm{vec}(d\mathbf{S}). \tag{2.2.4}$$

Here, $\mathbf{I}$ is an $n \times n$ identity matrix. Recall that there are m distinct elements in the symmetric matrix $\mathbf{E}$. For a vector $\{d\varepsilon\}$ consisting of those m distinct elements of $d\mathbf{E}$ (diagonal plus subdiagonal elements), it can be shown that there exists an $m \times n^2$ matrix $\mathbf{D_E}$ such that:

$$\underset{m\times 1}{\{d\varepsilon\}} = \begin{Bmatrix} d\varepsilon_{11} \\ d\varepsilon_{22} \\ \vdots \\ d\varepsilon_{nn} \\ \\ \vdots \\ d\varepsilon_{n,1} \\ d\varepsilon_{n,2} \\ \vdots \\ d\varepsilon_{n,(n-1)} \end{Bmatrix}_{m\times 1} = \underset{m\times n^2}{\mathbf{D_E}}\ \underset{n^2\times 1}{\mathrm{vec}\,(d\mathbf{E})}\,. \tag{2.2.5}$$

Equation (2.2.5) can also be written in the reverse order by employing a certain right-inverse of $\mathbf{D_E}$:

$$\underset{n^2\times 1}{\mathrm{vec}\,(d\mathbf{E})} = \underset{n^2\times m}{\tilde{\mathbf{D}}_\mathbf{E}}\ \underset{m\times 1}{\{d\varepsilon\}}, \tag{2.2.6}$$

where $\tilde{\mathbf{D}}_\mathbf{E}$ consists of n^2 unit rows of size $1 \times m$.

In books on Matrix Algebra, the matrix $\tilde{\mathbf{D}}_\mathbf{E}$ in (2.2.6) is typically referred as the Duplication Matrix (see e.g. Magnus & Neudecker 1988, pp. 48–53). Note that $n^2 > m$ for $n > 1$. Hence, the matrix $\mathbf{D_E}$ here can be regarded as a transformation operator that maps a vector from a higher-dimensional space $\mathcal{R}_{n^2}$ to a lower-dimensional space $\mathcal{R}_m$. There are multiple choices of this operator that can fulfil (2.2.5). However, its reverse transformation defined in (2.2.6) is unique, and so is matrix $\tilde{\mathbf{D}}_\mathbf{E}$. Hence, for the uniquely determined $\tilde{\mathbf{D}}_\mathbf{E}$, one can pick a unique selection for the matrix $\mathbf{D_E}$ by using the pseudo-inverse of $\tilde{\mathbf{D}}_\mathbf{E}$, namely:

$$\mathbf{D_E} = \tilde{\mathbf{D}}_\mathbf{E}^{+} = \left(\tilde{\mathbf{D}}_\mathbf{E}^T\tilde{\mathbf{D}}_\mathbf{E}\right)^{-1}\tilde{\mathbf{D}}_\mathbf{E}^T. \tag{2.2.7}$$

From (2.2.7), one can immediately verify that:

$$\mathbf{D_E}\tilde{\mathbf{D}}_\mathbf{E} = \mathbf{I}. \tag{2.2.8}$$

For the $n \times n$ diagonal matrix $d\mathbf{\Lambda}$, the vec of its n distinct elements can be written as:

$$\underset{n\times 1}{\{d\boldsymbol{\lambda}\}} = \begin{Bmatrix} d\lambda_1 \\ \vdots \\ d\lambda_n \end{Bmatrix} = \underset{n\times n^2}{(\mathbf{I}\odot\mathbf{I})^T}\ \underset{n^2\times 1}{\operatorname{vec}}\,(d\mathbf{\Lambda}), \tag{2.2.9}$$

where $\odot$ denotes the Khatri–Rao product defined by $\mathbf{A}\odot\mathbf{B} = [\mathbf{A_1}\otimes\mathbf{B_1}, \ldots, \mathbf{A_p}\otimes\mathbf{B_p},]$ if $\mathbf{A_j}$ and $\mathbf{B_j}$ $(j = 1, \ldots, p)$ are (column) portioned matrices of $\mathbf{A}$ and $\mathbf{B}$, respectively (see Rao & Mitra 1971, pp. 12–13).

By applying the known relation $(\mathbf{I}\odot\mathbf{I})^T(\mathbf{I}\odot\mathbf{I}) = \mathbf{I}$ (Schaffrin 1985, pp. 548–597), (2.2.9) can be written in the reverse order:

$$\underset{n^2\times 1}{\operatorname{vec}}\,(d\mathbf{\Lambda}) = \underset{n^2\times n}{(\mathbf{I}\odot\mathbf{I})}\ \underset{n\times 1}{\{d\boldsymbol{\lambda}\}} \tag{2.2.10}$$

For the principal rotation matrix, it can easily be verified that:

$$\underset{n^2\times 1}{\operatorname{vec}}\left(d\mathbf{S}^T\right) = \underset{n^2\times n^2}{\mathbf{D_S}}\ \underset{n^2\times 1}{\operatorname{vec}}\,(d\mathbf{S}) = \underset{n^2\times n^2}{\mathbf{D_S}}\ \underset{n^2\times 1}{\{d\mathbf{S}\}}, \tag{2.2.11}$$

where $\mathbf{D_S}$ is a square matrix transformation operator, and

$$\underset{n^2\times 1}{\{d\mathbf{S}\}} = \operatorname{vec}(d\boldsymbol{S}) = \begin{Bmatrix} ds_{11} \\ ds_{21} \\ \vdots \\ ds_{nn} \end{Bmatrix}. \tag{2.2.12}$$

Substituting (2.2.6), (2.2.10) and (2.2.11) into (2.2.4), one obtains:

$$\begin{aligned}\tilde{\mathbf{D}}_{\mathbf{E}}\{d\boldsymbol{\varepsilon}\} &= ((\mathbf{\Lambda S})^T\otimes\mathbf{I})\mathbf{D_S}\{d\mathbf{S}\} + (\mathbf{S}^T\otimes\mathbf{S}^T)(\mathbf{I}\odot\mathbf{I})\{d\boldsymbol{\lambda}\} + (\mathbf{I}\otimes(\mathbf{S}^T\mathbf{\Lambda}))\{d\mathbf{S}\} \\ &= (\mathbf{S}^T\otimes\mathbf{S}^T)(\mathbf{I}\odot\mathbf{I})\{d\boldsymbol{\lambda}\} + (((\mathbf{\Lambda S})^T\otimes\mathbf{I})\mathbf{D_S} + \mathbf{I}\otimes(\mathbf{S}^T\mathbf{\Lambda}))\{d\mathbf{S}\}.\end{aligned} \tag{2.2.13}$$

Using the known properties of the Kronecker product and the Khatri–Rao product, it can be shown that (see Rao & Mitra 1971, pp. 12–13):

$$(\mathbf{S}^T\otimes\mathbf{S}^T)(\mathbf{I}\odot\mathbf{I}) = (\mathbf{S}^T\odot\mathbf{S}^T). \tag{2.2.14}$$

In addition, the matrix transformation operator $\mathbf{D_S}$ here is typically referred as a Commutation Matrix (Magnus & Neudecker 1988, pp. 46–48), which gives the following relation:

$$((\mathbf{\Lambda S})^T\otimes\mathbf{I})\mathbf{D_S} = \mathbf{D_S}(\mathbf{I}\otimes(\mathbf{\Lambda S})^T) = \mathbf{D_S}(\mathbf{I}\otimes(\mathbf{S}^T\mathbf{\Lambda})). \tag{2.2.15}$$

Substituting (2.2.14) and (2.2.15) into (2.2.13), which becomes:

$$\tilde{\mathbf{D}}_{\mathbf{E}}\{d\boldsymbol{\varepsilon}\} = (\mathbf{S}^T\odot\mathbf{S}^T)\{d\boldsymbol{\lambda}\} + (\mathbf{D_S}+\mathbf{I})(\mathbf{I}\otimes(\mathbf{S}^T\mathbf{\Lambda}))\{d\mathbf{S}\}. \tag{2.2.16}$$

Pre-multiplying by $\mathbf{D_E}$ both sides of (2.2.16), and recalling that $\mathbf{D_E}\tilde{\mathbf{D}}_{\mathbf{E}} = \mathbf{I}$, one has:

$$\begin{aligned}\underset{m\times 1}{\{d\boldsymbol{\varepsilon}\}} &= \mathbf{D_E}((\mathbf{S}^T\odot\mathbf{S}^T)\{d\boldsymbol{\lambda}\} + (\mathbf{D_S}+\mathbf{I})(\mathbf{I}\otimes(\mathbf{S}^T\mathbf{\Lambda}))\{d\mathbf{S}\}) \\ &= \mathbf{D_E}\left(\mathbf{S}^T\odot\mathbf{S}^T\ \vdots\ (\mathbf{D_S}+\mathbf{I})(\mathbf{I}\otimes(\mathbf{S}^T\mathbf{\Lambda}))\right)\begin{Bmatrix}\{d\boldsymbol{\lambda}\}\\ \cdots \\ \{d\mathbf{S}\}\end{Bmatrix} \\ &= \mathbf{F}\,\{d\boldsymbol{\beta}\},\end{aligned} \tag{2.2.17}$$

with

$$\underset{m\times n(n+1)}{\mathbf{F}} = \mathbf{D_E}\left(\mathbf{S}^T\odot\mathbf{S}^T\ \vdots\ (\mathbf{D_S}+\mathbf{I})(\mathbf{I}\otimes(\mathbf{S}^T\mathbf{\Lambda}))\right), \tag{2.2.18}$$

and

$$\underset{n(n+1)\times 1}{\{d\boldsymbol{\beta}\}} = \begin{Bmatrix}\{d\boldsymbol{\lambda}\}\\ \cdots \\ \{d\mathbf{S}\}\end{Bmatrix}. \tag{2.2.19}$$

Equation (2.2.17) defines the differential relationship between an n-D symmetric tensor and its eigenvalues and eigenvectors. However, one should not use this relationship to propagate covariance matrices between them, without taking into account that not all the parameters on the right-hand side of (2.2.17) are independent. Recall that the matrix $\mathbf{S}$ is essentially the product of $(m-n)$ successive rotation matrices and, thus, consists of only $(m-n)$ independent parameters. As a result, the number of independent variables in $\{d\boldsymbol{\beta}\}$ should be $(m-n)+n = m$ $(< n^2)$. If one directly applies the covariance propagation rule to (2.2.17), the covariance matrix propagated from the dependent variables in $\{d\boldsymbol{\beta}\}$ will become unrealistic (see Section 3).

In order to make all the parameters on the right hand side of (2.2.19) be independent, we use a known relationship for the first derivative of an orthogonal matrix, which is an immediate result of a standard Cartan relation (Cartan 1951, pp. 19–20), namely:

$$d\mathbf{S} = -\mathbf{S}\mathbf{\Omega}, \tag{2.2.20}$$

where $\underline{\boldsymbol{\Omega}}$ is an $n \times n$ antisymmetric matrix with $(m-n)$ independent infinitesimal elements $(\Omega_1, \Omega_2, \ldots, \Omega_{m-n})$. Applying (2.2.2) on (2.2.20), one arrives at:

$$\underset{n^2\times 1}{\{d\mathbf{S}\}} = -\underset{n^2\times n^2}{(\mathbf{I}\otimes\mathbf{S})}\ \underset{n^2\times 1}{\mathrm{vec}\,(\underline{\boldsymbol{\Omega}})} = -\underset{n^2\times n^2}{(\mathbf{I}\otimes\mathbf{S})}\ \underset{n^2\times(m-n)}{\mathbf{D}_{\boldsymbol{\Omega}}}\ \underset{(m-n)\times 1}{\{\boldsymbol{\Omega}\}}\ , \tag{2.2.21}$$

where $\{\boldsymbol{\Omega}\}$ consists of the $(m-n)$ independent (off-diagonal) elements in the matrix $\underline{\boldsymbol{\Omega}}$. $\mathbf{D}_{\boldsymbol{\Omega}}$ is a transformation operator that maps the $(m-n)$ elements in $\{\boldsymbol{\Omega}\}$ to the n^2 elements in $\underline{\boldsymbol{\Omega}}$.

Substituting (2.2.21) into (2.2.17), one obtains:

$$\begin{aligned}\underset{m\times 1}{\{d\boldsymbol{\varepsilon}\}} &= \underset{m\times n(n+1)}{\mathbf{F}} \underset{n(n+1)\times 1}{\begin{Bmatrix} \{d\boldsymbol{\lambda}\} \\ \cdots \\ -(\mathbf{I}\otimes\mathbf{S})\,\mathbf{D}_{\boldsymbol{\Omega}}\,\{\boldsymbol{\Omega}\} \end{Bmatrix}} = \underset{m\times n(n+1)}{\mathbf{F}} \underset{n(n+1)\times m}{\begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -(\mathbf{I}\otimes\mathbf{S})\,\mathbf{D}_{\boldsymbol{\Omega}} \end{bmatrix}} \underset{m\times 1}{\begin{Bmatrix} \{d\boldsymbol{\lambda}\} \\ \cdots \\ \{\boldsymbol{\Omega}\} \end{Bmatrix}}, \\ &= \underset{m\times m}{\tilde{\mathbf{F}}} \underset{m\times 1}{\begin{Bmatrix} \{d\lambda\} \\ \cdots \\ \{\boldsymbol{\Omega}\} \end{Bmatrix}},\end{aligned} \tag{2.2.22}$$

where

$$\begin{aligned}\underset{m\times m}{\tilde{\mathbf{F}}} &= \underset{m\times n(n+1)}{\mathbf{F}} \underset{n(n+1)\times m}{\begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -(\mathbf{I}\otimes\mathbf{S})\,\mathbf{D}_{\boldsymbol{\Omega}} \end{bmatrix}} \\ &= \mathbf{D}_{\mathbf{E}}\big(\mathbf{S}^T\odot\mathbf{S}^T \ \underset{m\times n(n+1)}{\vdots}\ (\mathbf{D}_{\mathbf{S}}+\mathbf{I})(\mathbf{I}\otimes(\mathbf{S}^T\boldsymbol{\Lambda}))\big) \underset{n(n+1)\times m}{\begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -(\mathbf{I}\otimes\mathbf{S})\,\mathbf{D}_{\boldsymbol{\Omega}} \end{bmatrix}} \\ &= \mathbf{D}_{\mathbf{E}}\left(\mathbf{S}^T\odot\mathbf{S}^T \ \vdots\ -(\mathbf{D}_{\mathbf{S}}+\mathbf{I})(\mathbf{I}\otimes(\mathbf{S}^T\boldsymbol{\Lambda}))(\mathbf{I}\otimes\mathbf{S})\mathbf{D}_{\boldsymbol{\Omega}}\right).\end{aligned} \tag{2.2.23}$$

Furthermore, from Rao & Mitra (1971), pp. 11, it is shown that:

$$(\mathbf{A}\otimes\mathbf{C})\,(\mathbf{B}\otimes\mathbf{D}) = (\mathbf{AB}\otimes\mathbf{CD})\,. \tag{2.2.24}$$

By successfully applying the relation in (2.2.24), (2.2.23) can be reduced in a more compact form:

$$\begin{aligned}\underset{m\times m}{\tilde{\mathbf{F}}} &= \mathbf{D}_{\mathbf{E}}\left(\mathbf{S}^T\odot\mathbf{S}^T \ \vdots\ -(\mathbf{D}_{\mathbf{S}}+\mathbf{I})(\mathbf{I}\otimes(\mathbf{S}^T\boldsymbol{\Lambda}\mathbf{S}))\mathbf{D}_{\boldsymbol{\Omega}}\right) \\ &= \mathbf{D}_{\mathbf{E}}\left(\mathbf{S}^T\odot\mathbf{S}^T \ \vdots\ -(\mathbf{D}_{\mathbf{S}}+\mathbf{I})(\mathbf{I}\otimes\mathbf{E})\mathbf{D}_{\boldsymbol{\Omega}}\right).\end{aligned} \tag{2.2.25}$$

Now we have the same number of parameters on both sides of (2.2.22), with all of them independent on the right hand side. Applying the principle of covariance propagation (Hamilton 1964, pp. 149–150), one obtains:

$$\boldsymbol{\Sigma}_{\{\varepsilon\}} = \tilde{\mathbf{F}}\boldsymbol{\Sigma}_{\{\lambda,\bar{\Omega}\}}\tilde{\mathbf{F}}^T, \tag{2.2.26}$$

where $\{\boldsymbol{\varepsilon}\} = \{\,\varepsilon_{11}\ \varepsilon_{22}\ \cdots\ \varepsilon_{nn}\ \varepsilon_{21}\ \varepsilon_{31}\ \ \cdots\ \ \varepsilon_{n1}\ \varepsilon_{32}\ \cdots\ \varepsilon_{n(n-1)}\,\}^T$ is a vector that consists of the m distinct elements in the symmetric matrix $\mathbf{E}$ on and below its diagonal, and $\bar{\boldsymbol{\Omega}}$ is defined such that $d\{\bar{\boldsymbol{\Omega}}\} = \{\boldsymbol{\Omega}\}$.

Since $\tilde{\mathbf{F}}$ is a square matrix of full rank, equation (2.2.26) can also be written as its reverse version:

$$\boldsymbol{\Sigma}_{\{\lambda,\bar{\Omega}\}} = \tilde{\mathbf{F}}^{-1}\boldsymbol{\Sigma}_{\{\varepsilon\}}\tilde{\mathbf{F}}^{-T}. \tag{2.2.27}$$

From (2.2.21), one can write:

$$\boldsymbol{\Sigma}_{\mathrm{vec}(\mathbf{S})} = ((\mathbf{I}\otimes\mathbf{S})\mathbf{D}_{\boldsymbol{\Omega}})\boldsymbol{\Sigma}_{\{\hat{\Omega}\}}((\mathbf{I}\otimes\mathbf{S})\mathbf{D}_{\boldsymbol{\Omega}})^T. \tag{2.2.28}$$

Now by combining (2.2.21) and (2.2.22), one obtains the following equation:

$$\begin{aligned}\underset{(n^2+n)\times 1}{\begin{Bmatrix} \{d\boldsymbol{\lambda}\} \\ \cdots \\ \{d\mathbf{S}\} \end{Bmatrix}} &= \underset{(n^2+n)\times m}{\begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -(\mathbf{I}\otimes\mathbf{S})\,\mathbf{D}_{\boldsymbol{\Omega}} \end{bmatrix}} \underset{m\times m}{\tilde{\mathbf{F}}^{-1}}\ \underset{m\times 1}{\{d\boldsymbol{\varepsilon}\}} \\ &= \underset{(n^2+n)\times m}{\mathbf{K}}\ \underset{m\times 1}{\{d\boldsymbol{\varepsilon}\}}\,,\end{aligned} \tag{2.2.29}$$

with

$$\underset{(n^2+n)\times m}{\mathbf{K}} = \underset{(n^2+n)\times m}{\begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -(\mathbf{I}\otimes\mathbf{S})\mathbf{D}_{\boldsymbol{\Omega}} \end{bmatrix}} \underset{m\times m}{\tilde{\mathbf{F}}^{-1}} \tag{2.2.30}$$

Thus the covariance propagation model can be written as:

$$\boldsymbol{\Sigma}_{\{\lambda,\mathrm{vec}(\boldsymbol{S})\}} = \mathbf{K}\boldsymbol{\Sigma}_{\{\varepsilon\}}\mathbf{K}^T. \tag{2.2.31}$$

By using (2.2.31), one is able to obtain the propagated covariance matrix for the eigenvalues and eigenvectors from an n-D symmetric tensor with random entities. Different values should be assigned to the scalar matrices $\mathbf{D_E}$, $\mathbf{D_S}$ and $\mathbf{D_\Omega}$ depending on the dimension of the symmetric tensor. For a 3-D case, the values for these transformation operators are given in Section 3.

3 CASE STUDY FOR A 3-D SYMMETRIC TENSOR

3.1 Model for a general 3-D case

For a 3-D symmetric tensor $\underset{3\times3}{\mathbf{E}}$, $n = 3$ and $m = 6$. Equation (2.2.31) can be applied to perform the covariance propagations from a tensor to its eigenvalues and eigenvectors. The dimension of the matrix $\mathbf{K}$ is 12×6, and the following transformation operators are defined only for a general 3-D case:

$$\underset{9\times6}{\tilde{\mathbf{D}}_\mathbf{E}} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}, \tag{3.1.1}$$

$$\underset{6\times9}{\mathbf{D}_\mathbf{E}} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0.5 & 0 & 0.5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.5 & 0 & 0 & 0 & 0.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.5 & 0 & 0.5 & 0 \end{bmatrix}, \tag{3.1.2}$$

$$\underset{9\times9}{\mathbf{D_S}} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \tag{3.1.3}$$

and

$$\underset{9\times3}{\mathbf{D}_\mathbf{\Omega}} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{3.1.4}$$

3.2 Numerical simulation

Here a 3-D coordinate transformation problem for a 587-site network is used to illustrate the capability of the proposed approach. First, the original coordinates $\mathbf{x}$ of all sites with simulated principal scales $\mathbf{\Lambda}$ and rotations $\mathbf{S}$ are used to compute the new coordinates $\mathbf{x}'$ in the transformed frame using the following coordinate transformation equation:

$$\mathbf{x}' = \mathbf{S}^T \mathbf{\Lambda S x}, \tag{3.2.1}$$

or

$$\mathbf{x}' = \mathbf{E x}. \tag{3.2.2}$$

To simulate uncertainties, a ±5 mm random error is added to the positional coordinates. Then, we use the original and transformed coordinates as observations to estimate the principal scales and rotations and their covariance matrices.

In (3.2.1), there are 12 parameters (three in $\mathbf{\Lambda}$ and nine in $\mathbf{S}$) to be estimated. However, $\mathbf{S}$ is a rotation matrix with only three independent (rotation) parameters in it. In such a case, it will be easier if we use (3.2.2) instead of (3.2.1) to perform the parameter estimation, which will directly give us the estimates for the six independent parameters in $\{\varepsilon\}$ which represents the full symmetric matrix $\mathbf{E}$. Then, by using (2.1.1), we can obtain the parameter estimates for $\mathbf{\Lambda}$ and $\mathbf{S}$. The covariance matrix for $\{\boldsymbol{\lambda}\}$ and vec $(\mathbf{S})$ can be propagated from the estimated covariance matrix $\Sigma_{\{\varepsilon\}}$ by applying (2.2.31).

The same procedure is performed using a classical covariance propagation approach, however, assuming that all the elements in $\mathbf{S}$ are independent. The approach is as follows:

Suppose we have:

$$\{\boldsymbol{\varepsilon}\} = f\left(\{\boldsymbol{\lambda}\}, \operatorname{vec}(\mathbf{S})\right) = f\left(\{\boldsymbol{\beta}\}\right) \tag{3.2.3}$$

Here $\underset{6\times 1}{\{\boldsymbol{\varepsilon}\}} = \{\, \varepsilon_{11} \quad \varepsilon_{22} \quad \varepsilon_{33} \quad \varepsilon_{21} \quad \varepsilon_{31} \quad \varepsilon_{32} \,\}^T$ represents the six distinct elements in $\mathbf{E}$; $\underset{3\times 1}{\{\boldsymbol{\lambda}\}} = \{\, \lambda_1 \quad \lambda_2 \quad \lambda_3 \,\}^T$ denotes the three principal scales; $\underset{9\times 1}{\operatorname{vec}(\mathbf{S})} = \{\, s_{11} \quad s_{21} \quad \cdots \quad s_{33} \,\}^T$ denotes the nine elements in the rotation matrix $\mathbf{S}$; $\underset{12\times 1}{\{\boldsymbol{\beta}\}} = \begin{Bmatrix} \{\boldsymbol{\lambda}\} \\ \cdots \\ \operatorname{vec}(\mathbf{S}) \end{Bmatrix}$.

The covariance propagation model is then:

$$\mathbf{\Sigma}_{\{\varepsilon\}} = \mathbf{J}_{\{\varepsilon\},\{\beta\}} \mathbf{\Sigma}_{\{\beta\}} \mathbf{J}^T_{\{\varepsilon\},\{\beta\}}, \tag{3.2.4}$$

and

$$\mathbf{\Sigma}_{\{\beta\}} = \mathbf{J}^+_{\{\varepsilon\},\{\beta\}} \mathbf{\Sigma}_{\{\varepsilon\}} \left(\boldsymbol{J}^+_{\{\varepsilon\},\{\beta\}}\right)^T, \tag{3.2.5}$$

with

$$\mathbf{J}_{\{\varepsilon\},\{\beta\}} = \left[\frac{\partial\{\varepsilon\}}{\partial\{\boldsymbol{\beta}\}^T}\right] = \left[\frac{\partial\{\varepsilon\}}{\partial\{\boldsymbol{\lambda}\}^T} \;\vdots\; \frac{\partial\{\varepsilon\}}{\partial\{vec(\mathbf{S})\}^T}\right] = \begin{bmatrix} \frac{\partial\varepsilon_{11}}{\partial\lambda_1} & \frac{\partial\varepsilon_{11}}{\partial\lambda_2} & \frac{\partial\varepsilon_{11}}{\partial\lambda_3} & \vdots & \frac{\partial\varepsilon_{11}}{\partial s_{11}} & \frac{\partial\varepsilon_{11}}{\partial s_{12}} & \frac{\partial\varepsilon_{11}}{\partial s_{13}} & \cdots & \frac{\partial\varepsilon_{11}}{\partial s_{33}} \\ \frac{\partial\varepsilon_{22}}{\partial\lambda_1} & \frac{\partial\varepsilon_{22}}{\partial\lambda_2} & \frac{\partial\varepsilon_{22}}{\partial\lambda_3} & \vdots & \frac{\partial\varepsilon_{22}}{\partial s_{11}} & \frac{\partial\varepsilon_{22}}{\partial s_{12}} & \frac{\partial\varepsilon_{22}}{\partial s_{13}} & \cdots & \frac{\partial\varepsilon_{22}}{\partial s_{33}} \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\partial\varepsilon_{32}}{\partial\lambda_1} & \frac{\partial\varepsilon_{32}}{\partial\lambda_2} & \frac{\partial\varepsilon_{32}}{\partial\lambda_3} & \vdots & \frac{\partial\varepsilon_{32}}{\partial s_{11}} & \frac{\partial\varepsilon_{32}}{\partial s_{12}} & \frac{\partial\varepsilon_{32}}{\partial s_{13}} & \cdots & \frac{\partial\varepsilon_{32}}{\partial s_{33}} \end{bmatrix}_{6\times 12}. \tag{3.2.6}$$

Note that, the Jacobian matrix $\mathbf{J}_{\{\varepsilon\},\{\beta\}}$ here is a 6×12 matrix with rank six. Its pseudo-inverse can be computed analytically by (see e.g. Graybill 1983, p.112):

$$\boldsymbol{J}^+_{\{\varepsilon\},\{\beta\}} = \mathbf{J}^T_{\{\varepsilon\},\{\beta\}} \left(\mathbf{J}_{\{\varepsilon\},\{\beta\}} \mathbf{J}^T_{\{\varepsilon\},\{\beta\}}\right)^{-1}. \tag{3.2.7}$$

Then equation (3.2.5) can be applied to perform the covariance propagation.

Table 1 lists the parameter estimates and the corresponding standard deviation values after imposing a ±5 mm random error to the observables. From the results, it can be seen that the proposed approach gives significantly different uncertainty estimates compared with those from a classical approach without considering any parameter dependency. If we compare the estimated parameters to the true (simulated)

Table 1. Uncertainty estimates for the eigenvalues and eigenvectors of a 3-D symmetric tensor.

Parameters (unit)	Simulated parameter values	Estimated parameter values[a]	Estimated standard deviations	
			From the proposed approach, Eq. (2.2.27)[a]	From a classical approach without considering parameter dependencies, Eq. (3.2.5)[a]
λ_1(ppb)[b]	−10.860	−10.991	±0.198	±0.040
λ_2 (ppb)[b]	−5.260	−5.733	±0.175	±0.035
λ_3 (ppb)[b]	−6.330	−6.470	±0.194	±0.039
s_{11}	−0.500326	−0.462850	±0.020362	±5.5710e − 011
s_{12}	−0.517359	−0.502740	±0.007322	±7.2990e − 011
s_{13}	−0.694272	−0.730084	±0.015051	±8.3755e − 011
s_{21}	−0.754406	−0.777826	±0.013053	±5.7840e − 011
s_{22}	−0.133022	−0.164684	±0.014526	±6.3629e − 011
s_{23}	−0.642788	−0.606519	±0.019101	±7.8306e − 011
s_{31}	−0.424905	−0.425155	±0.007800	±6.2683e − 011
s_{32}	−0.845367	−0.848606	±0.003740	±7.6546e − 011
s_{33}	−0.323744	−0.314820	±0.010128	±7.2661e − 011

[a] ±5 mm random errors are added to observations.
[b] part per billion (=10^{-9}).

values, it is obvious that those uncertainty estimates from the proposed approach are more realistic. The uncertainty estimates without considering any parameter dependency are underestimated, especially for the parameters associated with the orientation part (i.e. the rotation matrix).

It can be verified that the comparison approach here is identical to the one that uses (2.2.17) to perform the covariance propagation; in both cases the parameter dependencies in the principal orientations are neglected. As a result, the covariance matrix is propagated from a 'lower-rank' vector space to a 'higher-rank' vector space. $\mathbf{\Sigma}_{\{\beta\}}$ will be singular (in this 3-D example, its rank is six), and the corresponding covariance will be degenerated (Hamilton 1964). The proper covariance propagation of a symmetric tensor using the classical approach has been mentioned in Xu & Grafarend (1996a, b), Cai (2004) and Cai *et al.* (2005), in which the relationships between the tensor entries and principal values and orientation parameters (principal rotation angles) are required.

REMARKS

The proposed approach is proven for its ability to determine a correct and, thus, more realistic covariance propagation of the eigenparameters by using a direct analytical expression which works for symmetric tensors of any dimensions. In the classical approach, the parameter dependencies of the principal components need to be resolved first, or the relationships between the entries in an n-D tensor with its principal values and corresponding rotation angles need to be known. Then, one still needs to take care of the differentiations while preparing the Jacobian matrix whose size follows the dimension of the symmetric tensor. For the cases where the dimension of a symmetric matrix is substantially large (e.g. applications in remote sensing), preparing the Jacobian matrix becomes laborious. Furthermore, situations could become more complicated when additional constraints are imposed (e.g. the zero-trace constraint in geophysical applications). By using the formulation introduced here, one only needs the three matrix transformation operators $\mathbf{D}_{\mathbf{E}}$, $\mathbf{D}_{\mathbf{S}}$ and $\mathbf{D}_{\mathbf{\Omega}}$, which can be easily determined from the linear relationships between vectors. Additional constraints can also be imposed by adequately rearranging the values of these operators. However, most important of all are the parameter dependencies between the principal orientations have been correctly resolved and implemented in this new model.

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