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Guideline for uncertainty quantification of rock mechanical properties

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REPORT

ACT SHARP Project

GUIDELINE FOR UNCERTAINTY QUANTIFICATION OF ROCK MECHANICAL PROPERTIES

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Summary

This report introduces some practical methods that can be used to quantify the uncertainties involved in geomechanical properties estimation. Among the various aspects of uncertainties, this report mainly focuses on uncertainties involved in regression when deriving mechanical properties from empirical correlations and spatially-averaged properties. In addition, it also briefly introduces other types of uncertainties that can be involved in the entire process of geomechanical properties estimation with conceptual methods. In overall context of a risk assessment, the information described in this report can be used to prepare statistical inputs for the hazard assessment phase of CO_2 containment risk assessment. The main contents of this report can be summarized as follows:

- A depth profile of geomechanical inputs are mostly estimated indirectly from acoustic waves or petrophysical properties using semi-empirical models and calibrated by laboratory or field measurements. The indirect estimations are mainly based on empirical correlations from field/laboratory measurements and/or simplified physical understandings. Thus, the estimations can naturally involve uncertainty caused by the simplification and lack of physical understanding in the empirical correlation.
- When the depth-averaged geomechanical properties are estimated from a well-log or petrophysical information, the estimation can involve the following uncertainties:
    - Statistical parameter uncertainty, which can be associated with limited number of observations or field measurements;
    - Model uncertainty, which can be associated with imperfection of a physical model – for example model used to transform well-log information to rock mechanical inputs – and a probabilistic model, which is related to the form of the statistical parametric distribution and regression model;
    - Spatial variability, which is related to natural randomness of a parameter varying from one point in space to another; and
    - Observation (measurement) error, which is related to imprecisions associated with measurements such as limitations of equipment or operational conditions.
- A few quantification methods for uncertainties listed in the previous bullet point are introduced in this report. As a method to quantify statistical parameter uncertainties, a confidence and prediction interval is introduced. Then, the concept of Bayesian approach is introduced as a means for quantifying model uncertainties. For quantification of spatial variability, a simplified approach using random fields is presented.
- Finally, the uncertainty quantification procedure introduced in this report is demonstrated using a dataset from the North Sea.

This report clearly demonstrates that statistics can be a helpful tool to estimate reliable ranges of geomechanical input that cover an area of interest. Furthermore, it can be useful to determine likelihoods of the data's upper and lower limits in a systematic way

without relying entirely on engineering judgement. Note that this report only addresses basic approaches for uncertainty quantification with simplified assumptions. In future studies, more advanced uncertainty quantification methods (e.g., Bayesian approaches) should be actively adopted for uncertainty quantification of rock mechanical property estimation.

Contents

Review and reference page

1 Introduction

This document provides a brief introduction on how to quantify uncertainties involved in spatially-averaged inputs required for geomechanics modelling. This work has been carried out through ACT SHARP project (EC Project no. 691712), Deliverable D5.1: Internal guidelines for input uncertainties quantification.

1.1 Background and motivation

The subsurface is inherently heterogeneous because of spatially varying geological processes involving natural randomness. In addition, data processing and interpretation process can also result in errors or uncertainties in the estimated or interpreted rock-mechanical properties because of our lack of knowledge on the physical phenomena. Usually, a geomechanical model needs rock mechanical properties that may cover a large range of interest (e.g. from less than a few metres of a wellbore to a few km of reservoir). The estimation of the rock mechanical properties thus relies on upscaling of point source measurements (e.g., laboratory mechanical tests, leak-off tests from fields, etc.) by combining with indirect measurements (e.g., sonic logging, 2D or 3D geophysical survey) covering the area of interest. This upscaling process using indirect measurements needs a model that can transform the measured parameters to mechanical properties of interest (e.g., from acoustic wave velocity to static mechanical properties). The transformation model usually includes assumptions and simplifications, and the imperfect nature of the transformation models can result in uncertainties or errors in the estimation. Figure 1 shows a typical example of estimated profile of best-, low-, high-estimate of Young's modulus along the depths. The profiles in the figures were estimated by indirect measurement using the sonic log (left figure). Because of the heterogenous nature of the subsurface, the 1D profile of the sonic log shows significant fluctuation. When the model transforms the measured sonic velocity to the static Young's modulus, the estimation (i.e., the yellow solid line in the right figure) shows discrepancy with measured lab-data (i.e., a red dot) because of simplification and idealization involved in the transformation model. The fluctuated features of the inputs are typically averaged for each layer or represented as a trend line using 1D regression. Usually, geomechanical stability assessment is mostly governed by weak points that are related to high- or low-estimates rather than its average. However, it is quite rare to estimate the likelihoods of the data's upper and lower limits using a systematic statistical approach without engineering judgement. Consequently, the uncertainties in geomechanical proprieties resulting from lack of knowledge and subsurface randomness can result in inaccurate assessment of CO_2 storage integrity (e.g., caprock integrity, fault stability, etc.). It is thus important to have a better understanding of the possible types of uncertainties in the geomechanical properties estimation and associated quantification methods to estimate reliable ranges of geomechanical input for the area of interest and problem of concern.

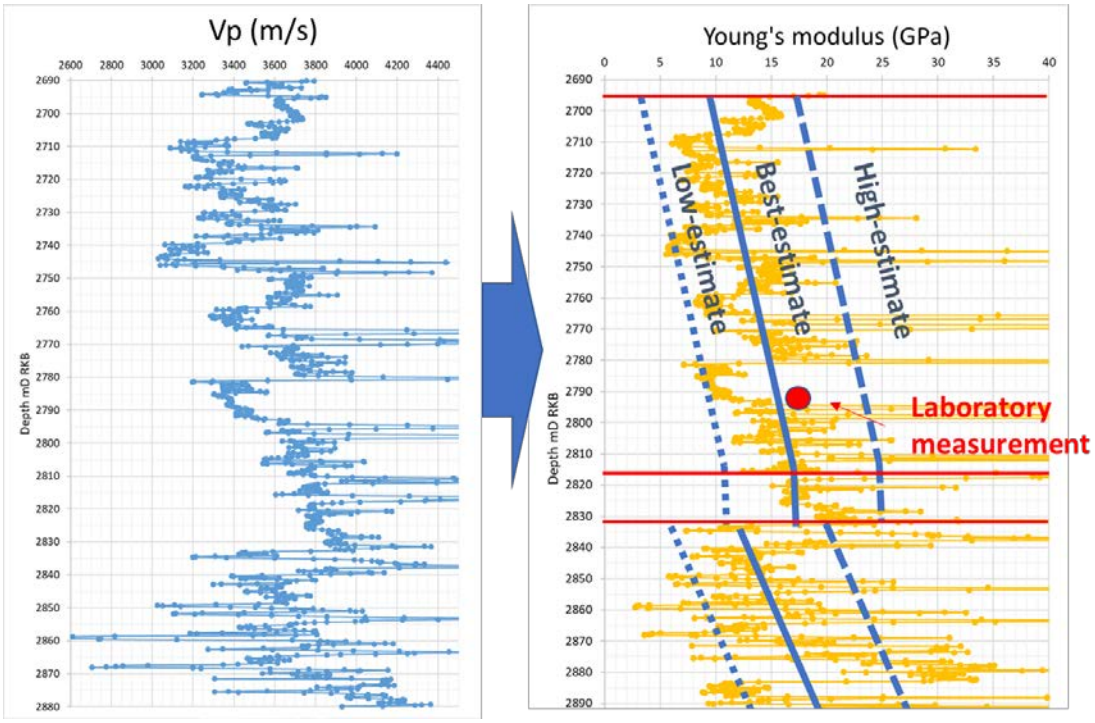

Figure 1 Example of typical 1D profile of Young's modulus estimated from sonic log.

1.2 Objective and scope of work

This report aims to introduce some practical methods that can be used to quantify the uncertainties involved in geomechanical properties estimation. Among the various aspects of uncertainties, this report mainly focuses on uncertainties involved in regression when deriving mechanical properties from empirical correlations and spatially-averaged properties. In addition, it also briefly introduces other types of uncertainties that can be involved in the entire process of geomechanical properties estimation with conceptual methods. In overall context of a CO_2 containment risk assessment, the information described in this report can be used to prepare the statistical inputs for a hazard assessment.

This document consists of following sections:

- Section 2 describes some examples of methodology for estimating the input required for geomechanics modelling.
- In Section 3, typical types of uncertainty that can be involved in estimating geomechanical properties are introduced.
- Section 4 describes methods on how to covert the inputs uncertainties that came from different sources defined in Section 3 to statistical parameters (e.g., mean, standard deviation, lower and upper bounds). This section mainly focuses on the uncertainties from the limited number of data (i.e. statistical uncertainty) and the natural variability.

- In Section 5, an example showing how to quantify spatial variability involved in depth-averaged parameters is demonstrated using a dataset from the North Sea.
- Summary and suggestions for further studies are addressed in Section 6.

2 Input properties for geomechanics modelling

This chapter briefly describes how to estimate a depth profile of geomechanical input properties, which are used for geomechanical assessment of reservoir and seal integrity, from indirect measurement (e.g., sonic logs). In-situ stress conditions, elastic properties and strength properties are considered crucial input. Access to data for estimating these parameters may vary considerably depending on the development stage of the project and numbers of wells available. This section focuses on the Norwegian North Sea practices and the correlations typically used for site development when one well has been drilled and well logs, rock mechanical data and formation stress tests are available. Note that this section only covers basic properties that can be used to demonstrate the uncertainty quantification methods in the following sections. A comprehensive review of the rock mechanical property estimation methods is beyond the scope of this report.

2.1 In-situ stress condition

In the following, we will outline few example methods that are widely used to derive depth profiles for the stress conditions based on combining information from well logs and one or more stress tests in the reservoir such as extended leak off tests (XLOT).

In-situ stress conditions are defined as three principal stress orientations and their magnitudes. Within the North Sea sedimentary basin, although some variations are observed, it is common to assume a normal faulting regime (Andrews et al., 2016). In a normal faulting regime, the maximum principal stress σ_1 is vertical ($\sigma_1 = \sigma_v$) and the intermediate principal stress σ_2 and minimum principal stress σ_3 are horizontal ($\sigma_2 = \sigma_H$ and $\sigma_3 = \sigma_h$). In order to assess the effective stress σ' conditions, the pore pressure (p) is used.

Vertical stress σ_V is determined from integration of density logs. The accuracy will depend on the coverage of density log for the site. Normally, the upper stratigraphy is not logged and one would need to assume a density for those layers. Vertical stress generally increases with depth with a gradient between 20–22 kPa/m. This is equal to an average density for sedimentary rocks on Norwegian Continental Shelf (NCS) of between 2.04–2.24 kg/m^3 (Andrews, 2016).

Minimum horizontal stress is often determined by extended leak off tests (XLOT) in combination with sonic log method (Andrews and de Lesquen, 2019). The XLOT test is the most accurate test method for measuring the minimum horizontal stress and has a

coverage of a few metres, while sonic log method gives variation along the well. The XLOT test measures the minimum horizontal stresses by measuring the pressure recorded at the instance the fractures in a wellbore close. A typical pressure record for XLOT is shown in Figure 2. When XLOT data are not available for a specific field, XLOT trends from nearby areas may be utilized. In other cases, when XLOT data are not available, then leak off pressure (LOP) from leak off tests (LOT) can be an indicator for the minimum horizontal stress. However, LOP-value has large uncertainties and normally varies between fracture closure pressure (FCP) and formation breakdown pressure (FBC).

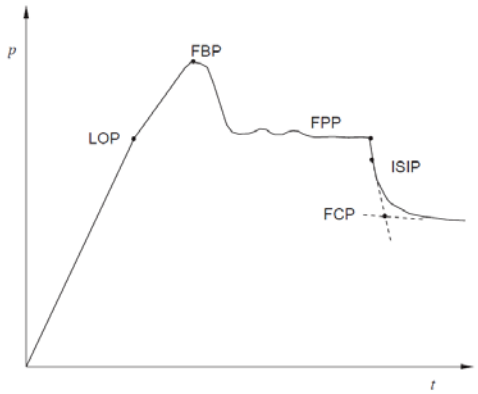

Figure 2 Illustration of pressure records for a XLOT test (from Raaen et al., 2006).

The horizontal stress profile can be calculated from the vertical stress σ_v, initial pore pressure p_o, the ratio between effective horizontal and vertical stress (K_0). When we assume that the horizontal stresses are primarily governed by elastic depositional history, the K_0 value and dynamic undrained Poisson's ratio (μ) can be calculated from equations 2.1 and 2.2, which again are derived based on the compressional and shear wave velocities (V_p and V_s) using elastic equation from Eq.2.3;

$$\sigma_h = K_o(\sigma_v - p_o) + p_o \tag{2.1}$$

$$K_0 = \frac{\mu}{1-\mu} \tag{2.2}$$

$$\mu = \frac{1}{2}\frac{\left(\frac{V_p}{V_s}\right)^2 - 2}{\left(\frac{V_p}{V_s}\right)^2 - 1} \tag{2.3}$$

The stress estimation methods described above may involve some uncertainties because of our lack of knowledge about the factors affecting the in-situ stresses. The estimate of the vertical stresses is relatively accurate because of the robust theoretical basis about the relationship between the overburden loading and the density. However, the pore pressure and the horizontal stress estimation from well-logs involves uncertainties

related to simplification behind its estimation model. Although the estimates of horizontal stresses are based on simplified physical models (e.g., elasticity and uniaxial strain conditions during compaction), the horizontal stresses can be governed by visco-plastic behaviour during complex geological histories and tectonic stresses. A limitation of the model is that sometimes S-wave logs are missing. Estimating S-wave velocity from other log information can result in another layer of uncertainties in the stress estimation.

2.2 Static rock mechanical properties

This section will outline a few example methods that are widely used to derive depth profiles of geomechanical properties by combining information from well logs and laboratory-measured properties.

Triaxial tests are the most common and standard method to measure geomechanical properties directly. A standard triaxial test typically uses small cores that are 1.0 – 1.5 inches (0.0254 – 0.0381 m) in diameter and twice the diameter in height. The test setup can control stresses/deformation in the vertical and horizontal directions and pore pressures to simulate various in-situ stresses and stress paths. The static elastic modulus is typically estimated from a tangential slope of a stress-strain curve at a 50% peak stress level. The shear strength can be measured by the peak stress during shear loading. Because of the relatively high cost of coring from a wellbore and triaxial tests, the number of tests is typically limited to 1 or 2 tests for a specific layer, and the tests are commonly used to calibrate the preliminary results estimated from indirect measurement(s).

Empirical correlations between rock mechanical properties and the acoustic or petrophysical properties are commonly used for preliminary estimation of rock mechanical properties. The coefficients of the empirical correlation are typically determined by a regression model using multiple observations from laboratories and fields. Wave velocity, resistivity, and petrophysical properties (e.g., porosity) are pair attributes widely used as inputs for empirical correlations. For example, undrained Young's modulus and uniaxial compressive strength (UCS) can be derived from a compressional sonic log by the empirical correlation from Horsrud (2001). The correlations are based on laboratory-measured rock-mechanical properties and V_p in km/s using the North Sea mudstones and shales. The correlations for the undrained Young's modulus in GPa and the UCS in MPa are expressed in equations 2.4 and 2.5, respectively.

$$E = 0.076 \cdot V_p^{3.23} \tag{2.4}$$

$$UCS = 0.77 \cdot V_p^{2.93} \tag{2.5}$$

Dynamic- to static-modulus conversion is also one of the widely used method to get a static elastic property profile from wave velocities. The equations for dynamic Young's

modulus (E_{dyn}) and dynamic Poisson's ratio (ν_{dyn}) using wave velocities (V_p and V_s) and a density (ρ) are:

$$E_{dyn} = \frac{\rho V_s{}^2 \left(3V_p{}^2 - 4V_s{}^2\right)}{\left(V_p{}^2 - V_s{}^2\right)} \tag{2.6}$$

$$\nu_{dyn} = \frac{\left(V_p{}^2 - 2V_s{}^2\right)}{2\left(V_p{}^2 - V_s{}^2\right)} \tag{2.7}$$

The dynamic modulus is typically several times higher than a static modulus. The reason for the observed significant discrepancy between dynamic and static properties is known to be from various reasons, including the effect of strain rate, drainage condition, heterogeneities, anisotropy, strain amplitude, etc. (Fjær, 2019). Because of its complexity related to factors affecting the elastic properties, it is not straightforward to include all factors into the model that can convert dynamic to elastic properties. Instead, it is common to use a ratio between dynamic- and static- stiffness. According to Grande and Cuisiat (2008), static undrained shear modulus of shale from the North Sea is 3-5 times lower than that from lab-measured dynamic stiffness. For a sandstone from the North Sea, the weak rock tends to have higher discrepancy between static and dynamic stiffness (e.g., an order of magnitude difference) than a stiff cemented rock (e.g., 20-30% discrepancy for well cemented Berea sandstone) (Fjær et al., 2008). The differences between dynamic- and static- stiffness decreases with higher confining stresses.

Similar to the limitation mentioned earlier about the in-situ stress profile estimation, the models used to estimate the rock mechanical properties partly or fully rely on empirical correlations. Hence, they naturally involve uncertainty stemming from simplifications and missing/incomplete physical understanding in the empirical correlation. In particular, the discrepancy between laboratory and field condition can result in uncertainties in the estimation. Most correlations between velocity and mechanical properties have been calibrated based on observation pairs from laboratories (e.g., laboratory-measured V_p vs. static properties), but are used to make predictions based on field observation *of velocity(V_p)* from a well log. The different conditions between the field and the laboratory (e.g., temperature, heterogeneity and anisotropy from microfractures, borehole quality, mud invasion) can result in estimation errors.

3 Types of uncertainty

Quantifying and propagating uncertainties in engineering problems requires recognizing and identifying sources and types of uncertainty. This section discusses these. Section 3.1 briefly introduces a more philosophically-oriented epistemic/aleatory classification of uncertainties. Understanding this distinction is important because, to some degree, it shapes one's strategies for dealing with uncertainties in practice. Section 3.2 then discusses a more application-oriented classification of uncertainties. The goal is to present a comprehensive overview of the key uncertainty types and not an exhaustive

discussion of all components involved in geomechanical assessment of reservoir and seal integrity. Section 3.3 provides more context by discussing predicting modulus of elasticity from sonic log data.

When discussing uncertainty quantification for a problem in a specific domain, a careful use of terminology is warranted to prevent confusions between the mathematical uncertainty quantification and statistical terminology on one hand and the domain-specific terminology on the other. For instance, the term "parameter" may be understood as soil or rock property (e.g., friction angle or UCS) in an engineering context, while in a statistical modelling context "parameter" usually refers to unknown, un-observable quantities that are estimated from data (e.g. mean, variance or regression coefficients are statistical parameters). Therefore, when considering uncertainty quantification, UCS would be referred to as observable data (or random variable), while *mean* UCS would be a (statistical) parameter. The coefficients of the regression models in Equations 2.4 and 2.5 are also parameters.

Finally, it is noted that in this section, the term geotechnical engineering refers to both soil and rock engineering as there is considerable overlap between the uncertainty quantification literature on the two.

3.1 Aleatory and epistemic uncertainties

Uncertainty is often characterised as either *epistemic* or *aleatory*, according to its source: epistemic uncertainty is attributed to imperfect knowledge while aleatory uncertainty arises from the inherent randomness or variability in systems (e.g., Ferson and Ginzburg, 1996; O'Hagan and Oakley, 2004; see also, e.g., Baecher and Christian (2005) for a discussion in the context of geotechnical engineering). The term epistemic is derived from the Greek word "episteme", which means knowledge, and aleatory is derived from the Latin "alea" – meaning rolling of dice. Also, epistemic and aleatory uncertainties are sometimes thought of as reducible and irreducible uncertainties, respectively. That is, by definition, epistemic uncertainty can be reduced by obtaining better or more information about the system while the natural randomness in the system cannot be reduced.

Among others, O'Hagan and Oakley (2004) discuss a more nuanced point of view where it is argued that what is referred to as irreducible randomness in a system would be eliminated (or at least reduced) if we were able to recognise and specify more conditions within our description of the system. Therefore, any uncertainty reduced in such a manner must really have been epistemic. As an example, consider the uniaxial compressive strength (UCS) of intact rock for which we have many laboratory tests on intact rock specimens from the same formation. We can construct a simple probabilistic model, say, a normal distribution with two parameters mean and variance. It is noted a normal distribution is used here as an example because it admits the possibility of negative values at the left hand tail of the distribution, which for properties like stress or young's modulus are generally non-physical. The randomness or "residual variance" estimated by such model is considered to be natural variability and thus irreducible.

However, it is possible to argue that by adopting for example a micro-mechanics framework and considering contributions of individual constituents of the material to its macro-scale properties, one could "explain" some of the above-mentioned randomness and obtain more accurate predictions of UCS for individual specimens. This is essentially the argument of *determinism* that *if we knew the exact position and velocity of every particle, we could predict the future exactly, and thus all uncertainty is epistemic in nature*. O'Hagan and Oakley (2004) further add that perhaps true randomness exists in some phenomena as suggested by quantum physics. However, this does not extend to the scales on which most models (including those used in engineering) operate. Therefore, although philosophically somewhat disputed, it is useful to maintain the conceptual aleatory/epistemic distinction in the context of engineering problems:

- it is important to quantify aleatory uncertainty for quantities whose measurements exhibit variation and no effort is made in gaining better understanding of the factors contributing to this uncertainty (or, it is impractical to do so at an engineering scale); and,

- identifying the epistemic portions of uncertainty is equally important, for instance to address the issue of parameter uncertainty due to limited data. Furthermore, quantifying epistemic uncertainty allows for better allocation of resources for uncertainty reduction.

Other than the aleatory/epistemic classification, there are also taxonomies of uncertainty that are more application-oriented and hence more suitable for engineering practice. The following section discusses such classifications in more detail.

3.2 An application-oriented classification of uncertainties

Engineering reliability, risk and decision problems are solved within the confines of a *model universe* (Der Kiureghian and Ditlevsen, 2009). The model universe contains a set of physical and probabilistic models, which are mathematical idealizations of reality employed to render a solution for the problem at hand. This is also comparable to the concept of the *small world* from foundations of statistics and decision theory which refers to the self-contained logical world of a model (Savage, 1972). The model universe may contain inherently uncertain quantities; e.g. there is variation in laboratory measurements of modulus of elasticity of intact rock. Another possibility is that a quantity might be measured with insufficient precision, or indirectly, i.e. estimated from other (proxy) physical properties; an example of this is finding modulus of elasticity E from in-situ P-wave data Vp. The sub-models in the model universe are also imperfect, giving rise to additional uncertainties. For instance, the empirical regression model used for transforming Vp data to modulus of elasticity is not perfect. Therefore, quantification and propagation of uncertainties should address these uncertainties. Furthermore, as mentioned earlier in the UCS example, the nature and character of uncertainties should be discussed within the confines of the model universe.

There is no unique taxonomy of uncertainties, but most of the existing ones include classifications such as parameter uncertainty, model inadequacy (or method

uncertainty), residual variability, parametric variability, observation (measurement) error and code or computational uncertainty (e.g. Kennedy and O'Hagan, 2001), all of which are relevant and understood to some degree in engineering. Sections 3.2.1-3.3.3 discuss parameter, model, measurement and computational uncertainty in more detail and with reference to data involved in risk assessment for CO_2 storage containment. Furthermore, context-dependent comments about aleatory or epistemic nature of each of these uncertainties are provided. To facilitate these discussions, first terminology and a rather simple notation are introduced.

We refer to basic random variables as those that are input to the engineering model(s) (e.g., geo-material strength and stiffness properties, in-situ stresses and geometrical data). They can be scalar or vector and are denoted as $\boldsymbol{Y}$. Parameters on the other hand are the unknown quantities (e.g. mean, standard deviation, regression coefficients) that are estimated from data, and denoted $\boldsymbol{\theta}$. There are other random variables that are not necessarily direct input to the engineering models but are used (e.g. as proxy measures) to predict basic random variables. An example of this is in-situ P-wave velocity well log data used to predict static rock mechanical properties. These are denoted $\boldsymbol{X}$.

When measured directly, basic random variables are characterised using probabilistic sub-models $f_{\boldsymbol{Y}}$ with (statistical) parameters $\boldsymbol{\theta}_f$, denoted $f_Y(\mathbf{Y}; \boldsymbol{\theta}_f)$. For example, f could be a normal distribution with parameters $\boldsymbol{\theta}_f$ mean and standard deviation and used for modelling the basic random variable UCS.

Due to high costs and difficulties involved with direct measurements, it is common to establish and use empirical relationships between proxy variables $\boldsymbol{X}$ and the random variables of interest $\boldsymbol{Y}$. That is, the variable of interest $\boldsymbol{Y}$ is obtained by *transforming* the easier-to-measure variable(s) $\boldsymbol{X}$, usually via empirical relationships that are commonly referred to as empirical transformations or correlations in the geotechnical literature. This can be thought of as *indirect measurement* of $\boldsymbol{Y}$. Transformation models are denoted $T_{\boldsymbol{Y}}$ with parameters $\boldsymbol{\theta}_T$, hence $T_{\boldsymbol{Y}}(\boldsymbol{Y}, \boldsymbol{X}; \boldsymbol{\theta}_T)$. Empirical relationships addressed in Section 2 (e.g., relationship between wave velocities and the in-situ stresses/static rock mechanical properties) are examples of commonly used transformation in reservoir geomechanics.

Finally, the (directly measured or transformed) basic random variables are used as input to engineering model $M(\mathbf{Y}; \boldsymbol{\theta}_M)$; predicting caprock integrity during CO_2 injection, a 3D field-scale geomechanical model or an analytical approach using Mohr-Coulomb failure criterion are examples of the engineering model $M(\mathbf{Y}; \boldsymbol{\theta}_M)$. This aspect of models is not the focus of this document and is merely mentioned for completeness.

3.2.1 Parameter uncertainty

There is inherent uncertainty (aleatory randomness) associated with the directly measured basic random variables $\boldsymbol{Y}$. This randomness is captured by the dispersion parameter (e.g. standard deviation, variance, coefficient of variation) of the distribution $f_Y(\boldsymbol{Y}; \boldsymbol{\theta}_f)$. For a given statistical model $f_Y(\boldsymbol{Y}; \boldsymbol{\theta}_f)$, this uncertainty does not reduce with

obtaining more data, and only better (more precise) estimates of the dispersion parameter could be obtained.

The (statistical) parameters $\boldsymbol{\theta}_f$ (including the dispersion parameter) are *estimated* from observed data and are thus uncertain. This uncertainty is usually referred to as (statistical) parameter uncertainty and is epistemic in nature: it reduces as we obtain more data. For instance, the standard error[1] of the sampling distribution of the mean is proportional to $1/\sqrt{n}$ where n is the sample size (see also section 4.1). That is, as more data become available, the mean is estimated with a higher precision. This possibility of reduction in uncertainty implies epistemic uncertainty.

It is emphasized again that such discussions of aleatory/epistemic uncertainty are only justified within the confines of the specified model. For instance, a statistical model that accounts for spatial variability of UCS may result in smaller residual variance, and hence implies smaller unmodelled randomness. Such a model would also have different parameters and thus different epistemic uncertainty compared to the simple parametric distribution $f_{\boldsymbol{Y}}(\boldsymbol{Y}; \boldsymbol{\theta}_f)$.

Similar arguments could be made for transformed variables $\boldsymbol{Y}$. The transformation $T_{\boldsymbol{Y}}(\boldsymbol{Y}, \boldsymbol{X}; \boldsymbol{\theta}_T)$ is usually formulated as a regression model with $\boldsymbol{Y}$ as the response (also known as outcome or dependent) variable and $\boldsymbol{X}$ as the predictors (also known as independent or regressor) variables. The vector $\boldsymbol{\theta}_T$ includes the regression coefficients and the residual variance of $\boldsymbol{Y}$ and is estimated with less uncertainty as larger data become available.

3.2.2 Model uncertainty

Models are abstract mathematical idealizations of real-world processes. They are based on assumptions and simplifications, and thus no model can really be said to be perfect or correct. This is perhaps best stated by Box and Draper (1987) in their famous statement "*all models are wrong, but some are useful*". This is particularly true from a practical engineering point of view where many models give sufficiently accurate predictions that allow analysis and design. Model uncertainty is undoubtedly epistemic: it is always possible to improve the model and hence reduce the uncertainty by, for example, including more descriptive parameters, adopting more realistic assumptions, or employing a different functional form all together.

Model uncertainty – also called model error, model bias, method bias, method uncertainty, or model omissions in different fields of science and engineering – is generally defined as the difference between the true mean value of the real-world process and the model output at the true values of the inputs (e.g. Kennedy and O'Hagan, 2001; Der Kiureghian and Ditlevsen, 2009). This difference is often characterised using a random variable, the statistical properties (usually mean and standard deviation) of

[1] The term "standard error" is used in the frequentist statistics literature and refers to the standard deviation of the sampling distribution of parameters; the term "standard deviation" is used when discussing variability of observed data. In the Bayesian context (see section 4.2.1) the term standard deviation is used for both.

which are estimated from data gathered on the real-world process, and further used as a correction or modifying factor when using the model for making predictions, or for design in an engineering context.

The terms “model” and “model uncertainty” could refer to different things as discussed in the following.

Physical models
A model $M(\boldsymbol{Y}; \boldsymbol{\theta}_M)$ could describe a physical or mechanical phenomena. For example, using the theory of elasticity, the Kirsch solution allows determination of the stresses and displacements around a circular excavation. A basic soil engineering example is calculating the total stress as the sum of the effective stress and pore water pressure. Models could also be considerably more complex mathematical descriptions of much larger engineering problems, e.g. a finite element model for caprock integrity assessment. In geomechanical engineering practice, reliable quantification of the modelling error arising in such complex models could be very challenging or even impossible due to our inability in obtaining sufficiently large number of measurements of the model output to be compared with model predictions. It is noted that model calibration procedures could themselves involve other types of uncertainty, e.g., measurement error, transformation uncertainty and parameter uncertainty; these are usually neglected when quantifying the uncertainty in geotechnical models.

Probabilistic models
Model could also refer to statistical/probabilistic models, and thus model error (uncertainty) could result from selection of the form of the parametric probability density function (PDF) $f_{\boldsymbol{Y}}(\boldsymbol{Y}; \boldsymbol{\theta}_f)$, or the functional form of the transformation equation $T_{\boldsymbol{Y}}(\boldsymbol{Y}, \boldsymbol{X}; \boldsymbol{\theta}_T)$, or the choice of which predictors $\boldsymbol{X}$ to include in the model. For example, one could choose among many distributions – say normal, lognormal, gamma, weibull, and student *t*-distribution – for statistical modelling of modulus of elasticity of intact rock. In case of transformed variables, one example from rock engineering is the numerous available choices of empirical equations relating modulus of elasticity *E* of intact rock and its UCS where some of them are linear and some non-linear; some include only UCS and *E* while others include various combinations of parameters such as unit weight of the rock, point load test, P-wave velocity, Schmidt hammer rebound values and void ratio (e.g., Feng and Jimenez, 2014). Another example is the diverse collection of empirical relationships for predicting undrained shear strength of soils from CPT and other soil engineering data (e.g., Paniagua et al., 2019).

In a practical setting, when dealing with the above-described statistical model uncertainty, it is important to check the goodness-of-fit of individual models to the data. Note that this should ideally go beyond statistical tests that are based on null hypothesis testing (e.g. Anderson-Darling or Kolmogrov-Smirnov) designed to reject/fail-to-reject a hypothesized distribution type. In doing so, we suggest following Gelman et al. (2013) who recommended judging model flaws by their practical implications for the inference or prediction of interest. Another step is to consider multiple models with reasonable fits and compare their predictive accuracy. Then, either model selection or statistical model

averaging should be considered. Detailed discussions of model checking, comparison and selection are beyond the scope of this document and may be found in e.g. the seminal text by Gelman et al. (2013) or the overview provided by Bozorgzadeh and Bathurst (2019) with geotechnical applications in mind. It is nevertheless noted that, unfortunately, rigorous statistical model checking, model comparison, model selection and model averaging are not routinely performed for geotechnical applications. When dealing with statistical model uncertainty, it is common to not explore the model uncertainty associated with f_Y and select a distribution due to convenience or convention.

Transformation uncertainty
Empirical transformations are essentially regression models, and thus all the above-mentioned probabilistic model uncertainties apply to them. In geotechnical literature however, *the residual variation of the regression is referred to as transformation (or correlation) uncertainty*. For example, when predicting *E* from *Vp*, Equation 2.4 gives the mean (i.e. best) prediction of *E*, and the residual standard deviation of the regression is considered to be the uncertainty in *E* arising from using this equation. Furthermore, it is noteworthy that the uncertainties in the parameters of the model (i.e. the regression coefficients) is typically ignored in current practice. Quantifying this uncertainty is crucial for updating generic empirical correlations with site-specific data using Bayesian techniques. Essentially, estimations (with uncertainty) of parameters of the empirical equation using generic data are used for specifying "prior" distributions in Bayesian analysis of site-specific data. For more details see Section 4.2.

3.2.3 Other types of uncertainty

Measurement error
Measurement error refers to imprecisions associated with measuring variables of interest due to reasons such as limitations of equipment or operational conditions. Another related error is the between-equipment variation; that it, any systematic differences (on average) between measurements of the same quantity obtained by different equipment.

Computational uncertainty
There are also numerical approximation and computational errors. For instance, using finite difference for solving a differential equation, or errors arising from convergence tolerances in a finite element analysis. Monte Carlo error is another example of common computational errors.

In the context of geotechnical engineering in general, and CO_2 storage risk assessment in particular, the above measurement and computational uncertainties are expected to be negligible compared to the (aleatory) residual uncertainty in variables, (epistemic) statistical parameter uncertainty, and model uncertainty (including transformation uncertainty).

3.3 An illustrative example

This section provides more context to the uncertainties discussed in section 3.2 by exploring the key steps involved in estimating static Young's modulus E from P-wave velocity V_p log data. Figure 3 gives a visual summary of the procedures and uncertainties; both direct and indirect measurements are considered.

3.3.1 Indirect measurement

Indirect measurement refers to the situation where semi-continuous V_p well log data are available. The 1D profile of V_p is typically obtained from a well log and exhibits variation with depth. In the schematic of Figure 3, this spatial variability is carried over to the next step of analysis and dealt with in a future step.

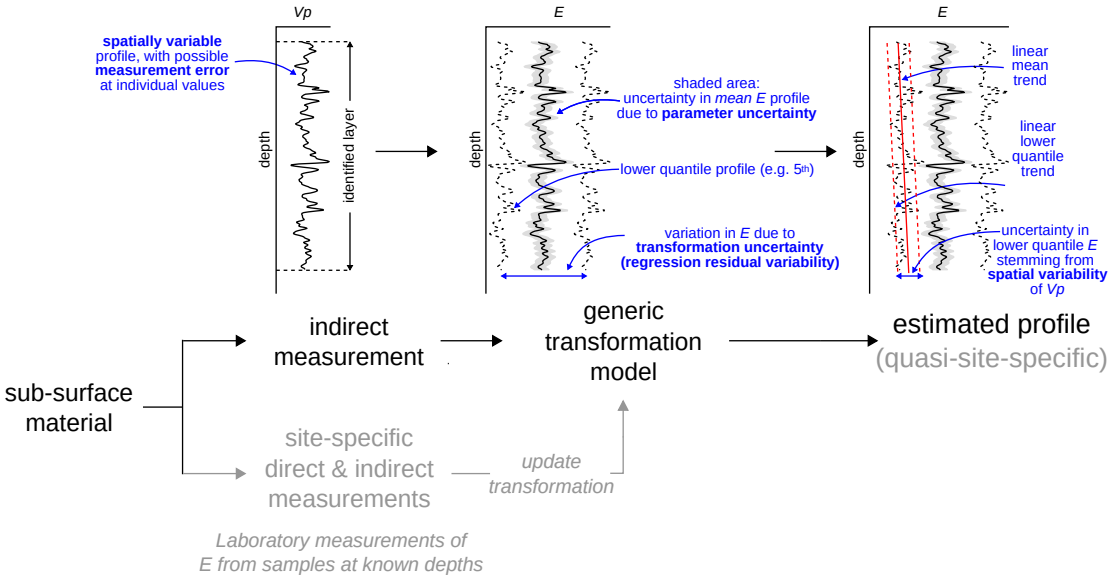

Figure 3 Schematic overview of uncertainties involved in obtaining E from Vp.

The V_p data are input to generic empirical transformations for obtaining E (e.g. Equation 2.4). As mentioned earlier in section 3.2.2, unfortunately uncertainties arising from multiple regression models being available (i.e. multiple functional forms of the transformation, what predictors (independent variables) to include in the regression model, and what probability distribution to use for the residual error) are overlooked in engineering practice. In such situations, at least a brief engineering justification of applicability of the selected empirical equation should be presented. An alternative approach, especially where such the justifications are not compelling, is to apply other empirical equation(s) as sensitivity studies, with the aim of understanding the associated variation.

With a single transformation equation selected, two components of uncertainty should be considered. First is the parameter uncertainty associated with the coefficients of the generic empirical transformation equation. When incorporated correctly, this uncertainty translates to uncertainty in *mean* modulus of elasticity and is depicted as the shaded grey area in Figure 3. Moreover, quantifying this uncertainty is crucial for situations where site-specific measurements of E are available and it is intended to combine them with a generic correlation. Second, the residual variability associated with the empirical transformation equation should be considered. As mentioned in section 3.2.2, this is generally referred to as transformation uncertainty in the geotechnical literature and quantifies the variability in E when predicted from a proxy predictor like V_p and can be used to obtain the quantiles of the distribution of E at each depth.

As Figure 3 shows, the uncertain transformed E can be summarized with five profiles: mean, lower and upper bounds of the confidence interval for the mean (shaded grey area) and lower and upper quantiles of the probability distribution of E (dashed profiles). All such profiles exhibit variation with depth due to spatial variability of the regression input V_p. As will be discussed in section 4.3, each profile can be modelled as the sum of a deterministic trend component, a randomly fluctuating term and measurement error. As an example, Figure 3 shows a best fit (mean) linear trend and a lower quantile linear trend to the spatially variable lower quantile E. Note that the spatially variable lower quantile profile is influenced by the transformation uncertainty, and the lower linear quantile further includes the effect of spatial variation with depth. The variance required for calculating the former is the residual variance of the transformation equation and the variance required for obtaining the latter is usually estimated from a simplified procedure from random field theory as discussed in section 4.3.1.

It is equally valid to perform the spatial analysis on the input V_p in the first step, i.e. obtain best fit and lower bound linear trends, and transform those into E. The illustrated procedure in Figure 3, however, gives a more comprehensive visual summary because the actual spatial variability of each of the five profiles can be shown alongside the simplified spatial model.

3.3.2 Direct and indirect measurement

Direct measurement of E refers to laboratory testing of rock specimens that are obtained from specific depths of a borehole at the site of the current project for which the corresponding in-situ V_p is also known. Therefore, the data consist of site-specific pairs of E and V_p. These data can be used in a Bayesian analysis (see section 4.2) to *update* the generic transformation to obtain quasi-site-specific profiles of E. As more site-specific data become available, the transformation becomes more site-specific and less generic.

4 Methods for quantifying uncertainty involved in spatially-averaged inputs

The uncertainties stemming from sources discussed in section 3 should be quantified using probabilistic models and statistical data analysis techniques. To this end, this section briefly discusses statistical concepts and methods that are required for analysing a profile of geomechanical model inputs listed in section 2. It should be noted that, for any of the discussed cases, there is a multitude of approaches and methodologies to be adopted and not all of them are discussed here.

Section 4.1 introduces confidence intervals for the mean of a scalar random variable. Section 4.2 points out a number of frequently arising situations that call for more nuanced statistical approaches. Finally, section 4.3 discusses 1-dimensional spatially variable data.

4.1 Confidence in estimated values

It was discussed in section 3 that when statistical parameters (e.g., mean) are estimated from noisy and variable data (e.g., lab measurements of UCS), there will be uncertainty associated with them. In the classical or frequentist statistics framework this uncertainty is quantified using confidence intervals[2]. Confidence intervals have the general form

$$\text{point estimate} \pm \text{critical statistics value} \times \text{standard error} \tag{4.1}$$

The critical statistics and standard error are related to the sampling distribution of the parameter that is being considered, e.g., a student *t*-distribution for the mean and a Chi-squared distribution for the variance of a normally distributed random variable. The critical statistics value also depends on the selected target level of confidence.

A 100(1-α) % confidence interval for the mean of random variable *Y* is

$$\bar{y} \pm t_{\left(n-1,\frac{\alpha}{2}\right)} \times \frac{s}{\sqrt{n}} \tag{4.2}$$

Where $\bar{y}$ is the estimated mean, $t_{(n-1,\alpha/2)}$ is the 100(1-α)-*th* quantile of a student *t*-distribution with *n*-1 degrees of freedom, *s* is the sample standard deviation and *n* the sample size; $s/\sqrt{n}$ is the standard error, i.e. the standard deviation of the sampling distribution of the mean. For example, if n = 10 UCS measurements with mean $\bar{y} =$

[2] Strictly speaking, this is incorrect. Confidence intervals quantify confidence in the procedure and not the parameter; they should be interpreted with respect to a hypothetical long-run sequence of repeated similar experiments. For instance, a 95% confidence interval does not imply that there is 95% probability that the parameter lies between the lower and upper bounds of the interval. Rather, it means that if we would have repeated the experiment many times and constructed a confidence interval from the data obtained in each experiment, then 95% of these confidence intervals would contain the true value of the parameter. However, it is common in practice to adopt the first (incorrect) interpretation for confidence intervals. This is sometimes justifiable by assuming that such confidence intervals are more-or-less the same as Bayesian credible intervals obtained with non-informative priors.

10.0 MPa and standard deviation s = 2.0 MPa, then the 95% confidence interval for the mean is calculated as $10.0 \pm 2.26 \times \frac{2.0}{\sqrt{10}}$, thus (8.57, 11.43). It is clear from the above equation that obtaining more data (i.e. larger n) results in narrower confidence intervals, hence reduced uncertainty.

A 100(1-α) % prediction interval (i.e. a likely range for a future observation) for a normally distributed random variable Y is

$$\bar{y} \pm t_{\left(n-1,\frac{\alpha}{2}\right)} \times \mathrm{s} \sqrt{1+\frac{1}{n}} \tag{4.3}$$

In the previous UCS tests example, assuming UCS is normally distributed, a 95% prediction interval for UCS is (5.69, 14.31) which is wider than the confidence interval for the mean (8.57, 11.43). The confidence interval includes uncertainties in determining the mean. The prediction interval covers data scatter or data variability around the mean in addition to uncertainties in determining mean. Thus, the prediction interval tends to be wider than a confidence interval.

Analytical formulations of confidence and prediction intervals do not exist for all parameters and models, e.g. for non-linear regression models. One powerful alternative for such situations is bootstrapping which involves re-sampling with replacement from the original data to estimate the properties of an estimator. Exploring the bootstrap method is beyond the scope of this report. More information may be found in e.g., Efron (1992) and Efron and Tibshirani (1994).

It is also possible to adopt a Bayesian framework instead of the classical (frequentist) statistics. Suitability of Bayesian methods for rock and soil engineering applications has been long recognized (see for example review papers Baecher (2017), Juang and Zhang (2017), and Zhang et al. (2017)), with a considerable increase in their usage in the past decade or so. The following section discusses some situations where Bayesian methods are particularly useful.

4.2 Combining data and other sources of information

There are many instances in soil and rock engineering projects where site-specific data are available. These data are usually limited in quantity and do not allow for fully site-specific parameter estimations. Nevertheless, it is desirable to include these data in the statistical analyses, e.g. in conjunction with generic empirical correlations. Another example is information about in-situ stress data. Information could be available at different levels, e.g. qualitative descriptions by geologists, historical data, data from more recent adjacent projects, and expert engineering judgement. The Bayesian approach to statistics provides a framework for tackling such challenges.

4.2.1 A brief introduction to Bayesian statistics

Bayesian statistics is not different from the classical (frequentist) statistical methods in the sense that the purpose of both is to make statistical inference. However, there is a fundamental theoretical difference between the two approaches. The frequentist methods treat observations (data) as random variables, and the unobservable quantities that one wishes to learn about (i.e. statistical parameters such as mean and standard deviation) as constant unknowns that are estimated from the data and accompanied by confidence intervals as a measure of reliability of these estimates. On the other hand, in Bayesian statistics probability models are applied to both the observations and the statistical parameters (Gelman et al., 2013). In other words, not only are the data treated as random variables but also the parameters of the statistical model are treated as such.

Assume the intention is to learn about a set of (unobservable) statistical parameters θ (e.g. the mean and variance of a normal distribution) in terms of a probability model by obtaining some data y. A Bayesian model is constructed by defining a full joint probability model for all observable (y) and unobservable quantities (θ)

$$f(\theta, y) = f(\theta) \cdot f(y|\theta) \tag{4.4}$$

where $f(\theta)$ is known as the prior distribution and summarises – in the form of a probability density function – all of the available information about the parameter θ before observing the data y. $f(y|\theta)$ is known as the likelihood function, and is the probability distribution of the data assuming they arise from the model with parameters θ. Obtaining new data y provides further information about the parameter θ. Consequently, the prior distribution $f(\theta)$ must be updated to account for the newly available data. To do so, the right-hand side of equation 4.4 could be rewritten to include the new known values of y – that is

$$f(\theta, y) = f(y) \cdot f(\theta|y) \tag{4.5}$$

Combining equations 4.4 and 4.5 and rearranging gives the Bayes' theorem

$$f(\theta|y) = \frac{f(\theta) \cdot f(y|\theta)}{f(y)} \tag{4.6}$$

The term $f(\theta|y)$ is known as the posterior distribution and reads as 'the probability distribution of θ given y'. $f(\theta|y)$ reflects the updated state of knowledge about θ after observing the data y. The f(y) term is a constant, as it only depends on the known values of data and ensures that the posterior distribution integrates to unity as required by the axioms of probability. One of the features of the Bayesian approach is that it allows common-sense interpretations of statistical conclusions. For instance, a Bayesian credible region or credible interval can be directly interpreted as containing an unknown parameter with a specified probability, in contrast to frequentist confidence intervals that must be strictly interpreted in relation to a sequence of similar inferences that might be made in repeated practice, as discussed in section 4.1.

Prior distributions

Another distinctive feature of the Bayesian approach is the requirement to specify the prior distribution f(θ). This allows other type of relevant information, e.g., historical data, engineering judgement, and regional information to be introduced into the analysis for a specific project/site. For example, the posterior distribution from one analysis can be used, directly or modified by an expert, as a prior distribution for a subsequent analysis. This feature of the Bayesian framework can be used in soil and rock engineering to augment project-specific data logically with related available information from elsewhere.

Prior distributions that are based on sources of information other than current data are known as informative prior distributions, and through application of equation 4.6 they strongly influence the posterior f(θ|y). On the other hand, vague (also known as non-informative) priors are those that convey little knowledge, have minimal influence on the posterior and allow the data to dominate the posterior distributions. Thus, vague priors result in inferences and predictions similar to those obtained from frequentist (classical) models, in which there is no possibility of using prior information. Loosely speaking, vague priors can be defined using flat probability distributions (i.e. no distinct peak to the probability density function) – for example, a uniform distribution or a normal distribution with a very large variance (relative to the range of the data) – but they must be selected considering the physical or mathematical limitations of the parameters of the model. For instance, compressive strength of rock is physically restricted to be positive, and variance is positive by definition.

Specifying informative or weakly informative prior distributions is neither an automatic nor a straightforward task (Lunn et al., 2012). If expert judgment is to be used, a series of techniques generally known as "expert elicitation" should be followed. In simple terms, expert elicitation guidelines provide a framework for expressing expert knowledge in a probabilistic format while guarding against known cognitive biases and heuristics (e.g., O'Hagan et al., 2006).

Another suggestion for specifying prior distributions in the geotechnical literature is using uniform prior distributions over typical ranges of the parameter of interest reported in the literature (e.g., Cao et al., 2016). This approach usually results in priors that are very wide relative to the limited site-specific data and thus not really informative.

However, if data from multiple sources (other than project-specific data) are considered, then hierarchical Bayesian models could be used for formulating informative prior distributions. Although hierarchical modelling has a long history in the Bayesian statistics literature, they have only recently been considered seriously for geotechnical applications. Using strength of intact rock as an example, Bozorgzadeh et al. (2019) discuss how informative priors can be constructed from relevant historical data. Ching and Phoon (2019) and Ching et al. (2022) are recent examples of application of hierarchical models for predicting soil engineering parameters from empirical relationships based on Cone Penetrate Test (CPT) data. Bozorgzadeh and Bathurst

(2020) discuss similar procedures for updating site-specific model uncertainty using mechanically stabilized earth walls as an example.

No matter what source of information, there is always subjectivity involved in specifying informative priors and thus transparency is key in communicating them. It is important to document any selected and left-out data, the reasoning and assumptions, and elicitation procedures.

More details on mathematical issues, and discussions on practical considerations for selecting prior distributions, may be found in key texts, e.g. Lunn et al. (2012) and Gelman et al. (2013).

Bayesian computation
Analytically tractable posterior distribution calculations (i.e. the right-hand side of Equation 4.6 simplifies to a known parametric distribution) only exist for a limited number of simple Bayesian models, most of which involve cases where the prior distributions for the parameters of the likelihood give posterior distributions of the same family as the prior distributions. Such a prior is said to be conjugate for the likelihood function. For example, the normal and gamma distributions are conjugate priors for the mean and precision (reciprocal of variance) of the normal likelihood, respectively.

The concept of conjugacy is mostly of theoretical and historical importance and not particularly relevant in modern practical Bayesian data analysis. Modern Bayesian model fitting is dominantly performed using a class of sampling algorithms known as Markov chain Monte Carlo (MCMC). Probabilistic programming languages and software such as Stan (Stan Development Team, 2022) are widely used for this purpose.

4.3 1-D trend data

Spatial variability is not another type of uncertainty like parameter and model uncertainties, but rather a challenge that calls for a special class of statistical models, and thus there is merit in discussing it in more detail. Properties of geo-material vary from one point in space to another. This is usually referred to as spatial variability. Furthermore, these properties exhibit strong spatial correlations both vertically and horizontally. In other words, and informally, the points closer to each other show more similarity in properties. Spatial variability of geo-material is usually modelled using methods such as random fields, time series data analysis techniques, or kriging. These methods are relatively involved and difficult to employ in a practical setting. The following discusses a simplified approach from random fields for dealing with 1-D vertical spatial variability.

Consider a CPT profile or sonic log *Vp* measurements that show variation with depth (e.g. see Figure 3). This spatial variability, $\varepsilon(z)$, can be modelled as the sum of a deterministic trend component, $t(z)$, a randomly fluctuating term $w(z)$ and measurement error $e(z)$ (Baecher, 1985; Nadim, 1988; Phoon and Kulhawy, 1999):

$$\varepsilon(z) = t(z) + w(z) + e(z) \tag{4.7}$$

The mean u and standard deviation σ for the property can be determined as follows:

$$u_\varepsilon = t(z) \tag{4.8}$$

$$\sigma_\varepsilon^2 = \sigma_w^2 + \sigma_e^2 \tag{4.9}$$

Therefore, the coefficient of variation (COV) of $\varepsilon(z)$, defined as $\sigma_\varepsilon / u_\varepsilon$, is given by

$$COV_\varepsilon^2 = COV_w^2 + COV_e^2 \tag{4.10}$$

The residuals of the trend $w(z)$ tend to exhibit remaining spatial correlation. Spatial averaging is a concept with which spatial variability is averaged to approximate a random variable that represents a spatially varying parameter (Vanmarcke, 1977). In random field theory, the spatial variability of a parameter can be described statistically by the mean, variance, and the scale of fluctuation, δ (Vanmarcke, 1977). The scale of fluctuation defines the distance over which there is a significant correlation of property values. While the mean and variance (or standard deviation) are easily obtained using equations from statistics, the scale of fluctuation has specific data requirements and, generally, its evaluation requires more complex analyses.

The main requirement for evaluating the scale of fluctuation is the stationarity of data. Data are stationary if they satisfy the following conditions: (a) the mean is constant with distance (that is, no trend exists in the data); (b) the variance is constant with distance; and (c) there are no irregular fluctuations. Vanmarcke (1983) suggested that the scale of fluctuation be defined as twice the area under the autocorrelation function of the stationary random variable (see Figure 4):

$$\text{Scale of fluctuation } \delta = 2\int_0^\infty \rho(\tau)d\tau \tag{4.11}$$

where ρ is the autocorrelation function of the random process.

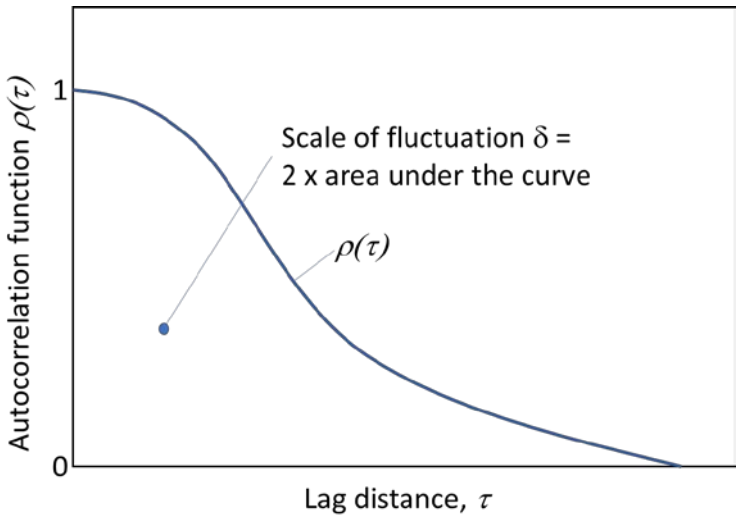

Figure 4 *Derivation of scale of fluctuation from the autocorrelation function* (Vanmarcke, 1983).

A variance reduction factor Γ is derived in terms of a scale of fluctuation δ and an averaging distance L. The scale of fluctuation, sometimes called correlation length within the framework of the random field, defines the distances over which there is a significant correlation of the geotechnical parameter in question. Small and large scales of fluctuation define rough and smooth random fields, respectively. In the limits, a scale of fluctuation of zero indicates no spatial correlation (infinitely rough field, white noise) while a scale of fluctuation of infinity indicates a completely uniform field. The averaging distance is defined as the interval over which the parameter of interest is averaged.

The following approximate variance reduction function was proposed by (Vanmarcke, 1983) for practical applications:

$$\Gamma^2(L) = \begin{cases} 1 & for\ L = \delta_v \\ \dfrac{\delta_v}{L} & for\ L > \delta_v \end{cases} \tag{4.12}$$

where δ_v is the scale of fluctuation in the vertical direction.

Fenton and Griffiths (2008) suggested the following approximation for Γ, which is more accurate for small values of L:

$$\Gamma^2(L) \approx \frac{\delta}{\delta + \mathrm{L}} \tag{4.13}$$

There are various statistical techniques available in the geotechnical literature for the estimation of scale of fluctuation. Several studies have reported values of scale of

fluctuation for soil properties, using either geostatistics (DeGroot and Baecher, 1993; Keaveny et al., 1990; Lacasse and Nadim, 1996), or random field modelling (Dasaka and Zhang, 2012; Fenton, 1999). For practical applications, Vanmarcke (1997) proposed an approximate relationship between the scale of fluctuation, δ_v, and average distance, $\bar{d}$, between intersections of the fluctuating property and its trend function, as shown in Figure 5. This simplified random field approach can be adopted to estimate the spatial correlation structure in the vertical direction in e.g. in *Vp* and *Vs* profiles.

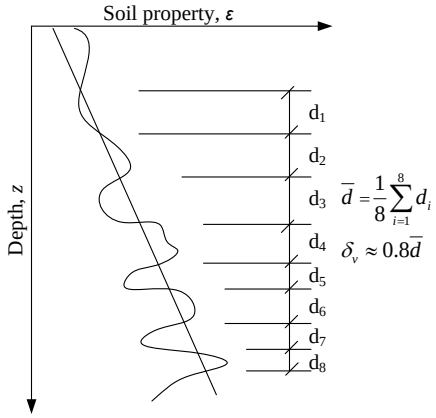

Figure 5 Estimation of vertical scale of fluctuation (after Vanmarcke, 1977).

The *Vp* logs can sometimes be divided into layers. To maintain the required stationarity assumption when using random fields, a trend is generally removed from the data for each and the *detrended data* (i.e. fluctuating component) are considered to be a zero mean stationary process (Liu et al., 2015). The variance of the spatial average, $\sigma^2_{Vp,a}$, and the spatial averaged COV of *Vp* are then given by:

$$\sigma^2_{V_{p,a}} = \Gamma^2(L)\sigma^2_w + \sigma^2_e \tag{4.14}$$

$$COV^2_{V_{p,a}} = \Gamma^2(L)COV^2_w + COV^2_e \tag{4.15}$$

A critical question when dealing with spatial data and models is if engineering behaviour depends on the properties of an isolated weak zone or the average property value within the ground volume being considered. A widely used example of this from soil engineering is the axial capacity of piles (e.g. Bond and Harris, 2008; Orr, 2000). The shaft friction resistance of a pile is influenced by a large volume of ground along the length of the pile, and thus governed by average soil strength. On the other hand, the end bearing influences an isolated zone below and in the vicinity of the pile tip, and thus the possibility of that locality being weak should be considered. The distinction further dictates if the quantity of interest should be chosen as the basic random variable or as its average. Although not common practice, it is important to provided similar reasoning and arguments when dealing with spatially variable data in rock engineering problems.

In other words, it is particularly important to establish if the above-mentioned variance reduction due to spatial averaging is relevant for the problem at hand (Cami et al., 2020).

4.4 3-D spatial data

Finally, a challenging and less-studied problem is that of 3D spatially variable data in soil and rock engineering where the spatial data are horizontally sparse (large distance between CPTs or boreholes). A discussion of this topic is beyond the scope of this document. See e.g. Ching et al. (2021, 2020) as examples of recent developments in analysing CPT data.

5 Field application

This chapter briefly demonstrates how to quantify spatial variability involved in depth-averaged parameters using the statistical methods described in Section 4 and data from EOS well 31/5-7 in the North Sea.

5.1 Data examples from the EOS well 31/5-7 in the North Sea

5.1.1 In-situ stress conditions

Example of P-wave velocity log and the stress data from EOS Well 31/5-7 and the stress data from EOS Well 31/5-7 are shown in Figure 6. The example shows minimum horizontal stress estimated from XLOT fracture closure stress, including two interpretations with stress gradients of 1.43 sg (specific gravity) and 1.55 sg. The XLOT data in the Drake formations are considered to be of high quality. A regional trendline from XLOT data and LOP data in Horda platform area is also included in the Figure 6. The in-situ stress conditions are summarized in Table 1 based on data from Thompson et al. (2022) and a published Eos well 31/5-7 data by Equinor (Meneguolo et al., 2021). The range of values, mean value and uncertainties are indicated in Table 1. It is noted that the variation described in Table 1 is from the interpretation by the Thompson et al., (2022), not from the methods described in Section 4.

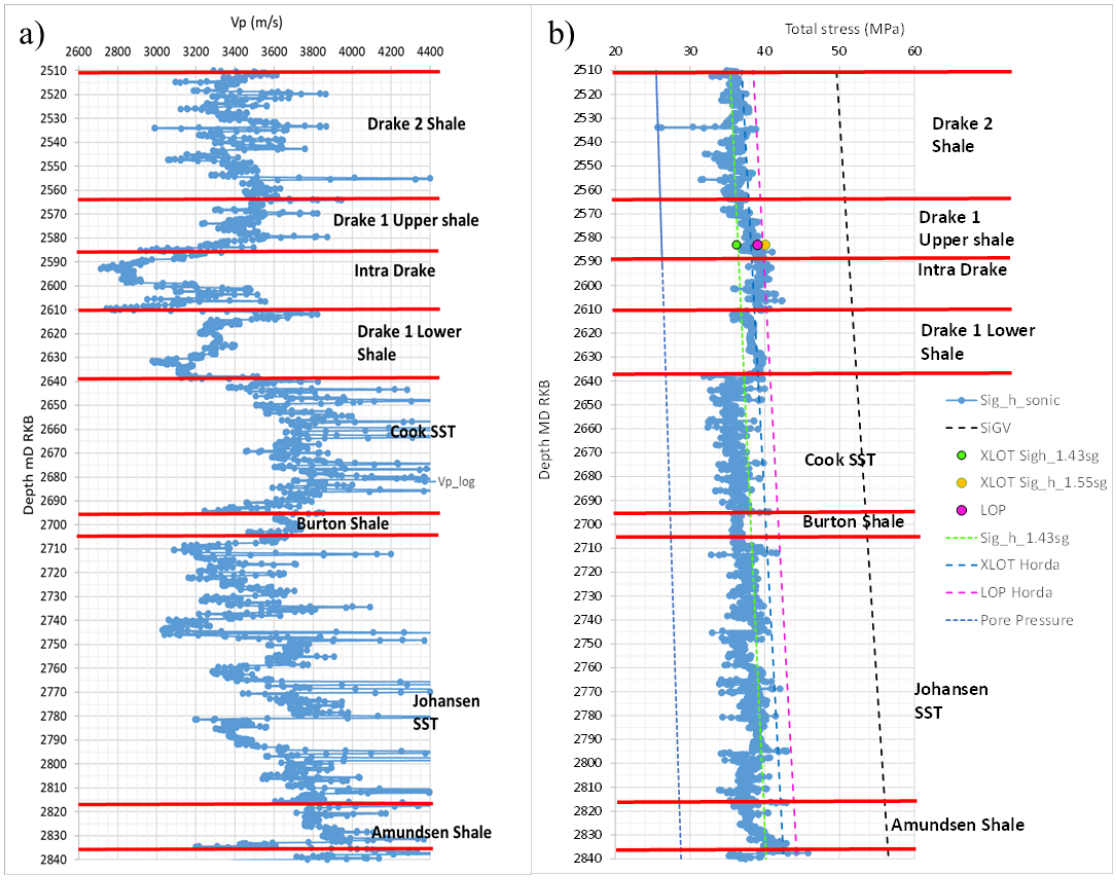

Figure 6 a) P-wave velocity profile for EOS well 31/5-7 (left), and b) Minimum horizontal stress from XLOT test and sonic log method for EOS well 31/5-7 (right). Depth profile indicating base interpretation stress gradients 1.43sg and alternative high value of 1.55 sg, and reginal XLOT trend for Horda platform (data from Thompson, et.al. 2022).

Table 1 Example of stress estimation for Drake cap rock in the Aurora field. Mean values are at depth of XLOT and within Drake. The variation and uncertainties are roughly judged from correlation lines and the spread in data in Figure 6.

Parameter	**Method**	**Range (MPa)**	**Mean (MPa)**	**% variation (+/-) around mean**	**Comments**
Vertical stress	Density log	49.6-52.3	51.2	low	Not quantified. Normally low, however, depends on log coverage
	Global trend	55.4-60.6	58	5%	Trend for Norwegian Continental Shelf based on Andrews et.al 2016
Minimum horizontal stress	XLOT	36.2 (40 MPa)	36.2	1%	Normally <0.5MPa error for high quality XLOT data. Alternative interpretation 1.55sg= 40MPa is 11% higher
	Sonic log	34-40	37	9%	Reflects vertical variations
	LOP	36.2-40.5	39	4-7%	Reported LOP value NPD. Closure pressure and FBP in XLOT used as lower and upper limit respectively.
	Horda XLOT	37-39	38	8%	Trend from Thompson et. al. 2022
	Horda LOP	38.5-40.5	39	20%	
	Lateral variations sonic logs	32-43	37.6	14%	Lateral variations based on 17 logs. S-wave was calculated based on Machine Learning Technique
Pore pressure	RPM	25.5-26.8	26.1	Low	Assumed Hydrostatic. No measurements in shale.
Maximum horizontal stress	Backcalculated value	36.2-39.8	36.6	Medium	S_H/S_h=1.05 is normal assumption. S_H/S_h= 1.01, 1.05 an 1.1 back calculated Thomson et al 2022.
Maximum Stress orientation	FMI	83-89	87	Low	Based on EOS well induced fractures
	FMI and BO	35-177	89.9	19	Equinor database
	FMI , BO, FMS	13-160	92.8	25.2	World Stress Map 2016

From Table 1, it is clear the uncertainties vary depending on the methods used (LOP, XLOT, log based method) and the dataset available (local vs. regional trends of XLOT and LOT), and whether accounting for detailed variation of stress with depth or laterally. When using regional trends, effects of pore pressure, well inclination, operational effect, lithology and geological history can give increased uncertainties in the trends. Maximum horizontal stress σ_H is often uncertain due to lack of method for direct measurement, but generally σ_H is assumed to be close to σ_h in the North Sea ($\sigma_H/\sigma_h < 1.05$). Stress path during injection will depend on material properties, pore pressure and temperature changes.

5.1.2 Elastic properties

Example of elastic properties of Drake sealing shale formation derived from p-wave velocity log from EOS well 31/5-7 is shown in Figure 7, along with histogram of the dynamic Poisson's ratio derived from sonic logs strength and histogram of Young's modulus from Horsrud correlation (Horsrud, 2001), which is expressed in Equation 2.4. A regional trend of dynamic Young's modulus and Poisson's ratio for the Drake formation from 17 wells compared with data from the EOS well is shown in Figure 7d, showing also lateral variations in the elastic properties.

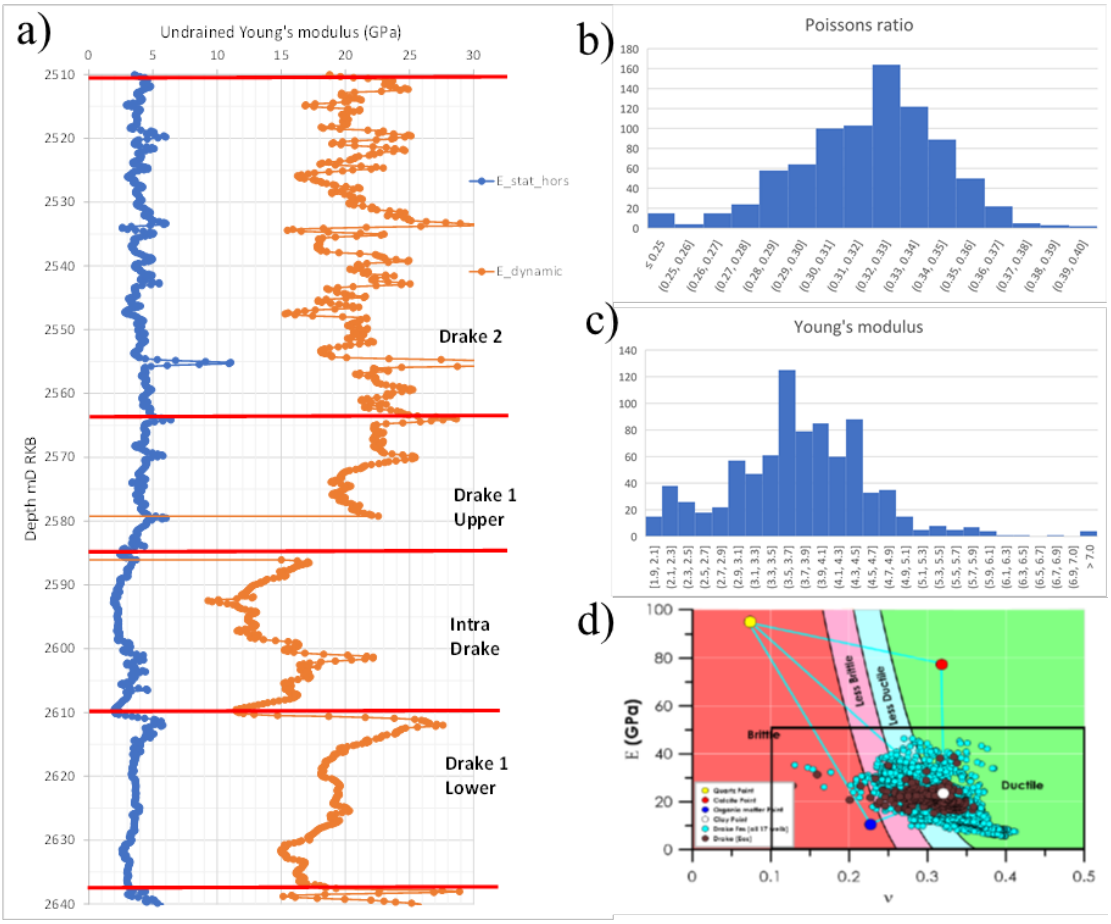

Figure 7 Youngs modulus vs. depth for Drake sealing formation in EOS well 31/5-7, showing static undrained Young's modulus from Horsrud empirical correlation and dynamic Youngs's modulus from sonic log data. b) Histogram of dynamic undrained Poisson's ratio c) Histogram of undrained Young's modulus in MPa from Horsrud correlation. Note for Histograms: x-axis is the horizontal stress value, and y-axis indicates the number of logged values in Drake d) Lateral variation in Dynamic Young's modulus (E) and Poisson's ratio (v) form Drake formation from a range of Wells around EOS (Mondol et al., 2022)

5.2 Example calculation for Young's modulus profile

This section demonstrates an example of obtaining a lower quantile linear trend of profile of Young's modulus derived from V_p data illustrated in Figure 6. Transformation uncertainty and spatial variability of the 1D profile are considered. For the former, this example uses only information reported by Horsrud (2001) and no additional statistical analyses are performed. Shortcomings arising from solely relying on information reported in the literature will be discussed.

5.2.1 Transformation uncertainty

By applying Equation 2.4, the V_p profile of Figure 6a can be transformed into a best estimate or *mean* profile of Young's modulus *E*. This is shown as the grey solid line profile in Figure 8. Also shown are layer-specific *mean* linear trends obtained from simple linear regression. As discussed previously, a statistically rigorous calculation of a lower quantile of interest requires constructing a prediction interval for *E*. Unfortunately, this is not possible with the available information. Horsrud (2001) reports the point estimates (best fit values) of the regression parameters and a residual standard deviation of σ_{tr} = 0.4 GPa. Missing are a more detailed description of the regression model and its assumptions (e.g. distribution type of the error), sample size, and the variance-covariance matrix of the parameters. In absence of these required information, it is not possible to quantify the uncertainty in *mean E* and in turn its contribution to *predictions of E*.

Here, a rough estimation of a spatially variable *lower profile E* is obtained by subtracting two[3] times the residual standard deviation of the transformation (i.e., $2 \times 0.4 = 0.8$) from the mean profile. The resulting profile is shown as dashed grey; the dashed blue line is the corresponding linear trend. It should be noted that it is not possible to say what quantile exactly such lower bounds are because of missing details about the regression model, i.e. error distribution type, number of data points, mean of *Vp* data used in the regression, and variance-covariance of the parameters.

As mentioned earlier, the above calculations provide *a lower trendline* for these data. A sound statistical quantification, however, should account for uncertainty in the parameters of the transformation as well as the number of observations used for fitting the regression model. Furthermore, if it is desired to *update* such generic transformations with site-specific measurements of *E*, quantification of the parameter uncertainty in the regression analysis is absolutely necessary. In other words, it is not possible to perform a Bayesian updating with the information provided by Horsrud (2001). The straightforward solution to this problem is to obtain the database used for fitting the regression model, refit the regression model and extract the necessary information. It is emphasized that the above criticism are not a reflection on the research presented by

[3] Note that the 95% probability interval for the standard normal distribution is (−1.96, 1.96).

Horsrud (2001). Rather, they are merely an example of typical reporting of regression results in many soil and rock engineering publications. With increasing interest in quantitative uncertainty quantification, this should be done more carefully taken into account explicitly.

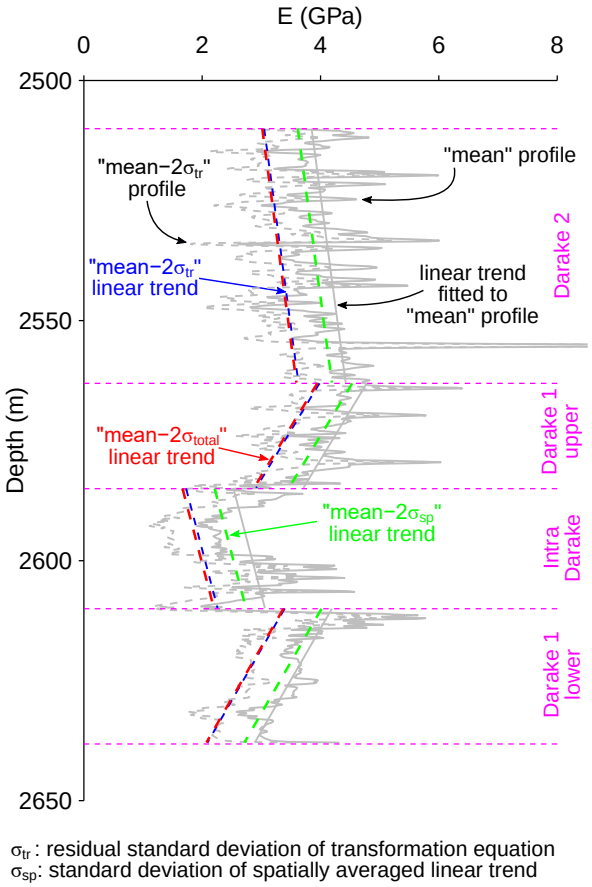

Figure 8 Profiles and conservative estimates of Young's modulus vs. depth for Drake formation EOS well 31/5-7, showing strength from Horsrud (2001) empirical correlation.

5.2.2 Spatial variability

The next step is to consider the spatial variability exhibited by the profiles. Table 2 summarizes layer-specific estimated scales of fluctuation and variance reduction factors obtained using the approach described in Figure 4. For each layer, the dashed green lines in Figure 8 are obtained by subtracting two (spatial) standard deviations from the mean trend line.

Table 2 Variance reduction factor for spatially averaged E

Layer	Thickness (m)	σ_w^2	δ_v (m)	$\Gamma^2(L)$	$\Gamma^2(L)\sigma_w^2$
Drake 2	52.88	0.73	0.98	0.019	0.0136
Drake 1 upper	21.80	0.30	1.11	0.051	0.0151
Intra Drake	24.84	0.35	1.80	0.072	0.0256
Drake 1 lower	27.90	0.24	0.88	0.032	0.0077

5.2.3 Total variation

The total variance for each layer is calculated as the sum of the two variance components. For example, for the Drake 2 layer, the variance of the transformation is $0.4^2 = 0.16$ and the variance of the spatially averaged linear trend is 0.0136. The total variance and standard deviation are 0.1736 and 0.42, respectively. The dashed red lines in Figure 8 represent linear trends obtained by subtracting two times total standard deviation from the mean trend line. It is noted that the transformation variance is dominant in this illustration. Finally, it is emphasized that the above analysis is valid for situations where it is reasonable to assume that the measurements involve spatial averaging, and thus detailed differences in the spatially varying field are averaged out, and the variance of the averaged field is smaller than that of the original field. This seems to be a reasonable assumption for large-scale engineering analyses that require an estimate of modulus of elasticity of sedimentary rock layers that are few metres to few tens of metres thick.

6 Summary and recommendations

This report introduced methods for uncertainty quantification that can be involved in geomechanical properties estimation, especially for depth-profile indirectly estimated from acoustic wave velocities. The main findings from this report can be summarized as follows:

- According to section 2 on the estimation methods for a depth profile, indirect estimation of rock mechanical properties and in-situ stress condition using well-log or petrophysical information are mainly based on empirical correlations from field/laboratory measurements and/or simplified physical understandings. Thus, the estimations can naturally involve an uncertainty caused by its simplification and lack of physical understanding in the empirical correlation.
- Section 3 introduced various type of uncertainties, including philosophically-oriented epistemic/aleatory classification of uncertainties and application-oriented classification. When the depth-averaged geomechanical properties are estimated from a well-log or petrophysical information, the estimation can involve following uncertainties:

  - Statistical parameter uncertainty, which can be associated with limited number of observation or field measurements;
  - Model uncertainty, which can be associated with imperfection of a physical model – which transform well-log information to rock mechanical inputs – and a probabilistic model which is related to a form of the statistical parametric distribution and regression model;
  - Spatial variability, which is related to nature randomness varying from one point in space to another; and
  - Observation (measurement) error, which is related to imprecisions associated with measurements such as limitations of equipment or operational conditions.
- Section 4 introduced a few quantification methods for uncertainties listed in section 3. As a method to quantify statistical parameter uncertainties, a confidence and prediction interval is introduced. Then, the concept of Bayesian approach is introduced as a means of quantifying model uncertainties. For quantification of spatial variability, a simplified approach using random fields is presented.
- Finally, in section 5, the uncertainty procedure described in sections 3 and 4 was demonstrated using data from the North Sea.

As addressed in this report, statistical modelling is a helpful tool to estimate reliable ranges of geomechanical input that can cover an area of interest. Also, it can be useful to determine likelihoods of the data's upper and lower limits using a systemic approach without an engineering judgement. In spite of its usefulness, the statistical approaches have been less highlighted in geomechanics for CO_2 storage. It should be kept in mind that this report addressed only basic approaches for uncertainty quantification with simplified assumptions. In reality, the uncertainties listed in section 3 are closely linked and sometimes difficult to separate as independent components. Thus, it is recommended to adopt more advanced methods (e.g., Bayesian approaches) for quantification of uncertainty in estimated rock mechanical properties.

The feasibility of the methods described in this report will be investigated with WP1 of the SHARP project, which is related to the in-situ stress modelling and interpretation, and potentially reported in the D5.4 deliverable.

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