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Multivariate distribution model for stress variability characterisation

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ABSTRACT

In situ stress is an important parameter in rock mechanics, but localised measurements of stress often display significant variability. For improved understanding of *in situ* matrices that satisfy both Eq. stress it is important that this variability be correctly characterised, and for this a robust statistical distribution model – one that is faithful to the tensorial nature of stress – is essential. Currently, variability in stress measurements is customarily characterised using separate scalar and vector distributions for principal stress magnitude and orientation respectively. These customary scalar/vector approaches, which violate the tensorial nature of stress, together with other quasi-tensorial applications found in the literature that consider the tensor components as statistically independent variables, may yield biased results. To overcome this, we propose using a multivariate distribution model of distinct tensor components to characterise the variability of stress tensors referred to a common Cartesian coordinate system. We discuss why stress tensor variability can be sufficiently and appropriately characterised by its distinct tensor components in a multivariate manner, and demonstrate that the proposed statistical model gives consistent results under coordinate system transformation. Transformational invariance of the probability density function (PDF) is also demonstrated, and shows that stress state probability is independent of the coordinate system. Thus, stress variability can be characterised in any convenient coordinate system. Finally, actual *in situ* stress results are used to confirm the multivariate characteristics of stress data and the derived properties of the proposed multivariate distribution model, as well as to demonstrate how the quasi-tensorial approach may give biased results. The proposed statistical distribution model not only provides a robust approach to characterising the variability of stress in fractured rock mass, but is also expected to be useful in risk- and reliability-based rock engineering design.

1. Introduction

In situ stress is an important parameter in many aspects of rock mechanics, including hydraulic fracturing propagation, rock mass permeability analysis and earthquake potential evaluation.[1–5] Because of the inherent complexity of fractured rock masses in terms of varying rock properties and the presence of discontinuities, *in situ* stress in rock often displays significant variability.[4,6–8] Also, with the increasingly widespread application of probabilistic or reliability-based design in rock engineering,[9–14] robustly incorporating stress variability in these analyses is becoming a necessity and for this a statistical distribution model is a prerequisite. However, stress is a second order tensor, and it appears that a robust statistical distribution model that characterises the variability of stress data – one that is faithful to the tensorial nature of stress – is not available. To address this deficiency, and to assist probabilistic-related analyses that need to consider the inherent variability of *in situ* stress, we propose using a multivariate distribution model for stress variability characterisation.

Currently in rock mechanics, stress magnitude and orientation are customarily processed separately (e.g. Fig. 1). This effectively decomposes the stress tensor into scalar (principal stress magnitudes) and vector (principal stress orientations) components, to which non-tensor related approaches such as classical statistics[15] and directional statistics,[16] respectively, are applied.[6,9,17–32] However, such applications imply a statistical distribution model that is an *ad hoc* combination of distributions of scalars and vectors, and therefore in general are erroneously applying statistical tools to process data that are referred to different geometrical bases. They thus violate the tensorial nature of stress, and as a result may yield biased results.[33–40] Additionally, these non-tensor related statistical models render it difficult to incorporate stress variability into reliability-based geotechnical engineering design codes such as Eurocode 7.[41]

As an alternative to the separate analysis of principal stress magnitude and orientation, and to be faithful to the tensorial nature of stress, analyses of stress variability should be conducted on the basis of stress tensors referred to a common Cartesian coordinate system.[34,38–40]

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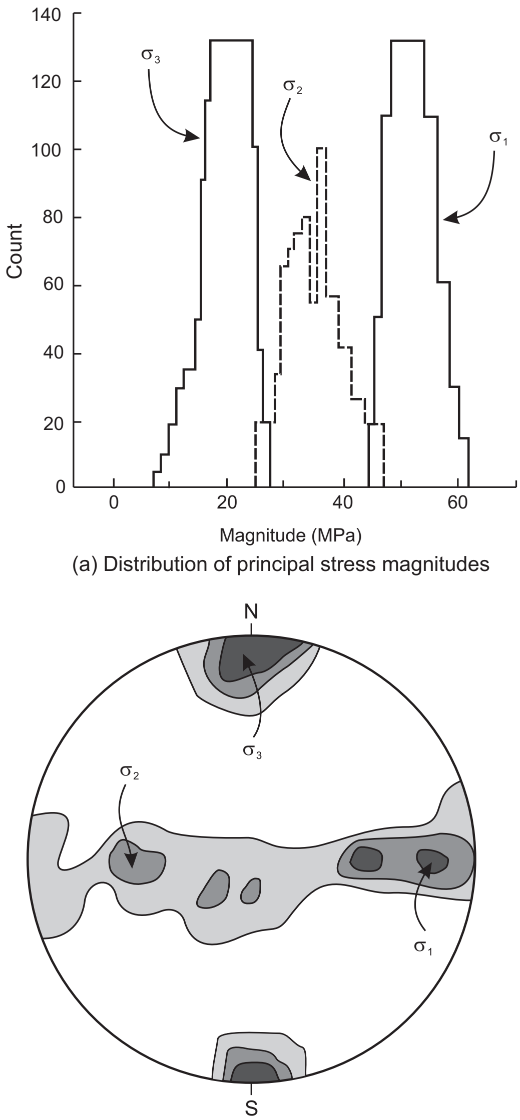

(a) Distribution of principal stress magnitudes

(b) Contouring of principal stress orientations

Fig. 1. Customary analyses of stress processes principal stress magnitude and orientation separately using classical statistics and directional statistics, respectively (after Brady & Brown[31]).

Several researchers have followed this technique when calculating the mean[36,42–45] and variance[36,43,45,46] of stress tensors, as well as for random stress tensor generations.[43,46,47] However, in this previous work the stress tensor components are treated as statistically independent variables, which implies an underlying statistical distribution model that is a combination of several independent univariate distributions in which the effect of correlation between tensor components is ignored.[39] As with earlier non-tensorial customary scalar/vector approaches, these quasi-tensorial applications may also yield unreasonable results. We have previously discussed the inappropriateness of customary scalar/vector and quasi-tensorial approaches for stress variability characterisation.[38–40]

In order to improve on these oversimplified statistical distribution models, some work has attempted to apply multivariate statistics to analyses of stress variability.[36,48,49] However, multivariate statistics is generally only suitable for vector data, not tensors.[50] We therefore suggest that these previous applications of multivariate techniques have taken place in an empirical setting, in that the applicability of multivariate statistics to stress variability analysis has not been formally demonstrated. Thus, to date there seems to have been no mathematically rigorous proposal for, and systematic analysis of, a statistical distribution model for stress variability characterisation in rock mechanics. The principal aim of this article is to provide this formal framework.

Stress tensors, which are 2×2 or 3×3 symmetric matrices, together with other matrix-valued quantities, play a pivotal role in many subjects such as solid mechanics, physics, earth science, medical imaging and economics.[51] To explicitly account for the inherent variability of such matrix-valued quantities, matrix variate statistics – as a generalisation of multivariate statistics – has been developed.[51] Although this has been demonstrated to be appropriate for stress variability analysis,[52] application of it is not straightforward and some essential components remain to be developed.[53,54] Fortunately, the statistical equivalence between matrix variate and multivariate statistics implies that, for stress variability analysis, multivariate statistics can be used in certain circumstances as an easily-applicable alternative to matrix variate statistics. Indeed, matrix variate statistics and multivariate statistics are occasionally used interchangeably.[51,54–56]

Among many statistical distributions, the normal distribution is particularly important as physical observations are often seen to be approximately normally distributed.[51] Thus, to provide an easily applicable approach, and as an extension of our previous work,[33,52] here, based on matrix variate statistics and using the normal distribution as an example, a multivariate distribution model for characterising the variability of stress tensors obtained in a common Cartesian coordinate system is presented and examined systematically. We also derive the reason why stress tensor variability can be adequately represented by variability of distinct tensor components in a multivariate manner.

In the present paper, the multivariate distribution model of complete tensor components is presented first, and difficulties faced in application to the analysis of stress variability discussed. To overcome these difficulties the multivariate distribution of distinct tensor components is introduced. We then analytically demonstrate the transformational consistency and invariance of this statistical distribution model in terms of mean, covariance matrix and probability density function (PDF). Finally, using actual *in situ* stress data, the multivariate characteristics of stress data is confirmed and inappropriateness of a quasi-tensorial distribution model discussed. Some relevant contents and derivations are shown in the Appendices. The notation adopted here generally follows the convention of bold uppercase, bold lowercase and normal lowercase letters denoting matrix, vector and scalar, respectively, unless otherwise noted.

2. Multivariate distribution model

Generally, a tensor is a quantity that can be represented by an organised array of numerical values. The order of a tensor is the dimension of the array needed to represent it, or equivalently the number of indices needed to label a component of that array. Thus, scalars, being single numbers, are zero order tensors, and vectors, being one-dimensional arrays, are tensors of the first order. Stress tensors are represented by 2×2 or 3×3 two-dimensional arrays, and therefore are second order. Unless otherwise noted, here the term "tensor" is specifically used to denote a symmetric 2×2 or 3×3 second order tensor. As stress is a second order tensor, the explicit and intuitive approach to characterise stress variability is to use a matrix variate distribution, as these characterise the variability of matrices by considering each matrix as a single entity.[51] However, current limitations of and application difficulties associated with matrix variate statistics require the more applicable approach of multivariate statistics to be used, as the two techniques can be shown to be equivalent.[51]

Here, we first introduce the matrix variate normal distribution to demonstrate the equivalence between the matrix variate statistics of a stress tensor and the multivariate statistics of the complete tensor components. Then, by making use the symmetric structure of the stress tensor and to avoid the singularity caused by repeated rows and columns in the covariance matrix of complete tensor components, we apply the symmetric matrix variate normal distribution in order to simplify the multivariate distribution model into a distribution of only the distinct tensor components.

2.1. Multivariate normal distribution of all tensor components

Matrix variate statistics has been developed to explicitly quantify the inherent variability of matrix-valued quantities. Of the many matrix variate distributions available, the matrix variate normal distribution is the most widely used.[51] A detailed description of this matrix variate normal distribution and its parameter estimation are presented in Appendix A. As this Appendix shows, the PDF of this distribution is[51(p.55)]

$$f(\mathbf{X}) = \frac{1}{\sqrt{(2\pi)^{pq}|\boldsymbol{\Sigma}|}}\mathrm{etr}\left(-\frac{1}{2}\mathbf{U}^{-1}(\mathbf{X}-\mathbf{M})\mathbf{V}^{-1}(\mathbf{X}-\mathbf{M})^T\right), \tag{1}$$

where $\mathbf{U}$ and $\mathbf{V}$ result from separating the covariance matrix $\boldsymbol{\Sigma}$ using the decomposition

$$\boldsymbol{\Sigma} = \mathbf{U}\otimes\mathbf{V}, \tag{2}$$

and $\otimes$ denotes the Kronecker product.[57]

Unfortunately, separability of covariance matrices cannot be easily satisfied since it imposes a number of strict and difficult to meet constraints on the variances of, and correlations between, the observed variables.[53] Additionally, a separability test must be conducted for each specific data group as separability depends on the matrix-valued data themselves,[53,58,59] and such tests are not yet generally available.[53,58–60] To compound matters, the components $\mathbf{U}$ and $\mathbf{V}$ cannot be explicitly calculated and numerical iterative approaches have to be employed to determine them.[54] All these factors significantly limit the distribution's application to stress variability characterisation, and thus it is appropriate to investigate the applicability of multivariate statistics to the problem.

Matrix variate statistics and multivariate statistics are seen to be used interchangeably,[51,54–56] and the matrix variate normal and multivariate normal distributions are known to be statistically equivalent even though they appear dissimilar in terms of covariance matrix and PDF.[51,52] Indeed, the PDF of the matrix variate normal distribution shown in Eq. (1) is equivalent to that of the multivariate normal distribution of all matrix components [51 (p.56),55], which is

$$f(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^{pq}|\boldsymbol{\Sigma}|}}\exp\left(-\frac{1}{2}(\mathbf{x}-\mathbf{m})^T\cdot(\boldsymbol{\Sigma})^{-1}\cdot(\mathbf{x}-\mathbf{m})\right), \tag{3}$$

where the maximum likelihood estimation (MLE) of the mean vector $\mathbf{m}$ is

$$\hat{\mathbf{m}} = \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_i = \bar{\mathbf{x}} = \mathrm{vec}(\bar{\mathbf{X}}^T), \tag{4}$$

and the covariance matrix can be estimated by Eq. (A.10), i.e.

$$\hat{\boldsymbol{\Sigma}} = \mathrm{cov}(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_i-\bar{\mathbf{x}})\cdot(\mathbf{x}_i-\bar{\mathbf{x}})^T. \tag{5}$$

Thus, for a stress tensor, to avoid the limitations and application difficulties of the matrix variate normal distribution identified above, a multivariate normal distribution of all matrix components can be used instead. However, symmetric matrices such as stress tensors lead to duplicated rows and columns in the covariance matrix, and the resulting singularity of this matrix precludes use of Eq. (3). To overcome this problem, we propose using a multivariate distribution of the distinct tensor components, the derivation of which is presented next.

2.2. Multivariate normal distribution of distinct tensor components

The multivariate normal distribution of distinct tensor components is the multivariate analogue of the symmetric matrix variate normal distribution. Details of this matrix distribution are presented in Appendix B, and its suitability for characterising the variability of stress tensors has been demonstrated previously.[52]

As with the matrix variate normal distribution, the symmetric matrix variate normal distribution requires separability of the covariance matrix $\boldsymbol{\Sigma}$, i.e. $\boldsymbol{\Sigma} = \mathbf{U}\otimes\mathbf{V}$, and as noted above this renders calculation of the PDF difficult. However, the PDF of the symmetric matrix variate normal distribution (Eq. (B.10)) is known to be equivalent to the PDF of the multivariate normal distribution of distinct tensor components $\mathbf{s}_d$ (Eqs. 2.5.6-2.5.8 in Gupta & Nagar [51(p.70)], which is

$$f(\mathbf{s}_d) = \frac{1}{\sqrt{(2\pi)^{\frac{1}{2}p(p+1)}|\boldsymbol{\Omega}|}}\exp\left(-\frac{1}{2}(\mathbf{s}_d-\mathbf{m}_d)^T\cdot(\boldsymbol{\Omega})^{-1}\cdot(\mathbf{s}_d-\mathbf{m}_d)\right), \tag{6}$$

where the MLE of the mean vector $\mathbf{m}_d$ is

$$\hat{\mathbf{m}}_d = \frac{1}{n}\sum_{i=1}^{n}\mathbf{s}_{d_i} = \bar{\mathbf{s}}_d = \mathrm{vech}(\bar{\mathbf{S}}), \tag{7}$$

and the covariance matrix can be estimated (see Eq. (B.12)) as

$$\hat{\boldsymbol{\Omega}} = \mathrm{cov}(\mathbf{s}_d) = \frac{1}{n}\sum_{i=1}^{n}(\mathbf{s}_d-\bar{\mathbf{s}}_d)\cdot(\mathbf{s}_d-\bar{\mathbf{s}}_d)^T. \tag{8}$$

This equivalence means that the variability of symmetric matrix-valued data can be appropriately and adequately represented by the multivariate distribution of the distinct components.

A benefit of only considering the distinct components is that the minimum sample size required for MLE of the covariance matrix $\boldsymbol{\Omega}$ is reduced from (p^2+1) to $\left(\frac{1}{2}p(p+1)+1\right)$. For example, for three-dimensional stress tensors and when considering all nine tensor components, the minimum sample size required is 10, but when only the six distinct components are considered the sample size is reduced to 7. Although this is a small reduction, it is helpful for rock stress analysis since *in situ* stress measurements are difficult and hence expensive to perform, with the result that most rock engineering projects usually do not have the luxury of large samples. Thus, when the sample size $n > \frac{1}{2}p(p+1)$, the multivariate distribution of distinct tensor components can be used to characterise the stress variability. For the case of $n \le \frac{1}{2}p(p+1)$, and once an appropriate covariance matrix separability test for symmetric matrices has been developed, it will be possible to employ the symmetric matrix variate distribution with a separable covariance matrix.

In the above analyses, the stress vector $\mathbf{s}_d$ containing the distinct tensor components obtained by function $\mathrm{vech}(\mathbf{S})$ (see Appendix B) has the component sequence shown in Eq. (B.2), i.e.

$$\mathbf{s}_d = [\sigma_x \quad \tau_{xy} \quad \tau_{xz} \quad \sigma_y \quad \tau_{yz} \quad \sigma_z]^T \tag{9}$$

and all subsequent multivariate analyses presented here use this sequence. In fact, and as will be demonstrated below using actual stress data, the component sequence has no effect on the characteristics (e.g. the determinant) of the covariance matrix $\boldsymbol{\Omega}$, and thus does not influence the PDF of Eq. (6). Therefore, any convenient sequence of the distinct tensor components can be used when characterising stress variability using multivariate statistics in engineering applications.

3. Transformational consistency and invariance of multivariate normal distribution

It is well known that, for any given stress state, the magnitudes of the components of a stress tensor are dependent on the coordinate system in use. By extension, and recognising that it is common for many different coordinate systems to be in use when characterising stress variability,[61] it is critical that the PDF and parameters such as the mean and covariance matrix display transformational consistency and invariance. Here the transformational consistency is defined such that a quantity obtained in one coordinate system can be linked to the one obtained in another system by the transformation matrix, and the transformational invariance means that no matter which coordinate system in use, the quantity always has the identical results. It is known that the mean and covariance matrix of the symmetric matrix variate normal distribution subjected to a general transformation are consistent (p.73, Gupta & Nagar[51]), and here we demonstrate both the consistency and invariance for the multivariate normal distribution of the distinct components subject to the transformation

$$\mathbf{S}' = \mathbf{R}\mathbf{S}\mathbf{R}^T, \tag{10}$$

where $\mathbf{R}$ denotes a $p \times p$ orthogonal transformation matrix. This is the customary stress transformation equations, relating a stress tensor $\mathbf{S}$ in one Cartesian coordinate system to a tensor $\mathbf{S}'$ in another system.[61]

When $\mathbf{S}$ follows the symmetric matrix variate normal distribution in one coordinate system, the transformed tensor $\mathbf{S}'$ will also follow the symmetric matrix variate normal distribution and can be denoted as[51(p.73)]

$$\mathbf{S}' \sim SN_{p,p}(\mathbf{M}', \mathbf{\Omega}'), \tag{11}$$

where the mean stress tensor is

$$\mathbf{M}' = \mathbf{R}\mathbf{M}\mathbf{R}^T \tag{12}$$

and the covariance matrix is

$$\mathbf{\Omega}' = \mathbf{B}_p^T\mathbf{\Sigma}'\mathbf{B}_p. \tag{13}$$

Here $\mathbf{B}_p$ is the "transition matrix" defined in Appendix B, and $\mathbf{\Sigma}'$ is the covariance matrix of all transformed tensor components, which in decomposed matrix form is[51(p.73)]

$$\mathbf{\Sigma}' = \mathbf{U}' \otimes \mathbf{V}', \tag{14}$$

where

$$\mathbf{U}' = \mathbf{R}\mathbf{U}\mathbf{R}^T \tag{15}$$

and

$$\mathbf{V}' = \mathbf{R}\mathbf{V}\mathbf{R}^T. \tag{16}$$

Therefore, the transformed covariance matrices $\mathbf{\Sigma}$ and $\mathbf{\Omega}$ are

$$\mathbf{\Sigma}' = \mathbf{U}' \otimes \mathbf{V}' = (\mathbf{R}\mathbf{U}\mathbf{R}^T) \otimes (\mathbf{R}\mathbf{V}\mathbf{R}^T) \tag{17}$$

and

$$\mathbf{\Omega}' = \mathbf{B}_p^T \cdot ((\mathbf{R}\mathbf{U}\mathbf{R}^T) \otimes (\mathbf{R}\mathbf{V}\mathbf{R}^T))\cdot\mathbf{B}_p, \tag{18}$$

respectively.

Based on Eq. (11) and the definition of the symmetric matrix variate normal distribution, the transformed distinct tensor components $\mathbf{s}'_d = \text{vech}(\mathbf{S}')$ will follow a multivariate normal distribution with the mean vector

$$\mathbf{m}'_d = \text{vech}(\mathbf{M}') = \text{vech}(\mathbf{R}\mathbf{M}\mathbf{R}^T). \tag{19}$$

Now, for the four general matrices $\mathbf{A}$, $\mathbf{C}$, $\mathbf{P}$ and $\mathbf{Q}$, if the matrix products $\mathbf{AP}$ and $\mathbf{CQ}$ exist then the following identity holds[57(p.32)]:

$$(\mathbf{AP}) \otimes (\mathbf{CQ}) = (\mathbf{A} \otimes \mathbf{C}) \cdot (\mathbf{P} \otimes \mathbf{Q}). \tag{20}$$

Using this identity the covariance matrix $\mathbf{\Sigma}'$ in Eq. (17) may be changed to a version that does not require its decomposition:

$$\begin{aligned}\mathbf{\Sigma}' &= \mathbf{U}' \otimes \mathbf{V}' = (\mathbf{R}\mathbf{U}\mathbf{R}^T) \otimes (\mathbf{R}\mathbf{V}\mathbf{R}^T)\\ &= (\mathbf{R} \otimes \mathbf{R})\cdot((\mathbf{U}\mathbf{R}^T) \otimes (\mathbf{V}\mathbf{R}^T))\\ &= (\mathbf{R} \otimes \mathbf{R})\cdot(\mathbf{U} \otimes \mathbf{V})\cdot(\mathbf{R}^T \otimes \mathbf{R}^T)\\ &= (\mathbf{R} \otimes \mathbf{R})\cdot\mathbf{\Sigma}\cdot(\mathbf{R}^T \otimes \mathbf{R}^T).\end{aligned} \tag{21}$$

Thus, the transformed covariance matrix $\mathbf{\Omega}'$ of the distinct components in terms of the original covariance matrix $\mathbf{\Omega}$ is

$$\mathbf{\Omega}' = \mathbf{B}_p^T\mathbf{\Sigma}'\mathbf{B}_p = \mathbf{B}_p^T\cdot(\mathbf{R} \otimes \mathbf{R})\cdot\mathbf{\Sigma}\cdot(\mathbf{R}^T \otimes \mathbf{R}^T)\cdot\mathbf{B}_p. \tag{22}$$

The multivariate PDF of the transformed distinct tensor components can be written as

$$f(\mathbf{s}'_d) = \frac{1}{\sqrt{(2\pi)^{\frac{1}{2}p(p+1)}|\mathbf{\Omega}'|}}\exp\left(-\frac{1}{2}(\mathbf{s}'_d - \mathbf{m}'_d)^T\cdot(\mathbf{\Omega}')^{-1}\cdot(\mathbf{s}'_d - \mathbf{m}'_d)\right). \tag{23}$$

However, since

$$\begin{aligned}&(\mathbf{s}_d - \mathbf{m}_d)^T\cdot(\mathbf{\Omega})^{-1}\cdot(\mathbf{s}_d - \mathbf{m}_d)\\ &= (\text{vech}(\mathbf{S} - \mathbf{M}))^T\cdot\mathbf{B}_p^+(\mathbf{U} \otimes \mathbf{V})^{-1}(\mathbf{B}_p^+)^T\cdot\text{vech}(\mathbf{S} - \mathbf{M}),\\ &= (\text{vec}(\mathbf{S} - \mathbf{M}))^T\cdot(\mathbf{U} \otimes \mathbf{V})^{-1}\cdot\text{vec}(\mathbf{S}-\mathbf{M})\\ &= \text{tr}(\mathbf{U}^{-1}(\mathbf{S} - \mathbf{M})\mathbf{V}^{-1}(\mathbf{S} - \mathbf{M}))\end{aligned} \tag{24}$$

(Eqs. 2.5.6–2.5.8 in Gupta & Nagar[51(p.71)]), the argument to the exp(·) function in Eq. (23) can be changed to

$$(\mathbf{s}'_d - \mathbf{m}'_d)^T\cdot(\mathbf{\Omega}')^{-1}\cdot(\mathbf{s}'_d - \mathbf{m}'_d) = \text{tr}((\mathbf{U}')^{-1}(\mathbf{S}' - \mathbf{M}')(\mathbf{V}')^{-1}(\mathbf{S}' - \mathbf{M}')). \tag{25}$$

The invariance of this expression can be demonstrated as follows. For non-singular matrices $\mathbf{P}$ and $\mathbf{Q}$ of the same size we have

$$(\mathbf{PQ})^{-1} = \mathbf{Q}^{-1}\mathbf{P}^{-1}, \tag{26}$$

and for an orthogonal matrix $\mathbf{R}$

$$\mathbf{R}^T = \mathbf{R}^{-1}. \tag{27}$$

Using these, the right hand side of Eq. (25) can be written in terms of $\mathbf{S}$, $\mathbf{M}$, $\mathbf{U}$ and $\mathbf{V}$ thus:

$$\begin{aligned}&\text{tr}((\mathbf{U}')^{-1}(\mathbf{S}' - \mathbf{M}')(\mathbf{V}')^{-1}(\mathbf{S}' - \mathbf{M}'))\\ &= \text{tr}((\mathbf{R}\mathbf{U}\mathbf{R}^T)^{-1}\cdot(\mathbf{R}(\mathbf{S} - \mathbf{M})\mathbf{R}^T)\cdot(\mathbf{R}\mathbf{V}\mathbf{R}^T)^{-1}\cdot(\mathbf{R}(\mathbf{S} - \mathbf{M})\mathbf{R}^T))\\ &= \text{tr}((\mathbf{R}\mathbf{U}^{-1}\mathbf{R}^T)\cdot(\mathbf{R}(\mathbf{S} - \mathbf{M})\mathbf{R}^T)\cdot(\mathbf{R}\mathbf{V}^{-1}\mathbf{R}^T)\cdot(\mathbf{R}(\mathbf{S} - \mathbf{M})\mathbf{R}^T)).\\ &= \text{tr}(\mathbf{R}\cdot\mathbf{U}^{-1}(\mathbf{S} - \mathbf{M})\mathbf{V}^{-1}(\mathbf{S} - \mathbf{M})\cdot\mathbf{R}^T)\\ &= \text{tr}(\mathbf{U}^{-1}(\mathbf{S} - \mathbf{M})\mathbf{V}^{-1}(\mathbf{S} - \mathbf{M}))\end{aligned} \tag{28}$$

Hence, using Eqs. (24), (25) and (28), the transformational invariance of the argument to the exp(·) function in Eq. (23) is confirmed:

$$\begin{aligned}&(\mathbf{s}'_d - \mathbf{m}'_d)^T\cdot(\mathbf{\Omega}')^{-1}\cdot(\mathbf{s}'_d - \mathbf{m}'_d)\\ &= \text{tr}((\mathbf{U}')^{-1}(\mathbf{S}' - \mathbf{M}')(\mathbf{V}')^{-1}(\mathbf{S}' - \mathbf{M}'))\\ &= \text{tr}(\mathbf{U}^{-1}(\mathbf{S} - \mathbf{M})\mathbf{V}^{-1}(\mathbf{S} - \mathbf{M}))\\ &= (\mathbf{s}_d - \mathbf{m}_d)^T\cdot(\mathbf{\Omega})^{-1}\cdot(\mathbf{s}_d - \mathbf{m}_d)\end{aligned} \tag{29}$$

In addition, we have analytically derived in Appendix C the transformational invariance of the determinant of the covariance matrix $\mathbf{\Omega}$, i.e.

$$|\mathbf{\Omega}| = |\mathbf{\Omega}'|. \tag{30}$$

This transformational invariance of the determinant of the covariance matrix $\mathbf{\Omega}$, together with Eq. (29), gives the transformational invariance of the PDF of the multivariate normal distribution of distinct tensor components (Eq. (6)):

$$\begin{aligned}&\frac{1}{\sqrt{(2\pi)^{\frac{1}{2}p(p+1)}|\mathbf{\Omega}|}}\exp\left(-\tfrac{1}{2}(\mathbf{s}_d - \mathbf{m}_d)^T\cdot(\mathbf{\Omega})^{-1}\cdot(\mathbf{s}_d - \mathbf{m}_d)\right)\\ &= \frac{1}{\sqrt{(2\pi)^{\frac{1}{2}p(p+1)}|\mathbf{\Omega}'|}}\exp\left(-\tfrac{1}{2}(\mathbf{s}'_d - \mathbf{m}'_d)^T\cdot(\mathbf{\Omega}')^{-1}\cdot(\mathbf{s}'_d - \mathbf{m}'_d)\right)\end{aligned} \tag{31}$$

Thus, it is seen that the PDF of distinct tensor components is independent of the coordinate system, and therefore characterisation of stress variability can be conducted in any convenient Cartesian coordinate system. This transformational invariance also demonstrates that the probability associated with a particular stress state is independent of the coordinate system, as would be expected when it is remembered that a stress state is a coordinate system independent point property.

4. Application to actual *in situ* stress data

The above analyses present a multivariate distribution model of distinct tensor components to characterise stress variability that is superior to the existing quasi-tensorial applications which consider tensor components as independent quantities. These analyses also give theoretical support to the few existing multivariate analyses of stress seen in the literature.[36,48,49] Here, to give an application of the proposed multivariate distribution model, 17 actual *in situ* stress data obtained on the 420 Level of the Atomic Energy of Canada Limited (AECL)'s Underground Research Laboratory (URL) in south-eastern Manitoba, Canada are analysed.[6] Geomechanics research was conducted at the AECL's URL during the period of about 1982 – 2004 to assess the feasibility of deep disposal of nuclear fuel waste in a plutonic rock mass.[6,62] These 17 stress data are part of the 99 *in situ* stress measurements presented by Martin,[6] which were made using a modified CSIR triaxial strain cell,[63] and are used here for the purpose of demonstrating the applicability and efficacy of the proposed statistical distribution model for stress variability characterisation from the mathematical and statistical points of view, rather than interpreting the stress conditions at the site. The 17 stress data were originally presented in the form of principal stress magnitudes and orientations. To allow the current application, we use Eq. (10) to transform these data into stress tensors referred to the common coordinate system of x East, y North and z vertically upwards. The components of the transformation matrix corresponding to each stress are the direction cosines of the principal stress orientations relative to the x, y and z directions. The distinct tensor components of the 17 stress tensors are shown in Table 1.

In what follows, the statistical dependence between distinct stress tensor components is firstly examined in terms of the correlation matrix. Following this, parameter estimates are obtained and transformational consistency of the proposed model verified. Finally, the effect of tensor component sequence on stress variability analysis is tested.

4.1. Statistical dependence between distinct stress tensor components

The statistical relationship between variables is formally determined by calculating their correlation coefficient, which for two variables x and y is[50(p.65)]

$$\rho = \frac{\mathrm{cov}(x, y)}{\sqrt{\mathrm{var}(x)\cdot\mathrm{var}(y)}}, \tag{32}$$

where $\mathrm{var}(\cdot)$ denotes the variance function. The correlation matrix[50(p.65)] of the six distinct tensor components of the stress data in Table 1 is presented in Table 2. When the correlation coefficient is close to zero there is no evidence of any relationship, i.e. the variates are independent. Thus, here only the relationships between σ_x and τ_{yz} ($\rho = 0.01$), and σ_y and τ_{yz} ($\rho = 0.03$) can be practically considered as independent, with the remaining pairs of stress components demonstrating some degree of dependence. The geological reasons for these dependencies is not known, nor is whether such dependencies exist in all fractured rock masses; we suggest these are subjects that warrant further investigation by the rock mechanics community.

Table 1
In situ stress tensor components in *x-y-z* coordinate system and the estimated mean.

Depth (m)	Stress number	Stress tensor components (MPa)					
		σ_x	τ_{xy}	τ_{xz}	σ_y	τ_{yz}	σ_z
416.55	$\mathbf{S}_1$	43.25	4.67	−3.44	32.67	−0.34	15.35
416.57	$\mathbf{S}_2$	41.20	6.59	−3.32	31.30	0.46	17.69
416.60	$\mathbf{S}_3$	42.92	8.80	−3.97	35.83	2.83	14.57
416.62	$\mathbf{S}_4$	45.11	5.42	−4.44	31.59	2.29	18.34
416.68	$\mathbf{S}_5$	42.57	4.36	−1.93	28.27	0.85	15.13
416.69	$\mathbf{S}_6$	53.78	5.26	−2.26	31.51	3.62	17.61
416.70	$\mathbf{S}_7$	26.05	−7.48	−2.57	38.40	1.74	12.35
416.71	$\mathbf{S}_8$	28.85	−12.01	−5.65	45.40	6.71	16.29
416.73	$\mathbf{S}_9$	30.96	−9.73	−3.86	42.67	0.45	14.56
416.77	$\mathbf{S}_{10}$	23.88	−9.88	−3.70	51.36	1.09	15.19
416.79	$\mathbf{S}_{11}$	34.97	−14.97	−4.51	57.51	1.80	11.74
416.81	$\mathbf{S}_{12}$	27.89	−10.89	−1.60	44.53	−0.24	14.22
417.17	$\mathbf{S}_{13}$	33.78	6.06	−2.19	46.27	0.19	14.59
417.17	$\mathbf{S}_{14}$	33.09	6.35	−5.77	45.00	0.10	18.15
417.17	$\mathbf{S}_{15}$	26.07	4.60	−3.30	42.37	3.14	12.69
417.17	$\mathbf{S}_{16}$	28.18	4.70	−3.89	40.82	3.72	18.25
417.17	$\mathbf{S}_{17}$	29.73	3.00	−4.92	40.55	−0.08	14.22
Estimated mean	$\bar{\mathbf{S}}$	34.84	−0.30	−3.61	40.36	1.67	15.35

Table 2
Correlation matrix of the distinct stress tensor components shown in Table 1.

	σ_x	τ_{xy}	τ_{xz}	σ_y	τ_{yz}	σ_z
σ_x	1.00	0.53	0.18	−0.67	0.01	0.42
τ_{xy}		1.00	0.08	−0.66	−0.12	0.48
τ_{xz}			1.00	−0.32	−0.29	−0.24
σ_y				1.00	0.03	−0.44
τ_{yz}		*sym.*			1.00	0.17
σ_z						1.00

To examine the significance of the correlation coefficients we use the null hypothesis that two tensor components are unrelated,[64] and test this using *p*-values. The *p*-values for each pair of tensor components of the stress data in Table 1 are tabulated in Table 3. Mathematical software packages such as MATLAB,[65] GNU Octave[66] and Excel's regression tool have functions to calculate the *p*-value, and in general values smaller than 0.05 can be deemed as significant. Thus, from Table 3 we observe that σ_x and τ_{xy}, σ_x and σ_y, σ_y and τ_{xy}, and σ_z and τ_{xy} are highly dependent. The first three of these have the greatest significance, and are between the stress components in the *xy* (i.e. horizontal) plane; we surmise that this is indicative of a systematic variation in the state of stress in this plane.

The non-zero correlation coefficients shown in Table 2 and the *p*-values presented in Table 3 demonstrate statistical dependence between distinct stress tensor components. As a result, simply treating all tensor components as independent quantities and using a collection of independent univariate distributions as a statistical distribution model in stress variability related analyses[36,43,45–47] is incorrect. Therefore, the proposed multivariate distribution model, which considers both the variances of and the correlations between tensor components, is more appropriate for characterising stress variability. Indeed, this observation prompts us to suggest that the term "six independent components", which is customarily used in rock mechanics to describe the stress tensor, should be replaced by "six distinct components" in order to both be statistically correct[67(p.56)] and avoid misinterpretations.[39]

4.2. Parameter estimations and their transformational consistency

For the data of Table 1, the MLE of the mean stress tensor (Eq. (B.11)) is

$$\hat{\mathbf{M}} = \begin{bmatrix} 34.84 & -0.30 & -3.61 \\ & 40.36 & 1.67 \\ sym. & & 15.35 \end{bmatrix} \text{MPa}, \tag{33}$$

and the MLE of the mean stress vector is

Table 3
p-values between the distinct stress tensor components shown in Table 1.

	σ_x	τ_{xy}	τ_{xz}	σ_y	τ_{yz}	σ_z
σ_x	1.00	0.03	0.50	0.00	0.98	0.09
τ_{xy}		1.00	0.77	0.00	0.65	0.05
τ_{xz}			1.00	0.21	0.26	0.35
σ_y				1.00	0.92	0.08
τ_{yz}		*sym.*			1.00	0.51
σ_z						1.00

$$\hat{\mathbf{m}}_d = [34.84 \ \ -0.30 \ \ -3.61 \ \ 40.36 \ \ 1.67 \ \ 15.35]^T \ \text{MPa}, \tag{34}$$

which are seen to have identical values. The covariance matrix of the distinct tensor components, by application of either Eqs. (B.9) or (8), is

$$\hat{\mathbf{\Omega}} = \begin{bmatrix} 67.59 & 34.96 & 1.74 & -42.09 & 0.11 & 7.01 \\ & 63.61 & 0.72 & -40.24 & -1.75 & 7.86 \\ & & 1.43 & -2.92 & -0.63 & -0.59 \\ & & & 58.29 & 0.38 & -6.85 \\ & sym. & & & 3.33 & 0.63 \\ & & & & & 4.13 \end{bmatrix} \text{MPa}^2. \tag{35}$$

The quasi-tensorial approach,[43,46,47] which treats distinct tensor components as independent quantities and ignores their covariances, produces the diagonal covariance matrix[39,40], i.e.

$$\text{diag}(\hat{\mathbf{\Omega}}) = \begin{bmatrix} 67.59 & 0 & 0 & 0 & 0 & 0 \\ & 63.61 & 0 & 0 & 0 & 0 \\ & & 1.43 & 0 & 0 & 0 \\ & & & 58.29 & 0 & 0 \\ & sym. & & & 3.33 & 0 \\ & & & & & 4.13 \end{bmatrix} \text{MPa}^2. \tag{36}$$

The leading diagonals of these two matrices are seen to be identical. The implication of ignoring the covariances in probability density calculation is demonstrated in a later section.

When using Eq. (5), the covariance matrix of all tensor components is

$$\hat{\mathbf{\Sigma}} = \begin{bmatrix} 67.59 & 34.96 & 1.74 & 34.96 & -42.09 & 0.11 & 1.74 & 0.11 & 7.01 \\ & 63.61 & 0.72 & 63.61 & -40.24 & -1.75 & 0.72 & -1.75 & 7.86 \\ & & 1.43 & 0.72 & -2.92 & -0.63 & 1.43 & -0.63 & -0.59 \\ & & & 63.61 & -40.24 & -1.75 & 0.72 & -1.75 & 7.86 \\ & & & & 58.29 & 0.38 & -2.92 & 0.38 & -6.85 \\ & & & & & 3.33 & -0.63 & 3.33 & 0.63 \\ & sym. & & & & & 1.43 & -0.63 & -0.59 \\ & & & & & & & 3.33 & 0.63 \\ & & & & & & & & 4.13 \end{bmatrix} \text{MPa}^2, \tag{37}$$

and comparison of Eqs. (35) and (37) demonstrates that the covariance matrix of all tensor components $\hat{\mathbf{\Sigma}}$ adds nothing to the covariance matrix of distinct tensor components $\hat{\mathbf{\Omega}}$ except for redundant data in the repeated second and fourth, third and seventh, and sixth and eighth rows and columns. In other words, $\hat{\mathbf{\Omega}}$ carries sufficient statistical information to allow the variability of stress tensors to be interpreted by their distinct tensor components.

To examine the transformational consistency of the mean and covariance matrix, the data of Table 1 are transformed into a new Cartesian coordinate system X-Y-Z that coincides with the orientations of the principal stresses of the estimated mean stress tensor in Eq. (33). The principal stress directions, the eigenvectors of the mean stress tensor, are

$$\mathbf{R}^T = \begin{bmatrix} 0.1037 & -0.9792 & -0.1743 \\ -0.9913 & -0.1160 & 0.0615 \\ -0.0805 & 0.1664 & -0.9828 \end{bmatrix}, \tag{38}$$

where the three column vectors correspond to the directions of σ_1, σ_2 and σ_3, respectively, referred to the x-y-z frame. Stress transformation into the X-Y-Z Cartesian coordinate system is performed using Eq. (10), and the transformed stresses are presented in Table 4.

The MLE of the mean vector of the 17 transformed stress tensors is

$$\hat{\mathbf{m}}'_d = [40.52 \ \ 0 \ \ 0 \ \ 35.42 \ \ 0 \ \ 14.61]^T \ \text{MPa}, \tag{39}$$

which is equal to that obtained by transforming the original mean in Eq. (33) using Eq. (19), i.e.

$$\text{vech}(\mathbf{RMR}^T) = [40.52 \ \ 0 \ \ 0 \ \ 35.42 \ \ 0 \ \ 14.61]^T \ \text{MPa}. \tag{40}$$

The MLE of the covariance matrix of the distinct tensor components of the 17 transformed stress tensors is

Table 4
In situ stress tensor components in X-Y-Z coordinate system and the estimated mean.

Depth (m)	Stress number	Stress tensor components (MPa)					
		σ_X	τ_{XY}	τ_{XZ}	σ_Y	τ_{YZ}	σ_Z
416.55	$\mathbf{S}_1$	31.71	3.36	−0.75	44.53	1.20	15.02
416.57	$\mathbf{S}_2$	30.09	5.10	0.66	42.97	0.61	17.13
416.60	$\mathbf{S}_3$	34.48	7.18	2.86	45.23	0.98	13.62
416.62	$\mathbf{S}_4$	30.97	3.22	2.29	46.78	0.40	17.29
416.68	$\mathbf{S}_5$	27.61	2.59	0.48	43.21	2.72	15.15
416.69	$\mathbf{S}_6$	31.20	2.19	3.15	54.27	4.20	17.44
416.70	$\mathbf{S}_7$	39.96	−6.08	−1.27	24.91	0.27	11.94
416.71	$\mathbf{S}_8$	48.66	−11.03	2.85	27.58	−2.03	14.29
416.73	$\mathbf{S}_9$	44.50	−8.20	−2.98	29.69	−0.56	13.99
416.77	$\mathbf{S}_{10}$	53.10	−6.72	−2.75	22.93	−1.70	14.41
416.79	$\mathbf{S}_{11}$	60.41	−12.16	−3.75	32.64	0.25	11.18
416.81	$\mathbf{S}_{12}$	46.38	−8.46	−4.14	25.79	1.03	14.47
417.17	$\mathbf{S}_{13}$	44.75	7.27	−0.81	35.50	0.79	14.39
417.17	$\mathbf{S}_{14}$	43.51	7.09	−0.17	36.15	−3.27	16.58
417.17	$\mathbf{S}_{15}$	41.62	5.65	2.10	27.92	−0.80	11.60
417.17	$\mathbf{S}_{16}$	40.23	5.14	3.23	30.27	−1.83	16.75
417.17	$\mathbf{S}_{17}$	39.71	3.87	−1.00	31.73	−2.26	13.05
Estimated mean	$\bar{\mathbf{S}}'$	40.52	0.00	0.00	35.42	0.00	14.61

$$\hat{\mathbf{\Omega}}' = \begin{bmatrix} 74.53 & -38.37 & -11.65 & -56.12 & -7.95 & -9.17 \\ & 45.74 & 9.07 & 32.75 & 0.97 & 5.46 \\ & & 5.79 & 10.52 & 0.43 & 2.01 \\ & & & 78.81 & 10.49 & 9.86 \\ & sym. & & & 3.35 & 0.62 \\ & & & & & 3.67 \end{bmatrix} \text{MPa}^2. \tag{41}$$

The covariance matrix obtained by using Eq. (22) to transform the covariance matrix $\mathbf{\Sigma}$ of the stress tensors in the x-y-z coordinate system is

$$\mathbf{B}_p^T \cdot (\mathbf{R} \otimes \mathbf{R}) \cdot \mathbf{\Sigma} \cdot (\mathbf{R}^T \otimes \mathbf{R}^T) \cdot \mathbf{B}_p = \begin{bmatrix} 74.53 & -38.37 & -11.65 & -56.12 & -7.95 & -9.17 \\ & 45.74 & 9.07 & 32.75 & 0.97 & 5.46 \\ & & 5.79 & 10.52 & 0.43 & 2.01 \\ & & & 78.81 & 10.49 & 9.86 \\ & sym. & & & 3.35 & 0.62 \\ & & & & & 3.67 \end{bmatrix} \text{MPa}^2, \tag{42}$$

which is identical to that of Eq. (41). These analyses confirm the transformational consistency of the mean and covariance matrix derived analytically in Section 3.

4.3. Transformational invariance of the PDF of the multivariate distribution

To test the transformational invariance of the PDF, we firstly examine the transformational invariance of the determinant of the covariance matrix $\mathbf{\Omega}$. The determinant of the covariance matrix in the x-y-z coordinate system (i.e. Eq. (35)) is

$$|\hat{\mathbf{\Omega}}| = 6.57 \times 10^5 \ \text{MPa}^{12}, \tag{43}$$

which is the same as the determinant of the covariance matrix in X-Y-Z coordinate system (i.e. Eqs. (41) or (42)):

$$|\hat{\mathbf{\Omega}}'| = 6.57 \times 10^5 \ \text{MPa}^{12}. \tag{44}$$

Calculations of the probability densities corresponding to the stress data shown in Table 1 and Table 4 using Eqs. (6) and (23), respectively, are tabulated in Table 5. The identical probability densities of the same stress states under these two coordinate systems confirms the transformational invariance of the PDF of the proposed multivariate distribution model. A large number of additional calculations using different coordinate systems, but not presented here for brevity, also confirm the transformational invariance. These analyses verify that the proposed multivariate distribution model can characterise stress variability in any convenient coordinate system.

Table 5
Probability densities of the stress tensors in *x-y-z* and *X-Y-Z* coordinate systems, and in *x-y-z* coordinate system using quasi-tensorial approach as well as using proposed approach but with changed tensor component sequence.

Stress number	Probability density			
	Coordinate system *x-y-z*	Coordinate system *X-Y-Z*	Quasi-tensorial approach	After tensor component sequence change
$\mathbf{s}_1$	1.01E-06	1.01E-06	2.88E-07	1.01E-06
$\mathbf{s}_2$	1.35E-06	1.35E-06	1.84E-07	1.35E-06
$\mathbf{s}_3$	4.85E-07	4.85E-07	3.55E-07	4.85E-07
$\mathbf{s}_4$	8.78E-07	8.78E-07	8.35E-08	8.78E-07
$\mathbf{s}_5$	7.37E-07	7.37E-07	9.49E-08	7.37E-07
$\mathbf{s}_6$	6.31E-08	6.31E-08	8.25E-09	6.31E-08
$\mathbf{s}_7$	2.75E-07	2.75E-07	1.53E-07	2.75E-07
$\mathbf{s}_8$	2.77E-08	2.77E-08	1.75E-09	2.77E-08
$\mathbf{s}_9$	1.08E-06	1.08E-06	5.60E-07	1.08E-06
$\mathbf{s}_{10}$	7.38E-07	7.38E-07	1.21E-07	7.38E-07
$\mathbf{s}_{11}$	1.59E-08	1.59E-08	4.15E-09	1.59E-08
$\mathbf{s}_{12}$	1.81E-07	1.81E-07	5.49E-08	1.81E-07
$\mathbf{s}_{13}$	1.28E-07	1.28E-07	3.23E-07	1.28E-07
$\mathbf{s}_{14}$	1.05E-07	1.05E-07	5.40E-08	1.05E-07
$\mathbf{s}_{15}$	1.12E-07	1.12E-07	2.43E-07	1.12E-07
$\mathbf{s}_{16}$	1.82E-07	1.82E-07	2.00E-07	1.82E-07
$\mathbf{s}_{17}$	3.81E-07	3.81E-07	4.08E-07	3.81E-07
Mean stress	4.97E-06	4.97E-06	1.81E-06	4.97E-06

Further calculation of the probability densities corresponding to the stresses shown in Table 1 but in a quasi-tensorial manner, i.e. using the covariance matrix shown in Eq. (36), is also presented in Table 5. The non-identical probability densities between the quasi-tensorial and proposed multivariate approach demonstrates that, by not considering the correlations between distinct tensor components, the former approach may yield incorrect results.

4.4. Effect of the sequence of distinct tensor components on stress variability analysis

The sequence of the distinct tensor components used above is that shown in Eq. (9). Here, the effect of changing the sequence of distinct tensor components on stress variability analysis is tested. For the distinct tensor components, if the shear components are put first, followed by the normal components, then a new stress vector is obtained:

$$\mathbf{s}_d'' = [\tau_{xy} \quad \tau_{xz} \quad \tau_{yz} \quad \sigma_x \quad \sigma_y \quad \sigma_z]^T. \tag{45}$$

Using this sequence for the stress tensors shown in Table 1 in *x-y-z* coordinate system, the new estimated mean is

$$\hat{\mathbf{m}}_d'' = [-0.30 \quad -3.61 \quad 1.67 \quad 34.84 \quad 40.36 \quad 15.35]^T \text{ MPa}, \tag{46}$$

and the covariance matrix is

$$\hat{\Omega}'' = \begin{bmatrix} 63.61 & 0.72 & -1.75 & 34.96 & -40.24 & 7.86 \\ & 1.43 & -0.63 & 1.74 & -2.92 & -0.59 \\ & & 3.33 & 0.11 & 0.38 & 0.63 \\ & & & 67.59 & -42.09 & 7.01 \\ & sym. & & & 58.29 & -6.85 \\ & & & & & 4.13 \end{bmatrix} \text{MPa}^2, \tag{47}$$

which has a determinant of

$$|\hat{\Omega}''| = 6.57 \times 10^5 \text{ MPa}^{12}. \tag{48}$$

Comparing Eq. (46) to Eq. (34), and Eq. (47) to Eq. (35) shows that the elements of the mean and covariance matrices are identical, although in a different sequence. The probability densities corresponding to the 17 stresses in the new tensor component sequence are shown in Table 5. The identical covariance matrix determinant obtained from Eqs. (48) and (43), and the same probability densities of the 17 stresses in the new tensor component sequence demonstrate that the sequence of stress components has no effect on the statistical properties of the stress data. Nevertheless, for consistency with the transition matrix $\mathbf{B}_p$ (i.e. Eq. (B.4)) the order given above in Eq. (9) is recommended.

In the above analyses, a multivariate normal distribution has been used. Additionally, statistical equivalence between matrix variate and multivariate statistics has been proved for Wishart, gamma and beta distributions.[51] However, it is not yet known what multivariate distribution type of distinct tensor components is best suited to *in situ* stresses. When information regarding the underlying probability distribution of *in situ* stress tensor components becomes available, the methodology presented here can be used but with the appropriate distribution being substituted for the multivariate normal distribution.

5. Conclusions and further comments

A multivariate distribution model of the distinct tensor components is presented here to characterise the variability of stress tensors obtained in a common Cartesian coordinate system when the sample size $n > \frac{1}{2}p(p+1)$. The proposed model is faithful to the tensorial nature of stress, in that it does not decompose the stress tensor into scalar (i.e. principal stress magnitude) and vector (i.e. principal stress orientation) components, and then process them separately. In addition to giving a systematic proposal for using a multivariate statistical distribution model for stress variability characterisation and demonstrating the reason why the variability of stress tensors can be characterised using a multivariate distribution of their distinct tensor components, we also analytically demonstrate the transformational consistency and invariance of the proposed statistical model under coordinate system transformation.

The discussion of the equivalence between the matrix variate normal distribution and the multivariate normal distribution of all matrix components shows that the variability of matrix-valued data can be characterised by its components in a multivariate manner. However, because of the symmetric nature of stress tensor, the repeated rows and columns in the covariance matrix render it singular and thus hinder the calculation of the PDF. By introducing a transition matrix and using the equivalence between the symmetric matrix variate normal distribution and the multivariate normal distribution of distinct tensor components, it is seen that the variability of stress tensors can be represented and interpreted in terms of the variability of their distinct tensor components in a multivariate manner.

The transformational consistency of both the mean and the covariance matrix of the proposed multivariate distribution model shows that the mean and covariance matrix in one coordinate system are related to those in another system by a transformation matrix. Additionally, the determinant of the covariance matrix is invariant with respect to coordinate system. The transformation invariance of the PDF is also derived, which demonstrates that the probability density of a stress state is invariant and leads to the observation that the variability of stress tensors can be characterised in any convenient coordinate system. This supports the understanding of the probability of a stress state, in that no matter in which coordinate system the stress tensor is obtained, there should be a particular probability associated with it. Applications of actual *in situ* stress data confirm the transformational consistency and invariance of the proposed distribution model and also demonstrate that the quasi-tensorial approach may give us biased results. The sequence in a multivariate analysis of the distinct tensor components is seen to have no effect on the characterisation of stress variability.

When applied to actual *in situ* stress data, the proposed multivariate model indicates differing degrees of statistical dependence between the six distinct tensor components. The geological basis for this dependence is not known, nor is whether similar dependence exists in other fractured rock masses. As such dependence may have ramifications for engineering design, particularly when reliability- or risk-based design approaches are being implemented, we suggest that these matters be investigated when appropriate *in situ* stress data become available.

The proposed statistical distribution model not only provides a robust approach to characterise the variability of stress in rock masses, but also gives a theoretical support to many aspects of rock mechanics involving stress variability. For example, based on the proposed multivariate statistical distribution model, random stress tensors can be generated using a multivariate random vector generation approach and used in Monte-Carlo simulation to incorporate stress variability into reliability-based rock engineering design.[39] However, one important question that continues to challenge the rock mechanics community is how many *in situ* stress measurements are necessary to characterise the state of stress in a specific engineering project. One suggestion is that, by using the proposed statistical distribution model, once the appropriate multivariate statistical distribution type has been determined a series of multivariate statistical tests could then be conducted to establish the minimum number of *in situ* stress measurements needed in order to reach a certain significance level. We are conducting further work to investigate this. Notwithstanding the results of this future work, the proposed statistical distribution model is expected to be helpful in the analysis of stress variability in rock mechanics and rock engineering.

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Appendix A. Matrix variate normal distribution

Following customary concepts,[51] the matrix $\mathbf{X}\,(p\times q)$ is said to follow a matrix variate normal distribution with mean matrix $\mathbf{M}\,(p\times q)$ and covariance matrix $\mathbf{\Sigma}\,(p\times q)$, i.e.

$$\mathbf{X}\sim N_{p,q}(\mathbf{M},\mathbf{\Sigma}), \tag{A.1}$$

if all components of $\mathbf{X}$ follow a multivariate normal distribution, i.e.

$$\mathbf{x}\sim N_{pq}(\mathbf{m},\mathbf{\Sigma}), \tag{A.2}$$

where

$$\mathbf{x}=\mathrm{vec}(\mathbf{X}^T) \tag{A.3}$$

is the vector containing all the matrix components, and the mean vector is

$$\mathbf{m}=\mathrm{vec}(\mathbf{M}^T). \tag{A.4}$$

Here, $\mathrm{vec}(\cdot)$ is the vectorisation function that vectorises a matrix into a column vector by stacking the columns.[68] For example, the general matrix

$$\mathbf{A}=\begin{bmatrix} a & c\\ b & d\end{bmatrix} \tag{A.5}$$

is vectorised to

$$\mathrm{vec}(\mathbf{A})=[a\quad b\quad c\quad d]^T. \tag{A.6}$$

with $[\cdot]^T$ denoting the matrix transpose.

The PDF of the matrix variate normal distribution is[51(p.55)]

$$f(\mathbf{X})=\frac{1}{\sqrt{(2\pi)^{pq}|\mathbf{\Sigma}|}}\mathrm{etr}\left(-\frac{1}{2}\mathbf{U}^{-1}(\mathbf{X}-\mathbf{M})\mathbf{V}^{-1}(\mathbf{X}-\mathbf{M})^T\right), \tag{A.7}$$

where $|\cdot|$ is the matrix determinant, $\mathrm{etr}(\cdot)$ is the matrix exponential trace, i.e. $\mathrm{etr}(\cdot)=\exp(\mathrm{tr}(\cdot))$, with $\mathrm{tr}(\cdot)$ denoting the trace of a matrix, and $\mathbf{U}\,(p\times p)$ and $\mathbf{V}\,(q\times q)$ are symmetric positive definite (SPD) matrices[55] obtained by decomposition of $\mathbf{\Sigma}$,

$$\mathbf{\Sigma}=\mathbf{U}\otimes\mathbf{V}, \tag{A.8}$$

where $\otimes$ denotes the Kronecker product.[57] Maximum likelihood estimation (MLE) of the mean matrix is[54]

$$\hat{\mathbf{M}}=\frac{1}{n}\sum_{i=1}^{n}\mathbf{X}_i=\overline{\mathbf{X}}. \tag{A.9}$$

For a sample size $n>pq$, the MLE of the covariance matrix is[51(p.47),54]

$$\begin{aligned}\hat{\mathbf{\Sigma}}&=\mathrm{cov}(\mathbf{x})\\&=\mathrm{cov}(\mathrm{vec}(\mathbf{X}^T))\\&=\tfrac{1}{n}\textstyle\sum_{i=1}^{n}\mathrm{vec}(\mathbf{X}_i^T-\overline{\mathbf{X}}^T)\cdot(\mathrm{vec}(\mathbf{X}_i^T-\overline{\mathbf{X}}^T))^T,\end{aligned} \tag{A.10}$$

where $\mathrm{cov}(\cdot)$ denotes the covariance function[69(p.428)]. The condition $n>pq$ signifies that only when this sample size is met can a meaningful MLE of the covariance matrix using Eq. (A.10) be obtained.[53]

Appendix B. Symmetric matrix variate normal distribution

The symmetric matrix variate normal distribution is derived from the matrix variate normal distribution shown in Appendix A. This derivation makes use of several special matrix operators. One is the half-vectorisation function $\mathrm{vech}(\cdot)$, which stacks only the lower triangular (i.e. on and below the diagonal) columns of a symmetric matrix[69(p.246)]. For example, for a symmetric matrix such as the 3×3 stress tensor

$$\mathbf{S} = \begin{bmatrix} \sigma_x & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_y & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_z \end{bmatrix}, \tag{B.1}$$

its half-vectorisation is

$$\begin{aligned} \mathrm{vech}(\mathbf{S}) &= [\sigma_x \;\; \tau_{yx} \;\; \tau_{zx} \;\; \sigma_y \;\; \tau_{zy} \;\; \sigma_z]^T \\ &= [\sigma_x \;\; \tau_{xy} \;\; \tau_{xz} \;\; \sigma_y \;\; \tau_{yz} \;\; \sigma_z]^T \end{aligned} \tag{B.2}$$

The vech(·) function thus forms a vector that contains only the distinct components of a symmetric matrix. The other required operator is the transition matrix $\mathbf{B}_p$, which allows elimination of duplicated elements in the vector obtained from the vec(·) functions, such that[51(p.11),69(p.246),70]

$$\mathrm{vech}(\mathbf{S}) = \mathbf{B}_p^T \mathrm{vec}(\mathbf{S}). \tag{B.3}$$

The transition matrices associated with two- and three-dimensional symmetric matrices are respectively

$$\mathbf{B}_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0.5 & 0 \\ 0 & 0.5 & 0 \\ 0 & 0 & 1 \end{bmatrix} \text{ and } \mathbf{B}_3 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.5 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.5 & 0 \\ 0 & 0 & 0.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}. \tag{B.4}$$

The symmetric matrix variate normal distribution and allied statistics are defined next.[51] For the symmetric matrix $\mathbf{S}\,(p \times p)$, if the $\frac{1}{2}p(p+1) \times 1$ vector

$$\mathbf{s}_d = \mathrm{vech}(\mathbf{S}) \tag{B.5}$$

containing the distinct components of $\mathbf{S}$ follows a multivariate normal distribution with mean $\mathbf{m}_d$ and covariance matrix $\boldsymbol{\Omega}$, i.e.

$$\mathbf{s}_d \sim N_{\frac{1}{2}p(p+1)}(\mathbf{m}_d, \boldsymbol{\Omega}), \tag{B.6}$$

where $\mathbf{m}_d$ is the vector of distinct mean components

$$\mathbf{m}_d = \mathrm{vech}(\mathbf{M}), \tag{B.7}$$

then matrix $\mathbf{S}$ is said to follow a symmetric matrix variate normal distribution with mean matrix $\mathbf{M}$ and covariance matrix $\boldsymbol{\Omega}$,

$$\mathbf{S} \sim SN_{p,p}(\mathbf{M}, \boldsymbol{\Omega}). \tag{B.8}$$

Here, the subscript "d" denotes "distinct". The covariance matrix of the distinct components is found from the covariance matrix of all matrix components (i.e. Eq. (A.10)) by application of the transition matrix:

$$\boldsymbol{\Omega} = \mathbf{B}_p^T \boldsymbol{\Sigma} \mathbf{B}_p. \tag{B.9}$$

Application of the transition matrix $\mathbf{B}_p$ is thus seen to form the non-singular covariance matrix $\boldsymbol{\Omega}$ through elimination of the repeated rows and columns in covariance matrix $\boldsymbol{\Sigma}$. The PDF of the symmetric matrix variate normal distribution is[51(p.70)]

$$f(\mathbf{S}) = \frac{1}{\sqrt{(2\pi)^{\frac{1}{2}p(p+1)}|\boldsymbol{\Omega}|}} \mathrm{etr}\left(-\frac{1}{2}\mathbf{U}^{-1}(\mathbf{S}-\mathbf{M})\mathbf{V}^{-1}(\mathbf{S}-\mathbf{M})\right), \tag{B.10}$$

where $\mathbf{U}$ and $\mathbf{V}$ are $p \times p$ SPD matrices that satisfy both Eq. (2) and the identity $\mathbf{UV} = \mathbf{VU}$. The MLE of the mean tensor $\mathbf{M}$ is

$$\hat{\mathbf{M}} = \frac{1}{n}\sum_{i=1}^{n}\mathbf{S}_i = \bar{\mathbf{S}}, \tag{B.11}$$

and when the sample size $n > \frac{1}{2}p(p+1) \times 1$, the MLE of the covariance matrix $\boldsymbol{\Omega}$ is[53]

$$\begin{aligned} \hat{\boldsymbol{\Omega}} &= \mathrm{cov}(\mathbf{s}_d) \\ &= \mathrm{cov}(\mathrm{vech}(\mathbf{S})) \\ &= \tfrac{1}{n}\textstyle\sum_{i=1}^{n} \mathrm{vech}(\mathbf{S}_i - \bar{\mathbf{S}})\cdot(\mathrm{vech}(\mathbf{S}_i - \bar{\mathbf{S}}))^T. \end{aligned} \tag{B.12}$$

Appendix C. Transformational invariance of the determinant of covariance matrix $\boldsymbol{\Omega}$

To derive the transformational invariance of the determinant of covariance matrix $\boldsymbol{\Omega}$, several matrix functions related to the transition matrix $\mathbf{B}_p$ need to be introduced first. Based on $\mathbf{B}_p$, Nel[56(Eqs. 2.5–2.8)] introduces a $p^2 \times p^2$ matrix

$$\mathbf{M}_p = \mathbf{B}_p \mathbf{B}_p^+, \tag{C.1}$$

where $(\cdot)^+$ denotes the Moore-Penrose pseudoinverse. For this the following identities hold:

$$\mathbf{B}_p^T = \mathbf{B}_p^T\mathbf{M}_p^T,$$
$$\mathbf{M}_p = \mathbf{M}_p^T,$$
$$\mathbf{B}_p^T = \mathbf{B}_p^T\mathbf{M}_p,$$
$$\mathbf{B}_p^+ = \mathbf{B}_p^+\mathbf{M}_p \text{ and}$$
$$\mathbf{B}_p = \mathbf{M}_p\mathbf{B}_p. \tag{C.2}$$

Also, the determinant of $\mathbf{B}_p^T\mathbf{B}_p$ is a constant[56 (Eq. 2.16)],

$$|\mathbf{B}_p^T\mathbf{B}_p| = 2^{-\frac{1}{2}p(p-1)}. \tag{C.3}$$

For a transformation matrix $\mathbf{R}$, the following identity can be obtained based on Eq. 2.9 in Nel[56]:

$$\mathbf{M}_p(\mathbf{R}\otimes\mathbf{R}) = (\mathbf{R}\otimes\mathbf{R})\mathbf{M}_p \text{ and}$$
$$(\mathbf{R}^T\otimes\mathbf{R}^T)\mathbf{M}_p = \mathbf{M}_p(\mathbf{R}^T\otimes\mathbf{R}^T). \tag{C.4}$$

Using Eq. (27) and Eq. 2.11 in Nel[56], then

$$\begin{aligned}(\mathbf{B}_p^+(\mathbf{R}\otimes\mathbf{R})\mathbf{B}_p)^{-1}\\ = \mathbf{B}_p^+(\mathbf{R}^{-1}\otimes\mathbf{R}^{-1})\mathbf{B}_p\\ = \mathbf{B}_p^+(\mathbf{R}^T\otimes\mathbf{R}^T)\mathbf{B}_p,\end{aligned} \tag{C.5}$$

and hence

$$(\mathbf{B}_p^+(\mathbf{R}\otimes\mathbf{R})\mathbf{B}_p)\cdot(\mathbf{B}_p^+(\mathbf{R}^T\otimes\mathbf{R}^T)\mathbf{B}_p) = \mathbf{I}. \tag{C.6}$$

Since two square matrices $\mathbf{A}$ and $\mathbf{C}$[69(p.58)] satisfy the identity

$$|\mathbf{AC}| = |\mathbf{A}|\cdot|\mathbf{C}|, \tag{C.7}$$

then the determinant of Eq. (C.6) is

$$|\mathbf{B}_p^+(\mathbf{R}\otimes\mathbf{R})\mathbf{B}_p|\cdot|\mathbf{B}_p^+(\mathbf{R}^T\otimes\mathbf{R}^T)\mathbf{B}_p| = 1. \tag{C.8}$$

Based on these matrix functions, the determinant of the covariance matrix $\boldsymbol{\Omega}$ becomes

$$\begin{aligned}|\boldsymbol{\Omega}| &= |\mathbf{B}_p^T\boldsymbol{\Sigma}\mathbf{B}_p| = |\mathbf{B}_p^T\mathbf{M}_p\boldsymbol{\Sigma}\mathbf{B}_p|\\ &= |\mathbf{B}_p^T\mathbf{B}_p\mathbf{B}_p^+\boldsymbol{\Sigma}\mathbf{B}_p|\\ &= |\mathbf{B}_p^T\mathbf{B}_p|\cdot|\mathbf{B}_p^+\boldsymbol{\Sigma}\mathbf{B}_p|\\ &= 2^{-\frac{1}{2}p(p-1)}\cdot|\mathbf{B}_p^+\boldsymbol{\Sigma}\mathbf{B}_p|\end{aligned} \tag{C.9}$$

and the determinant of the transformed covariance matrix $\boldsymbol{\Omega}$ is

$$\begin{aligned}|\boldsymbol{\Omega}'| &= |\mathbf{B}_p^T\cdot(\mathbf{R}\otimes\mathbf{R})\cdot\boldsymbol{\Sigma}\cdot(\mathbf{R}^T\otimes\mathbf{R}^T)\cdot\mathbf{B}_p|\\ &= |\mathbf{B}_p^T\mathbf{M}_p\cdot(\mathbf{R}\otimes\mathbf{R})\cdot\boldsymbol{\Sigma}\cdot(\mathbf{R}^T\otimes\mathbf{R}^T)\cdot\mathbf{M}_p\mathbf{B}_p|\\ &= |\mathbf{B}_p^T\mathbf{B}_p\mathbf{B}_p^+\cdot(\mathbf{R}\otimes\mathbf{R})\cdot\boldsymbol{\Sigma}\cdot(\mathbf{R}^T\otimes\mathbf{R}^T)\cdot\mathbf{M}_p\mathbf{B}_p|\\ &= |\mathbf{B}_p^T\mathbf{B}_p|\cdot|\mathbf{B}_p^+\cdot(\mathbf{R}\otimes\mathbf{R})\cdot\boldsymbol{\Sigma}\cdot(\mathbf{R}^T\otimes\mathbf{R}^T)\cdot\mathbf{M}_p\mathbf{B}_p|\\ &= 2^{-\frac{1}{2}p(p-1)}\cdot|\mathbf{B}_p^+\mathbf{M}_p\cdot(\mathbf{R}\otimes\mathbf{R})\cdot\boldsymbol{\Sigma}\cdot(\mathbf{R}^T\otimes\mathbf{R}^T)\cdot\mathbf{M}_p\mathbf{B}_p|\\ &= 2^{-\frac{1}{2}p(p-1)}\cdot|\mathbf{B}_p^+\cdot(\mathbf{R}\otimes\mathbf{R})\mathbf{M}_p\cdot\boldsymbol{\Sigma}\cdot\mathbf{M}_p(\mathbf{R}^T\otimes\mathbf{R}^T)\cdot\mathbf{B}_p|\\ &= 2^{-\frac{1}{2}p(p-1)}\cdot|\mathbf{B}_p^+(\mathbf{R}\otimes\mathbf{R})\mathbf{B}_p\cdot\mathbf{B}_p^+\boldsymbol{\Sigma}\mathbf{B}_p\cdot\mathbf{B}_p^+(\mathbf{R}^T\otimes\mathbf{R}^T)\mathbf{B}_p|\\ &= 2^{-\frac{1}{2}p(p-1)}\cdot|\mathbf{B}_p^+(\mathbf{R}\otimes\mathbf{R})\mathbf{B}_p|\cdot|\mathbf{B}_p^+\boldsymbol{\Sigma}\mathbf{B}_p|\cdot|\mathbf{B}_p^+(\mathbf{R}^T\otimes\mathbf{R}^T)\mathbf{B}_p|\\ &= 2^{-\frac{1}{2}p(p-1)}\cdot|\mathbf{B}_p^+\boldsymbol{\Sigma}\mathbf{B}_p|\end{aligned} \tag{C.10}$$

As the right hand side of both Eqs. (C.9) and (C.10) are identical, we see that

$$|\boldsymbol{\Omega}| = |\boldsymbol{\Omega}'|, \tag{C.11}$$

which confirms the transformational invariance of the determinant of covariance matrix $\boldsymbol{\Omega}$.

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