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Uncertainty quantification of in-situ horizontal stress with pressuremeter using a statistical inverse analysis method

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Abstract

Knowledge of in situ stress magnitude and orientation plays a very important role in geological/geotechnical engineering and in the development of energy resources, such as caprock integrity, waste fluid disposal, geological storage of CO₂, and geothermal energy extraction. The uncertainty of estimated parameters, especially horizontal stress, from in situ tests such as pressuremeter tests, is a long-existing challenge due to the existence of uncertainties from geomaterial spatial variability, measurement errors, limited information, and modelling method. Therefore, non-unique solutions are often encountered in the pressuremeter interpretation. In this research, a statistical inverse analysis method is proposed to solve this issue by combining the closed-form solution, finite-difference model, and selected optimization algorithms. The objective of the statistical inverse analysis is to determine the optimal parameters by minimizing the sum of squared errors while providing the confidence intervals of inversed parameters. Random variables generated in the optimization process reproduce the

potential parameter uncertainties. The Jacobian matrix and the confidence intervals are derived from the optimization process to evaluate the variability of predicted horizontal stress and ground properties. A workflow that demonstrates a statistical inverse method for analyzing pressuremeter results is presented that helps to quantify the uncertainties of the ground properties and in-situ stress magnitudes and orientations derived from a pressuremeter test.

Keywords: Pressuremeter; Uncertainty; Horizontal stress; Inverse analysis; Statistical assessment

1 Introduction

The pressuremeter was introduced by Louis Menard in 1955 for in-situ testing to provide an estimation of ground properties for geotechnical designs (Clarke 1995; Mair and Wood 1987; Schnaid 2009). In general, there are three types of pressuremeter devices in terms of their installation methods (Mair and Wood 1987): the Menard-type pressuremeter, the self-boring pressuremeter (SBP), and the push-in pressuremeter. Theoretically, an SBP device can achieve minimal disturbance to the adjacent soils by drilling its own testing pocket. In a pressuremeter test, both the applied pressure and volume or radial displacements are recorded. A typical pressuremeter testing curve includes two components, expansion and contraction, as well as loops if unloading–loading cycles are performed. Geotechnical properties, such as undrained shear strength and shear modulus, as well as in-situ horizontal stress, can be derived from pressuremeter testing curves.

Uncertainties that exist in ground properties and in-situ stress field are associated with the aleatory uncertainties (spatial variability) and the epistemic uncertainties (measurement errors, limited information, and model uncertainty) in a pressuremeter test (Nadim 2007). Uncertainty

quantification plays a vital role in assessing potential natural hazards (Chen et al. 2017; Cui et al. 2017; Liu et al. 2020). The quantified uncertainty helps to provide a more sophisticated design of hydraulic fracturing, tunnelling, and caprock integrity in subsurface development considering the spatial variability of geotechnical properties, stress, and pore pressure distributions (Yang et al. 2004; Ghassemi 2012; Ganesh et al. 2019; Zhang et al. 2020).

In general, the interpretation of pressuremeter tests is conducted using graphical plotting methods (Gibson and Anderson 1961; Houlsby and Withers 1988; Marsland and Randolph 1977) or curve fitting methods (Arnold 1981; Denby and Clough 1980). The graphical plotting methods involve the construction of a tangent line to the loading or unloading curve, which can determine geotechnical properties. However, one of the drawbacks of graphical methods is its subjectivity to personal judgements (Clark 1995). To fit measured points with predicted ones, a computational model, which can be either a closed-form solution or a numerical model, is required. Jefferies (1988) proposed a curve-fitting approach to identify horizontal stress and ground properties by extending the mathematical solution proposed by Gibson and Anderson (1961). However, the model fit was achieved through visual comparison, which may lead to non-unique solutions (Houlsby 1989). By extending the hyperbolic model (Duncan and Chang 1970), Ferreira (1992) fitted the pressuremeter curves numerically using the least square error curve fitting technique. Fahey and Carter (1993) performed finite element analyses to simulate the behaviour of pressuremeter tests in sand using a nonlinear elastic, plastic model. Fawaz et al. (2002) conducted the pressuremeter chamber tests in the sand and deduced the parameters using the finite element method. Huang et al. (1986) adopted the simplex algorithm in the least square error curve fitting process to solve the problem of repeatability. Levasseur et al. (2008)

identified the Mohr-Coulomb parameters using two optimization approaches based on a gradient method and the genetic algorithm (GA), respectively. In a recent publication, Obrzud et al. (2009) presented the application of the neural network technique in parameter identification from SBP measurements. Gaone et al. (2019) derived modified Cam clay parameters from SBP testing data by combining traditional interpretation methods, parameter sweeps, and a local minimizer based on the golden section search algorithm and parabolic interpolation. However, the uniqueness of a solution in parameter estimations discussed above has yet to be addressed in depth.

In general, there are two possible sources for non-uniqueness: 1) The initial parameters are arbitrarily chosen during the numerical curve fitting process (Arnold 1981). Houlsby (1989) pointed out that experimental data can be fitted by a wide range of different combinations of parameters and 2) the mathematical minimum is not necessarily the physical minimum. For example, the simplex algorithm (Nelder and Mead 1965; Huang et al. 1986) is sensitive to the initial values provided at the beginning of the optimization process, leading to different optimal results for each initial dataset. Consequently, the curve fitting process may produce mathematically optimal values rather than physically optimal ones (Papon 2012).

To deal with the issue of arbitrarily chosen parameters, the research presented in this paper introduces cut-offs of random parameter variables in the inverse analysis to filter unreasonable data points (Clark 1995). A priori knowledge of the ground properties is essential to define the physical bounds for a constrained optimization problem. Multiple optimizers shall be utilized in the inverse analysis. Notably, the statistical inverse analysis method can accommodate the parameter uncertainties during the interpretation of pressuremeter tests. A statistical assessment of the estimated parameters shows not only the optimal predicted dataset but also

the bounds of predicted values (e.g., 95% CIs). Furthermore, correlations between estimated values can be derived from the statistical assessment.

To overcome the disadvantages of conventional interpretation techniques for pressuremeter tests, a statistical inverse analysis framework is proposed and applied in the uncertainty quantification of the parameter estimation for an SBP test. Results demonstrate its capability in quantifying uncertainties for geotechnical design and research.

2 Methodology

In geotechnical engineering, inverse analysis has been widely applied in the calibration of constitutive models, identification of soil parameters, and geotechnical design optimization (Levasseur 2008; Papon 2012; Yin 2016). The objective of the proposed statistical inverse analysis of a pressuremeter test is to minimize the errors between the measured and predicted data under a statistical framework as opposed to the deterministic method adopted by Jefferies (1988) for parameter estimation of an SBP. The framework of the statistical inverse analysis includes, but is not limited to, the following steps: (1) a priori knowledge of initial values and uncertainty quantification of input variables; (2) selection of a computational model and coupling with an optimization algorithm; (3) establishing an objective function; (4) identification of the optimal dataset based upon the optimization criteria; and (5) execution of a statistical assessment on the identified parameters. The workflow for the proposed statistical inverse analysis for pressuremeter tests is illustrated in Fig. 1.

To begin the statistical inverse analysis, initial values must be selected for certain optimizers, e.g., Levenberg–Marquardt algorithm (LMA) and simplex algorithm. For other optimizers, e.g., Monte

Carlo simulation (MCS) and subset simulation (SS), independent and identically distributed (IID) parameter samples must be randomly drawn from a proposed probability density function (PDF) (e.g., uniform distribution, Gaussian distribution, lognormal distribution). The PDFs denote the initial probability distributions of formation properties and in-situ horizontal stress, which can be defined with a priori knowledge, such as laboratory and field tests, local experience and literature. The uniform distribution is adopted in the inverse analysis. These IID samples are used as input parameters in a computational model. Solving an objective function consists of coupling a computational model with an optimizer.

2.1 Objective functions

To minimize the subjective errors caused by the visual interpretation method proposed by Jefferies (1988), an unweighted nonlinear least squares (NLLS) performance function (also called error function) can be formulated. The NLLS performance function is formulated as the objective function in the searching process of optimization algorithms (Ahmed et al. 2015; Papon 2012; Yin 2016). The unweighted NNLS performance function is expressed as

$$SSE = \sum_{i=1}^n [Y_i - \hat{Y}_i(b_i)]^2, \quad (1)$$

where SSE denotes the sum of squared errors, Y_i denotes observed data, $\hat{Y}_i$ denotes predicted data, and b_i represents a parameter to be estimated (G, σ_h, S_u). G represents the shear modulus, σ_h indicates the total horizontal stress, and S_u denotes the undrained shear strength. $\hat{Y}_i(b_i)$ represents a nonlinear function of b_i for the simulation of a pressuremeter test. In the inverse analysis, an optimizer must be coupled with a computational model to find the minimization of the SSE as formulated in Eq. 1.

136 2.2 Optimization algorithms

137 The LMA and the trust-region reflective algorithm (TRRA), which are adopted in the statistical
 138 inverse analysis, are realized with the nonlinear least-squares solver *lsqnonlin* in Matlab
 139 (MathWorks 2019). To verify the conclusion made by the local optimizers (i.e., the LMA and the
 140 TRRA), a global optimization algorithm, the SS, is used in the inverse analysis. The SS code is
 141 modified from Li and Cao (2016) and implemented in the minimization of unweighted NNLS
 142 performance function as described by Eq. 1. Appendix A briefly introduces the theories about the
 143 three optimization algorithms.

144 2.3 Simulation of a pressuremeter test

145 A pressuremeter test can be simulated with either a closed-form solution or a numerical model.
 146 Based on the solution proposed by Gibson and Anderson (1961), Jefferies (1988) proposed the
 147 theoretical relationship between pressure and the ratio of initial radius to the current radius,
 148 a_0/a , at the stage of plastic loading:

$$149 \quad P = \sigma_{h0} + S_u \left[1 + \ln \left(\frac{G}{S_u} \right) \right] + S_u \ln \left[1 - \left(\frac{a_0}{a} \right)^2 \right] \quad (2)$$

150 To account for strength softening or hardening effect in unloading during the SBP contraction
 151 phase, Jefferies (1988) introduced a fraction β of the undrained shear strength S_u :

$$152 \quad S_{u_c} = \beta S_u \quad (3)$$

153 Then, the pressure that initiates plastic deformation during the contraction stage becomes $P =$
 154 $P_{max} - (1 + \beta)S_u$, and the relationship between P and a should be written as (Jefferies 1989):

$$155 \quad P = P_{max} - (1 + \beta)S_u - S_u \ln \left\{ \left[1 - \left(\frac{a}{a_{max}} \right)^2 \right] \left[\frac{G}{(1 + \beta)S_u} \right] \right\}$$

$$- \beta S_u \ln \left\{ \left[\left(\frac{a_{max}}{a} \right)^2 - 1 \right] \left[\frac{G}{(1 + \beta) S_u} \right] \right\} \quad (4)$$

where β denotes softening or hardening coefficient in unloading, and a_{max} represents the maximum radius.

Displacements measured in the field can be directly applied to Eqs. 2 and 4 after calibrations. The proposed inverse analysis of an SBP test in clay can be efficiently conducted using the NLLS curve fitting inverse analysis technique, as explained previously.

In addition to the closed-form solution introduced above, a two-dimensional numerical model, using the Finite Element Method (FEM) or the Finite Difference Method (FDM), can be built to simulate pressuremeter tests in clay, sand, and rock (Yeung and Carter 1990; Yu and Netherton 2000; Gaone et al. 2019). In the present study, FLAC (Fast Lagrangian Analysis of Continua), a commercial two-dimensional explicit finite-difference program (Itasca 2011), was applied to the modelling of an SBP test in clay. A properly-built numerical model can address the sources of inaccuracy from oversimplified assumptions in closed-form solutions about pressuremeter geometry, water drainage, and initial disturbance (Yu 2006). Although the numerical model may encounter convergence issues, it can detect the unreasonable initial estimates for the unconstrained optimization problem.

2.4 Statistical assessment of the identified parameters

To quantify the uncertainty in parameter estimates, statistical assessments should be conducted after the optimization process. The evaluation of uncertainty for an inverse analysis requires the definition of mean values, standard deviations (SDs), and confidence intervals (CIs). In the

proposed workflow, the covariance for the optimal parameters, b' , is calculated as (Knabe et al. 2012):

$$cov(b') = s^2(J^T J)^{-1}, \quad (5)$$

where b' represents the estimated optimal parameters, s^2 denotes the calculated error variance, and J indicates the Jacobian matrix, also called the sensitivity matrix.

The error variance, s^2 , asymptotically reaches the mean squared error, and is defined as:

$$s^2 = \frac{SSE}{(n-p)}, \quad (6)$$

where SSE represents the sum of squared errors, as calculated using Eq. 1, n represents the number of observations, p indicates the number of parameters, and $(n-p)$ denotes the degrees of freedom.

The standard deviation (SD) is the square root of diagonal elements of matrix $cov(b')$. With the derived SD, the $100(1-\alpha)\%$ CIs for the optimal parameters are

$$b' \pm t_{(1-\alpha/2, n-p)} \frac{SD(b')}{\sqrt{n}} \quad (7)$$

where $SD(b')$ represents the SD of b' , and $t_{(1-\alpha/2, n-p)}$ indicates $100(1-\alpha/2)^{th}$ percentile of t -distribution with $(n-p)$ degrees of freedom. The off-diagonal elements of matrix $cov(b')$ are covariance, which can be used to determine the correlation between the optimal parameters. For uncorrelated parameters, the covariance is zero. If parameters are correlated, then their covariance will be nonzero (Weisstein et al. n.d.). Knabe et al. (2012) pointed out that the matrix $cov(b')$ gives the reliability of estimated parameters in terms of their covariances.

The proposed statistical inverse method can accommodate parameter uncertainty into the interpretation of pressuremeter tests. With a statistical assessment, statistics on the estimated parameters provide the confidence bounds together with the optimal values. Also, correlations between estimated values can be derived from the statistical assessment.

3 Case study of an SBP test

The SBP test conducted at the test site Amauligak F-24 (Jefferies 1988) was re-analyzed using the proposed statistical inverse method. Parameter estimation accomplished by Jefferies was based on the curve fitting with visual comparison by trial-and-error. In the case study, the re-analysis of the SBP test was performed using the inverse method under a statistical framework. The model fit was evaluated with the coupling of the closed-form solution (Jefferies 1988) or a finite-difference model with the LMA, the TRRA, and the SS. Results were interpreted using the SSE for the unweighted residuals and statistics (mean and CIs).

3.1 Project background

The Amauligak F-24 site is located 32 m below sea level. The testing pocket was surrounded by stiff clay (unit D1) approximately 40 m below the mud line. The published SBP testing data (Jefferies 1988) are utilized for the re-analysis of the SBP testing in clay at this site.

3.2 Soil profile

The geotechnical profile below the mud line is illustrated in a study by Jefferies (1987). A 12 m layer of soft clay (units A1 and A2) overlies 24 m of dense to compact sand (unit C). The SBP testing pocket is located in the 15 m massive clay unit (D1) below unit C, which is horizontally bedded silty clay with medium to high plasticity. The water content for unit D1 ranges from 25%

to 32%, and the liquid index is close to zero. A priori information presented by Jefferies (1987) provides the geotechnical constraints for the following inverse analyses of the same SBP testing.

3.3 Numerical modelling of an SBP test

In addition to the analytical solution proposed by Jefferies (1988), FLAC modelling was used in inverse analyses. As the expanding length of the SBP instrument is approximately 0.5 m (Cambridge 2012), to simplify numerical modelling, the SBP testing in clay was treated as a cylindrical cavity expansion in a homogeneous, isotropic medium (Wroth 1984; Jefferies 1988; Yeung and Carter 1990; Yu and Netherton 2000). The studies were conducted using total stresses with an assumption of undrained conditions throughout the test considering a fast-loading rate (Windle and Wroth 1977; Jefferies 1988; Liu et al. 2020). Fig. 2 illustrates the two-dimensional plane-strain discretized domain and boundary conditions. Taking advantage of symmetry, only a quarter of the cylindrical cavity was modelled.

The Mohr-Coulomb model was implemented to calculate the elastic and plastic response of the SBP test. Under undrained conditions, the plastic strength of the clay in D1 is represented by the Tresca model with a unique S_u and $\varphi = 0^\circ$.

Random variables, horizontal stress (σ_{h0}), shear modulus (G), and undrained shear strength (S_u), were generated through parameter perturbation in the LMA and the TRRA, and randomly selected from IID samples in the SS. These random variables were used as input parameters for the analytical and finite-difference FLAC models. The minimization of the objective function formulated using Eq. 1 was solved by coupling the analytical or the FLAC model with the LMA, the TRRA, and the SS.

3.4 Criteria applied in the determination of the best-fit dataset

The goal of optimization is to determine the optimal dataset in an inverse analysis. The criteria used to determine the best-fit dataset are summarized as follows:

(1) Value of SSE: the value of SSE is considered as the primary index to determine the optimal dataset with the minimum SSE.

(2) Error bar: the length of the error bar shown in Figs. 4 and 5 represents the variability of estimated parameters, which can be treated as the secondary index to determine the optimal dataset.

(3) In general, there are three cases in the decision-making process from which the best-fit dataset is selected:

Case A: dataset with both the minimal SSE and error bar is considered as the best-fit dataset.

Case B: In the case of the same minimal SSEs, a dataset with a shorter error bar is preferred to one with a longer error bar.

Case C: Whereas if the SSE is minimal, its error bar is longer, which means an “accurate” fit but larger uncertainty in the curve fitting (or vice versa, the dataset with a greater SSE but a shorter error bar). In such cases, the assessment should be assisted with other statistical parameters, e.g., coefficient of determination and p-value, and the evidence from other independent tests, such as field vane test, triaxial test.

(4) Knowledge and experiences from experts are still important in the final determination of the best-fit dataset.

The flow chart of the criteria described above is illustrated in Fig. 3.

3.5 Statistical inverse analysis of the expansion curve

A complete pressuremeter test curve consists of both expansion and contraction parts. To examine the effects of the contraction part on the parameter estimation, the inverse analysis in this section is performed by considering the expansion part only. The inverse analysis of the complete curve is conducted in Section 3.6. Two local optimization algorithms (LMA and TRRA) together with a global optimization algorithm (SS) are implemented in the statistical framework. In the case of three input parameters, a gradient descent algorithm may be easily confined by local minima. Thus, other optimizers, such as the SS or the GA, need to be adopted to ensure the global minimum. However, these optimizers often require a large number of iterations to accomplish an optimization task, which becomes computationally costly for an inverse analysis using a numerical model. In some cases, a hybrid of local and global optimizers may be an alternative solution.

3.5.1 Inverse analysis of the expansion curve using the local optimizers

The inverse analyses of the SBP test AF85 P06-15 are conducted with the proposed inverse method and compared with the results presented by Jefferies (1988) and from conventional interpretation methods (Appendix B). The expansion part of the SBP test AF85 P06-15 is utilized. The initial parameters in the inverse analyses of the SBP test are listed in Table 1. Three sets of initial parameters are selected to estimate σ_{h0} , G , and S_u . Initial values of dataset A (Initial A) represent the parameters estimated by Jefferies (1988) using the complete expansion and contraction curve, and dataset B (Initial B) only considers the expansion part (refer to Figs. 10 and 12a in Jefferies, 1988). Dataset C (Initial C) was randomly generated to test the robustness

of the proposed method in the present study. Initial values of SSE shown in Table 1 have been evaluated using Eq. 1.

The optimal parameters from the inverse analysis of the expansion curve using the LMA are presented in Table 2. In terms of the SSE in Table 2, the optimal dataset using the closed-form solution corresponds to the optimal values of dataset A and dataset C, which are virtually identical. In dataset A, G measures 9,915 kPa, which is similar to the lower bound reported by Jefferies (1988, see Fig. 7a). Similarly, the optimal parameters using the numerical model can also be determined to be dataset A by examining the SSE in Table 2.

Fig. 4 illustrates the datasets of σ_h in Table 2 with error bars (one SD below and above the data points). The SDs for Initials A, B, and C were not provided in the study by Jefferies (1988). The lengths of error bars shown in Fig. 4 illustrate that the estimation uncertainty using numerical modelling appears to be higher than that using the closed-form solution, indicating that the numerical model is more sensitive to the variation of input parameters than the closed-form solution while simulating the expansion part due to the disturbance at the early stage.

The error bars for optimized dataset B in Fig. 4 are absent due to the ill-conditioned Jacobian matrix caused by the overestimated G . The computational model predicted using dataset B is unstable. A small change in the input leads to a significant difference in the output. Therefore, dataset B presented in Table 2 should be discarded, although the predicted curve fits the measured data quite well.

For a pressuremeter test, σ_{h0} draws the most attention as the soil stiffness and strength can be evaluated by other types of in-situ tests, such as the cone penetration test, standard penetration test, and field vane test. σ_{h0} measures 1,713 kPa, as identified from the numerical model in Table

301 2. Compared to the numerical model, the closed-form solution (1,736 kPa) seems to overestimate
302 σ_{h0} slightly as well as S_u and significantly underestimate G by 50%.

303 While using the LMA, the parameters are not constrained. Although the LMA is the most popular
304 algorithm for unconstrained NLLS curve fitting problems, the TRRA is still needed to constrain the
305 parameters in the optimization process. Specifically, limits of the soil stiffness and strength
306 should be well defined to derive reasonable horizontal stress, σ_{h0} , from the inverse analyses.

307 The TRRA was implemented in the minimization of objective functions for the inverse problems
308 as it can constrain the randomly generated variables within the defined bounds. Table 3 defines
309 the initial variabilities of geotechnical properties and the in-situ horizontal stress with lower and
310 upper bounds, which are calculated by assuming 50% deviations from the initial values in Table 1.

311 The TRRA conducted a search around the neighbourhood constrained by the bounds defined in
312 Table 3. The optimal parameters using the closed-form solution coupled with the TRRA were
313 determined to be dataset A and dataset C in Table 4. Although the Initial C (G, σ_h, S_u) differs from
314 the Initial A, only a negligible difference in G was observed between dataset A (9,920 kPa) and
315 dataset C (9,922 kPa). With bound constraints, the TRRA derived nearly identical optimal values
316 as the LMA.

317 By comparing the SSEs presented in Table 4, the optimal horizontal stress derived from the
318 closed-form solution using the TRRA can be determined as 1,736 kPa, and from the numerical
319 modelling as 1,703 kPa, respectively.

3.5.2 Inverse analysis of the expansion curve using the subset simulation algorithm

As a global optimization algorithm, the SS is implemented to compare the results from the two local optimizers, the LMA and the TRRA. Dataset A in Table 3 is also used to define the bounds for the SS. With the number of samples $N_s = 250$, intermediate conditional failure probability $P(F_i) = 0.1$, and the maximum number of simulation levels $N_l = 5$, the SS algorithm can derive the optimal parameters listed in Table 5. The global optimizer SS serves as a reliable reference that constrains the solution derived from the two local optimizers.

3.6 Statistical inverse analysis of the complete (expansion–contraction) curve

To study the effects of the contraction part on the inversed parameters, the complete expansion–contraction SBP testing curve AF85 P06-15 is utilized in the following inverse analyses.

Initial values of $(G, \sigma_{lv}, S_w, \beta)$ for datasets D, E, and F in Table 6 are adopted from Figs. 8a, 8b and 10 in Jefferies (1988) and β is defined as softening or hardening coefficient in unloading in the SBP test. The optimal parameters after inverse analyses using the closed-form solution and the numerical model are presented in Table 7. In terms of the SSE in Table 7, dataset D is preferred to datasets E and F as the optimal dataset using the closed-form solution and the numerical model coupled with the LMA. It can be observed that the SDs (see Fig. 5) using numerical modelling appear to be lower than those using the closed-form solution, indicating that the prediction made by the numerical model has less uncertainty than the closed-form solution while simulating the entire expansion–contraction curve.

Table 8 defines the lower and upper bounds for the TRRA. The optimal datasets using the TRRA are listed in Table 9. Similarly, Table 10 defines the bounds for the SS, and Table 11 confirms the global minimum predicted by the two local optimizers.

In terms of the derived values (G, σ_h, S_u) in Tables 7 and 9, different initial values of datasets D, E, and F have similar predictions with the closed-form solution or the numerical model, indicating the robustness of the inverse analysis approach used in this study.

Compared with Fig. 4, Fig. 5 indicates that prediction using the complete curve has lower uncertainty than using just the expansion curve for numerical models. There are two reasons to explain this advantage: (1) the complete curve provides more data points for the inverse analysis, leading to less uncertainty in prediction; and (2) the contraction curve is more reliable than the expansion part as the effect of installation disturbance becomes minimal at this stage (Ferreira 1992; Houlsby and Withers 1988).

The purpose of using the TRRA is to verify the conclusion made by the LMA and reduce the non-uniqueness caused by arbitrarily chosen parameters and local minimum values. Additionally, the uniqueness of the solution can be better addressed with statistical assessments on the derived parameters. Thus, it is more meaningful to derive narrow CIs rather than "true values" from the parameter estimation. The derived narrow CIs are valuable in quantifying the uncertainty of G, σ_h, S_u for geotechnical design.

3.7 Uncertainty quantification of optimal inversed results

With one global and two local optimizers, the optimal parameters are derived from initial datasets and their bounds. After the optimization process, uncertainties from parameter estimation can be quantified using the statistical assessment methods discussed in Section 2.4.

3.7.1 Summary of the optimal inversed parameters and statistical assessments

Table 12 summarizes the derived mean and 95% CIs of (G, σ_h, S_u) using the closed-form solution while Table 13 denotes the numerical model.

In Table 12, G appears to be underestimated while σ_h is overestimated in using the expansion curve only, and vice versa for the complete curve. The closed-form solution tends to be unconservative in interpreting pressuremeter tests due to oversimplifications in geometry and boundary conditions.

From Table 13, it is interesting to find that the numerical model provides similar mean values of (G, σ_h, S_u) between the expansion and the complete curves. In contrast, the estimated 95% CI for the expansion curve is much wider than the complete curve. Again, the wider CI band for the expansion curve accounts for the uncertainties at the early stage of the expansion part. Therefore, the complete curve can provide a more reliable prediction than the expansion curve.

3.7.2 Validation of the optimal inversed parameters

By examining Table B1, the value of σ_h (1,690 kPa) deduced from the modified inspection technique (Jefferies 1988) basically agrees with the corresponding values (1,713 kPa and 1,709 kPa) shown in Table 13. Table 12 illustrates a slightly higher or lower value of σ_h than Table B1. The mean of S_u (182 kPa) in Table B1, which was estimated from the SBP curve using the linear regression method, approximately coincides with those in Tables 12 and 13. The values of G

(13,730 kPa and 11,230 kPa) deduced from the triaxial test curve lie roughly within the 95% CI (between 11,638 kPa and 19,050 kPa) predicted by the complete curve (Table 13). At the same time, the gradient of the unloading–reloading loop in Fig. B3 illustrates a significant increase in stiffness, which may be resulted from the drainage taking place near the probe during this stage (Clarke 1995). The ratio of shear strength β is identified as 0.79, which approximately coincides with 0.8 given in Table B1.

Due to the advantages of runtime efficiency, it is recommended to conduct a closed-form solution coupled with an optimizer (LMA or TRRA) prior to running additional numerical simulations. To determine σ_h , the expansion part of the pressuremeter curve may be sufficient to conduct a proper inverse analysis. The complete expansion–contraction curve can be used to investigate the unloading effects on soil properties and provide a narrower 95% CIs.

3.7.3 Evaluation of the model fit with the coefficient of determination

Although the statistical values listed in Tables 12 and 13 provide the quantitative assessments of the inversed parameters, visual comparison of predicted and observed curves adopted by Jefferies (1988) is still meaningful in evaluating the model fit as a final check.

Figs. 6 and 7 illustrate the observed data from test AF85P06-15 (Jefferies 1988) and the predicted data using the analytical and numerical models. The goodness of fit can also be quantified with the coefficient of determination, R^2 , which is defined as:

$$R^2 = 1 - \frac{SSE}{SST} \quad (8)$$

where SSE represents the sum of squared errors, as defined in Eq. 1; and SST indicates the total sum of squares:

$$SST = \sum_{i=1}^n (Y_i - \bar{Y})^2 \quad (9)$$

where Y_i denotes observed data, and $\bar{Y}$ represents the mean of observed data.

R^2 can take any value between 0 and 1, with a value equal to 1 indicating the model prediction exactly matches the observed data. By only visual comparison, it is challenging to make an unbiased judgment of which dataset is the best fit. Therefore, the SSE, SD, and R^2 can evaluate the model fit numerically, which is independent of an observer.

In terms of R^2 in Figs. 6a and 7a, the best values predicted by the closed-form solution achieve a slightly better fit for the observed data compared to the estimates (initial A in Table 1) proposed by Jefferies (1988). Whereas there are significant deviations observed in Figs. 6b and 7b, implying that the best values predicted by the numerical model achieve a significantly better fit than the initial dataset A does. The best-fit dataset evaluated with the closed-form solution does not necessarily apply to the numerical model.

Jefferies (1988) emphasized the match at the early stage; however, the observed data may be significantly affected by the disturbance of the adjacent soil during the SBP installation. The 95% prediction interval (shaded band in Figs. 6 and 7) provides the lower and upper bounds of the predicted data. The wider band at the early stage of expansion reveals more uncertainties in the curve fitting due to the disturbance caused by tool installation. The narrow band at the later stage verifies the viewpoint proposed by Ferreira (1992) that the later part of the loading stage is more reliable. Thus, in terms of R^2 and the width of the band, Fig. 7b illustrates the best fit for the observed data and the corresponding prediction interval.

4 Discussion

Traditionally, interpretation of pressuremeter tests focuses on the derivation of soil properties using graphical plotting or curve fitting methods in a deterministic way. Therefore, the interpreted parameters are usually expressed as the "best" dataset, which may be biased as it fails to account for the uncertainty and errors related to soil or rock spatial variability, measurement errors, limited information, and model uncertainty. The proposed statistical approach can employ analytical and numerical models coupled with selected optimization algorithms to quantify the effects of uncertainty and errors on derived soil properties and horizontal stress. To perform the parameter estimation for an SBP test in clay, both the closed-form solution (Jefferies 1988) and numerical modelling coupled with three optimization algorithms were adopted in the inverse analyses. The closed-form solution was used for initial assessments due to its computational efficiency. The two-dimensional numerical model can provide more realistic estimates of in-situ parameters. To verify the parameters derived from the inverse analyses, data from the SBP test and the triaxial test were also interpreted using graphical plotting and the linear fit regression methods. Finally, the variability of optimized datasets derived from the inverse analysis can be described using the mean, SD, and 95% CIs. The quality of curve fitting can be quantified using R^2 and prediction intervals.

To minimize the non-uniqueness: (1) various optimization algorithms should be implemented; (2) the statistical assessment may be unable to improve the accuracy of the predicted mean but can give the precise lower and upper bounds within which the true values may lie; and (3) other types of laboratory and in-situ tests, such as triaxial test and field vane test, can provide more constraints on the predicted parameters with relatively narrow bounds.

Compared to an analytical solution, a numerical model can simulate an SBP test as a two-dimensional cylindrical cavity expansion, which is similar to a real pressuremeter test. As oversimplification and idealization in the closed-form solution could lead to significant errors in the derived soil properties (Yu 2006), the numerical model adopted here can identify reasonable combinations of parameters as presented in this research.

In future, the statistical inversion code will be extended to consider uncertainties from tool calibrations, installation disturbance, and irregular cavity geometry, as well as a more complex numerical model considering partial drainage, soil anisotropy and inhomogeneity using solid and fluid coupling method (Yin et al. 2021).

5 Conclusion

Compared to the conventional pressuremeter interpretation methods, the proposed statistical inverse analysis can quantify the potential uncertainty and errors from ground properties and in-situ horizontal stress. The minimization of the objective function with multiple optimizers can reduce the degree of non-uniqueness encountered using conventional methods. Compared to the expansion curve only, the complete curve can predict a more reasonable mean and narrower 95% CIs in the inverse analysis. The statistical assessments of the optimal parameters can evaluate the statistics defined by the SD and CIs. Also, the model fitness can be further evaluated with the R^2 and prediction intervals. The uncertainties propagated from ground properties and computational modelling can be quantified statistically.

461 The statistical methodology described above can be extended to other engineering inverse
462 analysis problems, such as the calibration of constitutive models and the inverse analysis of in-
463 situ stress field for horizontal drilling, tunnelling, and hydraulic fracturing, among others.

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Nomenclature

a_0	Initial radius of the instrument
a_{max}	Maximum radius of the instrument
a	Current cavity radius of the instrument
b	Estimated parameters
b'	Optimal parameters estimated
d	Trial step
G	Shear modulus
I	Identity matrix
J	Jacobian matrix
N	Region of trust
n	Number of observations
p	Number of parameters
$n - p$	Degrees of freedom
P	Total pressuremeter pressure
q	Approximation of the objective function $f(x)$
s^2	Calculated error variance
R^2	Coefficient of determination

S	Sum of squared errors, equivalent to the SSE in Eq. 1
S_u	Undrained shear strength
$SD(b')$	The standard deviation of b'
SSE	Sum of squared errors
SST	Total sum of squares
$t_{(1-\alpha/2, n-p)}$	$100(1-\alpha/2)^{th}$ percentile of t-distribution with n-p degrees of freedom
Y_i	Observed data
$\hat{Y}_i$	Predicted data
$\bar{Y}$	Mean of observed data
σ_h	Horizontal total stress
λ	Non-negative damping factor identity matrix
δ	Increment of the estimated parameter
φ	Friction angle
β	Softening or hardening coefficient in unloading

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Figures captions

Fig. 1 Flow chart of statistical inverse analysis of a pressuremeter test

Fig. 2 Boundary conditions for the FLAC model in the inverse analysis

Fig. 3 Flow chart of the criteria applied in the determination of the best-fit dataset

Fig. 4 Initial and best datasets of horizontal stresses derived from expansion curve using the closed-form solution and the numerical model coupled with the LMA and the TRRA. Note: the number displayed on the top of error bar is SD, unit: kPa

Fig. 5 Initial and best datasets of horizontal stresses derived from complete curve using the closed-form solution and the numerical model coupled with the LMA and the TRRA. Note: the number displayed on the top of error bar is SD, unit: kPa

Fig. 6 Fit of observed data to predicted data using the closed-form solution for test AF85P06-15 (Jefferies, 1988). Note: (a) is predicted with the closed-form solution, and (b) is predicted with the numerical model.

Fig. 7 Fit of observed data to predicted data using the numerical modelling for test AF85P06-15 (Jefferies, 1988). Note: (a) is predicted with the closed-form solution, and (b) is predicted with the numerical model.

Table

Table 1 Initial parameters for the inverse analysis of the expansion curve

Dataset	Initial values (Initial)			
	σ_{h0} (kPa)	G_0 (kPa)	S_{u0} (kPa)	SSE
A	1,690	18,000	160	1.08
B	1,525	45,000	165	0.96
C	1,882	19,900	178	71.27

Notes:

1. Initial values of A (Initial A) and B (Initial B) refer to Figs. 10 and 12a in Jefferies (1988).
2. Initial values of C (Initial C) are random values generated for the inverse analysis.

Table 2 Optimal parameters from the inverse analysis of the expansion curve using the LMA

Dataset	Optimal values using the closed-form solution				Optimal values using the numerical model			
	σ_h (kPa)	G (kPa)	S_u (kPa)	SSE	σ_h (kPa)	G (kPa)	S_u (kPa)	SSE
A	1,736	9,915	190	0.47	1,713	15,289	178	0.43
B	1,453	44,695	189	0.48	1,488	44,997	174	0.45
C	1,736	9,915	190	0.47	1,658	19,975	176	0.44

Table 3 Lower and upper bounds for the TRRA

Dataset	Horizontal stress (kPa)	Shear Modulus (kPa)	Undrained shear strength (kPa)
A	(1,267 2,113)	(9,000 27,000)	(80 240)
B		(9,000 50,000)*	
C		(9,000 27,000)	

***Note:** To compare with Jefferies (1988), the upper bound of shear modulus for dataset B is relaxed to 50,000 kPa

Table 4 Optimal parameters from the inverse analysis of the expansion curve using the TRRA

Dataset	Optimal values using the closed-form solution				Optimal values using the numerical model			
	σ_h (kPa)	G (kPa)	S_u (kPa)	SSE	σ_h (kPa)	G (kPa)	S_u (kPa)	SSE
A	1,736	9,920	190	0.47	1,695	17,962	173	0.45
B	1,456	44,116	189	0.48	1,489	42,840	176	0.44
C	1,736	9,922	190	0.47	1,703	16,314	178	0.43

Table 5 Optimal parameters from the inverse analysis of the expansion curve using the SS

Optimal values using the closed-form solution				Optimal values using the numerical model			
σ_h (kPa)	G (kPa)	S_u (kPa)	SSE	σ_h (kPa)	G (kPa)	S_u (kPa)	SSE
1,577	22,930	190	0.49	1,680	16,546	166	0.48

Table 6 Initial parameters for the inverse analysis of the complete curve

Dataset	Initial values (Initial)				
	σ_{h0} (kPa)	G_0 (kPa)	S_{u0} (kPa)	β	SSE
D	1,690	18,000	160	0.83	1.81
E	1,670	20,000	160	0.70	1.29
F	1,730	16,000	150	1.30	1.88

Notes:

1. Initial values of D (Initial D) refer to Fig. 10 in Jefferies (1988).
2. Initial values of E (Initial E) and F (Initial F) refer to Figs. 8a and 8b in Jefferies (1988).

Table 7 Optimal parameters from the inverse analysis of the complete curve using the LMA

Dataset	Optimal values using the closed-form solution					Optimal values using the numerical model				
	σ_h (kPa)	G (kPa)	S_u (kPa)	β	SSE	σ_h (kPa)	G (kPa)	S_u (kPa)	β	SSE
D	1,610	23,097	173	0.60	0.99	1,709	15,344	180	0.79	0.49
E	1,619	22,271	172	0.64	1.02	1,702	15,536	183	1.03	0.59
F	1,620	21,839	173	0.68	1.04	1,715	16,677	170	0.93	0.61

Table 8 Lower and upper bounds for the TRRA

Dataset	Horizontal stress (kPa)	Shear Modulus (kPa)	Undrained shear strength (kPa)	β
D	(1,267 2,113)	(9,000 27,000)	(80 240)	(0.4 1.5)
E				
F				

Table 9 Optimal datasets from the inverse analysis of the complete curve using the TRRA

Dataset	Optimal values using the closed-form solution					Optimal values using the numerical model				
	σ_h (kPa)	G (kPa)	S_u (kPa)	β	SSE	σ_h (kPa)	G (kPa)	S_u (kPa)	β	SSE
D	1,616	23,109	171	0.58	0.99	1,707	18,632	167	0.87	0.83
E	1,628	22,269	169	0.65	1.03	1,691	19,121	172	0.83	0.66
F	1,614	22,983	172	0.56	1.00	1,739	16,657	156	1.12	0.97

Table 10 Lower and upper bounds for the SS

Horizontal stress (kPa)	Shear Modulus (kPa)	Undrained shear strength (kPa)	β
(1,267 2,113)	(9,000 27,000)	(80 240)	(0.8 0.9)

Table 11 Optimal parameters from the inverse analysis of the complete curve using the SS

Optimal values using the closed-form solution					Optimal values using the numerical model				
σ_h (kPa)	G (kPa)	S_u (kPa)	β	SSE	σ_h (kPa)	G (kPa)	S_u (kPa)	β	SSE
1,616	24,124	169	0.88	1.04	1,725	14,826	174	0.85	0.49

Table 12 Optimized parameters after inverse analysis of the expansion curve using the closed-form solution

Type	Predicted values	Horizontal stress (σ_h) (kPa)	Shear modulus (G) (kPa)	Undrained strength (S_u) (kPa)	β
Expansion curve	mean	1,736	9,915	190	-
	95% CI	(1,652 1,820)	(5,412 14,418)	(180 199)	-
Complete curve	mean	1,610	23,097	173	0.60
	95% CI	(1,526 1,695)	(13,365 32,828)	(165 182)	(0.0 1.3)

Table 13 Optimized parameters after inverse analysis of the complete curve using the numerical model

Type	Predicted values	Horizontal stress (σ_h) (kPa)	Shear modulus (G) (kPa)	Undrained strength (S_u) (kPa)	β
Expansion curve	mean	1,713	15,289	178	-
	95% CI	(1,593 1,832)	(6,263 24,315)	(164 193)	-
Complete curve	mean	1,709	15,344	180	0.79
	95% CI	(1,649 1,769)	(11,638 19,050)	(172 188)	(0.53 1.05)

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Figures

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Fig. 6 Fit of observed data to predicted data using the closed-form solution for test AF85P06-15 (Jefferies, 1988). Note: (a) is predicted with the closed-form solution, and (b) is predicted with the numerical model.

Fig. 7 Fit of observed data to predicted data using the numerical modelling for test AF85P06-15 (Jefferies, 1988). Note: (a) is predicted with the closed-form solution, and (b) is predicted with the numerical model.

Appendix A Optimization algorithms for inverse analysis

To solve objective functions, the Gauss-Newton algorithm (GNA) can be used as a modified Newton's method for finding the minimum of a function. Here, the LMA is used to find the local minimum for the objective function (Levenberg 1944; Morrison 1960; Marquardt 1963):

$$(J^T J + I\lambda)\delta = J^T[y - f(b)] \quad (A1)$$

where I represents the identity matrix. The LMA can converge to a local minimum (Conn 2000) but not necessarily the global minimum. With the Jacobian matrix calculated in the iterative procedure, statistical assessment upon the identified parameter values can be efficiently conducted.

Rather than searching along a line in one direction in the LMA, the trust-region algorithm (TRA) explores the vicinity of the trust region. TRAs are a class of iterative methods for nonlinear optimization problems, which have been extensively studied for decades (Yuan 2015; Conn 2000). To minimize the objective function, $f(x)$, $x \in X$, a trial step can be computed by solving the following trust-region subproblem:

$$\min_s [q(d), d \in N] \quad (A2)$$

where q represents an approximation of the objective function $f(x)$, d indicates a trial step, and N denotes a region of trust.

Usually, q is approximated by a quadratic function, and the trust-region neighbourhood is generally spherical or ellipsoidal (Moré 1978). Due to the constraint of the trust region, the TRA can be applied in cases of negative curvature of an objective function and ill-conditioned problems (Yuan 2015). To accelerate the quadratic convergence, Coleman and Li (1994) proposed

a piecewise reflective line search at each iteration to modify the TRA. The modified TRA is called the trust-region reflective algorithm (TRRA).

SS was initially developed for seismic risk analysis of building structures subjected to stochastic earthquake motions (Au and Wang 2014). As an alternative to the MCS, SS is a Monte Carlo methodology that takes advantage of the Markov Chain Monte Carlo (MCMC) method and a simple evolutionary strategy (Schueller 2009). Like other optimization algorithms using heuristic techniques, the SS algorithm is based on a stochastic search algorithm for global optimization problems. SS is more efficient than MCS, particularly when using a computationally costly numerical model. In the SS algorithm, the failure probability of a rare event can be estimated by multiplication of a sequence of conditional failure probabilities of intermediate events, which can be evaluated as follows:

Given a failure event F , let $F_1 \supset F_2 \supset \dots \supset F_m = F$ be a decreasing sequence of failure events, P_F

$$= P(F_m) = P\left(\bigcap_{i=1}^m F_i\right) = P(F_1) \prod_{i=1}^{m-1} P(F_{i+1} | F_i) \quad (A3)$$

where P_F denotes the probability of failure; $P(F_i)$ represents the failure probability of an intermediate event; and $\{P(F_{i+1} | F_i); i = 1, 2, \dots, m-1\}$ denotes the conditional probabilities (Au and Wang 2014).

Appendix B Interpretation of SBP tests using conventional deterministic methods

Conventional methods are first applied to interpret the SBP tests, which can verify the effectiveness of the results from the inverse analysis. Geotechnical data from triaxial tests (Jefferies 1987) are also deduced to constrain the range of estimated parameters.

Interpretation of SBP tests using graphical plotting and linear fit regression methods

With the assistance of constructing lines, σ_{h0} , G , and S_u can be deduced by examining a pressuremeter testing curve (Gibson and Anderson 1961; Houlsby and Withers 1988; Marsland and Randolph 1977).

The lift-off method is usually applicable to identify the horizontal stress, σ_{h0} , for SBP tests, although it is criticized for its subjectivity (Clarke 1995; Mair and Wood 1987). To reduce the subjectivity, Jefferies (1987) improved the lift-off method by introducing a modified inspection technique. It is believed that σ_{h0} lies at a stress lower than the yield stress, σ_{hy} . Therefore, the method needs to identify σ_{hy} by the first observation of excess pore pressure change or inspection of the pressuremeter-displacement curve. Thus, σ_{h0} can be located from the intersection of the constructed instrument stiffness line and the gradient line determined by the unloading–reloading cycle. From Fig. B1, σ_{h0} is evaluated as 1,690 kPa using the modified inspection technique, which lies in the range of $1,670 \pm 30$ kPa reported by Jefferies (1987).

According to Mair and Wood (1987), S_u can be deduced from the slope of a straight line by plotting the SBP data as $p : \ln(\Delta V/V)$. Alternatively, the slope of a straight line can be determined through the linear fit regression by use of Origin 2020 (OriginLab 2020). The benefit of using this approach is to reduce the subjectivity, and therefore results become repeatable. The undrained shear strength S_u is identified in Fig. B2 as 182 ± 7.6 kPa. Similarly, the shear modulus, G , can be

determined as $49,540 \pm 1,378$ kPa, which is one half of the fitted slope value in Fig. B3 (Mair and Wood 1987).

Interpretation of triaxial tests using graphical plotting methods

Jefferies (1988) reported an anisotropically consolidated undrained triaxial test with shear stress reversal. The initial Young's modulus, E_i , and the secant modulus at 50% strength, E_{50} , can be inferred from the line construction on the triaxial testing curve. Fig. B4 indicates that E_i and E_{50} is 41,200 kPa and 33,700 kPa, corresponding to $G_i = 13,730$ kPa and $G_{50} = 11,230$ kPa, respectively. At the same time, the shear strength, S_w , in loading and unloading is identified as 238 kPa and 191 kPa from the peak positive and negative deviatoric stresses. In addition, the softening coefficient, β , defined in Eq. 3 is 0.8 by calculating the ratio of shear strength in loading to unloading.

Table B1 summarizes the results from the interpretation of both SBP and triaxial tests. Compared to the triaxial test, G deduced from the unloading–reloading loop seems to be overestimated. This may be due to the drainage taking place near the probe during this stage (Clarke 1995), which could exaggerate the deduced value of G . The undrained shear strength, S_w , can refer to Table B1.

Table B1 Results from the conventional interpretation of SBP and triaxial tests

Method	σ_{h0} (kPa)	G (kPa)	S_u (kPa)
Modified inspection on the SBP test curve	1,690	-	-
Linear fit regression of the SBP test curve	-	$49,540 \pm 1,378$	182 ± 7.6
Line construction on the triaxial test curve	-	13,730 (G_i) 11,230 (G_{50})	238 (loading)* 191 (unloading)

***Note:** The ratio of shear strength in loading to unloading β is calculated as $191/238 = 0.8$

Fig. B1 Identification of the horizontal stress σ_{h0} using graphical plotting method (reproduced from Jefferies, 1987)

Fig. B2 Identification of the undrained shear strength S_u using the linear fitting method

Fig. B3 Identification of the shear modulus G using the linear fitting regression method

Fig. B4 Identification of the Young’s modulus E using the line construction method