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Calibration of an elasto-plastic constitutive model by a constrained optimisation procedure

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Abstract

The presented paper deals with a constrained optimisation technique for the calibration of elasto-plastic model parameters in a rational and objective manner. The procedure consists in finding a set of model parameters which minimise the difference between the experimental data and the numerical simulations defined by an objective function. For this purpose, an optimisation routine, termed ParaID, has been developed which combines the quasi-Newton and stochastic methods. The optimisation technique was employed to calibrate a multi-mechanism elasto-plastic constitutive model. Using the results of three isotropically consolidated drained triaxial compression tests, a comparison between numerical and experimental results clearly shows the capability of the optimisation procedure to determine the model parameters correctly.

Keywords: Optimisation; Model parameters; Elasto-plasticity; Constitutive modelling; Sensitivity analysis

1. Introduction

Numerical methods are most often used for solving complex engineering problems. In geotechnical engineering, problems are very often encountered in situations where sophisticated constitutive laws, including kinematic hardening, are needed. Such constitutive models tend to become tremendously complex, including a considerable number of parameters which are generally assessed on the basis of laboratory test results. However, the determination of this potentially large number of parameters is difficult and quite often depends on the users' experience. In such circumstances, the numerical modelling of geomaterials is mainly based on computational approximation and empirical knowledge, which inevitably may lead to some inaccuracy. Thus, it is a challenging task to calibrate a potentially large number of model parameters while simultaneously satisfying the available experimental data. The minimum amount of experimental data required for the calibration depends on the complexity of the phenomena to be modelled. In this paper, an optimisation technique which allows the calibration of the model parameters in a more rational and objective manner is proposed. The procedure consists in solving the following problem: to find a set of model parameters which minimise the difference between the experimental data and the numerical simulations, starting from a given set of parameters. The problem is defined by an objective function which evaluates the discrepancy between the model predictions and the experimental data. The primary task is the selection of the optimisation strategy enabling the search for the minimum of this function. The parameters of the selected model play the role of optimisation variables. Most optimisation

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routines are only capable of searching for a local minimum, which is done here using the quasi-Newton method. In order to ensure that the optimised model parameters correspond to a minimum of the objective function over the entire domain considered, the stochastic method has also been employed. This is the most appropriate method for problems where the dimension of the space in which the optimisation takes place, made up of model parameters, is high. Starting from the initially imposed parameters, variables are randomly generated to try to minimise the objective function and the resulting value is then compared to the original one, restricting the admissible parameter ranges further and further as the calculation progresses. These two methods (quasi-Newton and stochastic) are included in the developed ParaID optimisation routine. The optimisation technique is employed to calibrate a multi-mechanism elasto-plastic constitutive model [1]. A sensitivity analysis was also conducted to explore the complexities quite often encountered in optimising highly non-linear functions.

A set of drained triaxial shear tests carried out on Kaolin clay [2] were used in the calibration procedure. Finally, a comparison between numerical and experimental results is presented to show the capability of the optimisation procedure to derive model parameters correctly.

2. Mathematical methodology

In conventional soil mechanics, model parameters are calibrated based on experimental results appropriate for the type of boundary value problem under examination. However, sometimes the number of available experimental results, as well as the type of experiments, are not sufficient for the calibration of the model parameters. The goal of model calibration is to find appropriate parameters which yield the best model response in relation to the available experimental results (Fig. 1). The mathematical methodology proposed here for the identification of model parameters is a rational procedure for the minimisation of error between experimental results and numerical predictions.

The mathematical procedure for optimisation used here basically consists of two main parts [3]:

- Formulation of an objective function, $F(\mathbf{p})$, which measures the difference between the theoretical and experimental results;
- Selection of an optimisation strategy enabling the search for the minimum of the objective function.

The difference between the experimental data and the numerical prediction for a given number of points is measured by a norm value, which, when summed, yields an objective function, $F(\mathbf{p})$. Thus, the function provides a scalar measurement of the error between the experimental and the numerical data. From a mathematical point of view, the problem can be stated as follows:

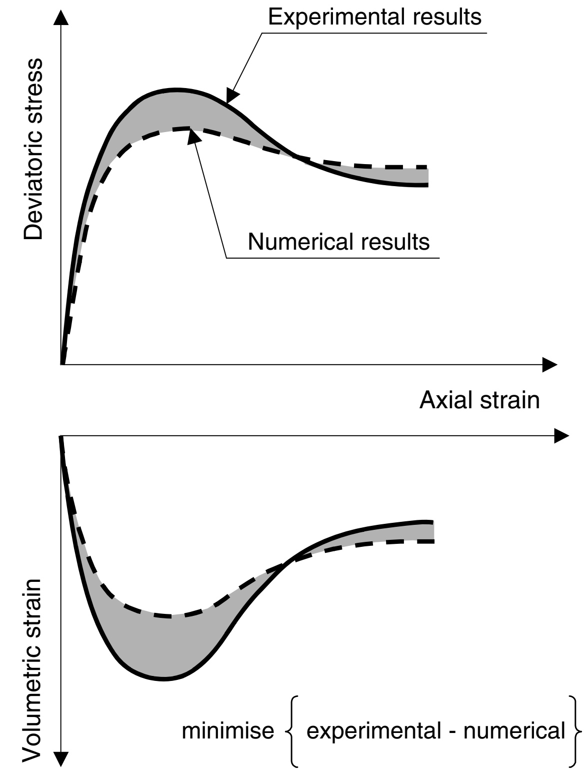

Fig. 1. Illustration of an optimization procedure used for the calibration of model parameters.

$$\text{minimise} \qquad F(\mathbf{p}) \tag{1}$$

$$\text{subject to constraints} \quad \mathbf{m} \leqslant \mathbf{p} \leqslant \mathbf{n} \tag{2}$$

where $\mathbf{p} \in \Re^n$ is a vector containing the model parameters; $\mathbf{m}$ and $\mathbf{n}$ are given bound vectors in $\Re^n$ and n is the number of variables to be optimised. The vectors $\mathbf{m}$ and $\mathbf{n}$ restrain the searching space for the vector $\mathbf{p}$ to a domain defined by reasonable parameter values. The solution of the optimisation problem is a vector $\mathbf{p}^*$, which satisfies the condition:

$$\forall \mathbf{p}: \quad \mathbf{m} \leqslant \mathbf{p} \leqslant \mathbf{n} \rightarrow F(\mathbf{p}^*) \leqslant F(\mathbf{p}) \tag{3}$$

Many algorithms have been proposed for solving small to medium-sized problems of the form (1) and (2) [4]. However, most optimisation routines are only capable of searching for a local minimum. One possibility to solve this problem is to start the search from different initial points and if the local minima become the same, they are most probably also the global minima.

However, it must be noted that even such a rational solution of model parameters, which may give satisfactory numerical results, requires a critical review. Based on experience and the physical meaning of the parameters, their suitability should be evaluated based on engineering judgement.

3. Objective function

The objective function can be defined as a function which evaluates, for a given set of parameters, the discrepancy between the model prediction and the experimental data. The function should include the stress/strain behaviour of the soil at every point involved in the optimisation and can be expressed as:

$$F(\mathbf{p}) = \frac{1}{t - t_0} \int \|Y^{\mathrm{e}} - Y^{\mathrm{n}}\| \mathrm{d}t \tag{4}$$

where $(t - t_0)$ is the duration of observation and $\|Y^{\mathrm{e}} - Y^{\mathrm{n}}\|$ represents a norm of the difference between the experimental data, Y^{e}, and numerical results, Y^{n}, for a given set of parameters.

In the formulation of an objective function, it is essential to construct a function of independent state variables represented by the principal total stresses σ_k $(k = 1,2,3)$, the principal strains ε_k $(k = 1,2,3)$ and the pore pressure, u. Since the measurements and the computed results are known only in discrete points, Eq. (4) can be replaced by a sum of individual norms at such points. Using the Euclidean norm and independent state variables, the objective function for only one point, $f(\mathbf{p})$, becomes:

$$f(\mathbf{p}) = \frac{1}{\sum_{k,l=1}^{3} w_{kl}} \left\{ \sum_{k=1}^{3} \frac{1}{\sigma_0^2} (\sigma_k^{\mathrm{e}} - \sigma_k^{\mathrm{n}}) w_{k1} (\sigma_k^{\mathrm{e}} - \sigma_k^{\mathrm{n}}) + \sum_{k=1}^{3} \frac{1}{\varepsilon_0^2} (\varepsilon_k^{\mathrm{e}} - \varepsilon_k^{\mathrm{n}}) w_{k2} (\varepsilon_k^{\mathrm{e}} - \varepsilon_k^{\mathrm{n}}) + \sum_{k=1}^{3} \frac{1}{u_0^2} (u^{\mathrm{e}} - u^{\mathrm{n}})^2 w_{k3} \right\} \tag{5}$$

where σ_k^{e}, $\varepsilon_k^{\mathrm{e}}$ and u^{e} are experimental values of deviator stress, volumetric strain and pore pressure, respectively; σ_k^{n}, $\varepsilon_k^{\mathrm{n}}$ and u^{n} are numerical values of deviator stress, volumetric strain and pore pressure for a given set of parameters; w_{kl} is a weighting matrix attributed to each state variable, $l = 1$ stresses, $l = 2$ strains and $l = 3$ pore pressure and $k = 1, 2, 3$.

Following the Critical State theory [5], stress invariants will be used: the deviator stress, $q = (\sigma_1 - \sigma_3)$ and mean effective stress, $p' = \frac{1}{3}(\sigma_1 + \sigma_2 + \sigma_3) - u$ and the corresponding strain invariants: volumetric strain $\varepsilon_{\mathrm{v}} = (\varepsilon_1 + \varepsilon_2 + \varepsilon_3)$ and distortional strain, $\varepsilon_{\mathrm{s}} = \frac{\sqrt{2}}{3}[(\varepsilon_1 - \varepsilon_2)^2 + (\varepsilon_2 - \varepsilon_3)^2 + (\varepsilon_3 - \varepsilon_1)^2]^{1/2}$. Thus, the experimental results may be represented in four planes: q vs. ε_1, q vs. p', ε_{v} vs. ε_1, e vs. p'; e is the void ratio. To describe either drained or undrained triaxial shear tests, two independent planes q vs. ε_1 and ε_{v} vs. ε_1 or u vs. ε_1 will be used. Thus, the optimisation procedure developed here considers only experimental results presented in these three planes. Of course, the procedure could be easily modified to include any another plane or to use other state variables. Using the above-mentioned constraints, for one experimental result, the objective function becomes:

$$f^k(\mathbf{p}) = \frac{1}{\sum_{j,k=1}^{m,3} w_{jk}} \left\{ \sum_{j=1}^{m} \frac{1}{q_0^2} \left(q_j^{\mathrm{e}} - q_j^{\mathrm{n}}\right) w_{j1} \left(q_j^{\mathrm{e}} - q_j^{\mathrm{n}}\right) + \sum_{j=1}^{m} \frac{1}{\varepsilon_{v0}^2} \left(\varepsilon_{vj}^{\mathrm{e}} - \varepsilon_{vj}^{\mathrm{n}}\right) w_{j2} \left(\varepsilon_{vj}^{\mathrm{e}} - \varepsilon_{vj}^{\mathrm{n}}\right) + \sum_{j=1}^{m} \frac{1}{u_0^2} \left(u_j^{\mathrm{e}} - u_j^{\mathrm{n}}\right) w_{j3} \left(u_j^{\mathrm{e}} - u_j^{\mathrm{n}}\right) \right\} \tag{6}$$

where q_j^{e}, $\varepsilon_{vj}^{\mathrm{e}}$ and u_j^{e} are experimental values of deviator stress, volumetric strain and pore pressure in point j, respectively; q_j^{n}, $\varepsilon_{vj}^{\mathrm{n}}$ and u_j^{n} are numerical values of deviator stress, volumetric strain and pore pressure at point j for a given set of parameters; m is the number of measurement points used in the optimisation procedure.

The values q_0, ε_{v0} and u_0 are scaling factors necessary to transform the observable variables into non-dimensional quantities. The scaling factors are chosen as the maximum absolute value of the corresponding variable at the discrete points involved in the computation:

$$\begin{aligned} q_0 &= \max\left\{q_j^{\mathrm{e}}\right\}, \quad j = 1, m \\ \varepsilon_{v0} &= \max\left\{\varepsilon_{vj}^{\mathrm{e}}\right\}, \quad j = 1, m \\ u_0 &= \max\left\{u_j^{\mathrm{e}}\right\}, \quad j = 1, m \end{aligned} \tag{7}$$

giving the inequalities

$$\begin{aligned} -1 &\leqslant \frac{1}{q_0^2}\left(q_j^{\mathrm{e}} - q_j^{\mathrm{n}}\right) w_{1j} \left(q_j^{\mathrm{e}} - q_j^{\mathrm{n}}\right) \leqslant 1 \\ -1 &\leqslant \frac{1}{\varepsilon_{v0}^2}\left(\varepsilon_{vj}^{\mathrm{e}} - \varepsilon_{vj}^{\mathrm{n}}\right) w_{2j} \left(\varepsilon_{vj}^{\mathrm{e}} - \varepsilon_{vj}^{\mathrm{n}}\right) \leqslant 1 \\ -1 &\leqslant \frac{1}{u_0^2}\left(u_j^{\mathrm{e}} - u_j^{\mathrm{n}}\right) w_{3j} \left(u_j^{\mathrm{e}} - u_j^{\mathrm{n}}\right) \leqslant 1 \end{aligned} \tag{8}$$

In Eqs. (5) and (6), the weighting matrix w_{ij} introduces the possibility of characterising the relative importance of the tests. Moreover, by using this weighting factor, confidence in the measured experimental variables q, ε_{v} and u is introduced. By doing this, we take into account different errors in measurement of state variables. Under undrained conditions, volumetric strain is negligible ($\varepsilon_{\mathrm{v}} \approx 0$) and its contribution should be removed from Eq. (6), while in drained conditions, the pore pressure is a constant ($\Delta u = 0$) and thus the third term disappears.

Calibration of model parameters in soil plasticity has been traditionally carried out based on the results of three shear tests at different confining (or normal) pressures. Therefore, the final form of the objective function is obtained by adding the objective functions computed for each experimental result included in the optimisation:

$$F(\mathbf{p}) = \sum_{s=1}^{3} f^s(\mathbf{p}) \tag{9}$$

where $F(\mathbf{p})$ is the sum of the norm value for the tests $s = 1{,}2$ and 3.

If necessary, in Eq. (9) a new weighting vector can easily be incorporated, giving:

$$F(\mathbf{p}) = \frac{1}{\sum_{s=1}^{3} w^s} \sum_{s=1}^{3} w^s f^s(\mathbf{p}) \tag{10}$$

which can introduce differences in the importance or confidence of the experimental results carried out at different stress states.

4. The optimisation strategy

The solution of the problem stated by Eqs. (1) and (2) requires the minimisation of a suitable function given by Eq. (9). It is emphasised that optimisation is meaningful only if the model predictions ($q_j^{\mathrm{n}}, \varepsilon_{vj}^{\mathrm{n}}$ and u_j^{n}) adequately describe the essential physical mechanism of the experimental tests [6]. According to the definition of the objective function, the minimisation can be achieved by means of a wide range of optimisation algorithms [7]. The methods can be divided into two groups: i) direct search methods in which the search strategy is based only on values of the objective function and ii) gradient methods, which also require computations of the derivatives of the objective functions. In general, the gradient methods are expected to be more powerful than those using only the values of the objective function [7]. On the other hand, the gradient methods are more complex to implement because of the requirements of having an objective function which is always differentiable and which possesses continuous derivatives over the considered domain. In general, the objective function, $F(\mathbf{p})$, is a highly non-linear function and may possess many local minima. However, the goal of the research is to find a point where $F(\mathbf{p})$ assumes its least value, or the global minimum, inside the considered domain. According to [6] there is no general way to determine whether a minimum point is global or not. To achieve the global minimum, a possible strategy could be to run the search algorithm as many times as possible, each time from a different point. Thus, the more runs, the higher the chance that the global minimum may be found. Another strategy would be to implement a global algorithm which aims at finding arguments corresponding to the global minimum.

In order to find the global minimum of the problem, a combination of stochastic and quasi-Newton methods have been employed in the developed optimisation program. The quasi-Newton method combines the advantages of the gradient method with those of the Newton approach. The method uses gradients of the objective functions, giving an inverse of the Hessien matrices indicating the precision of the obtained parameters. The other advantage of the quasi-Newton method is that there is no need to resolve the system of linear functions, which rapidly increases computation time. To obtain the direction of decrease of the objective function, the quasi-Newton method and the gradient method were used to treat inactive and active variables, respectively. The number of optimisations to be carried out is equal to the number of variables.

Stochastic methods belong to the category of direct search methods, while quasi-Newton methods belong to the gradient methods.

The stochastic method, here called the global method, is needed to ensure that the optimised model parameters correspond to a minimum of the objective function over the entire domain considered. Among the strategies tested, the stochastic method is the most appropriate one for problems where the dimension of the space in which the optimisation takes place, constituted of model parameters, is large. It requires fewer evolutions of the objective function in comparison with deterministic methods.

These two optimisation techniques were coupled and implemented in a program called ParaID, devoted to the parameter optimisation. ParaID permits the use of either a combination of the techniques employed or only one of them. The most common and recommended approach is to start with the stochastic method and to use the variables obtained as an input for the quasi-Newton method and, finally, to verify the optimum obtained by the stochastic method again.

4.1. Stochastic search strategy

The stochastic method is a class of the global optimisation procedure that drives the computation of global minima of nonlinear functions. Stochastic methods are designed for solving essentially unconstrained smooth problems where no additional structural properties are presented [8]. The random search strategy presented here is extremely simple to implement but may fail to locate any global minima. In general, a random search algorithm may be presented by the following steps:

(i) choose $\mathbf{p}^0$, set $k = 0$;

(ii) compute a trial point, $\mathbf{p}^{k+}$, according to the rule:

$$\mathbf{p}^{k+} = \mathbf{p}^k + \mathbf{r}^k \tag{11}$$

where $\mathbf{r}^k$ is a suitably-distributed random vector.

(iii) If $F(\mathbf{p}^{k+}) < F(\mathbf{p}^k)$ then:

$$\mathbf{p}^{k+1} = \mathbf{p}^{k+} \quad \text{otherwise} \quad \mathbf{p}^{k+1} = \mathbf{p}^k \tag{12}$$

(iv) $k = k + 1$ and go to step (ii).

A very important task is the selection of the vector $\mathbf{r}^k$: when $\mathbf{p}^k$ is far from $\mathbf{p}^*$, $\mathbf{r}^k$ should have a large variance to allow large displacements which might be necessary to escape the attraction by any local minimum. Otherwise, when $\mathbf{p}^k$ is near $\mathbf{p}^*$, $\mathbf{r}^k$ should have a small variance to allow finer exploration of the parametric space [9]. In order to satisfy these two conditions, Bekey and Masri [10] and Pronzato et al. [11] proposed an adaptive random search. The idea is to alternate variance-selection phases and variance-exploitation phases, during which the selected variance is used.

According to the notation in Eq. (2), the acceptable domain of the parameters is assumed to be the box:

$$\mathbf{p} | m_i \leqslant p_i \leqslant n_i, \quad i = 1, 2, \ldots n \tag{13}$$

where n is the number of variables to be optimised. The search is initialised at the centre of the admissible domain according to:

$$p_i^0 = \frac{m_i + n_i}{2}, \quad i = 1, 2, \ldots n \tag{14}$$

The displacement $\mathbf{r}^k$ is randomly generated according to the Gauss distribution:

$$\Sigma(\boldsymbol{\omega}) = \text{diag}\ \{\omega_i^2,\ i = 1, 2 \ldots n\} \tag{15}$$

For large displacements in the domain, the variance ω is generated:

$$^{1}\boldsymbol{\omega} = \mathbf{m} - \mathbf{n} \tag{16}$$

and for finer explorations:

$$^{i}\boldsymbol{\omega} = \frac{^{i-1}\boldsymbol{\omega}}{10}, \quad i = 2, 3, 4 \quad \text{and} \quad 5 \tag{17}$$

The best $^{i}\boldsymbol{\omega}$ in terms of the objective function is selected from the variance-exploitation phase. Starting from the best $\mathbf{p}$ obtained during the variance-selection phase, the basic algorithm is used with the covariance $\Sigma(\boldsymbol{\omega})$ for one hundred iterations before resuming a variance-selection phase. The algorithm ends when the maximum number of the objective function is reached or when $^{5}\boldsymbol{\omega}$ has been selected five times consequently. Then, the search may switch to local optimisation, which is explained in the following section.

4.2. The quasi-Newton algorithm

According to Chong and Zak [12], the Newton method is one of the more successful algorithms for local optimisation. If it converges, it has at least a quadratic order of convergence, but if the initial point is not sufficiently close to the solution, the algorithm may not be an adequate one.

Assuming that $F(\mathbf{p})$ is twice-continuously differentiable, the first derivative (gradient) and the second derivative of $F(\mathbf{p})$ are given by:

$$g(\mathbf{p}) = \frac{\partial F(\mathbf{p})}{\partial \mathbf{p}} \quad \text{and} \quad H(\mathbf{p}) = \frac{\partial^2 F(\mathbf{p})}{\partial^2 \mathbf{p}} \tag{18}$$

where $H(\mathbf{p})$ is the second derivative, known as a Hessien of $F(\mathbf{p})$. The sufficient conditions for a minimum in the optimisation problem are:

$$g(\mathbf{p}^*) = 0 \quad \text{and} \quad H(\mathbf{p}^*) > 0 \tag{19}$$

where $\mathbf{p}^*$ is a stationary point (i.e. local minimum). When both $g(\mathbf{p})$ and $H(\mathbf{p})$ can be evaluated directly, the Newton method is typically the most efficient for optimisation. In cases where the explicit expression of $g(\mathbf{p})$ and/or $H(\mathbf{p})$ are not available, the quasi-Newton algorithm using approximations for $g(\mathbf{p})$ and/or $H(\mathbf{p})$ can be employed [6]. The method adopted here is based on a subspace limited memory quasi-Newton algorithm proposed by Ni and Yuan [4]. The search direction consists of three parts: a quasi-Newton direction in the subspace spanned by inactive variables and two others, the gradient and modified gradient directions in the space spanned by active variables. The active $A(\mathbf{p})$ and inactive $B(\mathbf{p})$ variables are defined by:

$$\begin{aligned} &A(\mathbf{p}) = \{i : m_i \leqslant p_i \leqslant m_i + \delta_b \quad \text{or} \quad i : n_i - \delta_b \leqslant p_i \leqslant n_i\} \\ &B(\mathbf{p}) = \{1, \ldots, k\}/A(\mathbf{p}) = \{i : m_i + \delta_b < p_i < n_i - \delta_b\} \end{aligned} \tag{20}$$

The tolerance δ_b should be sufficiently small so that:

$$0 < \delta_b < \min_i \frac{1}{3}(n_i - m_i) \tag{21}$$

The search direction for inactive variables, $B(\mathbf{p})$, is chosen as:

$$-P_0^k H_k P_0^k \nabla F(p_k) \tag{22}$$

where P_0^k is the matrix whose columns are $\{e_i|\ i \in B(p_k)\}$ and H_k is an approximation of the reduced inverse Hessien matrix and ∇F the gradient of the objective function. For active variables, the search directions can be divided into three regions: (i) $A_1(\mathbf{p})$ where the steepest descent directions head towards the outside of the feasible region, (ii) $A_2(\mathbf{p})$ where the steepest descent directions move inside the region and (iii) $A_3(\mathbf{p})$ in which the steepest directions head towards the boundaries. If we define $P_j^{(k)}$ as the matrix whose columns are $\{e_i|i \in A_j(p_k)\}$, the search direction at the kth iteration is defined by

$$d_k = -\left(P_0^k H_k P_0^{kT} + P_2^k P_2^{kT} + P_3^k P_3^{kT} \Lambda_k\right)(g_k) \tag{23}$$

where $g_k = \nabla F(p)$

$$\Lambda_k = \text{diag}\ \{\lambda_1^k, \ldots, \lambda_n^k\} \tag{24}$$

which is given by:

$$\lambda_i^k = \begin{cases} 0, & \text{if } i \notin A_3(p) \\ \left(p_i^k - m_i\right)/g_i^k & \text{if } m_i < p_i \leqslant m_i + \delta_b \quad \text{and} \quad p_i^k - \nabla F\left(p_i^k\right) \leqslant m_i \\ \left(p_i^k - n_i\right)/g_i^k & \text{if } n_i - \delta_b \leqslant p_i \leqslant n_i \quad \text{and} \quad p_i^k - \nabla F\left(p_i^k\right) \geqslant n_i \\ 1, & \text{otherwise} \end{cases} \tag{25}$$

g_i^k is the component i of the vector g_k. The search direction given by Eqs. (23) and (24) ensures that $p_i^k + d_i^k$ holds inside the region $A_3(\mathbf{p})$.

In order to solve quadratic and nonlinear programming problems with simple bounds on the variables, a projected search has been used [13,14,4]. A projected search requires that a parameter α_k be chosen to satisfy the following condition:

$$\phi_k(\alpha) \leqslant (\phi_k(0) + \mu\phi_k.\alpha) \tag{26}$$

for constants $\mu \in (0,1/2)$. The function ϕ_k is a twice continuously-differentiable function defined by:

$$\phi_k(\alpha) = F(\mathbf{p})(P_\Omega[p_k + \alpha d_k]) \tag{27}$$

and

$$\Omega = \{\mathbf{p} \in \Re^n : \mathbf{m} \leqslant \mathbf{p} \leqslant \mathbf{n}\} \tag{28}$$

while P_Ω is the projection on the domain Ω defined by:

$$(P_\Omega \mathbf{p})_i = \begin{cases} p_i & \text{if } m_i \leqslant p_i \leqslant n_i \\ m_i & \text{if } p_i < m_i \\ n_i & \text{if } p_i > n_i \end{cases} \tag{29}$$

4.2.1. Inverse of the Hessien matrix

The inverse Hessien matrix, H, is commonly approximated using matrix-update methods such as the popular Broydon–Fletcher–Goldfarb–Shanno (BFGS) method [15]. The idea is to generate a matrix $\mathbf{H}_k$ that tends to the inverse of the Hessien without inverting a matrix. The following may be noted:

$$\mathbf{s}_k = \mathbf{p}_{k+1} - \mathbf{p}_k; \quad \mathbf{y}_k = \nabla F(\mathbf{p}_{k+1}) - \nabla F(\mathbf{p}_k) \tag{30}$$

$$a = \mathbf{s}_k^T \mathbf{y}_k; \quad b = \mathbf{y}_k^T \mathbf{H}_k \mathbf{y}_k \tag{31}$$

$$\rho_i = \frac{1}{s_i^T y_i}; \quad Q = I - \rho_i y_i s_i^T \tag{32}$$

According to the limited memory BFGS, an approximation of the full space inverse Hessien matrix is given by:

$$\begin{aligned}\overline{H}_{k+1} = {} & Q_k^T \ldots Q_t^T \overline{H}_0 Q_t \ldots Q_k \\ & + Q_k^T \ldots Q_{t+1}^T \rho_t s_t s_t^T Q_{t+1} \ldots Q_k \ldots \\ & + Q_k^T \rho_{k-1} s_{k-1} s_{k-1}^T Q_k + \rho_k s_k s_k^T\end{aligned} \tag{33}$$

where $t = \max\{0, k-q+1\}$, q is a given positive integer, $\overline{H}_0 = I$ is a given positive definite matrix. In order to retain $\mathbf{s}_k^T \mathbf{y}_k > 0$, $\mathbf{s}_k$ is replaced by $\mathbf{s}'_k$ defined by

$$\mathbf{s}'_k = \theta \mathbf{s}_k + (1-\theta) \mathbf{H}_k \mathbf{y}_k \tag{34}$$

where:

$$\theta = \begin{cases} 1 & \text{if } a \geqslant 0.2b \\ 0.8b/(b-a) & \text{otherwise} \end{cases} \tag{35}$$

In Eq. (34), $\mathbf{H}_k$ is the reduced matrix, defined as

$$\mathbf{H}_k = P_0^{(k)T} \overline{\mathbf{H}}_k P_0^{(k)} \tag{36}$$

where $\overline{\mathbf{H}}_k$ is an approximation of the full space inverse Hessien matrix.

4.2.2. The algorithm used

The subspace limited memory quasi-Newton (SLMQN) algorithm, proposed by Ni and Yuan [4], has been used for solving the optimisation problem at the local level. The procedure is as follows:

(i) Choose a constant $\mu \in (0,1/2)$ and $\mathbf{H}_0 = I$, variables $\mathbf{p}_0 \in \Re^n$ with respect to constraint $\mathbf{m} \leqslant \mathbf{p}_0 \leqslant \mathbf{n}$. If the SLMQN algorithm has been implemented after a stochastic search strategy then $\mathbf{p}_0 = \mathbf{p}_s$ where $\mathbf{p}_s$ is a solution obtained by the stochastic method.Compute $F(\mathbf{p}_0)$, $\nabla F(\mathbf{p}_0)$ and set $k = 0$.
(ii) Determine the search direction:compute $B(\mathbf{p})$ and $A_1(\mathbf{p})$, $A_2(\mathbf{p})$ and $A_3(\mathbf{p})$ and the search direction d_k from Eq. (23).
(iii) Determine a step length α_k and calculate $\mathbf{p}_{k+1} = P_\Omega[\mathbf{p}_k + \alpha_k d_k]$. Verify the termination condition; if it is satisfied stop the procedure.
(iv) Otherwise, calculate $\mathbf{H}_{k+1}$ according to the limited memory BFGS; impose $k = k+1$ and go to the first step.

5. Elasto-plastic constitutive model

It is obvious that the results of an optimisation process strongly depend on the ability of the chosen model to describe the soil behaviour. Thus, it is crucial to have knowledge about the range of application of the constitutive model. Herein, the constitutive model and parameters to be optimised are briefly summarised and more details can be found in the appropriate references.

Under the influence of mechanical loads, saturated soils experience non-linearity and plasticity. Elasto-plastic models using critical state formulations have been very successful in describing many of the more important aspects of the mechanical behaviour of soils. In this paper, the optimisation approach explained above is applied to an elasto-plastic model with isotropic and kinematical hardening developed by Aubry et al. [16] and Hujeux [1]. This model is a generalisation of the critical state theory in which the theory of coupled multi-mechanism elasto-plasticity, as in the Koiter–Mandel theory of elasto-plasticity [17], is introduced. The limit criterion is very close to that of Mohr–Coulomb and its yield function is similar to that of Cam Clay. In each plane (three planes), a plane plastic strain hypothesis is adopted. The orthotropic nature of the model stipulates that the physical coordinate axes be parallel to the principal stress directions. Two kinds of internal parameters are required: some subjected to a continuous flow rule and others obeying a discontinuous evolution, so that a double memory is built into the model. The second type of internal parameter is sometimes referred to as discrete memory internal parameters, as they represent only the last loading reversal in each plane. The irreversible phenomenon is represented by four coupled elementary elasto-plastic mechanisms: three deviatoric and one isotropic. These four mechanisms are activated during monotonic, as well as cyclic, loading. Each mechanism has its own hardening parameters related to distortion in the corresponding plane (k) and all four mechanisms are coupled by the isotropic hardening parameter, volumetric plastic strain,

$$\varepsilon_{\mathrm{v}}^{\mathrm{p}} = \sum_{k=1}^{4} \left(\varepsilon_{\mathrm{v}}^{\mathrm{p}}\right)_k.$$

In the following, because of the strain history dependence, the formulation is given in the incremental form. The total strain rate $\dot{\boldsymbol{\varepsilon}}$ is split into elastic and plastic parts.

5.1. Elastic and plastic formulations

The elastic strain, rate, $\dot{\varepsilon}^{\mathrm{e}}$, is given by:

$$\dot{\varepsilon}_{\mathrm{v}}^{\mathrm{e}} = \frac{\dot{p}'}{K} \tag{37}$$

$$\dot{\varepsilon}_{\mathrm{d}}^{\mathrm{e}} = \frac{\dot{\sigma}_{\mathrm{d}}}{G} \tag{38}$$

where $\dot{\varepsilon}_{\mathrm{v}}^{\mathrm{e}}$ is the volumetric strain rate ($\dot{\varepsilon}_{\mathrm{v}}^{\mathrm{e}} = tr(\dot{\varepsilon}^{\mathrm{e}})$) and $\dot{\varepsilon}_{\mathrm{d}}^{\mathrm{e}}$ the deviatoric strain rate $\left(\dot{\varepsilon}_{\mathrm{d}}^{\mathrm{e}} = \dot{\varepsilon}^{\mathrm{e}} - \frac{1}{3}\dot{\varepsilon}_{\mathrm{v}}^{\mathrm{e}} I\right)$; $\dot{\sigma}'_{\mathrm{d}}$ and $\dot{p}'$ are the deviatoric effective stress rate and rate of the mean effective pressure, respectively, expressed as:

$$\dot{\sigma}'_{\mathrm{d}} = \dot{\sigma}' - \dot{p}' I \tag{39}$$

$$\dot{p}' = tr(\dot{\sigma}')/3 \tag{40}$$

The hypo-elastic moduli are given by:

$$K = K_{\mathrm{ref}} \left(\frac{p'}{p_{\mathrm{ref}}}\right)^{\mathrm{n}} \quad G = G_{\mathrm{ref}} \left(\frac{p'}{p_{\mathrm{ref}}}\right)^{\mathrm{n}} \tag{41}$$

where K_{ref} and G_{ref} are the bulk and shear elastic moduli, respectively, at a reference pressure, p_{ref} (the value of the mean effective pressure at which the hypo-elastic moduli are measured); n being the non-linear elasticity exponent.

The plastic strain rate is given by:

$$\dot{\varepsilon}^{\mathbf{p}} = \lambda \cdot \Psi \tag{42}$$

with $\lambda(\boldsymbol{\sigma}, \alpha)$ being the plastic multiplier and Ψ $(\boldsymbol{\sigma}, \alpha)$ the direction of the strain increment. α represents the internal variables modifying the yield surfaces $f(\boldsymbol{\sigma}, \alpha)$.

5.2. Deviatoric yield limit

In order to take into account the anisotropy induced by the stress path, three deviatoric yield surfaces are written in three orthogonal planes (mechanisms k; $k = \{1,2,3\}$) of the stress space (Fig. 2). In each plane, a plane plastic strain hypothesis is assumed and a limit criterion very close to that of Mohr–Coulomb is obtained; its yield function is that of Cam Clay. Thus, the deviatoric yield surface for mechanism k is proposed as

$$f_{\text{d}} = q_k - p_k F_k r_k \sin\phi \tag{43}$$

where p_k and q_k are the reduced mean effective pressure and deviatoric stress, respectively, in the plane of each deviatoric mechanism k (Fig. 3), given as

$$\begin{aligned} q_k &= \|\mathbf{s}_k\| = \tfrac{1}{2}\left[\left(\sigma'_{ii} - \sigma'_{jj}\right)^2 + 4\sigma'^2_{ij}\right]^{1/2} \\ p_k &= \frac{\left(\sigma'_{ii} + \sigma'_{jj}\right)}{2} \\ k &= \{1,2,3\}; \quad i,j = \{2,3\},\{3,1\},\{1,2\} \end{aligned} \tag{44}$$

with the vector

$$\mathbf{s_k} = \left(\frac{1}{2}\left(\sigma'_{ii} - \sigma'_{jj}\right), \sigma'_{ij}\right)_k \tag{45}$$

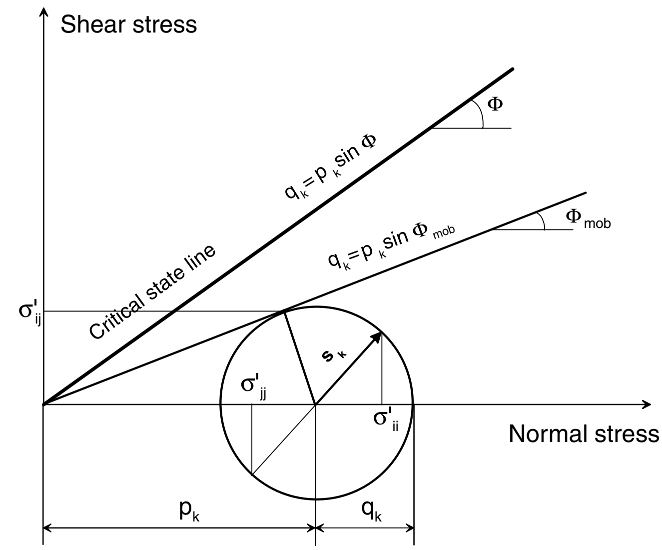

Fig. 3. Stress state in the (i,j) plane of the deviatoric mechanism k.

It may be noted that σ'_{ij} is a component of the tensor $\boldsymbol{\sigma}'$ (indicial notation is not used here). ϕ is the friction angle at the critical state.

The function F_k takes into account volumetric hardening or softening with respect to the critical state as:

$$F_k = 1 - b\left(\ln\frac{p_k}{p_{\text{c0}}} - \beta\varepsilon^p_{\text{v}}\right) \tag{46}$$

with b being a numerical parameter that controls the shape of the yield surface ($b = 0$ Mohr–Coulomb; $b = 1$ Cam Clay); β is the plastic compressibility modulus and p_{c0} the critical state pressure for the initial state.

The internal variable r_k represents the ratio of the mobilised friction over the maximum friction that may be mobi-

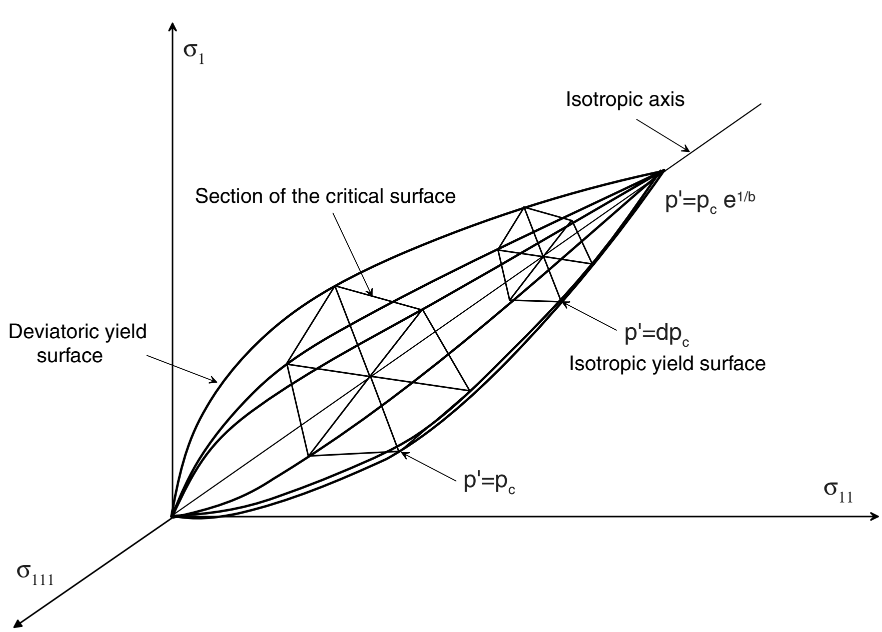

Fig. 2. Yield surfaces in the principal stress plane.

lised. It permits the decomposition of the behaviour domain into elastic, hysteretic and mobilised domains introduced by other model parameters termed r_{el}, r_{hys} and r_{mob} [1].

The variables F_k and r_k both introduce isotropic hardening but have different evolution rules and different origins. The first one introduces the isotropic hardening associated with plastic volumetric strain, as in the Cam clay model. The second one represents the isotropic hardening caused by the deviatoric plastic strain in each mechanism. The mechanisms are coupled only due to the first one, as the second is attached to each physical plane representing the deviatoric mechanism.

5.3. Isotropic yield limit

The development of plastic strain starts when the stress point reaches the yield limit. For isotropic paths, the preconsolidation pressure represents this yield limit.

The isotropic yield limit, f_i, can be expressed simply as:

$$f_i = p' - \sigma'_c \tag{47}$$

The preconsolidation pressure, σ'_c, can be related to volumetric plastic strain, ε_v^p, by:

$$\sigma'_c = \sigma'_{c0} \exp\left\{\beta \varepsilon_v^p\right\} \tag{48}$$

where β is the plastic compressibility (the slope of the plastic part of the $\varepsilon_v - \log \sigma'$) and σ'_{c0} the initial preconsolidation stress.

The complete expression of the isotropic yield limit is thus given by:

$$f_i = p' - \sigma'_{c0} \exp\left\{\beta \varepsilon_v^p\right\} \tag{49}$$

The proposed yield function will produce elastic deformations up to σ'_c and, beyond it, elasto-plastic ones. In such a case, the point that defines preconsolidation pressure corresponds to the abrupt change of the slope in the volumetric strain – $\ln p'$ plane. In order to have a smooth transition from the elastic to the plastic domain, which is realistic, the yield surface will be multiplied by a parameters r_i [1]:

$$r_i = r^e + \frac{\varepsilon_v^p}{c + \varepsilon_v^p} \tag{50}$$

where r^e is the radius of the elastic domain and c is the parameter which regulates the rate of the mobilisation of the isotropic mechanism.

Thus, the final form of the isotropic mechanism becomes:

$$f_i = p' - \sigma'_{c0} \exp\left\{\beta \varepsilon_v^p\right\} r_i \tag{51}$$

In this relation, the parameter r_i corresponds to the degree of mobilisation of the isotropic mechanism which is an hyperbolic function of ε_v^p; it varies from r^e, which defines the elastic domain, to 1 at a fully mobilised state (Fig. 4).

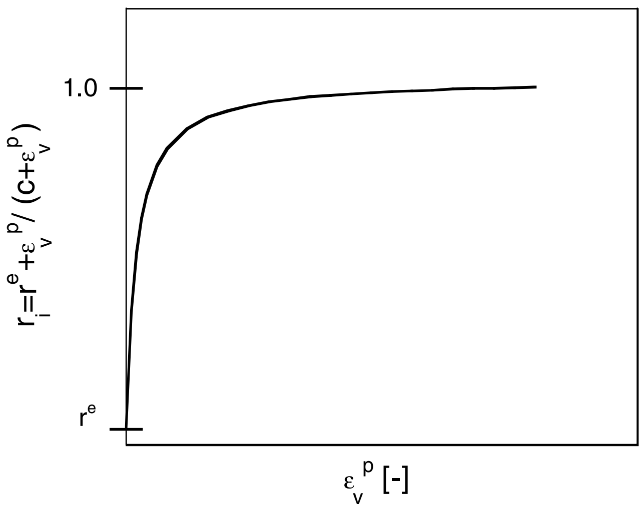

Fig. 4. Evolution of the parameter r_i with the volumetric plastic strain ε_v^p.

The isotropic mechanism presented above is coupled with the deviatoric parts. This coupling is driven by the volumetric plastic strain, ε_v^p. Thus, any variations of the

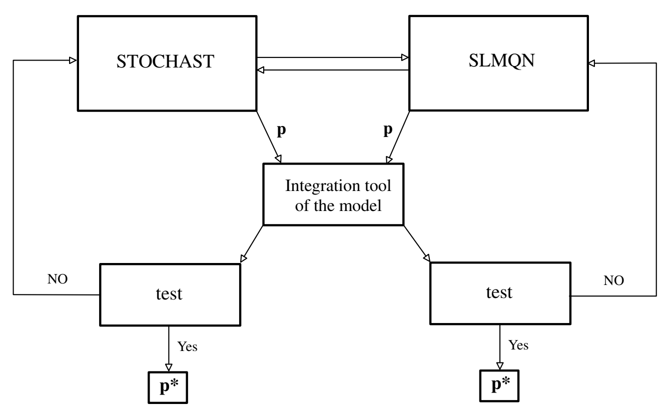

Fig. 5. Block diagram of the code ParaID.

Table 1
Optimisation domain for Hujeux model parameters

Optimization variable	Lower bound	Upper bound
Smooth variables		
ϕ [°]	0	30
β [–]	0	100
ψ [°]	0	30
α [–]	0	10
a [–]	1e–6	1
b [–]	0	1
r^e [–]	0	1
Neutral variables		
K [Pa]	1e5	1e9
G [Pa]	1e5	1e9
p_{c0} [Pa]	1e5	1e8
c [–]	1e–6	1
Irregular variables		
n [–]	0	1
r_{el} [–]	0	1
r_{hys} [–]	0	1
r_{mob} [–]	0	1

isotropic yield limit will also induce a modification of the deviatoric yield limit.

5.4. Model parameters

The model parameters to be determined can be split in the following groups:

(i) Elastic: the bulk modulus, K, the shear modulus, G, and the non-linear exponent, n, radius of elastic domain in deviatoric plane r_{el} and radius of elastic domain in isotropic plane, r^e,
(ii) Plastic: the friction angle, ϕ, the plastic compressibility modulus, β, the critical state pressure at the initial state, p_{c0}, internal variable α, numerical parameter b and dilatancy angle ψ,
(iii) hardening: a and c, radius of hysteretic and mobilised (r_{hys}, r_{mob}) domain, respectively. Thus, the total number of model parameters to be optimised is 15.

6. Numerical implementation

The optimisation techniques presented above (stochastic and quasi-Newton) have been coupled and implemented in the code ParaID, developed for parameter optimisation. The schematic block diagram of the code is presented in Fig. 5. The program is composed of an integration code of the constitutive law and two optimisation subroutines: STOCHAST which applies the stochastic search strategy and SLMQN which applies the quasi-Newton method. The ParaID code has been developed in a such way that it enables a combination of the employed techniques or use of only one of them. The most common and recommended approach is to start with the stochastic method (STOCHAST) and to use the obtained variables as an input for the quasi-Newton method (SLMQN) and then to verify this optimum by the stochastic method again. Moreover, it is recommended to repeat this procedure couple of times always changing the initial point. This

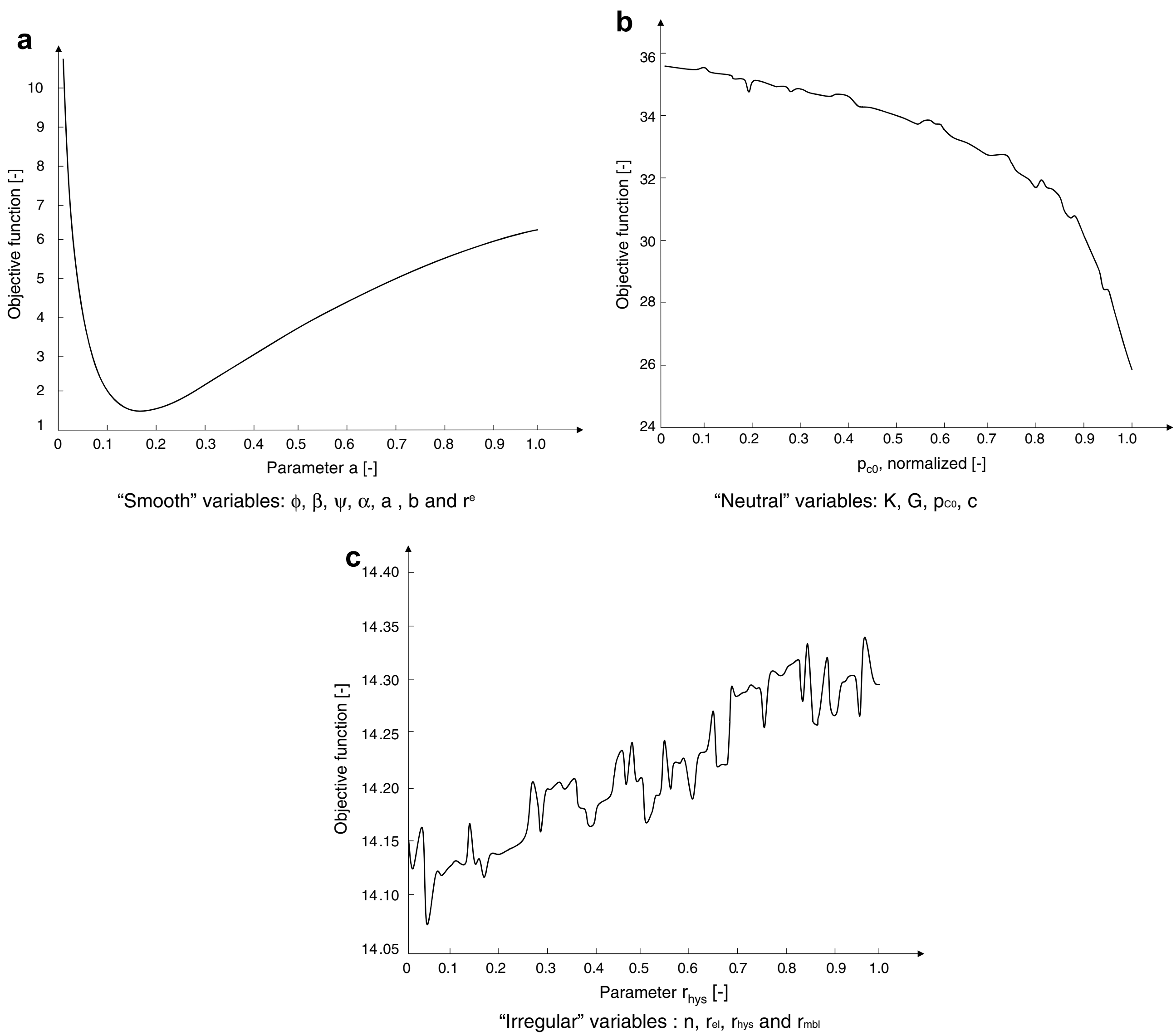

Fig. 6. Sensitivity of the objective function to different types of optimization variables: (a) "smooth", (b) "neutral" and (c) "irregular".

Table 2
Calibrated model parameters for MC clay (Kaolin)

Optimisation variable	Initial values	Optimised parameters based on		
		One experimental result	Two experimental results	Three experimental results
ϕ [°]	20.0	21.9	22.1	21.5
β [–]	21.0	26.1	30.4	31.8
ψ [°]	22.5	22.4	23.9	23.3
α [–]	3.80	3.71	1.88	2.05
a [–]	3.5e−3	3e−3	2.85e−3	3e−3
b [–]	0.550	0.550	0.524	0.509
c [–]	0.055	0.060	0.055	0.052
r^e [–]	1e−5	0.001	0.045	0.025

approach has been used in the present calculation in order to ensure that the global minimum be found over entire domain considered.

6.1. Parameter sensitivity analysis

A sensitivity analysis of the objective function for the parameters to be optimised has been carried out. For the analysis, each of the parameters was varied over the entire admissible domain (Table 1), while all other parameters were fixed, which allows the evaluation of the objective function. Based on this calculation, the parameters were divided into three classes: (i) smooth, (ii) neutral and (iii) irregular (Fig. 6).

It can be observed that for "smooth" variables, the objective function is always differentiable and possesses continuous derivations over the considered domain. It reaches a region of low values near the optimised parameter value and increases when the parameter values are far away (Fig. 6a; example for the parameter a). The model parameters, which show this pattern of behaviour, are:ϕ, β, ψ, α, a, b and r^e. In general, these parameters can easily be optimised by the quasi-Newton method.

The dependency of the objective function on "neutral" variables is a curved line with some irregularities (Fig. 6b, example for parameter p_{c0}). The derivatives of the objective function are not continuous, but its variation is relatively small. Instantaneous changes in derivatives or in wrong direction can be corrected in the next iteration, so, in general, optimisation of these parameters (K, G, p_{c0}, c) should not impose enormous difficulties.

The third group, i.e. "irregular" variables, shows a strong variation of the objective function, which does not have continuous derivatives (Fig. 6c, example for parameter r_{hys}). The influence of the "smooth" variables can be hidden, which imposes difficulties for optimisation by the quasi-Newton method. Therefore, these parameters (n, r_{el}, r_{hys} and r_{mbl}) can be successfully optimised by the stochastic method and with difficulty by using the quasi-Newton method.

6.2. Optimisation examples

Results from three isotropically consolidated drained triaxial shear tests were used in optimising the determination of the Hujeux model parameters. These results are part of an extensive experimental program on the behaviour of fine soils [2]. The triaxial tests were performed on CM clay, commercially known as Kaolin. The grain size distribution reveals that about 97% by weight was smaller than

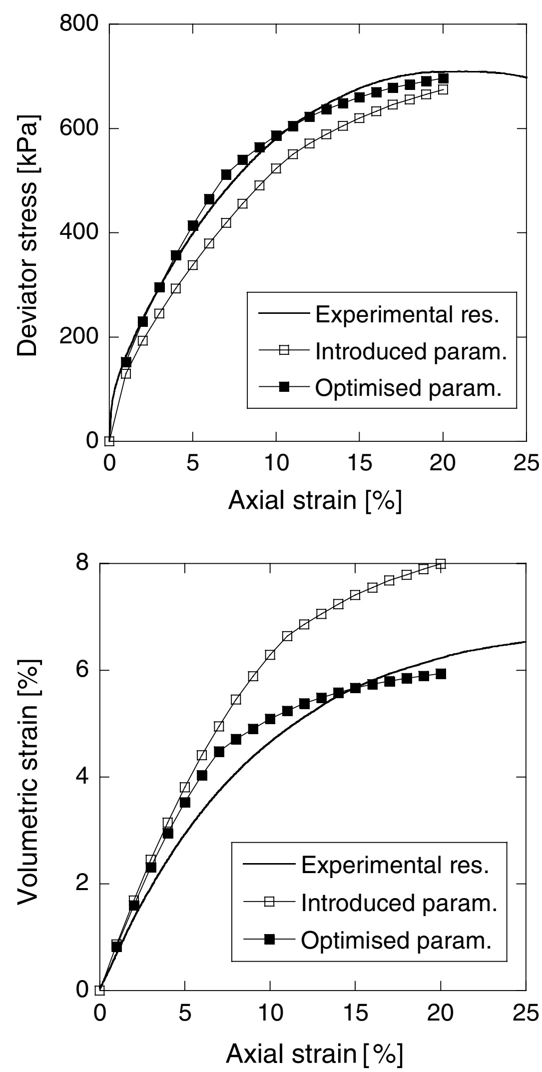

Fig. 7. Comparison between experimental results of drained shear test carried out at NC state (S2-T5) and numerical simulations; the model parameters were calibrated using the optimisation technique presented above.

0.06 mm and 45% was smaller than 0.002 mm. The liquid limit was $w_L = 45\%$ and plasticity limit was $w_P = 24\%$.

The procedure for carrying out the tests in triaxial conditions was as follows. The specimens were first consolidated at a pressure of 600 kPa followed by isotropoic unloading to different values of OCR (S2-T5, OCR = 1; T18, OCR = 3 and T28, OCR = 6). Thereafter, the specimens were sheared by applying a standard triaxial sharing path, $\partial q/\partial p' = 3$.

The optimisation procedure presented above was used to determine the model parameters based on one, two and three drained triaxial shear tests.

A first example has been made using a shear test in a NC state (S2-T5). The initial values of the optimisation variables (model parameters) were chosen to have average values between the lower and upper bounds (Table 1). The duration of the observation was limited to axial deformation of 20% and divided into 10 points. The analysis was started by using the weighting values of $w_{ij} = 1.0$ for $i = 1, 2$ and $j = 1, 2 \ldots 10$. Final values of the model parameters are given in Table 2 and comparisons between experimental and numerical results obtained for the initial and final set of parameters are given in Fig. 7. It may be observed that the numerical results are very close to the experimental ones. However, it should be noted that such a set of parameters cannot be used to predict the behaviour of soils at stress states different from the conditions used for calibration.

In the case of using two experimental results for the calibration procedure, it is possible to introduce additional weighting values w^k ($k = 1, 2$), which correspond to each of the tests. Using w^k values different from one, it is possible to give different amounts of importance to the experimental results. The experimental results used in this example (S2-T5 and T28) have been carried out in similar conditions (same experimental tools and the same operator) imposing the same confidence on the measured values and consequently weighting values have been taken to be 1 ($w^k = 1, k = 1, 2$). Similar to the previous example, weighting values w_{ij} ($i = 1, 2; j = 1, 2, \ldots, 10$) have been taken equal to 1. Initial values of model parameters were the same as in the previous case, while the final values were different (Table 2). Fig. 8 reveals that the numerical results

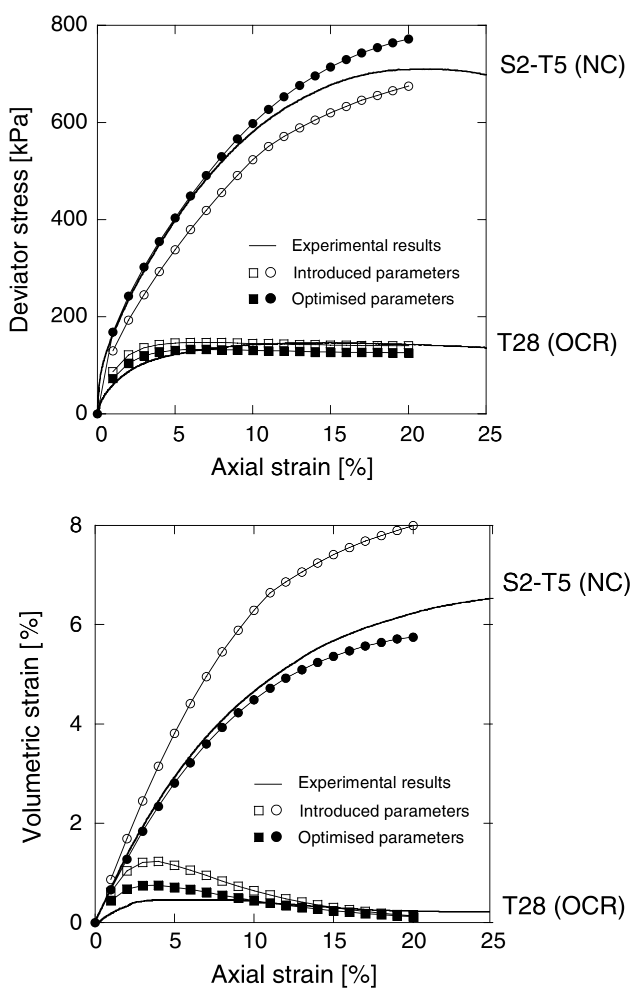

Fig. 8. Comparison between experimental results of drained shear tests carried out at NC (S2-T5) and OC (T28, OCR = 6) state and numerical simulations; the model parameters were calibrated using the optimisation technique presented above.

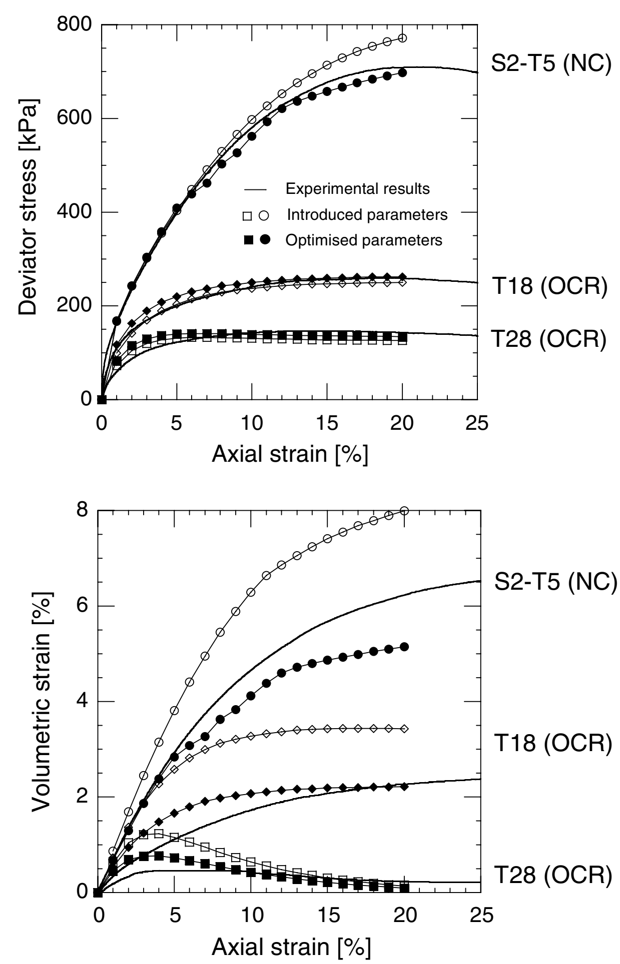

Fig. 9. Comparison between experimental results of drained shear tests carried out at NC (S2-T5) and OC states (T18, OCR = 3; T28, OCR = 6) and numerical simulations; the model parameters were calibrated using the optimisation technique presented above.

obtained for two tests give very satisfactory results in both considered planes (q versus ε_1; ε_v versus ε_1).

Finally, the optimisation procedure was carried out using the three drained shear tests. As in the previous case, weighting values for experiments (S2-T5, T28 and T18) were taken to be one. The model parameters and initial values obtained are given in Table 2. In comparison to values which may be obtained by a classical procedure, in regard to the physical meaning of the variables, the optimised values appear very realistic. The optimised combination of parameters gives numerical results which compare very well with experimental ones, ranging from normally consolidated (S2-T5) to highly overconsolidated samples (T28), Fig. 9. Of course, the obtained values must be carefully examined in the light of geotechnical practical experience.

7. Conclusions

The paper presents an optimisation technique for the calibration of model parameters in a rational and objective manner. The procedure consists in finding a set of model parameters which minimise the difference between the experimental data and numerical simulations defined by an objective function. From the mathematical point of view, the goal is to minimise the optimisation function on the domain constrained by boundary values of the model parameters. For this purpose, an optimisation routine, termed ParaID, that combines the quasi-Newton and stochastic methods, was developed. The quasi-Newton method combines the advantages of the gradient method with those of the Newton approach. The method uses gradients of the objective functions which yield inverted Hessien matrices, indicating the precision of the obtained parameters. The other advantage of the quasi-Newton method is that there is no need for a resolution of the system of linear functions. To obtain the direction of decrease of the objective function, the quasi-Newton method and gradient method were used to treat inactive and active variables, respectively.

The stochastic method, called the global method, is needed to ensure that the optimised model parameters correspond to a minimum of the objective function over the entire considered domain. Among the tested strategies, the stochastic method is the most appropriate one for problems where the dimension of the space in which the optimisation takes place, constituted of model parameters, is large.

The optimisation technique was employed to calibrate a multi-mechanism elasto-plastic constitutive model using the results of three isotropically consolidated drained triaxial compression tests. The procedure was tested on three numerical examples, using one, two and three experimental results for model calibration. A comparison between numerical and experimental results clearly shows the capability of the optimisation procedure to derive model parameters correctly.

However, it must be noted that even such a rational method for model calibration requires evaluation of the obtained results based on engineering judgement.

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