Inspection of ratcheting models for pathological error sensitivity and overparametrization

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Abstract Accurate analysis of plastic strain accumulation under stress-controlled cyclic loading is vital for numerous engineering applications. Typically, models of plastic ratcheting are calibrated against available experimental data. Since actual experiments are not exactly accurate, one should check the identification protocols for pathological dependencies on experimental errors. In this paper, a step-by-step algorithm is presented to estimate the sensitivities of identified material parameters. As a part of the sensitivity analysis method, a new mechanics-based metric in the space of material parameters is proposed especially for ratcheting-related applications. The sensitivity of material parameters to experimental errors is estimated, based on this metric. Moreover, a relation between pathological error sensitivity and overparametrization is established. This relation gives rise to a new criterion of overparametrization. The advantages of the new overparametrization criterion are exposed and its plausibility is checked by alternative criteria, like the consideration of correlation matrices and validation of identified parameters on “unseen” data. For demonstration purposes, the accumulation of irreversible strain in the titanium alloy VT6 (Russian analog of Ti-6Al-4V) is analysed. Three types of phenomenological models of plastic ratcheting are considered. They are the Armstrong-Frederick model as well as the first and the second Ohno-Wang models. Based on real data, a new rule of isotropic hardening is proposed for greater accuracy of simulation. The ability of the sensitivity analysis to determine reliable and unreliable parameters is demonstrated.

Keywords Parameter identification · Ratcheting · Error-sensitivity analysis · Overparametrization · Mechanics-based metric · Armstrong Frederick · Ohno Wang

1 Introduction

Accurate simulation of the stress-strain curves in a broad range of loading scenarios is essential for fatigue strength assessments. Proper models of elastoplasticity are back-bone of many advanced modelling approaches, including purely phenomenological models of continuum damage mechanics and microstructure-motivated models. Moreover, some simplified engineering methods allow for assessments of fatigue life, based on the parameters of the stress-strain hysteresis loops [11, 50, 51].

Both phenomenological and microstructure-based models are calibrated against experimental data. In general, the low sensitivity of material parameters to experimental errors means that the problem of parameter identification is stable, and the identified parameters can be used to solve practical problems.
However, the high sensitivity, also called pathological sensitivity, means that even a slight noise in experimental data may cause essential changes in the identified parameters. This sensitivity renders the obtained parameters unreliable and useless. In this regard, the following questions arise: (i) Are the material constants pathologically dependent on the measurement errors? (ii) How to quantify the sensitivity of a certain identification procedure? (iii) How to estimate the sensitivity? To answer these questions, we further develop the methodology from [37, 38], used to study the sensitivity of material parameters respective to the noise in experimental data. A step-by-step algorithm is presented allowing to estimate the sensitivity in a mechanically reasonable way. As a part of the approach, a new mechanics-based metric in the space of material parameters is developed especially for ratcheting-related applications. The sensitivity of parameters is then evaluated concerning this metric.

Many modelling concepts allow for the introduction of an unlimited number of material parameters towards improved accuracy. The obvious flaw of using too many parameters is that eventually the model becomes overparametrized with respect to given observations. Although some formal definitions of overparametrization have been suggested in the literature [10], it is difficult to provide a precise definition of overparametrization. Thus, the proposed criteria should be viewed as general guidelines based on experience and intuition. In this paper, the drawbacks of the standard criteria of overparametrization are discussed, and a new formal criterion is proposed. The plausibility of the new definition is checked by comparison with the classical ones.

As a demonstration example, we analyse the ratcheting of the titanium alloy VT6. The main focus is on accurate modelling of the thermo-mechanical response at mid-life and the corresponding sensitivities to measurement errors. In the case of uniaxial cyclic loading, considered here, nonlinear kinematic hardening must be accounted for due to the presence of the Bauschinger effect.¹ Three models are considered in this study: the Armstrong-Frederick model (AF), the first, and the second Ohno-Wang models (OW-I and OW-II). The isotropic hardening is modelled according to a new rule, based on the accumulated total strain and the Odqvist parameter.

Since we focus on the initial stage and mid-life, ductile damage is not incorporated into the considered models. However, this can be made based on principles from [4, 9, 23, 36]. Application of ductile damage models to ratcheting of metals is found in [21, 45].

To determine the optimal set of material parameters, we implement a nested identification procedure. Owing to the new rule of isotropic hardening, all models enable accurate simulations in agreement with the experimental data. The simulation accuracy increases with increasing number of parameters. Validation of the parameters and models is carried out by comparing the simulated and “unseen” experimental data regarding strain accumulation and dissipative heating. Moreover, for various identification problems correlations between unknown parameters are computed.

The paper is organized as follows. Section 2 presents the general algorithm of the sensitivity analysis; the main ingredients and ideas are shown and a new criterion of overparametrization is suggested. In Section 3, new models of ratcheting accounting for cyclic mechanical loading are presented. Their novelty lies in the advanced rule of isotropic hardening. The heat conduction equation is developed using the first law of thermodynamics. The experimental results for the alloy VT6, corresponding parameter identification protocols, and validation of parameters are shown in Section 4. Section 5 is devoted to the sensitivity analysis for the specific models of ratcheting. The implemented stochastic model of noise and the mechanics-based metric are presented, and the parameter sensitivities are estimated, depending on the complexity of the model. The occurrence of overparametrized models is exposed and the plausibility of the new overparametrization criterion is demonstrated. Section 6 discusses the results, and final conclusions are presented in Section 7.

¹ Dealing with a general non-proportional loading, advanced models of directional distortional hardening are needed [12, 35, 42]. Moreover, simplified J2 yield conditions can be replaced by their anisotropic counterparts [2].
2 Error sensitivity and overparametrization

2.1 Basic steps of sensitivity analysis

To formulate the general algorithm, we consider an arbitrary material model of ratcheting. Assume that the model contains \( n \) real-valued material parameters, subject to identification. By \( \vec{p} \in \mathbb{R}^n \), we denote the unknown parameter vector. The available experimental data are packed into the vector \( \text{Exp} \in \mathbb{R}^{N_{\text{exp}}} \), \( N_{\text{exp}} \geq n \). For ratcheting-related applications, such measured data can be total strains, strain amplitudes, displacements at individual points or even discretized displacement fields. Let \( \text{Mod}(\vec{p}) \) be the corresponding model prediction of \( \text{Exp} \).

Identification Following the standard approach [5], the error functional \( \Phi \) is built and the required parameter vector \( \vec{p}^* \) is its minimizer:

\[
\Phi(\vec{p}) = (\text{Exp} - \text{Mod}(\vec{p})) \cdot W \cdot (\text{Exp} - \text{Mod}(\vec{p})),
\]

\[
\vec{p}^* = \arg\min_{\vec{p}} \Phi(\vec{p}).
\]

Here, \( W \) is a fixed, symmetric, positive-definite weighting matrix. In the simplest case when all the experimental data are uncorrelated and equally important, one typically takes the identity matrix in place of \( W \) [5, 37].

Distance between parameter sets For sensitivity studies, a reasonable metric is needed in the space of material parameters. In the following sections, a mechanics-based distance is introduced such that dist\((\vec{p}_1, \vec{p}_2)\) is a deviation of parameter sets \( \vec{p}_1 \) and \( \vec{p}_2 \) from each other.

Stochastic model of noise To account for eventual presence of experimental errors, we introduce a stochastic model of experimental noise. Assuming that the model is additive [5, 15, 16], the real experimental data \( \text{Exp} \) are replaced by the noisy data \( \text{NoisyData} = \text{Exp} + \text{Noise} \). Here, \( \text{Noise} \) is a random vector in \( \mathbb{R}^{N_{\text{exp}}} \); its distribution is defined by the stochastic model, discussed later.

Monte Carlo computations The presented ideas behind the sensitivity analysis are rather general. The core of the method relies on Monte Carlo computations, a general tool, suitable even for integration of irregular functions in multiple dimensions [6]. Let \( N_{\text{noise}} \) be a sufficiently large number of draws of noisy data and the \( j \)th draw be denoted as \( \text{Noise}^{(j)} \). For each draw we consider a new optimization problem with the error function

\[
\Phi^{\text{noisy}}(\vec{p}) = (\text{Exp} + \text{Noise}^{(j)} - \text{Mod}(\vec{p})) \\
\cdot W \cdot (\text{Exp} + \text{Noise}^{(j)} - \text{Mod}(\vec{p})), \quad \vec{p}^{(j)} = \arg\min_{\vec{p}} \Phi^{\text{noisy}}(\vec{p})).
\]

A highly efficient way of solving this optimization problem is presented in Appendix A. The set of vectors \( \vec{p}^{(j)}, \ j = 1, 2, ..., N_{\text{noise}} \) is called the “cloud of parameters”. The center of the cloud is the average of all \( \vec{p}^{(j)} \) and the size of the cloud is the average distance to the center:

\[
\vec{p}^{\text{center}} = \frac{1}{N_{\text{noise}}} \sum_{j=1}^{N_{\text{noise}}} \vec{p}^{(j)},
\]

\[
\text{CloudSize} = \frac{1}{N_{\text{noise}}} \sum_{j=1}^{N_{\text{noise}}} \text{dist}(\vec{p}^{\text{center}}, \vec{p}^{(j)}).
\]

If we assume that the probability density function (PDF) of noise is symmetric with respect to zero (PDF\((\vec{x}) = \text{PDF}(\vec{-x}) \) for all \( \vec{x} \in \mathbb{R}^{N_{\text{exp}}} \)), then \( \vec{p}^* \) is located roughly at the center of the parameter cloud. In this case the definition of the CloudSize simplifies to

\[
\text{CloudSize} = \frac{1}{N_{\text{noise}}} \sum_{j=1}^{N_{\text{noise}}} \text{dist}(\vec{p}^*, \vec{p}^{(j)}).
\]

The procedure is summarized in Fig. 1

The CloudSize is the measure of the sensitivity of identified material parameters. Small CloudSize for realistic noise indicates that the sensitivity is low and the strategy is stable. If CloudSize is finite even for very small noise, then the identification protocol is unreliable and the dependence on measurement errors is pathological. In this study we show that such a pathological dependence is characteristic of overparametrized models.

For reproducibility of results and faster convergence of Monte Carlo computations, the quasi-Monte Carlo method is implemented in the current study (cf. [29, 38]). The quasi-Monte Carlo method differs from the classical in using a low-discrepancy sequence of random numbers. In the current paper, the Sobol sequence is implemented [43].
2.2 Formal criteria of overparametrization: old and new

Flexible modelling concepts allow for the introduction of unlimited number of material parameters for greater accuracy. For instance, the approach of Chaboche implies the incorporation of evolving backstresses with two scalar parameters per backstress. However, the model refinement must be limited at a certain moment to avoid the misuse of additional parameters. This decision can be made based on known practical criteria of overparametrization:

I Virtually no gain in accuracy occurs when increasing the number of material parameters (Fig. 2(top left)).

II The validation of the model on “unseen” data shows deteriorating predictive capabilities as the number of parameters increases (Fig. 2(top right)).

III There is a significant correlation among parameters, which is seen by inspecting the correlation matrices (Fig. 2(bottom left)).

IV The sensitivity of material parameters to experimental error becomes too high (Fig. 2(bottom right)), while the sensitivity is measured in terms of CloudSize.

Here, the “unseen” data are those experimental results that were not used for the parameter identification. In Fig. 2, the “unseen” data and the corresponding simulation results are denoted as Unseen-Exp and Simul. An algorithm for the computation of the correlation matrix is presented in Appendix B.

In this paper, we suggest the fourth criterion of overparametrization:

In the following sections, the usefulness of this new criterion is analysed. Toward that end, the basic steps of the sensitivity analysis are demonstrated on concrete examples. The applicability of the algorithm is demonstrated and the plausibility of the results is assessed by comparison with criteria I, II, and III. The qualitative analysis and comparison of the four criteria are presented in Sect. 5.4.
3 Material models

3.1 Strains, stresses, and entropy

For simplicity, the small strain framework is implemented. However, the developed models can be generalized to large strains using the methodology from [26, 39, 41, 47]. For phenomenological material description, three types of combined isotropic-kinematic hardening models are used here: the models of Armstrong-Frederick (AF), the first, and the second Ohno-Wang models (OW-I and OW-II). To control the complexity of each modelling approach, we introduce two, three, and four rheological branches. These branches are the following: the rate-independent Maxwell body for the AF-model, elasto-plastic model of Prandtl-Reuss for the OW-I-model, and a modified Maxwell body for the OW-II-model.

All the models share the same kinematics. First, the total strain tensor $\varepsilon$ is additively decomposed into the thermal part $\varepsilon_\theta$ and the mechanical part $\varepsilon_m$ (Fig. 3 left):

$$\varepsilon = \varepsilon_\theta + \varepsilon_m.$$  (5)

---

**Fig. 2** Criteria of overparameaterized material models for increasing number of parameters. Criterion I: inadequate gain in accuracy. Criterion II: deteriorating predictive capabilities tested on “unseen” data. Criterion III: high correlation among parameters. Criterion IV: large CloudSize meaning unacceptably high sensitivity of parameters to measurement errors.

**Fig. 3** Rheological interpretation of the ratcheting models with $N_{\text{branches}} = 2$. Left: introduced strains. Right: summary of material parameters.
The temperature-induced strain is purely volumetric; it is given by \( \varepsilon_\theta = \frac{1}{3} a(\theta - \theta_0) \cdot 1 \), where \( a \) is the (volumetric) thermal expansion coefficient and \( \theta_0 \) is the reference temperature. The mechanical strain is decomposed into the elastic part \( \varepsilon_e \) and the inelastic part \( \varepsilon_i \), such that \( \varepsilon_m = \varepsilon_e + \varepsilon_i \). Let \( N_{\text{branches}} = 2, 3, 4 \) be the number of rheological branches. The case of two branches is shown in Fig. 3(left). For each branch we introduce conservative (\( \varepsilon_{c_l} \)) and dissipative (\( \varepsilon_{d_l} \)) components of strain, such that

\[
\varepsilon_i = \varepsilon_{c_l} + \varepsilon_{d_l}, \quad \text{for all} \quad l = 1, \ldots, N_{\text{branches}}. \tag{6}
\]

The Helmholtz free energy per unit mass is computed as:

\[
\Psi = \Psi_e(\varepsilon_e) + \sum_{l=1}^{N_{\text{branches}}} \Psi_{\text{kin}}(\varepsilon_{c_l}) + \Psi_\theta(\theta), \tag{7}
\]

\[
\rho \Psi_e(\varepsilon_e) = \frac{k}{2} (\varepsilon_e) : \varepsilon_e + \mu \varepsilon_{\text{D}} : \varepsilon_{\text{D}}, \tag{8}
\]

\[
\rho \Psi_{\text{kin}}(\varepsilon_{c_l}) = \frac{c_l}{2} \varepsilon_{c_l} : \varepsilon_{c_l}, \quad l = 1, \ldots, N_{\text{branches}}, \tag{9}
\]

\[
\rho \Psi_\theta(\theta) = -c_{\theta 0} (\theta \ln \frac{\theta}{\theta_0} - (\theta - \theta_0)). \tag{10}
\]

Here, \( k > 0 \) and \( \mu > 0 \) are the bulk and shear moduli; \( c_l > 0 \) is the stiffness of the substructure, described by branch \( l \); \( c_{\theta 0} \) is material’s heat capacity per unit mass; \( \varepsilon_{\text{D}} = \mathbf{A} - \frac{2}{3} \text{tr} (\mathbf{A}) 1 \) is the deviatoric part of a tensor.

Note that alternative assumptions regarding energy storage \( \Psi_\theta \) are also possible, cf. [4]. The stress tensor \( \sigma \) is computed through Hooke’s law; the backstresses \( \varepsilon_i \) in branches \( l = 1, \ldots, N_{\text{branches}} \) are linear isotropic functions of \( \varepsilon_{c_l} = \varepsilon_i - \varepsilon_{d_l} \):

\[
\sigma = \frac{\partial \Psi_e}{\partial \varepsilon_e} = k \text{tr} (\varepsilon_m - \varepsilon_i) 1 + 2 \mu (\varepsilon_m - \varepsilon_i)^D, \tag{11}
\]

\[
X_i = \frac{\partial \Psi_{\text{kin}}}{\partial \varepsilon_{c_l}} = c_l (\varepsilon_i - \varepsilon_{d_l})^D, \quad l = 1, \ldots, N_{\text{branches}}. \tag{12}
\]

The effective stress \( \sigma_{\text{eff}} \) equals

\[
\sigma_{\text{eff}} = \sigma - \sum_{l=1}^{N_{\text{branches}}} X_i. \tag{13}
\]

In a similar fashion, we compute the entropy per unit mass as:

\[
\zeta = -\frac{\partial \Psi}{\partial \varepsilon_{\text{D}}} |_{\text{const}} = -\frac{\partial \Psi_e}{\partial \varepsilon_e} + \frac{\alpha}{3 \rho} \text{tr} \sigma = \frac{c_{\theta 0}}{\rho} (\theta \ln \frac{\theta}{\theta_0} - (\theta - \theta_0)) + \frac{\alpha}{3 \rho} \text{tr} \sigma. \tag{14}
\]

In the following, relations (11), (12), and (14), along with implemented evolution equations, will be sufficient for thermodynamic consistency of the models.

Let \( K > 0 \) be the initial uni-axial yield stress. By \( R \in \mathbb{R} \) we denote the isotropic hardening. Then the yield function \( f \) and the Kuhn-Tucker conditions for computing the inelastic strain rate \( \lambda_i = ||\varepsilon_i|| \) are as follows:

\[
f := ||(\sigma_{\text{eff}})^D|| - \sqrt{\frac{2}{3} (K + R)}, \quad \lambda_i \geq 0, \quad f \leq 0, \quad f \lambda_i = 0. \tag{15}
\]

3.2 New rule of isotropic hardening

According to (15), \( \sqrt{\frac{2}{3}(K + R)} \) is the current radius of the yield surface in the deviatoric stress space. In metal plasticity, the standard assumption is that the radius is a function of the accumulated arc-length \( s \).

In strain-controlled cyclic tests, the cyclic hardening (softening) response corresponds to monotonically increasing (decreasing) \( R(s) \) (cf. [46]). In stress-controlled tests there are also experimental observations of ratcheting with initial hardening, followed by softening (cf. [19]).

This situation is covered by a non-monotonic function \( R(s) \).

As will be shown in Sect. 4.3, the standard assumption \( R = R(s) \) is too restrictive for some applications. Toward a more flexible approach, the evolution of the isotropic hardening \( R \) is modelled by an extended ansatz. Along with the Odqvist parameter \( s \) we introduce the accumulated total deviatoric strain \( s_x \), and assume that the yield strength is a function of these two variables:

\[
\dot{s} = \sqrt{\frac{2}{3} ||\varepsilon_i||}, \quad \dot{s_x} = \sqrt{\frac{2}{3} ||\varepsilon_{\text{D}}||}, \quad R = R(s, s_x). \tag{16}
\]

2 Under stress-controlled cyclic loading, cyclic softening refers to a growth in cyclic strains under constant amplitude imposed cyclic stress.

3 This was also shown in [22].
Among all alternatives, the preference is given to \( s_e \) since it has a structure similar to \( s \). From the mechanical standpoint, the parameter \( s_e \) is reasonable for materials where some structural changes occur even in the elastic range. Moreover, in the strain-driven context, \( s_e \) is known. Thus, numerical algorithms developed for \( R = R(s) \) can be straightforwardly adopted to the new hardening rule (16). Note that the classical assumption \( R = R(s) \) is covered by (16) as a particular case.

Since \( R(s, s_e) \) is assumed to be smooth, we approximate it by the linear ansatz

\[
R = \gamma s - \beta s_e,
\]

where \( \gamma \in \mathbb{R} \) and \( \beta \in \mathbb{R} \) are material constants. The term \( \beta s_e \) comes with a negative sign since we assume its relation to strain softening.

### 3.3 Plastic flow rule and kinematic hardening

In all the models, the global flow rule governs the inelastic strain rate \( \dot{\varepsilon}_l \) according to the normality rule:

\[
\dot{\varepsilon}_l = \lambda_i \frac{\sigma_{\text{eff}}^D}{||\sigma_{\text{eff}}^D||},
\]

(18)

**Armstrong–Frederick hardening** For the model of AF-type the constitutive equations of each branch correspond to a rate-independent Maxwell model:

\[
\dot{\varepsilon}_l = \lambda_i \chi_l X_l, \quad l = 1, \ldots, N_{\text{branches}}.
\]

(19)

Here, \( \chi_l \geq 0 \) is the material parameter controlling the saturation of the backstress \( X_l \).

**Remark 1** Differentiating (12) with respect to time and using (19), we obtain a well-known form of the Armstrong-Frederick equation:

\[
\dot{X}_l = c_i (\dot{\varepsilon}_l - \dot{\varepsilon}_l^D) = c_i (\dot{\varepsilon}_l - \chi_l \dot{\varepsilon}_l X_l).
\]

(20)

Although (19) and (20) are equivalent, we prefer using strain-based relation (19) rather than the stress-based formula (20).

**First Ohno–Wang hardening** For the OW-I model, each branch corresponds to elastic-perfectly plastic body, also known as the Prandtl–Reuss body. The constitutive equations are

\[
\dot{X}_l = \lambda_i \frac{X_l}{||X_l||}, \quad \lambda_i \geq 0, \quad ||X_l|| \leq \sqrt{\frac{2}{3}} r_l.
\]

(21)

Here \( \lambda_i \) is the inelastic strain rate in the \( l \)th branch, \( r_l > 0 \) is the corresponding yield stress. Moreover, the Kuhn-Tucker conditions must be satisfied:

\[
\lambda_i \left(||X_l|| - \sqrt{\frac{2}{3}} r_l\right) = 0.
\]

(22)

The historical stress-based evolution law (cf. [30]) can be obtained by combining (12), (21), and (22).

**Second Ohno–Wang hardening** For the OW-II model we use

\[
\dot{X}_l = \left(\sqrt{\frac{2}{3}} \frac{||X_l||}{r_l}\right)^m \left(\dot{\varepsilon}_l - \lambda_i \frac{X_l}{||X_l||}\right) \frac{X_l}{||X_l||}.
\]

(23)

Here, the parameter \( r_l \) has a similar meaning as in the OW-I model. The exponent \( m \) governs the degree of nonlinearity.

**Remark 2** Differentiating (12) with respect to time and substituting (23) into the result, we obtain the historical stress-based form of the evolution equation (cf. [30]):

\[
X_l = c_i \left(\dot{\varepsilon}_l - \lambda_i \left(\sqrt{\frac{2}{3}} \frac{||X_l||}{r_l}\right)^m \frac{\sigma_{\text{eff}}^D}{||\sigma_{\text{eff}}^D||} \frac{X_l}{||X_l||}\right) \frac{X_l}{||X_l||}.
\]

(24)

Again, we prefer dealing with the strain-based equation (23).

**Remark 3** Another popular ratcheting model was proposed by Abdel-Karim and Ohno in [1]. This model combines dynamic recovery terms from the AF and OW-I models. However, it is not considered in the current study since it contains too many material parameters.
Using (8), (9), (11), and (14) we obtain the reduced form of the mechanical dissipation:

$$\delta_i = \frac{1}{\rho} \sigma_{\text{eff}} : \dot{\varepsilon}_i + \frac{1}{\rho} \sum_{j=1}^{N_{\text{branches}}} X_j : \dot{\varepsilon}_{\text{hi}} \geq 0. \quad (26)$$

Substituting evolution equations into the reduced form, we can check that (26) is indeed satisfied:

$$\sigma_{\text{eff}} : \dot{\varepsilon}_i \geq 0, \quad X_j : \dot{\varepsilon}_{\text{hi}} \geq 0. \quad (27)$$

The non-negativity of the dissipation indicates that all the models are thermodynamically consistent. In addition, we postulate the first law of thermodynamics in the local form:

$$\dot{\theta}^c = \delta_i - \frac{1}{\rho} \text{div} \mathbf{q} + r. \quad (28)$$

Here, $\mathbf{q}$ is the heat flux vector and $r$ represents local heat sources per unit mass. To simulate the heating of the sample in the gauge area, we implement the following simplified heat-exchange scheme (cf. [34])

$$-\frac{1}{\rho} \text{div} \mathbf{q} + r = \omega (\theta - \theta_0). \quad (29)$$

Here, $\theta$ is the sample temperature in the gauge area; the temperature of the surrounding medium is assumed to be equal to the reference temperature $\theta_0$; $\omega$ is the heat-exchange coefficient, depending on the shape and dimensions of the sample as well as on the heat conduction properties of involved components.\(^4\) Now we differentiated (14) with respect to time to obtain the rate of entropy:

$$\dot{\zeta} = \frac{c_{\text{th}}}{\rho} \frac{\dot{\theta}}{\theta} + \frac{ak}{\rho} \text{tr} \dot{\varepsilon} - \frac{\alpha^2}{\rho} k \dot{\theta}. \quad (30)$$

Multiplying both sides with $\theta$, we have

$$\theta \dot{\zeta} = \frac{c_{\text{th}}}{\rho} \frac{\dot{\theta}}{\theta} \theta + \frac{ak}{\rho} \text{tr} \dot{\varepsilon} \theta - \frac{\alpha^2}{\rho} k \theta \dot{\theta}. \quad (31)$$

Using the heat capacity parameter $c_\theta = \frac{c_{\text{th}}}{\rho} - \frac{\alpha^2}{\rho} k \theta$ we arrive at

$$\theta \dot{\zeta} = c_\theta \frac{\dot{\theta}}{\theta} + \frac{ak}{\rho} \text{tr} \dot{\varepsilon}. \quad (32)$$

Substituting this into (28), we obtain the heat conduction equation:

$$c_\theta \frac{\dot{\theta}}{\theta} = -\frac{ak}{\rho} \text{tr} \dot{\varepsilon} + \delta_i - \omega (\theta - \theta_0). \quad (33)$$

On the right side of this equation, the first term is responsible for the thermoelastic effect, the second term describes dissipation-induced heating, and the third term is the heat flux from the sample into the environment.

The thermal part is introduced into the modeling framework to validate the model by available experimental results on sample heating. In this work, the temperature dependence of the constants is neglected, since in the considered application the temperature increase is insignificant.

The system of constitutive equations is closed by specifying initial conditions. For simplicity, we assume that the initial state of the material is isotropic:

$$\mathbf{e}_{|t=0} = \mathbf{e}_{|t=0} = \ldots = \mathbf{e}_{|t=0} = \mathbf{0}, \quad s_{|t=0} = s_{|t=0} = 0, \quad \theta_{|t=0} = \theta_0. \quad (34)$$

As is common in engineering literature, the constitutive equations are formulated explicitly. However, there is an elegant alternative framework of generalized standard materials [14, 24, 27]. Within this framework, a thermodynamically consistent material model is uniquely defined by two convex scalar-valued functions.

### 4 Parameter identification for VT6

#### 4.1 Experimental data

We use experimental data from [22] on the ratcheting of samples from the titanium alloy VT6. In each test, the loading program consists of four stages (Fig. 4): quasi-static monotonic loading, holding under constant stress, harmonic cyclic loading with linearly increasing stress amplitude, and unloading. The third stage of each test contains 2400 stress-controlled cycles. During this stage, the mean stress $\sigma_m$ is held fixed and the stress amplitude is monotonically

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\(^4\) Since the temperature changes are small in this study, we linearize the heat exchange term near $\theta_0$. For example, the radiative heat transfer is proportional to $\theta^4 - \theta_0^4 \approx 4 \theta_0^3 (\theta - \theta_0)$. As a result, the simple ansatz (29) is obtained.
increasing; the maximum stress amplitude in each test is denoted as $a_{\text{max}}$.

Here we consider three tests where the maximum and the minimum axial strains at each cycle are recorded; for 2400 cycles this makes 4800 values per test. Tests with $a_m = 420$ MPa, $a_{\text{max}} = 470$ MPa (Fig. 5(left)) and $a_m = 635$ MPa, $a_{\text{max}} = 255$ MPa (Fig. 5(right)) are used for parameter identification. The test with $a_m = 530$ MPa, $a_{\text{max}} = 360$ MPa (Fig. 5(middle)) is reserved for validation. Thus, we refer to this test as “unseen” data. The maximum achievable stress for all tests is the same: it equals $a_m + a_{\text{max}} = 890$ MPa.

### 4.2 Identification procedure

The elastic constants of VT6 are fixed to $k = 98,037$ MPa, $\mu = 37,593$ MPa. AF-type models contain 7, 9, and 11 unknown parameters for variants with two, three and four Maxwell branches, respectively. The number of free parameters in models of OW-I-type is always less by one than in corresponding AF-models. Namely, to ensure that the material retains its carrying capacity, one of the branches needs to remain purely elastic all the time. Therefore, the corresponding local yield stress $r_1$ has to be sufficiently large. Since this parameter is undefinable using the available data, it is fixed to a pre-defined large value and it is excluded from the identification procedure. In contrast, each of the OW-II models contains one additional parameter, namely, the exponent $m$.

In this section, we describe the identification procedure for models with $N_{\text{branches}} = 4$. For convenience, we introduce the following notation:

$$\vec{p}_c = (\gamma, \beta, c_1, c_2, c_3, c_4).$$

$$\vec{p}_K = \begin{cases} (x_1, x_2, x_3, x_4, K) & \text{for AF,} \\ (r_1, r_2, r_3, K) & \text{for OW-I,} \\ (r_1, r_2, r_3, r_4, K, m) & \text{for OW-II.} \end{cases}$$

---

**Fig. 4** Loading program implemented in the experiment [22]

**Fig. 5** Experimental data from [22] on the ratcheting of the VT6 alloy
The sets $\vec{p}_c$ and $\vec{p}_K$ correspond to conservative and dissipative parameters. To identify parameters, tests with $\sigma_m = 420$ MPa and $\sigma_m = 635$ MPa are used. Denote by $\bar{\text{Exp}} \in \mathbb{R}^{9600}$ the vector of the experimental data. For each model, the vector of the model response $\bar{\text{Mod}}(\vec{p}_c, \vec{p}_K)$ contains the simulation results, corresponding to $\text{Exp}$. Following the previously discussed standard procedure we build an error function $\Phi(\vec{p}_c, \vec{p}_K)$ as the average deviation of the simulation results from the experimental data:

$$\Phi(\vec{p}_c, \vec{p}_K) = (\bar{\text{Exp}} - \bar{\text{Mod}}(\vec{p}_c, \vec{p}_K)) \cdot (\bar{\text{Exp}} - \bar{\text{Mod}}(\vec{p}_c, \vec{p}_K)).$$  \hspace{1cm} (36)

**Remark 4** All the experimental data enter the error function (36) with the same weight. This is the special case of (1) where $\mathbf{W}$ is the identity matrix. However, in some applications it is advisable to provide weighting factors or even weighting matrices [5, 37].

The standard identification procedure minimizes the error function $\Phi(\vec{p}_c, \vec{p}_K)$. However, due to the large number of material parameters, the error function $\Phi$ may exhibit numerous local minima. Therefore, optimization algorithms may provide a bad fit of simulation to experiment. To solve this issue, we use a nested identification procedure. It consists of internal and external optimization problems. The internal optimization problem is as follows. For a fixed set $\vec{p}_K$, the parameters $\vec{p}_c$ are identified from the following partial minimization:

$$\vec{p}_c = \text{argmin}_{\vec{p}_c} \Phi(\vec{p}_c, \vec{p}_K).$$  \hspace{1cm} (37)

The external optimization problem is formulated using the function $\vec{p}_c(\vec{p}_K)$, which was introduced in (37):

$$\vec{p}_K = \text{argmin}_{\vec{p}_K} \Phi(\vec{P}_c(\vec{p}_K), \vec{p}_K).$$  \hspace{1cm} (38)

After the external problem is solved, the parameters $\vec{p}_K$ are known. The remaining parameters are computed as $\vec{p}_c = \vec{P}_c(\vec{p}_K)$.

The advantage of the nested procedure is that instead of a relatively complex problem, two simpler optimization problems have to be considered with a smaller number of parameters. In particular, eventual correlations between conservative parameters $\vec{p}_c$ and the dissipative parameters $\vec{p}_K$ cannot spoil the internal optimization (37). Subproblems (37) and (38) are solved using the gradient-free Nelder-Mead method [28]. The solution of the internal optimization problem (37) with fixed $\vec{p}_K$ is standard. Within the external optimization (38), each call of the target function $\Phi(\vec{P}_c(\vec{p}_K), \vec{p}_K)$ involves the solution of the internal optimization problem to obtain $\vec{P}_c(\vec{p}_K)$, followed by the simulation of the model response $\bar{\text{Mod}}(\vec{P}_c(\vec{p}_K), \vec{p}_K)$. After the nested identification procedure is complete, the obtained set of material parameters is refined using the gradient-based Levenberg-Marquardt method [25]. Within the Levenberg-Marquardt step, general identification is carried out where all parameters are identified simultaneously. Such a refinement is necessary to make the gradient of the error function equal to zero. As will be seen from the following, zero gradient is essential for efficient algorithms implemented in the sensitivity analysis.

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**Table 1 Material parameters for AF models**

| $N_{\text{branches}}$ | $\gamma$ [MPa] | $c_1$ [MPa] | $c_2$ [MPa] | $c_3$ [MPa] | $c_4$ [MPa] |
|-----------------------|----------------|-------------|-------------|-------------|-------------|
| 2                     | 8094.2         | 12005       | 143832      | –           | –           |
| 3                     | 5736.0         | 7777.4      | 18789       | 109793      | –           |
| 4                     | 4176.2         | 4294.6      | 8232.5      | 21724       | 117736      |

Dissipative parameters

| $N_{\text{branches}}$ | $\beta$ [1/MPa] | $\kappa_1$ [1/MPa] | $\kappa_2$ [1/MPa] | $\kappa_3$ [1/MPa] | $\kappa_4$ [1/MPa] | $K$ [MPa] |
|-----------------------|-----------------|--------------------|--------------------|--------------------|--------------------|----------|
| 2                     | 3.7978          | 0.0360             | 0.0906             | –                  | –                  | 862.86   |
| 3                     | 3.5277          | 0.0352             | 0.0527             | 0.0866             | –                  | 847.26   |
| 4                     | 4.0121          | 0.0227             | 0.0366             | 0.0646             | 0.0797             | 846.73   |
### Table 2 Material parameters for OW-I models

| \(N_{\text{branches}}\) | \(\gamma\,[\text{MPa}]\) | \(c_1\,[\text{MPa}]\) | \(c_2\,[\text{MPa}]\) | \(c_3\,[\text{MPa}]\) | \(c_4\,[\text{MPa}]\) |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 2               | 4527.7          | 7329.5          | 4714.3          | –               | –               |
| 3               | 2109.3          | 10004           | 17306           | 7962.7          | –               |
| 4               | 6475.8          | 14915           | 19164           | 9673.5          | 3765.9          |

### Dissipative parameters

| \(N_{\text{branches}}\) | \(\beta\,[-]\) | \(r_1\,[\text{MPa}]\) | \(r_2\,[\text{MPa}]\) | \(r_3\,[\text{MPa}]\) | \(r_4\,[\text{MPa}]\) | \(k\,[\text{MPa}]\) |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 2               | 4.0919          | 30.702          | –               | –               | –               | 884.69          |
| 3               | 3.7940          | 22.206          | 31.518          | \(\infty\)     | –               | 852.41          |
| 4               | 3.8239          | 7.6188          | 17.099          | 29.030          | \(\infty\)     | 856.30          |

### Table 3 Material parameters for OW-II models

| \(N_{\text{branches}}\) | \(\gamma\,[\text{MPa}]\) | \(c_1\,[\text{MPa}]\) | \(c_2\,[\text{MPa}]\) | \(c_3\,[\text{MPa}]\) | \(c_4\,[\text{MPa}]\) |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 2               | 8957.3          | 214914          | 18441           | –               | –               |
| 3               | 8785.4          | 498547          | 10857           | 70184           | –               |
| 4               | 8805.0          | 140688          | 11377           | 443284          | 74932           |

### Dissipative parameters

| \(N_{\text{branches}}\) | \(\beta\,[-]\) | \(r_1\,[\text{MPa}]\) | \(r_2\,[\text{MPa}]\) | \(r_3\,[\text{MPa}]\) | \(r_4\,[\text{MPa}]\) | \(k\,[\text{MPa}]\) | \(m\,[-]\) |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 2               | 3.6190          | 101.26          | 39.032          | –               | –               | 757.30          | 2.9817          |
| 3               | 3.6194          | 99.053          | 27.750          | 58.154          | –               | 713.53          | 3.0173          |
| 4               | 3.6195          | 18.853          | 28.665          | 86.949          | 59.896          | 704.02          | 3.0490          |

**Fig. 6** Experimental data and simulation results by AF models for various number of branches (rheological bodies)

**Fig. 7** Experimental data and simulation results by OW-I models for various number of branches (rheological bodies)
4.3 Results of identification and validation

The identification results for AF, OW-I, and OW-II are given in Tables 1, 2 and 3, respectively. The best fit of AF models to experiment is shown in Fig. 6(left and right); best identification results for OW-I models are shown in Fig. 7(left and right); best results for OW-II are in Fig. 8(left and right). For validation against “unseen” data, the cyclic test with $\sigma_m = 530$ MPa is used, see Fig. 6(middle), Fig. 7(middle) and Fig. 8(middle).

All the considered models show a good correspondence between the simulation and the experiment. Naturally, as the number of rheological branches grows large, the accuracy increases. However, the validation of AF models on “unseen” data shows slightly decreasing predictive capabilities for larger $N_{\text{branches}}$.

Comparison of isotropic hardening rules: In many theoretical and applied studies, the classical Voce rule of isotropic hardening is used

$$R = R_{\text{Voce}}(s) = \frac{V_1}{V_2} (1 - e^{-V_2 s}),$$  \hspace{1cm} (39)

where $V_1$ and $V_2$ are material constants and $s$ is the Odqvist parameter. Another popular ansatz is the rule of Ludvig, employing parameters $L_1$ and $L_2$:

$$R = R_{\text{Ludvig}}(s) = L_1 s^{L_2}.$$  \hspace{1cm} (40)

The best possible fit of simulation to actual experiment (Fig. 9) reveals the poor performance of the classical rules (39) and (40). To explain this effect, note that the tests with $\sigma_m = 420$ MPa and $\sigma_m = 635$ MPa exhibit similar ranges of $s$. Thus, any ansatz of type $R = R(s)$ implies similar values of the isotropic hardening $R$ in both tests. However, the Voce and the Ludvig rules overestimate the strength of the material in the test with $\sigma_m = 420$ MPa (Fig. 9, left) and underestimate the strength in the test with $\sigma_m = 420$ MPa (Fig. 9, right). This conflict indicates that the assumption $R = R(s)$ is too restrictive.\(^5\) The new rule (17), however, relies on a more general ansatz $R = R(s, s_e)$. The parameter identification shows that the new rule (17) yields much better results than the classical rules (Fig. 9), although it contains the same number of

\(^5\) See also the discussion in [22].
material parameters. The high accuracy is achieved since the new rule resolves the conflict between the tests with $\sigma_m = 420 \text{ MPa}$ and $\sigma_m = 635 \text{ MPa}$.

Validation based on temperature evolution For an additional validation of the developed models, we use experimental data on the temperature evolution of the sample in the gauge area. Temperature measurements were carried out using the thermographic camera Infratec ImageIR 8305 (Germany). Note that these experimental data were not used during the identification. The temperature-related parameters adopted in the simulations are as follows: the reference temperature $\theta_0 = 293.35 \text{ K}$, the volumetric thermal expansion $\alpha = 1.59 \cdot 10^{-5} [1/\text{K}]$, the heat capacity per unit volume $c_{00}/\rho = 1.2058 [\text{J/(kg \cdot K)}]$, the mass density $\rho = 4,550 [\text{kg/m}^3]$. The heat exchange coefficient $w = 2.5 \cdot 10^{-2} [\text{J/(s \cdot kg \cdot K)}]$ is chosen to provide a realistic fit during cooling of the sample.

As is seen from Figs. 10, 11, and 12, all the simulation results agree with the experimental data. In these figures, $\Delta T = \theta - \theta_0$. The simulation reproduces the thermoelastic effect and the dissipation-induced heating. AF-type models are the most realistic regarding the temperature evolution. OW-I and OW-II models differ essentially from the experimental data...
for $N_{\text{branches}} = 2$, but the results are plausible for $N_{\text{branches}} = 4$.

Criticism of the OW-I models A pathological error-sensitivity is observed even for simple OW-I models. In Table 4 the vector of parameters $\vec{p}_1$ corresponds to the identification procedure, described earlier, and $\vec{p}_2$ is obtained by a single iteration of the Gauss-Newton method starting from $\vec{p}_1$. Although the gradient of the error function $\Phi$ is virtually zero at $\vec{p}_1$, a single step of the Gauss-Newton method yields a huge increment of the parameter vector (Table 4). In Fig. 13 we show the experimental data and simulation results for the OW-I model with $N_{\text{branches}} = 2$, corresponding to parameter vectors $\vec{p}_1$ and $\vec{p}_2$; the simulation results for $\vec{p}_2$ are obtained by the linearization of the model response near $\vec{p}_1$. The deviation of

\[ \text{Fig. 12} \quad \text{Experimental data on temperature evolution and simulation results, } N_{\text{branches}} = 4 \]

\[ \text{Fig. 13} \quad \text{Experimental data and simulation results by OW-I model obtained for } \vec{p}_1 \text{ and } \vec{p}_2; N_{\text{branches}} = 2 \]

\begin{table}[h]
\centering
\caption{Material parameters of the OW-I model}
\begin{tabular}{cccccccc}
\hline
& $\gamma$ [MPa] & $c_1$ [MPa] & $c_2$ [MPa] & $\beta$ [-] & $r_1$ [MPa] & $r_2$ [MPa] & $K$ [MPa] \\
\hline
$p_1$ & 0.0926 & 67,285 & 10,040 & 3.681 & 84.088 & $\infty$ & 825.43 \\
p_2 & 18,001,000 & 70,563 & 14,692,000 & 4.508 & 91.289 & $\infty$ & 832.01 \\
\hline
\end{tabular}
\end{table}

 Recall that the Gauss-Newton method corresponds to the minimization of an auxiliary error functional, obtained by linearization of the model response.
the simulation results from the experiment is nearly the same for both simulations. This example shows that the identification procedure for the OW-I model with this set of experimental data is unstable; it cannot provide reliable parameters for use in practical applications. The ill-posedness of the identification problem for the models of OW-I type is also visible from correlation matrices (Appendix B). As seen from Tables 10, 11, and 12, the correlation coefficient between some of the parameters are precisely equal to one. Loosely speaking, the reason for high correlation and unreliable optimization is as follows: the optimization algorithm “does not know” which values of the micro yield stresses $r_i$ should be taken for the best correspondence between simulation and experiment. Since the identification procedure for the OW-I model is clearly unreliable, its error-sensitivity is not studied any further.

5 Analysis of error sensitivity and overparametrization

5.1 Stochastic model of noise

As mentioned in Sect. 2, the actual experimental data contain errors. Following [5, 15, 16], the errors are additive. Therefore, the vector of noisy data $\text{NoisyData}$ is the sum of given experimental data $\text{Exp}$ and the noise $\text{Noise}$: $\text{NoisyData} = \text{Exp} + \text{Noise}$. In this work a simple stochastic model is implemented:

$$\text{NoisyData}_i = \text{Exp}_i + \sum_{k=1}^{20} \epsilon_k \cdot \text{Mode}_k(t_i), \quad \text{(41)}$$

$$\text{Mode}_k(t) = \sin\left(\frac{k\pi t}{T}\right), \quad \epsilon_k \in \mathcal{N}(0, \sigma^2).$$

Here, $\epsilon_k \in \mathcal{N}(0, \sigma^2)$ are independent, normally distributed random values with zero mean and the variance $\sigma^2$; $\text{Mode}_k(t)$ is the $k$th mode of noise with $t \in [0, T]$; $T$ is the duration of observations; $t_i$ is the time instance of $i$th measurement. Since the measured strains are non-dimensional, so is $\sigma$. In the current computations, the standard deviation is $\sigma = 10^{-6}$.

Remark 5 The stochastic model (41) corresponds to correlated noise. Correlated errors are typical in actual measurements [5, 15, 16]. The correlation may stem from systematic measurement errors or mechanical effects like wave propagation and synchronization. The reader interested in other stochastic models of noise is referred to [3, 13, 33, 37]. In many practical situations the real stochastic model of noise is unknown. In that case, the maximum entropy principle is helpful in creating realistic models [44, 48].

Remark 6 In the stochastic model (41), the vector $\text{Exp}$ corresponds to actual measurements, possibly carrying some errors. However, we study the error sensitivity near $\text{Exp}$, thus, in the context of error-sensitivity analysis, the vector $\text{Exp}$ is understood as noise-free (cf. [5, 16]).
Remark 7 The stochastic model (41) uses 20 modes of noise. Higher frequency modes with \( k > 20 \) are not important since they have a zero mean value. The most essential modes correspond to small \( k \).

Note that the implemented probability density function of noise is symmetric: \( \text{PDF}(\vec{x}) = \text{PDF}(−\vec{x}) \) for all \( \vec{x} \in \mathbb{R}^N \). Thus, simplified definition of the CloudSize is valid and equation (4) is used instead of (3).

As mentioned in Sect. 2, quasi Monte Carlo computations are based on Sobol’s sequence instead of pseudo-random numbers. A step-by-step procedure for computing coefficients \( \epsilon_k \) which appear in (41) is described in Appendix C (Fig. 14).

5.2 Mechanics-based metric for ratcheting models

To estimate the sensitivity of material parameters to the experimental errors, we introduce a new mechanics-based metric. This metric gives the distance between two sets of material parameters. The metric idea is to simulate the same stress-controlled ratcheting process using two sets of parameters. The distance is the maximum discrepancy between the strain trajectories:

\[
\text{dist}(\vec{p}^{(1)}, \vec{p}^{(2)}) := \max_{t \in [0, T_{\text{metric}}]} |\epsilon_{11}(t, \vec{p}^{(1)}) − \epsilon_{11}(t, \vec{p}^{(2)})|.
\]

(42)

Here, \( T_{\text{metric}} \) is the overall duration of the stress-controlled ratcheting process; \( \epsilon_{11} \) is the solution of the uniaxial ratcheting problem. The stress-controlled loading history does not have to coincide with the actual loading history used in the experiment:

Reasonable results are expected when the metric (42) utilizes a loading history which is close to the actual application. To be definite, cyclic loading with \( \sigma_{\text{min}} = 0 \) and monotonically increasing \( \sigma_{\text{max}} \) (Fig. 15) is used to define the metric in this study. The load intensity should be chosen such that the accumulated plastic strain \( s \) would not exceed the values of \( s \) obtained in real experiments.

Remark 8 The metric defined by (42) is similar to the one introduced for plasticity models in [37]. The main difference is as follows: For the plasticity models, the metric relies on the assumption that the material model obtains the strain history as input and provides the stress history as output. Thus, the plasticity-related metric is computed in terms of stresses [37]. In ratcheting-related applications, however, the model obtains the stress history as input and provides the total strain as output. Therefore, the proposed distance (42) is a non-dimensional number.

Remark 9 Any similarities between equations (1) and (42) defining the error function \( \Phi(\vec{p}) \) and the metric \( \text{dist}(\vec{p}^{(1)}, \vec{p}^{(2)}) \) are misleading. The error function \( \Phi(\vec{p}) \) describes the deviation of the simulation results from the actual experimental data and the metric \( \text{dist}(\vec{p}^{(1)}, \vec{p}^{(2)}) \) is the distance between \( \vec{p}^{(1)} \) and \( \vec{p}^{(2)} \). Even more, the loading histories used in (1) and (42) are different: The problem (1) employs the loading history which was used in the actual experiment, and the metric (42) should be based on any loading history, close to the chosen application.

The advantages of the new mechanics-based metric are the following:
Table 5 Sizes of the parameter clouds for AF and OW-II models in terms of the mechanics-based metric

| Model | $N_{\text{branches}}$ = 2 | $N_{\text{branches}}$ = 3 | $N_{\text{branches}}$ = 4 |
|-------|-----------------|-----------------|-----------------|
| AF    | 0.000284        | 0.00114         | 0.00342         |
| OW-II | 0.0000142       | 0.000299        | 0.000440        |

- the metric is invariant under reparametrization of the material model;
- the metric accounts for changes in those parameters which have a substantial impact on the mechanical response; less important parameters are automatically disregarded;
- the metric is independent of constants, used to obtain non-dimensional parameters (cf. [37]);
- the metric can be adjusted to specific applications by choosing application-dependent stress-controlled loading history.

The adjustment of the metric to particular applications is of great practical importance. Having an application-related metric, equation (42) makes it possible to study the propagation of an error through the entire modelling chain “experiment → material parameters → solution of the applied problem”.

5.3 Size of the parameter cloud

Let $\tilde{p}^*$ be the set of optimal parameters, obtained from the minimization of the error function $\Phi$. For given experimental data, the set $\tilde{p}^*$ is deterministic. Recall that the sensitivity analysis relies on the (quasi) Monte Carlo method. Let $N_{\text{noise}}$ be the number of draws of noisy data. Each draw is made according to the stochastic model (41). Let $\tilde{p}^{(j)}$ be the set of parameters for the $j$th draw of noisy experimental data, $j = 1, 2, \ldots, N_{\text{noise}}$. Each $\tilde{p}^{(j)}$ is obtained by the computationally efficient procedure in Appendix A.

**Remark 10** Reasonable $\tilde{p}^{(j)}$ are computed only when the noise-free optimal solution $\tilde{p}^*$ is highly accurate. At $\tilde{p}^*$, the gradient of the original error function $\Phi$ must be as close to zero as possible. This is the reason why the refined optimization procedure was implemented in Sect. 4 to find $\tilde{p}^*$.

Recall that the size of the parameter cloud is

\[
\text{CloudSize} = \frac{1}{N_{\text{noise}}} \sum_{j=1}^{N_{\text{noise}}} \text{dist}(\tilde{p}^*, \tilde{p}^{(j)}). \tag{43}
\]

Here, $N_{\text{noise}} = 10,000$. Fast computation of $\text{dist}(\tilde{p}^*, \tilde{p}^{(j)})$ is explained in Appendix D.

It is important that the mechanics-based metric is used here. Thus, CloudSize inherits the physical meaning of the distance function and the invariance under re-parametrization. By definition, CloudSize depends on $\sigma$, the intensity of noise (cf. (41)). For small $\sigma$, this dependence is linear. For brevity of notation, we omit the dependence of CloudSize on $\sigma$.

Table 5 shows the error-sensitivity of AF and OW-II models based on the available experimental data. Clearly, the OW-II models are calibrated much more reliably than the AF models. We discuss this unexpected effect in Appendix E.

5.4 Qualitative comparison of overparametrization criteria

Recall that three formal criteria I–III of overparametrization were listed in Sect. 2.2. They are related to gain in accuracy (criterion I), validation on “unseen” data (criterion II), and correlation among parameters (criterion III). In addition, a new criterion was introduced, based on the CloudSize (criterion IV). Typically, the transition between well parametrized and overparametrized states is smooth and various criteria may yield different results [10]. Therefore, one needs to compare these criteria qualitatively.

Criteria I–III share a common drawback: these criteria say nothing about the propagation of an error through the modelling chain “experiment → material parameters → solution of the applied problem”. Moreover, criterion II strongly depends on the choice of additional “unseen” data. In particular, this criterion cannot be used when “unseen” data are not available. Criterion III depends on the specific choice of parameters since new correlation matrices are obtained for a different parametrization of the same model. The correlation matrices are usually introduced for relatively simple stochastic noise models, like the multivariate normal distribution. Nevertheless, general stochastic models are also compatible with the concept. In that case, the correlation matrices are based on the Fisher information matrix.
The advantages of the newly proposed criterion IV are due to beneficial features of CloudSize, relying on the mechanics-based metric $\text{dist}(\vec{p}_1, \vec{p}_2)$:

- CloudSize is invariant under re-parametrization of the material model.
- CloudSize provides information about the propagation of the error through the entire modelling chain “experiment $\rightarrow$ material parameters $\rightarrow$ solution of the applied problem”. Thus, CloudSize delivers insights into how the experimental noise affects the final simulation results.
- CloudSize can be used with any stochastic model of noise.

Table 6 summarizes the general properties of the overparametrization criteria. Next, we assess the performance of these criteria in terms of concrete material models.

**Overparametrization of AF models** Figure 6 summarizes the results of calibration for the AF models. First, there is virtually no gain in accuracy when refining the model from $N_{\text{branches}} = 3$ to $N_{\text{branches}} = 4$. Thus, according to criterion I, the AF model is overparametrized with respect to given observations for $N_{\text{branches}} = 4$. The validation on “unseen” data shows that predictive capabilities of AF-type models are deteriorating as the number of rheological branches $N_{\text{branches}}$ increases to 4 (Fig. 6, middle). Therefore, criterion II says that the model is not overparametrized even for $N_{\text{branches}} = 4$. Moreover, the correlation among the parameters remains smaller than 0.98 for all $N_{\text{branches}}$ (Tables 13, 14, and 15). The bounded correlation means that criterion III is not active.

The parameter CloudSize is much smaller than for the corresponding AF models (Table 5). Thus, the calibration of models with a larger number of parameters is more sensitive to measurement errors than their simpler counterparts. For the chosen small intensity of noise, the CloudSize ranges up to 0.342 %. This error is of the same order of magnitude as the elastic strains in the VT6 alloy. Such a large error in prediction of the total strain is close to unacceptable. Thus, criterion IV also becomes active. In conclusion, the commonly used criteria I-III are consistent with the new criterion IV; there is a clear relation between overparametrization and pathological error-sensitivity in the case of AF-models.

**Overparametrization of OW-II models** Fig. 8 shows the calibration results for the OW-II models. First, note that the increase of $N_{\text{branches}}$ from three to four does not increase accuracy. Thus, the OW-II model is overparametrized according to criterion I when $N_{\text{branches}} = 4$. Next, for increasing $N_{\text{branches}}$ the predictive capabilities tested on “unseen” data are not deteriorating (Fig. 8, middle). Therefore, criterion II says that the model is not overparametrized even for $N_{\text{branches}} = 4$. Moreover, the correlation among the parameters remains smaller than 0.98 for all $N_{\text{branches}}$ (Tables 13, 14, and 15). The bounded correlation means that criterion III is not active.

The parameter CloudSize is much smaller than for the corresponding AF models (Tables 5). Therefore, according to criterion IV, the OW-II model is not overparametrized even for $N_{\text{branches}} = 4$. In conclusion, the newly proposed criterion IV is consistent with criteria II and III for the OW-II models but not consistent with criterion I.

### Table 6 Basic properties of overparametrization criteria I–IV

| criterion | provides estimates of error propagation | does not require “unseen” data | invariant under re-parametrization | compatible with arbitrary stochastic models |
|-----------|----------------------------------------|-------------------------------|-----------------------------------|-------------------------------------------|
| I         | No                                     | Yes                           | Yes                               | Noise not used                            |
| II        | No                                     | No                            | Yes                               | Noise not used                            |
| III       | No                                     | Yes                           | No                                | Yes                                       |
| IV        | Yes                                    | Yes                           | Yes                               | Yes                                       |

6 Discussion

In phenomenological material modelling, the standard procedure is as follows. First, the model and
numerical algorithm are created, followed by calibration and validation of the model against experimental data. In this study we propose an additional step, namely, the analysis of the sensitivity of identified material parameters with respect to errors contained in experimental data. Based on quasi Monte Carlo computations, the procedure gives insights into the error propagation through the simulation chain. Computationally efficient numerical schemes allow for a significant number of draws without any analytical or numerical difficulties. In particular, the approach is compatible with any stochastic model of noise.

Following the classical protocol of parameter identification, the problem is reduced to minimization of the error functional $\Phi$. As error-resistant solution of optimization problems is imperative in many engineering applications, various alternative approaches were also developed [48]. The advantage of the method advocated in the current study lies in its simplicity and practical use: While choosing among different protocols of parameter identification, the preference should be given to those which are noise resistant.

We show that for increasing number of parameters, the modelling becomes more accurate, but the error-sensitivity increases (Table 5). Thus, a conflict between accuracy and stability appears. A similar conflict was previously reported in [37] for plasticity-related applications.

The general drawback of conventional plasticity models is the kink of the stress-strain curve at the elastic-plastic boundary. One elegant way to solve this problem is introduction of subloading yield surfaces [17, 18]. A simpler way to smoothen the stress-strain curve, used by many, is to take a very large stiffness $c_k$ in one of the rheological branches ($c_k \gg \mu$). The undesired side effect is that an unacceptably large correlation appears among parameters (Appendix B). Thus, dealing with $c_k \gg \mu$, special regularization is needed to avoid the undesired correlations. Probably, the simplest regularization method relies on introduction of additional information, treated as equality constraints [40], which is a special case of the design variable linking technique [31].

Interestingly, when $N_{\text{branches}} = 4$ all three models perform equally well in describing the temperature evolution of the sample (Fig. 12). This similarity is due to convergence of the stress-strain curves to the same limit for large number of rheological branches. Since the dissipation-induced heating depends on the area of hysteresis loops, the temperature evolution in the tested models is nearly identical.

In the tests considered, the models of OW-II type are more stable to experimental errors than the AF-models. This stability is especially unexpected since OW-II models contain more parameters than the AF-models.

7 Conclusion

The paper presents a procedure for the sensitivity analysis of ratcheting models. The process is exemplified by actual experimental data and various kinematic hardening rules, like AF, OW-I, and OW-II. The paper’s main contribution is the new formal criterion of overparametrization, based on the sensitivity analysis (cf. criterion IV in Sect. 2.2). The plausibility of the new criterion is assessed by comparison with standard definitions of overparametrization (cf. criteria I–III in Sect. 2.2). Moreover, several auxiliary conclusions and contributions are made in this study:

- For models of ratcheting, a new mechanics-based metric is presented, allowing to measure the distance between sets of material parameters.
- A computationally efficient quasi Monte Carlo procedure is used to estimate the stability of the identified parameters; a large number of draws can be taken ($N_{\text{noise}} \geq 10,000$).
- A new rule of isotropic hardening is proposed. Dealing with the VT6 alloy, it is more accurate than the classical Voce and Ludvig rules based on the accumulated plastic arc-length $s$. Numerical algorithms originally developed for $R = R(s)$ can be straightforwardly generalized for the ansatz $R = R(s, s/\mu_1)$.
- For the increasing number of parameters, Cloud-Size grows large. Moreover, CloudSize reaches a threshold for overparametrized models. These two observations indicate that there is a relation between pathological error sensitivity and overparametrization.
- In the considered example, the calibration of OW-II models is more reliable than the calibration of AF and OW-I models.
The proposed criterion of overparametrization benefits from the implemented mechanics-based metric. The presented methodology is favourable for analysis of parameter identification protocols involving a large amount of noisy data, like heterogeneous data provided by digital image correlation or X-ray tomography. In particular, the methodology is promising for a flexible design of information-rich experiments.

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**Declarations**

**Conflict of interest** The authors declare that they have no conflict of interest.

**Appendix A: Fast computation of \( \vec{p}^{(j)} \)**

We discuss a quick computation of the parameter vectors \( \vec{p}^{(j)} \in \mathbb{R}^n \), corresponding to the \( j \)th draw of noisy data. The procedure is the same as in [38]. Recall that \( \vec{Exp} \in \mathbb{R}^{N_{exp}} \) is the vector of available experimental data, \( \vec{Mod}(\vec{p}) \in \mathbb{R}^{N_{exp}} \) is the corresponding modelling response, \( \vec{p} = (\vec{p}_c, \vec{p}_K) \in \mathbb{R}^n \) is the vector of unknown material parameters. Within the sensitivity analysis, the actual experimental data are replaced by the noisy data \( \vec{Exp} + \vec{Noise} \). The optimal set of parameters corresponding to noise-free data is denoted as \( \vec{p}^* \). The Jacobian of the model response at \( \vec{p}^* \) is the operator \( J := \frac{\partial \vec{Mod}(\vec{p})}{\partial \vec{p}} |_{\vec{p}^*} \in \mathbb{R}^{N_{exp} \times n} \).

Assuming only small changes in parameters, we linearize the model response near \( \vec{p}^* \):

\[
\vec{Mod}^{lin}(\vec{p}) := \vec{Mod}(\vec{p}^*) + J(\vec{p} - \vec{p}^*).
\]

Now, the parameter set \( \vec{p}^{(j)}, j = 1, 2, \ldots, N_{\text{noise}} \) is the minimizer of the error function for noisy data

\[
\Phi_{\text{noisy}}(\vec{p}) := \vec{Resid}^T \vec{Resid},
\]

\[
\vec{Resid} := \vec{Exp} + \vec{Noise} - \vec{Mod}^{lin} \vec{p}^{(j)}.
\]

Abbreviate by \( \vec{A} \) the following vector:

\[
\vec{A} := \vec{Exp} + \vec{Noise} - \vec{Mod}(\vec{p}^*) - J(\vec{p}^*).
\]

Then the error function is a quadratic form of \( \vec{p} \), given by

\[
\Phi_{\text{noisy}}(\vec{p}) = (\vec{A} - J\vec{p})^T (\vec{A} - J\vec{p}).
\]

Its derivative with respect to \( \vec{p} \) is a linear function of the unknown parameter vector \( \vec{p} \)

\[
\frac{\partial \Phi_{\text{noisy}}(\vec{p})}{\partial \vec{p}} = -2(\vec{A} - J\vec{p})^T J.
\]

The stationarity condition \( \frac{\partial \Phi_{\text{noisy}}(\vec{p})}{\partial \vec{p}} = 0 \) yields a system of linear algebraic equations with respect to \( \vec{p} \). Then the analytical solution is

\[
\vec{p}^{(j)} = (J^T J)^{-1} J^T \vec{A}.
\]

**Table 7** Correlation matrix for AF model with \( N_{\text{branches}} = 2 \)

|   | \( \gamma \) | \( \beta \) | \( c_1 \) | \( c_2 \) | \( x_1 \) | \( x_2 \) | \( K \) |
|---|-------------|-------------|--------|--------|--------|--------|-------|
| \( \gamma \) | 1.0000 | 0.4252 | 0.5607 | 0.1449 | -0.4514 | 0.2135 | -0.1029 |
| \( \beta \) | 0.4252 | 1.0000 | -0.0839 | -0.0260 | 0.0855 | -0.0555 | 0.0355 |
| \( c_1 \) | 0.5607 | -0.0839 | 1.0000 | 0.4708 | -0.9815 | 0.2795 | -0.3598 |
| \( c_2 \) | 0.1449 | -0.0260 | 0.4708 | 1.0000 | -0.5148 | -0.6415 | -0.9334 |
| \( x_1 \) | -0.4514 | 0.0855 | -0.9815 | -0.5148 | 1.0000 | -0.2535 | 0.3874 |
| \( x_2 \) | 0.2135 | -0.0555 | 0.2795 | -0.6415 | -0.2535 | 1.0000 | 0.7915 |
| \( K \) | -0.1029 | 0.0355 | -0.3598 | -0.9334 | 0.3874 | -0.7915 | 1.0000 |
In fact, this semi-analytical solution represents a single iteration of the Gauss-Newton method [49].

Unfortunately, due to matrix multiplication, the condition number of $A^{T}A$ can be very large. This effect may falsify the results of (51). To resolve this problem, QR decomposition of $A$ should be implemented:

$$J = QR \in \mathbb{R}^{N \times n}, \quad Q \in \mathbb{R}^{N \times n}, \quad Q^{T}Q = I \in \mathbb{R}^{n \times n}, \quad R \in \mathbb{R}^{n \times n}. \quad (52)$$

Here, $R$ is upper triangular. Substituting this into (51), we have after some computations

$$\tilde{p}^{(t)} = R^{-1}Q^{T}A.$$

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$$\tilde{p}^{(t)} = R^{-1}Q^{T}A.$$
Since the matrix $R^{-1}Q^{T}$ is pre-computed, the parameter cloud is evaluated extremely efficiently even for a large number of draws ($N_{\text{draws}} \geq 10,000$). The condition number of the matrix $R$ behaves like the square root of the condition number of $J^TJ$. Thus, (53) gives more robust solution than (51).

### Appendix B: Correlation matrices

Let $J$ be the Jacobian, defined in (44). The correlation matrix $\text{Corr} \in \mathbb{R}^{n \times n}$ is defined as follows [7]:

$$\text{Corr}_{ij} = \frac{P_{ij}}{\sqrt{P_{ii}P_{jj}}}, \quad \text{where} \quad P = (J^TJ)^{-1} \in \mathbb{R}^{n \times n}. \tag{54}$$

We say that there is a strong correlation between parameters $p_i$ and $p_j$, if $\text{Corr}_{ij} \approx \pm 1$. In that case, a
slight change in $p_j$ can be counteracted by a change in $p_j$, still leaving the model response $\hat{\text{Mod}}$ virtually the same. In such situations the minimum of the error functional $\Phi$ lies in a “horizontal ravine” (cf. Fig. 10 in [32]). In the sense of Euclidean metric, a large correlation between parameters is characteristic for ill-defined optimization problems.

Appendix C: Implementation of Sobol’s sequence

For each draw of the Monte Carlo method, the stochastic model (41) requires 40 independent random numbers $\varepsilon_k \in N(0, \sigma^2)$ (20 numbers to obtain noisy data for each test). Within the quasi Monte Carlo method, they are obtained in the following way. First, we set the properties of the Sobol sequence. $\text{Dimensions}$ is the number of terms of the Sobol sequence in each draw; we use $\text{Dimensions} = 40$. $\text{Skip}$ is the number of initial points to omit from Sobol’s sequence, we put $\text{Skip} = 10^3$. $\text{Leap}$ is the interval between points of the sequence; $\text{Leap} = 3 \cdot 10^2$ in our case.

Recall that $N_{\text{noise}}$ is the number of draws. Calling Sobol’ generator [8] we obtain a matrix $S \in \mathbb{R}^{N_{\text{noise}} \times \text{Dimensions}}$ of quasi-random numbers uniformly distributed over the interval [0, 1]. Then for

| $\gamma$ | $\beta$ | $c_1$ | $c_2$ | $c_3$ | $r_1$ | $r_2$ | $r_3$ | $K$ | $m$ |
|---|---|---|---|---|---|---|---|---|---|
| 1.0000 | 0.4060 | -0.0375 | 0.0314 | -0.1305 | 0.0886 | -0.0314 | -0.1304 | -0.0626 | 0.3707 |
| 0.4060 | 1.0000 | -0.0134 | -0.0080 | 0.0513 | -0.0149 | -0.0238 | 0.0591 | 0.0583 | -0.1065 |
| -0.0375 | -0.0134 | 1.0000 | 0.0995 | 0.1467 | 0.1197 | 0.0906 | 0.1162 | -0.3628 | -0.1244 |
| 0.0314 | 0.0134 | -0.0080 | 1.0000 | 0.5530 | -0.4165 | 0.9737 | -0.0008 | -0.0061 | -0.5962 |
| -0.1305 | 0.0513 | 0.1467 | 0.5530 | 1.0000 | -0.7498 | 0.5542 | 0.8072 | 0.0608 | -0.5079 |
| 0.0886 | -0.0149 | 0.1197 | -0.4165 | 0.7498 | 1.0000 | -0.4125 | -0.6502 | -0.5774 | 0.3668 |
| -0.0314 | -0.0238 | 0.0906 | 0.9737 | 0.5542 | -0.4125 | 1.0000 | 0.0072 | -0.0321 | -0.4958 |
| -0.1304 | 0.0591 | 0.1162 | -0.0008 | 0.8072 | -0.6502 | 0.0072 | 1.0000 | -0.0630 | -0.1636 |
| -0.0626 | 0.0583 | -0.3628 | 0.0061 | 0.0608 | -0.5774 | -0.0321 | -0.0630 | 1.0000 | -0.1395 |
| 0.3707 | -0.1065 | -0.1244 | -0.5962 | -0.5079 | 0.3668 | -0.4958 | -0.1636 | -0.1395 | 1.0000 |

| $\gamma$ | $\beta$ | $c_1$ | $c_2$ | $c_3$ | $c_4$ | $r_1$ | $r_2$ | $r_3$ | $r_4$ | $K$ | $m$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.0000 | 0.4135 | 0.0146 | -0.0427 | -0.0742 | -0.1835 | -0.0636 | -0.0987 | 0.1119 | -0.1729 | 0.0101 | 0.3868 |
| 0.4135 | 1.0000 | -0.0057 | 0.0157 | 0.0249 | 0.0627 | 0.0219 | -0.0002 | -0.0264 | 0.0659 | 0.0177 | -0.1092 |
| 0.0146 | -0.0057 | 1.0000 | -0.0283 | -0.0934 | -0.0367 | 0.1146 | -0.0258 | -0.0219 | -0.0299 | -0.0633 | 0.0384 |
| -0.0427 | 0.0157 | -0.0283 | 1.0000 | 0.1767 | 0.6513 | 0.1390 | 0.9773 | 0.3949 | 0.2469 | -0.0868 | -0.6823 |
| -0.0742 | 0.0249 | -0.0934 | 0.1767 | 1.0000 | 0.2426 | -0.2243 | 0.1614 | 0.3860 | 0.2175 | 0.6757 | -0.2207 |
| -0.1835 | 0.0627 | -0.0367 | 0.6513 | 0.2426 | 1.0000 | 0.2032 | 0.6453 | 0.6100 | 0.8789 | -0.1479 | -0.6251 |
| -0.0636 | 0.0219 | 0.1146 | 0.1390 | -0.2243 | 0.2032 | 1.0000 | 0.1270 | -0.6850 | 0.1890 | -0.1694 | -0.1789 |
| -0.0987 | -0.0002 | -0.0258 | 0.9773 | 0.1614 | 0.6453 | 0.1270 | 1.0000 | -0.3873 | 0.2435 | -0.0899 | -0.5964 |
| 0.1119 | -0.0264 | -0.0219 | -0.3949 | 0.3860 | -0.6100 | -0.6850 | -0.3873 | 1.0000 | -0.5637 | -0.3508 | 0.3794 |
| 0.1729 | 0.0659 | -0.0299 | 0.2469 | 0.2175 | 0.8789 | 0.1890 | 0.2435 | 0.5637 | 1.0000 | -0.1422 | -0.3655 |
| 0.0101 | 0.0177 | -0.0633 | -0.0868 | -0.6757 | -0.1479 | -0.1694 | -0.0899 | -0.3508 | -0.1422 | 1.0000 | 0.0506 |
| 0.3868 | -0.1092 | 0.0384 | -0.6823 | -0.2207 | 0.6251 | -0.1789 | -0.5964 | 0.3794 | -0.3655 | 0.0506 | 1.0000 |

Table 14 Correlation matrix for OW-II model with $N_{\text{branches}} = 3$

Table 15 Correlation matrix for OW-II model with $N_{\text{branches}} = 4$
Table 16 Condition numbers of $R$

| model | $N_{\text{branches}} = 2$ | $N_{\text{branches}} = 3$ | $N_{\text{branches}} = 4$ |
|-------|-----------------|-----------------|-----------------|
| AF    | $1.6 \cdot 10^4$ | $6.1 \cdot 10^4$ | $6.9 \cdot 10^4$ |
| OW-II | $5.3 \cdot 10^3$ | $8.4 \cdot 10^3$ | $7.3 \cdot 10^3$ |

Table 17 Condition numbers of $J^T J$

| model | $N_{\text{branches}} = 2$ | $N_{\text{branches}} = 3$ | $N_{\text{branches}} = 4$ |
|-------|-----------------|-----------------|-----------------|
| AF    | $1.6 \cdot 10^9$ | $2.2 \cdot 10^9$ | $1.8 \cdot 10^9$ |
| OW-II | $2.8 \cdot 10^7$ | $7.1 \cdot 10^7$ | $5.3 \cdot 10^7$ |

the $j$th draw, the corresponding quasi-random variables with the normal distribution are:

$$
\epsilon_{j,2i+1} = \cos(2\pi S_{j,2i+1}) \cdot \sqrt{-2 \ln S_{j,2i+1}},
$$

$$
\epsilon_{j,2i+2} = \sin(2\pi S_{j,2i+1}) \cdot \sqrt{-2 \ln S_{j,2i+1}},
$$

for $j = 1, 2, ..., N_{\text{noise}}$, $i = 1, 2, ..., \text{Dimensions}$.

Appendix D: Fast computation of the distance

The fast computation of the distance between two sets of parameters relies on the linearization of the strain response function $\epsilon_{11}(t)$ with respect to the material parameters. For the fixed stress-controlled loading history (Fig. 15) we evaluate the derivative

$$
\frac{d\epsilon_{11}(t, \vec{p})}{d\vec{p}}|_{\vec{p} = \vec{p}^*}, \quad t \in [0, T_{\text{metric}}].
$$

For the parameter set $\vec{p}$ close to the center of the cloud $\vec{p}^*$, the axial strain $\epsilon_{11}(t, \vec{p})$ is approximated as

$$
\epsilon_{11}(t, \vec{p}) = \epsilon_{11}(t, \vec{p}^*) + \frac{d\epsilon_{11}(t, \vec{p})}{d\vec{p}} \cdot (\vec{p} - \vec{p}^*),
$$

where $\epsilon_{11}(t, \vec{p}^*)$ is the strain history related to the center of the parameter cloud. Then the mechanics-based distance between $\vec{p}^*$ and $\vec{p}$ is

$$
\text{dist}(\vec{p}, \vec{p}^*) = \max_{t \in [0, T_{\text{metric}}]} |d\epsilon_{11}(t, \vec{p})|.
$$

Appendix E: AF versus OW-II regarding error sensitivities

Table 5 says that the material parameters of the AF models are more sensitive to experimental errors than the parameters of the OW-II models. To obtain an intuitive insight into this effect, recall that for each instance of noisy data the set $\vec{p}^{(i)}$ is computed through (48) and (53). Thus, the scatter of parameters $\vec{p}^{(i)}$ depends on the matrix $R \in \mathbb{R}^{n \times N}$. Recall that $R$ is obtained by the QR decomposition of the Jacobian $J \in \mathbb{R}^{N_{\text{param}} \times n}$ (Appendix A). The condition numbers of $R$ are listed in Table 16 for both models; they are evaluated with respect to the $l_2$ norm. Interestingly, the dependence of the condition number on $N_{\text{branches}}$ is not monotonic. However, the AF models exhibit much larger condition number than the OW-II models in all the cases. Therefore, in the Euclidean $l_2$ metric, the parameter vector of the AF models is more sensitive to the noise than for the OW-II models. This high sensitivity corresponds to the results shown in Table 5.

As noted in Appendix A, the condition number of the matrix $R$ behaves like the square root of the condition number of $J^T J$. The corresponding values are summarized in Table 17. Recall that the columns of $J$ are derivatives of the model response with respect to individual parameters. The large condition number of $J^T J$ means that the columns of the Jacobian $J$ are “close” to being linearly dependent. Geometrically, this means that the columns “almost” lie in an $(n - 1)$-dimensional subspace of $\mathbb{R}^{N_{\text{param}}}$. Table 17 suggests that this is likely the case for the AF model.

For the AF models, the minimum eigenvalues $\lambda_{\text{min}}$ of the matrix $R$ are shown in Table 18. Since the eigenvalues are close to zero, the corresponding eigenvectors represent certain directions in the space of parameters, such that the model response $\text{Mod}(\vec{p})$
is almost the same along those directions (Table 18). Recalling (35), we conclude that a small increase in \( c_1 \) can be compensated by an increase in \( \gamma \) and \( \beta \).

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