

Incorporating an assessment of uncertainty into estimates of *in situ* stress in rock as a function of depth

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ABSTRACT

Characterising the *in situ* stress state is important for all underground engineering projects, but is particularly so for safety-critical projects such as nuclear waste repositories. Although extensive campaigns are often mounted to robustly determine the *in situ* stress state, preliminary estimates may be apply the simple assumption that the state of stress is related to depth below ground. Such estimates are usually based on linear regression of principal stress magnitudes with depth, but as this ignores the tensorial nature of stress they are, strictly, incorrect. In this paper, we use Bayesian linear regression of stress components to obtain estimates of mean stress components and hence magnitudes and orientations of principal stresses. together with the uncertainty associated with these. The analysis is performed using over 100 overcoring data obtained at a potential nuclear waste repository site in granite in Sweden.

RÉSUMÉ

La caractérisation de l'état des contraintes *in situ* à une profondeur cible est importante pour tous les projets d'ingénierie souterrains, mais particulièrement critique pour les projets sensibles tels que les sites de stockage nucléaires. Même si des campagnes extensives sont souvent lancées dans le but d'estimer les contraintes *in situ*, les analyses préliminaires peuvent être basées sur la simple supposition d'une relation entre l'état des contraintes et la profondeur. Les estimations préliminaires basées sur la régression présument souvent une relation linéaire entre les contraintes principales et la profondeur, parfois en incluant l'orientation des contraintes principales. Comme ces méthodes ne respectent pas la nature tensorielle des contraintes, strictement, elles sont incorrectes. Pour cet article, nous utilisons la régression linéaire bayésienne des composantes des contraintes pour faire l'estimation des valeurs moyennes ainsi que l'incertitude reliée à ces valeurs. Par la suite, nous indiquons comment la régression des valeurs moyennes et des intervalles de crédibilité peut être utilisée pour estimer l'incertitude de l'état des contraintes, en ce qui concerne les composantes cartésiennes, ainsi que les contraintes principales (orientations et magnitudes). L'analyse est réalisée en utilisant plus de 100 échantillons de surcarottage en granite obtenus d'un site de stockage potentiel en Suède.

1 INTRODUCTION

In situ stress in rock is a key parameter in the design of underground structures, and is particularly significant for sensitive structures such as nuclear waste repositories. As a 3D stress state is defined by six distinct components of stress, characterisation of *in situ* stress is more complex than characterisation of scalar properties routinely used in rock mechanics and rock engineering. To date, there are no universally agreed and robust statistical methods to quantify variability and uncertainty in *in situ* stress measurements for the purpose of rock engineering design.

Direct methods of *in situ* stress measurement (e.g. hydraulic fracturing, CSIRO overcoring method) are expensive to perform, and indirect methods of stress estimation do not generate reliable estimates of the

complete stress state (Amadei & Stephansson 1997; Zang & Stephansson 2010). Consequently, large datasets of *in situ* stress measurements in rock are generally only obtained on specialized and critical projects such as nuclear waste repositories.

A commonly held assumption is that the state of stress in rock is significantly correlated with depth below ground surface, and thus linear regression of magnitudes of principal stresses against depth are often found in rock engineering literature. However, such regression methods that process principal stress magnitudes are strictly incorrect as they ignore the orientations of principal stresses, and thus violate the tensorial nature of stress. Therefore, complete characterisation of the uncertainty in *in situ* stress is not possible with these simplified regression methods.

Ordinary least squares regression obtains the maximum likelihood estimate of regression parameters (e.g. rate of stress increase with depth), and assumes there is no uncertainty in these. Conversely, Bayesian regression explicitly recognizes that such parameters are uncertain, and thus determines distributions – rather than single values – for them. In this paper, we present Bayesian linear regression analyses against depth of over 100 overcoring stress data obtained at the SKB Forsmark nuclear waste repository site in Sweden. The regression is performed using Cartesian stress components which honour the tensorial nature of stress. We also demonstrate, using informative priors, the benefit that Bayesian methods bring in being able to rationally incorporate prior knowledge.

2 BACKGROUND

2.1 Regression of principal stress magnitudes

As stress is a tensor it cannot be represented by principal stress magnitudes alone, as these do not contain any information on principal stress orientations. However, regression of principal magnitudes against depth continues to regularly appear in the rock engineering literature. Two such examples are shown in Figure 1, and these demonstrate that such scalar regressions have been in use for over forty years. Such regression can only be correct if principal stress orientations are invariant with depth, a severe constraint that is seldom, if ever, recognized in the literature.

2.2 Bayesian stress model

Gao & Harrison (2016; 2017; 2018) proposed a frequentist multivariate model to characterise the variability of *in situ* stress. This model is tensorial, but suffers from requiring a large number of *in situ* stress measurements to converge to stable values of statistical parameters such as mean and dispersion. To overcome this limitation, Feng & Harrison proposed a Bayesian stress model (Feng & Harrison 2019; Feng et al. 2020; Feng et al. 2021).

The Bayesian stress model assumes that the *in situ* stress data, $\mathbf{Y}_{\text{data}} = [\sigma_x \ \tau_{xy} \ \tau_{xz} \ \sigma_y \ \tau_{yz} \ \sigma_z]$, follow a multivariate normal distribution of

$$\mathbf{Y}_{\text{data}} \sim \text{MVN}(\boldsymbol{\mu}, \boldsymbol{\Omega}), \quad [1]$$

with prior distributions of

$$\boldsymbol{\mu} \sim \text{MVN}(\boldsymbol{\mu}_0, \boldsymbol{\Omega}_0), \quad [2]$$

and

$$\boldsymbol{\Omega}^{-1} \sim \text{Wishart}(\mathbf{S}, \nu). \quad [3]$$

Equations 2 and 3 show that the prior distributions have their own parameters $\boldsymbol{\mu}_0$, $\boldsymbol{\Omega}_0$, \mathbf{S} and ν ; these are the mean

stress vector, the covariance matrix, the Wishart distribution scale matrix and the degrees of freedom, respectively.

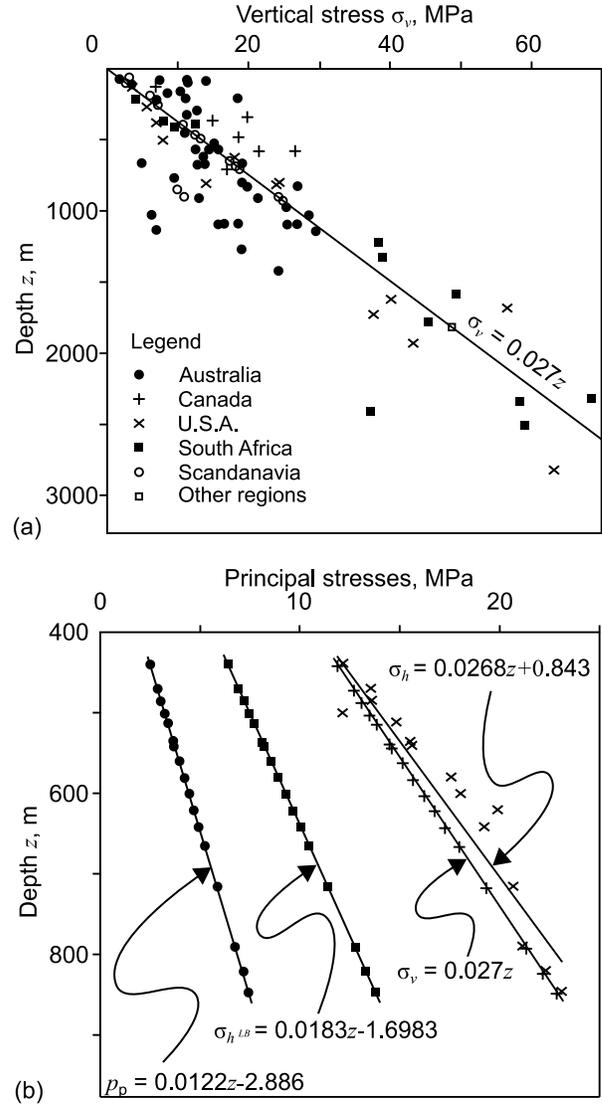


Figure 1. (a) 1978 example of vertical stress regression against depth (after Brown & Hoek 1978) and (b) 2021 example of regressing pore pressure, minimum horizontal and vertical stresses (after Shi et al. 2021)

In this paper we present a Bayesian linear regression for estimation of the mean stress vector $\boldsymbol{\mu}_0$ at any given depth, which honours the tensorial nature of stress and thus allows uncertainty in both the magnitudes and orientations of principal stresses to be obtained and characterized.

2.3 Bayesian linear regression

The Bayesian linear regression model can be written in generalized form as (Lunn et al. 2012)

$$y_i \sim \text{Normal}(\mu_i, \omega^2) \quad [4]$$

with

$$\mu_i = \beta_0 + \sum_{k=1}^p \beta_k x_{ki} \quad [5]$$

Here, y_i is the response variable (also known as the dependent variable) consisting of i data points, x_{ki} is the explanatory variable (also known as the independent variable) comprising k multivariate quantities of interest, μ_i is the mean relation between the variables of interest obtained by linear regression, β_0 and β_k are the intercepts and gradients respectively for the k quantities, and ω^2 is the variance around the mean regression line. The same value of variance is assumed to apply to all data, which represents the condition of homoscedasticity.

One significant advantage of a Bayesian approach is that it uses additional information in the form of prior distributions to augment limited measured values. In the above Bayesian linear regression model prior distributions for β_0 , β_k and ω are required, and these will be discussed in the next section.

3 METHODOLOGY

3.1 Bayesian linear regression of *in situ* stress

We present a Bayesian linear regression of 115 *in situ* stress data against depth below ground surface. These data were obtained at the SKB Forsmark site in Sweden, using overcoring measurement techniques, and comprise six distinct components of stress that are referred to arbitrarily selected Cartesian axes of x =East, y =North and z =Up.

The Bayesian stress model is

$$\mathbf{Y}_{ij} \sim \text{Normal}(\boldsymbol{\mu}_{ij}, \boldsymbol{\kappa}_j), \quad [6]$$

where

$$\boldsymbol{\mu}_{ij} = \boldsymbol{\beta}_{0j} + \boldsymbol{\beta}_j z_i, \quad [7]$$

with

$$\begin{aligned} \boldsymbol{\beta}_{0j} &= [\beta_{0_x} \ \beta_{0_y} \ \beta_{0_z} \ \beta_{0_{xz}} \ \beta_{0_{yz}} \ \beta_{0_{xy}}]^T \\ &= [\beta_{0_{\sigma_x}} \ \beta_{0_{\tau_{xy}}} \ \beta_{0_{\tau_{xz}}} \ \beta_{0_{\sigma_y}} \ \beta_{0_{\tau_{yz}}} \ \beta_{0_{\sigma_z}}]^T \end{aligned} \quad [8]$$

and

$$\boldsymbol{\beta}_j = [\beta_{\sigma_x} \ \beta_{\tau_{xy}} \ \beta_{\tau_{xz}} \ \beta_{\sigma_y} \ \beta_{\tau_{yz}} \ \beta_{\sigma_z}]^T. \quad [9]$$

The six distinct Cartesian stress components are individually regressed against depth below ground surface z in this regression model, and thus are regarded as independent response variables as shown in equations 7–9. We assume σ_z , τ_{xz} and τ_{yz} have magnitudes of zero at the ground surface, with the result that $\beta_{0_{\sigma_z}} = \beta_{0_{\tau_{xz}}} = \beta_{0_{\tau_{yz}}} = 0$.

We have performed Bayesian linear regression analyses using firstly uninformative priors, and then informative priors as explained in the following subsections.

3.1.1 Uninformative priors

Uninformative priors are often used in Bayesian statistics when we have no prior knowledge or a strong belief about the parameters of interest. For the case of uninformative priors, we have used

$$\beta_{0j} \begin{cases} \sim \text{Normal}(0, 0.0001) & \text{if } j \in (1, 2, 4) \\ 0 & \text{otherwise} \end{cases} \quad [10]$$

and

$$\beta_j \sim \text{Normal}(0, 0.0001). \quad [11]$$

For the precision parameter $\boldsymbol{\kappa}_j$ (the reciprocal of variance) we have used the uninformative priors

$$\boldsymbol{\kappa}_j = 1/\omega_j^2 \sim \text{Gamma}(0.0001, 0.0001), \quad [12]$$

where ω_j is the standard deviation of the j -th parameter of $\boldsymbol{\mu}_{ij}$.

3.1.2 Informative priors

The following Informative priors have been adopted for β_{σ_x} , $\beta_{\tau_{xz}}$ and $\beta_{\tau_{yz}}$:

$$\beta_{\sigma_x} \sim \text{Normal}(0.026, 1.0 \text{ E} + 06), \quad [13]$$

$$\beta_{\tau_{xz}} \sim \text{Normal}(0, 1.0 \text{ E} + 06), \quad [14]$$

$$\beta_{\tau_{yz}} \sim \text{Normal}(0, 1.0 \text{ E} + 06). \quad [15]$$

These priors reflect our increased belief in the reduced variability of the stress components σ_x , τ_{xz} and τ_{yz} . Priors on all the remaining regression parameters are uninformative as explained earlier in subsection 3.1.1.

The mean unit weight of 0.026 MN/m³ in equation 13 corresponds to a mean rock density of 2650 kg/m³ as determined from laboratory tests, and the precision of 1.0E +06 corresponds to an assumed standard deviation of 0.001 MN/m³ in the mean unit weight.

The flat ground surface at the SKB Forsmark site suggests that one of the three principal stresses will be vertical, which implies that both $\beta_{\tau_{xz}}$ and $\beta_{\tau_{yz}}$ should be zero; this is incorporated in equations 14 and 15 through use of a mean value of zero.

The posterior distributions of the regression parameters β_{0_j} , β_j and κ_j were obtained by performing 10,000 MCMC (Markov Chain Monte Carlo) simulations in the OpenBUGS software, with all pre- and post-processing carried out in R programming language.

3.2 Monte Carlo simulation

The MCMC samples of posterior distributions of β_{0_j} and β_j were subsequently substituted into equation 7 to obtain distributions of the mean of Cartesian stress components at selected depths in the interval 0 to 600m. These distributions were then randomly sampled to generate 10,000 random stress tensors at each depth value, and the eigenvalues and eigenvectors of each stress tensor extracted to obtain the principal stress magnitudes and orientations.

4 RESULTS AND DISCUSSIONS

The posterior distributions of the Cartesian stresses obtained using uninformative and informative priors are summarized in Table 1. Bayesian regression estimates of the individual Cartesian stress components using uninformative priors are shown in Figure 2, with regression plots for three normal stresses presented in the top row and the three shear stresses in the bottom row. Uncertainty in estimates of the individual mean Cartesian stress components relative to depth below ground surface are indicated by 95% credible intervals (C.I.) of the posterior distributions; these are obtained from MCMC simulations of

the mean values. The credible interval in Bayesian statistics is that interval which contains the mean with a particular probability (95% in our analysis), and 95% C.I. is obtained by equal tail method (i.e. 0-2.5% and 97.5-100% are discarded). Discussion on how C.I. fundamentally differs from the confidence interval used in frequentist statistics is given in many textbooks (e.g. Gelman et al. 2014).

Table 1 Summary of posterior distributions of Bayesian regression of Cartesian stresses

	Intercepts (uninformative priors)					
	$\beta_{0_{\sigma_x}}$	$\beta_{0_{\sigma_y}}$	$\beta_{0_{\sigma_z}}$	$\beta_{0_{\tau_{xy}}}$	$\beta_{0_{\tau_{xz}}}$	$\beta_{0_{\tau_{yz}}}$
Mean	6.629	6.191	0	0.267	0	0
Standard deviation	1.443	1.222	-	0.597	-	-
2.5% C.I.	3.823	3.801	-	-0.912	-	-
97.5% C.I.	9.459	8.564	-	1.450	-	-
	Gradients (uninformative priors)					
	β_{σ_x}	β_{σ_y}	β_{σ_z}	$\beta_{\tau_{xy}}$	$\beta_{\tau_{xz}}$	$\beta_{\tau_{yz}}$
Mean	0.057	0.066	0.037	-0.015	-0.003	-0.002
Standard deviation	0.007	0.006	0.003	0.003	0.001	0.002
2.5% C.I.	0.043	0.055	0.035	-0.021	-0.006	-0.005
97.5% C.I.	0.071	0.078	0.043	-0.009	0.0004	0.002
	Gradients (informative priors)					
	-	-	β_{σ_z}	-	$\beta_{\tau_{xz}}$	$\beta_{\tau_{yz}}$
Mean	-	-	0.027	-	-0.001	-4.5E-4
Standard deviation	-	-	9.5E-4	-	8.1E-4	8.6E-4
2.5% C.I.	-	-	0.016	-	-0.012	-0.011
97.5% C.I.	-	-	0.038	-	0.010	0.010

All three normal stresses show a positive correlation indicating that, as one would expect, they increase with depth. The C.I. for σ_x and σ_y appears to be much larger than that for σ_z , which suggests that σ_z can be estimated

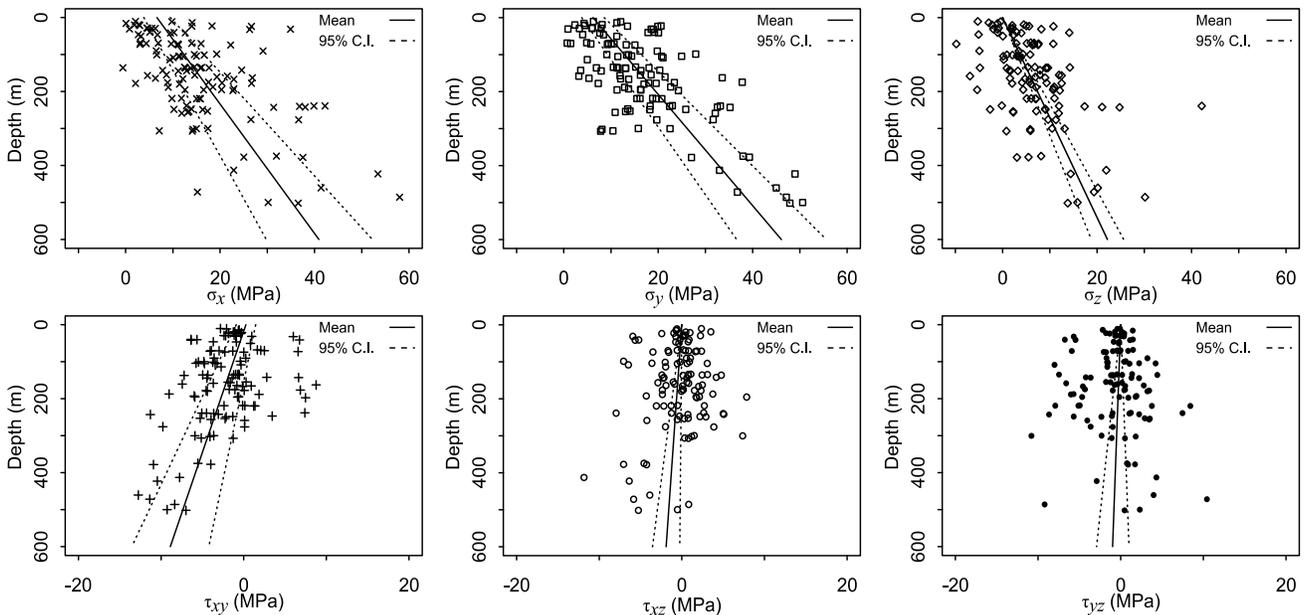


Figure 2. Bayesian linear regression of Cartesian stress components

with greater certainty than can σ_x and σ_y . The 95% C.I. for the mean values of σ_x and σ_y at 600m depth are approximately 30 to 52 MPa and 37 to 55 MPa respectively. For the stresses acting in a horizontal direction at 600m depth, the mean values are about $\bar{\sigma}_x=41$ MPa, $\bar{\sigma}_y=46$ MPa and $\bar{\tau}_{xy}=-9$ MPa, indicating a rotation of principal stress orientation of about $0.5 \arctan \left[\frac{2 \times -9}{46 - 41} \right] = -37^\circ$ from the x -axis. However, the wide C.I.s in these stress components indicate that there will be significant variability in this rotation angle, suggesting that it is quite wrong to assume the orientations of the horizontal principal stresses well known. This should not be ignored during design calculations.

Both τ_{xz} and τ_{yz} show a near zero posterior mean, with probabilities of about 98% and 88% respectively that the posterior mean is zero, and a relatively narrow C.I. This implies that one of the principal stresses will be vertical or near vertical. Conversely, the mean value of τ_{xy} is seen to change with depth, which indicates rotation of the sub-horizontal principal stresses with depth. However, as noted above, the wide 95% C.I. of τ_{xy} indicates significant uncertainty in this component, and this will propagate into uncertainty in the orientations of the sub-horizontal principal stress.

A comparison of two approaches to estimating variation of principal stress magnitude with depth – namely, Bayesian regression of individual principal stress magnitudes and principal stress magnitudes obtained by random sampling from the results of Bayesian regression of Cartesian stress components – is shown in Figure 3. It is important to recognise that although all three plots in Figure 3 show principal stress magnitudes, only the analyses in Figure 3b (uninformative priors) and Figure 3c (informative priors) are based on regression of Cartesian stress components and thus linked to principal stress orientations. A noteworthy effect of this is seen in the non-linear variation of principal stress magnitude with depth, particularly for σ_2 between depths 0-200m. Although generally similar, there are subtle but important differences among the three diagrams. For example, the C.I.s for σ_1 and σ_2 in 3(b) and 3(c) are narrower than those in 3(a); this shows that regression based on Cartesian components leads to smaller uncertainty than regression based on principal stress components. Also, the difference between the mean values of σ_1 and σ_3 (i.e. the differential stress $\bar{\sigma}_1 - \bar{\sigma}_3$), is smaller for 3(b) and 3(c) than for 3(a); as differential stress is a key factor in assessing the stability of rocks, this suggests that regression of Cartesian components will lead to stress states that are less critical than will regression of principal stresses. Note also how the mean and C.I. of σ_3 reduces from 3(b) to 3(c) through the use of informative priors.

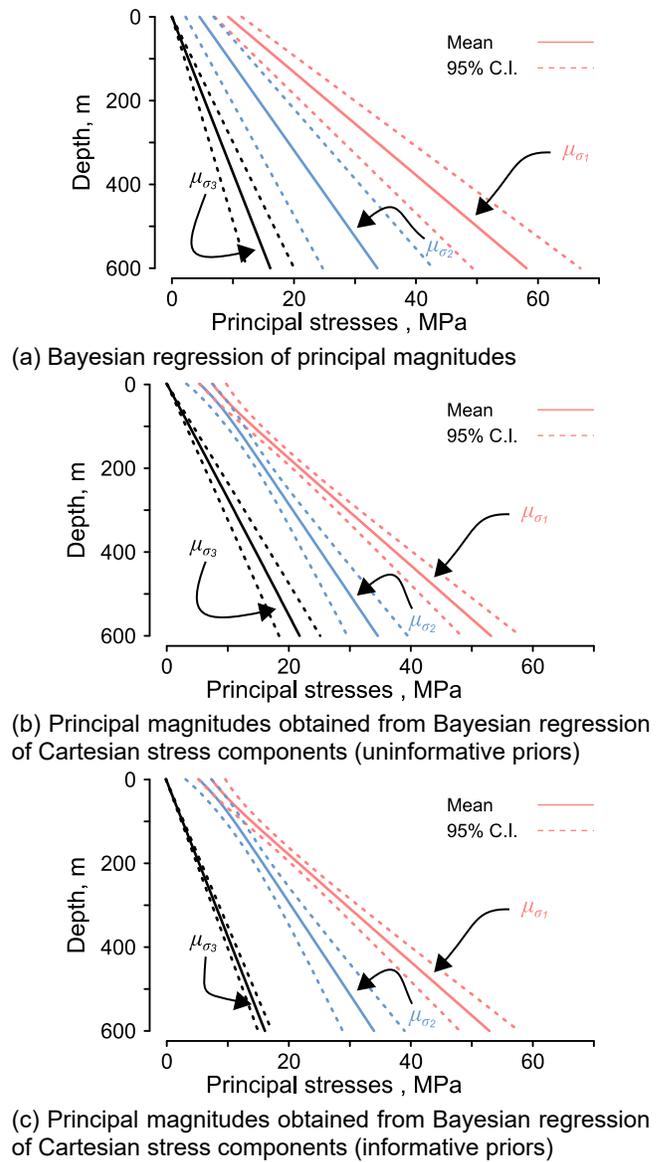


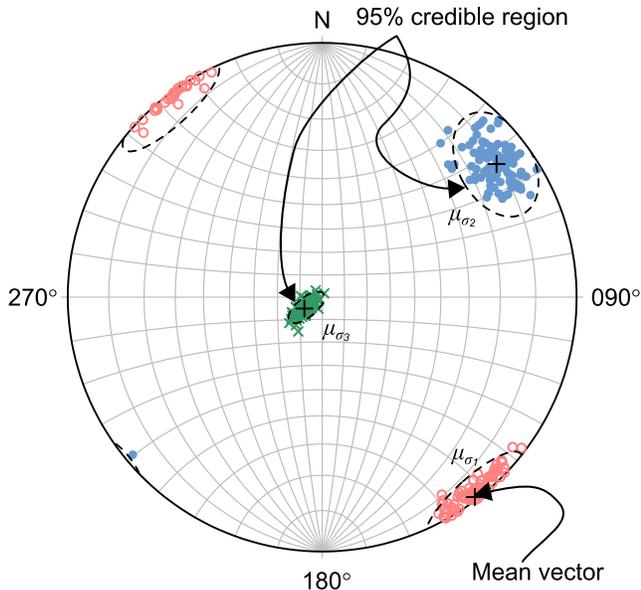
Figure 3. Estimated variation of principal stress magnitudes with depth

Figure 4 gives the distributions of both the orientations and magnitudes of the principal stresses obtained by random sampling from the results of uninformative Bayesian regression of Cartesian stress components at 450m (near to the planned repository depth). The credible regions of orientation shown in Figure 4(a) have been determined using the procedure proposed by Feng et al. (2021), which uses statistical depth of multivariate data. Here, we have used the R package *ddalpha* (Pokotylo et al. 2019) to compute Mahalanobis statistical depth in order to find a 95% credible region around the mean vectors. The plot shows a near vertical orientation for σ_3 and near horizontal orientations for σ_1 and σ_2 at trends of about 145° and 055° , respectively. Distributions of principal stress magnitudes obtained from Monte Carlo simulation are shown in Figure 4(b). The most probable mean values at

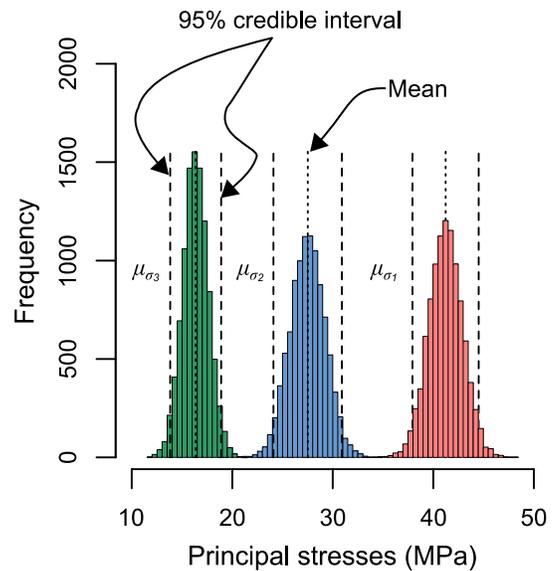
450m depth for σ_1 , σ_2 and σ_3 are approximately 41 MPa, 28 MPa and 16 MPa, and the 95% C.I. are approximately 38 to 45 MPa, 24 to 31 MPa and 14 to 19 MPa, respectively. These wide C.I.s should be accounted for in design calculations.

Figure 5 shows the results of using informative priors as discussed earlier, and clearly demonstrates the benefits of them. Thus, not only have the orientations of σ_1 and σ_2 moved closer to being horizontal, and that of σ_3 to vertical, but also the uncertainty in orientations of all three principal stresses is significantly reduced. For the magnitudes of

principal stresses, it should be noted that the distribution of σ_3 has shifted to the left (i.e. reduced). The most probable mean values of σ_2 and σ_3 calculated from samples of Cartesian stresses using informative priors are respectively about 27 MPa and 12 MPa, as opposed to 28 MPa and 16 MPa estimated using uninformative priors. This updated estimate of $\sigma_3=12$ MPa corresponds to a stress gradient of 0.027 MPa/m, i.e. a unit weight of 0.027 MN/m³. Furthermore, informative priors lead to a significant reduction in 95% C.I. for the magnitude of σ_3 , although the

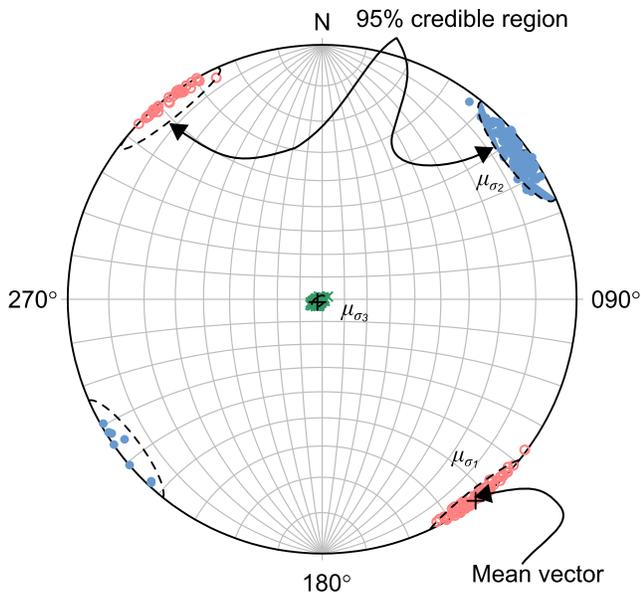


(a) orientations (100 random samples shown)

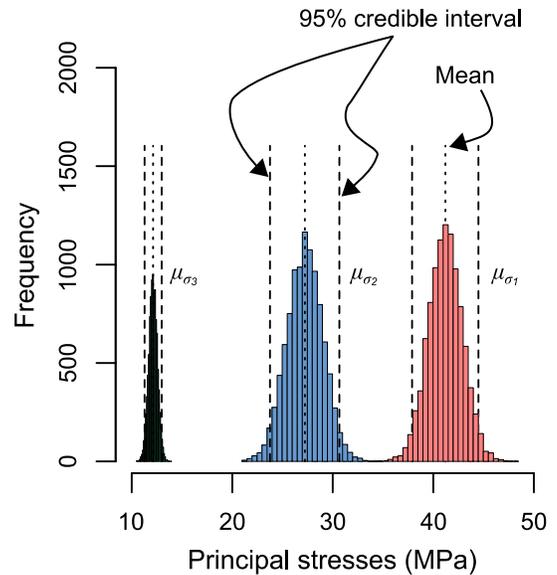


(b) magnitudes

Figure 4. Results of Monte Carlo simulation at a depth of 450m (using uninformative priors)



(a) orientations (100 random samples shown)



(b) magnitudes

Figure 5. Results of Monte Carlo simulation at a depth of 450m (using informative priors)

mean and 95% C.I. of the magnitude of σ_1 remains almost unchanged.

5 CONCLUSIONS

Linear regression of principal stress magnitudes against depth continues to appear in the rock mechanics and rock engineering literature, despite this analysis not honouring the tensorial nature of stress and thus being strictly incorrect. Furthermore, this regression suffers the considerable deficiency of being unable to determine principal stress orientations.

We have presented a method of Bayesian linear regression of Cartesian stresses against depth that is fully faithful to the tensorial nature of stress. This Bayesian regression method allows us to estimate the posterior distributions of mean Cartesian stresses using MCMC computations, and random sampling from these distributions allows the magnitudes and orientations of principal mean stress to be determined.

We have demonstrated the applicability of the method using 115 overcoring results performed at a range of depths at the SKB Forsmark site in Sweden. For the entire depth range of 0–600m we have shown profiles of both Cartesian stress components and principal stress magnitudes, and 95% credible intervals associated with these. These results show that it is reasonable to assume one principal stress is vertical, but there is significant uncertainty about the magnitudes and orientations of the horizontal principal stresses. We also have demonstrated how this uncertainty in the orientations and magnitudes of the sub-vertical principal stresses can be reduced by using appropriately chosen informative priors for the Bayesian regression analysis. Additionally, we have shown that the variation of principal stress magnitudes with depth is non-linear. For the planned repository depth of 450m we have presented distributions of both the magnitudes and orientations of the principal stresses, together with the associated credible intervals (for magnitudes) and credible regions (for orientations). These results demonstrate the superiority of this method over the customary linear regression of principal stress magnitudes, and its potential usefulness in rock engineering design.

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