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Research article / *Article de recherche*

On the formulation and convergence of Data-Driven Identification

Sur la formulation et la convergence de l'identification guidée par les données

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Abstract.
Background: The Data-Driven Identification(DDI) method is a model-free approach to the identification of the mechanical stress in parts subject to statically indeterminate stress states. Although the method has been applied in many studies, no theoretical analysis of its convergence has been proposed so far.
Purpose: The aim of this manuscript is to propose a first study of the DDI properties in order to increase the confidence in the results and guide the selection of optimal parameters.
Methods: A new formulation compared to the original one is proposed to explicitly define a minimization problem that is more amenable to analysis. The algebraic characteristics of the new formulation are studied to derive properties of interest.
Results: A simple criterion for the uniqueness of the DDI estimate is derived. In the case of elastic material behavior, an estimate of the error on the identified stress field is proposed. These results are illustrated using a synthetic dataset.
Conclusion: This work proposes a first analysis of the DDI and demonstrates the ability of the method to compute a model-free estimation of the stress field. The developed criteria and estimator open the door to further developments for the improvement of the method, the design of sample geometries and loading path and extension to other classes of material behavior.

Résumé.
Contexte : La méthode d'Identification Guidée par les Données (Data-Driven Identification — DDI) est une approche sans modèle pour l'identification des contraintes mécaniques dans des pièces soumises à des états de contrainte statiquement indéterminés. Bien que cette méthode ait été appliquée dans de nombreuses études, aucune analyse théorique de sa convergence n'a encore été proposée.
Objectif : Ce manuscrit a pour but de proposer une première étude des propriétés de la méthode DDI, afin de renforcer la confiance dans les résultats obtenus et de guider la recherche de paramètres optimaux.
Méthodes : Une nouvelle formulation, différente de celle d'origine, est proposée afin de définir explicitement un problème de minimisation plus favorable à l'analyse. Les caractéristiques algébriques de cette nouvelle formulation sont étudiées pour en déduire des propriétés pertinentes.
Résultats : Un critère simple d'unicité de l'estimation DDI est établi. Dans le cas d'un comportement élastique du matériau, une estimation de l'erreur sur le champ de contraintes identifié est proposée. Ces résultats sont illustrés à l'aide d'un jeu de données synthétiques.
Conclusion : Ce travail propose une première analyse théorique de la méthode DDI et démontre sa capacité à estimer le champ de contraintes sans recours à un modèle. Les critères développés et l'estimateur présenté ouvrent la voie à de futurs développements : amélioration de la méthode, conception de géométries d'échantillons et de chemins de chargement, ainsi qu'extension à d'autres types de comportement matériau.

Keywords. Data-driven identification, Material characterization, Full-field identification.

Mots-clés. Identification guidée par les données, Caractérisation des matériaux, Identification plein champ.

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1. Introduction

The identification of the mechanical response of materials from full-field kinematic measurements on geometrically complex samples is a rich field where numerous numerical approaches have been proposed. This ill-posed problem is typically regularized using a constitutive model of the material under study. Methods such as the virtual field methods, the Finite Element Model Updating (FEMU) method, the modified Constitutive relation error (mcre) propose efficient settings for the identification of the model parameters [1,2]. The constitutive model at the core of these approaches is however also one of the weak links. Since the model must be postulated a priori, testing an alternative model often incurs high computational costs while evaluating the relevance of a specific model can be challenging.

Alternative approaches have been proposed to circumvent these issues. Flaschel et al. [3] have suggested the use of sparse regression techniques to select relevant building blocks in a library of models while adjusting the parameters. Other methods, based on Machine Learning technology propose to replace the constitutive model by a phenomenological surrogate model that can adapt itself to the data [2,4,5]. Depending on the specific choice of surrogate model, it is possible to enforce constraints on its thermodynamic properties. This line of research is very active as the tools of artificial intelligence mature and gradually diffuse to the computational mechanics community.

Inspired by the Data-Driven Computational Mechanics (DDCM) method introduced by Kirchdoerfer and Ortiz [6], the Data-Driven Identification (DDI) [7] method is a model free method for estimating the mechanical response of materials and the heterogeneous Cauchy stress fields on test samples. Both DDCM and DDI differ from traditional computational mechanics as they do not account for the material behavior through a set of equations (closed form, implicit, neural network, ...) but through a discrete database of points that sample the material response in a well chosen space.

Although DDI has been successfully applied to synthetic and real data in various settings-including elasticity [7], hyperelasticity [8], elastoplasticity [9]—no theoretical analysis of the method has been conducted to demonstrate its ability to correctly estimate and converge to the mechanical stress. As a consequence its parameters have usually been chosen empirically, possibly leading to suboptimal estimation or some form of overfitting.

In this manuscript:

(1) we propose a reformulation of the DDI method in a way that is more prone to its mathematical analysis. The complex optimization problem lying at the core of DDI and usually solved through alternated minimization is discussed.
(2) We propose a criterion for characterizing the uniqueness of the problem solution upon convergence. This criterion can be used to assess the possible over parametrization of the DDI database.
(3) We show that it is possible to derive an error bound for the identified stress field therefore showing that the DDI can indeed be used to estimate the stress field. These results are illustrated in the absence of noise on synthetic data for a nonlinear elastic behavior.

2. DDI formulation

In this section, we recall the original DDI as introduced in [7] using different notations in order to ease its understanding and the subsequent analysis proposed in this manuscript.

2.1. *Formulation*

The stress field $\boldsymbol{\sigma}$ identified with DDI is constrained to satisfy mechanical equilibrium. In the quasi-static case, the discretized equations are linear with respect to the stress and read:

$$\sum_{e'=1}^{m} \mathbf{D}_{ke'} \cdot \boldsymbol{\sigma}_{e'} - \mathbf{f}_k = 0 \quad \forall k \in 1 \dots n. \tag{1}$$

If the Finite Element method is used to discretize the problem e' is an index over the m quadrature points, while k is an index over the n nodes. The vectors $\mathbf{f}_k$ denote nodal forces arising from body forces or boundary conditions. Guidelines for the robust construction of $\mathbf{D}_{ke}$ and $\mathbf{f}_k$ taking into account experimental limitations such as the unavailability of kinematic data close to boundaries can be found in [10].

In most cases Equation (1) is statically indeterminate, meaning it has multiple solutions because there are more unknowns than independent equations. DDI uses the infinitesimal strain field $\boldsymbol{\epsilon}$, to regularize the problem and select a particular stress field. The strain field is assumed to be available at each quadrature point and is usually obtained from full-field kinematic measurements methods as Digital Image Correlation (DIC).

The input data for the DDI method consists of the following:

(1) the equilibrium operator $\mathbf{D}_{ke}$ and associated force vector $\mathbf{f}_k$,
(2) the strain at all quadrature points, $\boldsymbol{\epsilon}_e$.

Following the Data-Driven Computational Mechanics framework introduced by Kirchdoerfer and Ortiz [6], the material behavior is represented by a discrete set of $N_{\mathscr{D}}$ strain($\mathscr{E}$)–stress($\mathscr{S}$) pairs, referred to as material states, that sample the mechanical response of the material and are collected into a material database $\mathscr{D}$:

$$\mathscr{D} = \{(\mathscr{E}_i, \mathscr{S}_i)\}_{i=1\dots N_{\mathscr{D}}}. \tag{2}$$

At each quadrature point e in the domain, the mechanical state is defined as the strain–stress pair $(\boldsymbol{\epsilon}_e, \boldsymbol{\sigma}_e)$. It is associated to a single material state through a $m \times N_{\mathscr{D}}$ binary pairing matrix P_{ei}:

$$P_{ei} \in \{0, 1\} \quad \text{for } 1 \le e \le m \text{ and } 1 \le i \le N_{\mathscr{D}}, \tag{3}$$

$$\sum_{i'=1}^{N_{\mathscr{D}}} P_{ei'} = 1 \quad \forall e. \tag{4}$$

The position of the single non-zero entry of line e identifies the index of the material state associated to the mechanical state e. Inversely, the non-zero entries of a column correspond to all the mechanical states associated to a specific material state. The columns of matrix P_{ei} induce a natural partitioning of the mechanical states into $N_{\mathscr{D}}$ clusters:

$$\Omega_i = \{e \mid P_{ei} = 1\} \quad \forall i. \tag{5}$$

Since each mechanical state corresponds to a quadrature point, each Ω_i can also be viewed as a subdomain of the whole computational domain. We assume that all Ω_i are non-empty. The number of elements N_i in each cluster is given by:

$$N_i = |\Omega_i| = \sum_{e'=1}^{m} P_{e'i} = \sum_{e'=1}^{m} P_{e'i} P_{e'i} \quad \forall i. \tag{6}$$

The material database and the pairing matrix are used to build the material strain field:

$$\boldsymbol{\epsilon}^*_e = \sum_{i'=1}^{N_{\mathscr{D}}} P_{ei'} \boldsymbol{\mathscr{E}}_{i'} \quad \forall e, \tag{7}$$

and the material stress field:

$$\boldsymbol{\sigma}^*_e = \sum_{i'=1}^{N_{\mathscr{D}}} P_{ei'} \boldsymbol{\mathscr{S}}_{i'} \quad \forall e. \tag{8}$$

By construction, all material fields are constant over each Ω_i.

In DDI, the mechanical stress field $\boldsymbol{\sigma}_e$, the material database $\mathscr{D}$ and the material–mechanical pairing P_{ei} are determined from the intuition that similar strain values should yield similar stress values. Since the material database provides a coarse sampling of the material response the following loss function is used for minimizing the quadratic distance between the mechanical and the material fields (strain and stress):

$$\begin{aligned}\mathscr{F}(\boldsymbol{\sigma}_e, \boldsymbol{\mathscr{E}}_i, \boldsymbol{\mathscr{S}}_i, P_{ei}) = &\frac{1}{2} \sum_{e'=1}^{m} w_{e'} (\boldsymbol{\epsilon}_{e'} - \boldsymbol{\epsilon}^*_{e'}) : \mathbb{C} : (\boldsymbol{\epsilon}_{e'} - \boldsymbol{\epsilon}^*_{e'}) \\ &+ \frac{1}{2} \sum_{e'=1}^{m} w_{e'} (\boldsymbol{\sigma}_{e'} - \boldsymbol{\sigma}^*_{e'}) : \mathbb{C}^{-1} : (\boldsymbol{\sigma}_{e'} - \boldsymbol{\sigma}^*_{e'}),\end{aligned} \tag{9}$$

which is identical to the penalty function of DDCM [6]. The loss function $\mathscr{F}$ is parametrized through w_e and $\mathbb{C}$. The weights w_e were originally [6,7] defined as the quadrature weights but this can actually be relaxed to reflect, for example, the level of confidence in the input data. The fourth order positive definite tensor $\mathbb{C}$ is a pseudo-stiffness tensor that should not be interpreted as describing a tangent material behavior. It serves several purposes:

(1) it gives the same units to all terms of Equation (9),
(2) its magnitude provides the weighting between the terms of Equation (9) involving the strain and the terms involving the stress,
(3) it provides a weighting between the different components of the strain and stress tensors to go beyond the 2-norm.

In several studies [10,11] $\mathbb{C}$ was simply taken as the identity tensor.

Finally, DDI can be written as the following equilibrium-constrained minimization problem:

$$\{\boldsymbol{\sigma}_e, \boldsymbol{\mathscr{E}}_i, \boldsymbol{\mathscr{S}}_i, P_{ei}\} = \arg\min \mathscr{F}(\boldsymbol{\sigma}'_e, \boldsymbol{\mathscr{E}}'_i, \boldsymbol{\mathscr{S}}'_i, P'_{ei})$$

with,

$$\begin{aligned}\boldsymbol{\epsilon}^*_e &= \sum_{i'=1}^{N_{\mathscr{D}}} P_{ei'} \boldsymbol{\mathscr{E}}_{i'} \quad \forall e, \\ \boldsymbol{\sigma}^*_e &= \sum_{i'=1}^{N_{\mathscr{D}}} P_{ei'} \boldsymbol{\mathscr{S}}_{i'} \quad \forall e, \\ \sum_{e'=1}^{m} \mathbf{D}_{ke'} \cdot \boldsymbol{\sigma}_{e'} - \mathbf{f}_k &= 0 \quad \forall k.\end{aligned}$$

The parameters of the method are: the scalar $N_{\mathscr{D}}$, the fourth order tensor $\mathbb{C}$ and the scalar weights w_e.

2.2. *Solution*

The above problem contains both real valued unknowns ($\{\boldsymbol{\sigma}_e, \boldsymbol{\mathscr{E}}_i, \boldsymbol{\mathscr{S}}_i\}$) and discrete valued unknowns (P_{ei}). As shown by Kanno [12], the minimization of DDCM problems, for which the material database $\mathscr{D}$ is known falls into the Mixed Integer Quadratic Programming (MIQP) problem

class. In the case of DDI this is no longer the case since both P_{ei} and $\boldsymbol{\mathscr{S}}_i$ are unknown. The loss function therefore involves the square of the product of unknowns. As the pairing matrix is binary the combinatorial nature of the problem remains. The main consequence is that for almost all large enough problems, the global minimum cannot be efficiently computed and heuristics are doomed to converge to local minima. In DDI as in DDCM the minimization is carried out by alternatively performing the minimization with respect to the discrete valued variables and real valued variables, until a fixed point is reached. Each step is detailed below.

The minimization over P_{ei} for given $\{\boldsymbol{\sigma}_e, \boldsymbol{\mathscr{E}}_i, \boldsymbol{\mathscr{S}}_i\}$ is carried out independently for each e:

$$P_{ei} = \delta_{ii^*} \quad \forall e, \tag{10}$$

with,

$$i^* = \arg\min_{i'} (\boldsymbol{\epsilon}_e - \boldsymbol{\mathscr{E}}_{i'}) : \mathbb{C} : (\boldsymbol{\epsilon}_e - \boldsymbol{\mathscr{E}}_{i'}) + (\boldsymbol{\sigma}_e - \boldsymbol{\mathscr{S}}_{i'}) : \mathbb{C}^{-1} : (\boldsymbol{\sigma}_e - \boldsymbol{\mathscr{S}}_{i'}). \tag{11}$$

This amounts to pairing each mechanical state with the closest database point according to the metric defined by $\mathbb{C}$.

The minimization over $\{\boldsymbol{\sigma}_e, \boldsymbol{\mathscr{E}}_i, \boldsymbol{\mathscr{S}}_i\}$ for a given pairing P_{ei} is carried out in two steps: first over the material database $\{\boldsymbol{\mathscr{E}}_i, \boldsymbol{\mathscr{S}}_i\}$, and the result is then substituted for the minimization over the mechanical stress $\boldsymbol{\sigma}_e$. Stationarity conditions with respect to the material database read:

$$\boldsymbol{\mathscr{E}}_i = \frac{1}{W_i} \sum_{e'} P_{e'i} w_{e'} \boldsymbol{\epsilon}_{e'} \quad \forall i, \tag{12}$$

and,

$$\boldsymbol{\mathscr{S}}_i = \frac{1}{W_i} \sum_{e'} P_{e'i} w_{e'} \boldsymbol{\sigma}_{e'} \quad \forall i, \tag{13}$$

with

$$W_i = \sum_{e'} P_{e'i} w_{e'} \quad \forall i. \tag{14}$$

These simply define the material database strain (resp. stress) as the w_e-weighted average of the mechanical strain (resp. stress) over each cluster, independently of the tensor $\mathbb{C}$. Equation (13) can be substituted into (8) to eliminate $\boldsymbol{\mathscr{S}}_i$ in the definition of the material stress field:

$$\boldsymbol{\sigma}^*_e = \sum_{i'} P_{ei'} \boldsymbol{\mathscr{S}}_{i'} = \sum_{a'} M_{ea'} \boldsymbol{\sigma}_{a'} \quad \forall e, \tag{15}$$

with the matrix M_{ea} defined as:

$$M_{ea} = \sum_i \frac{1}{W_i} P_{ei} P_{ai} w_a \quad \forall e, a. \tag{16}$$

The material stress field is thus directly expressed as constant over each cluster and equal to the w_e-weighted cluster average of the mechanical stress field.

Defining the matrix H_{ea} as:

$$H_{ea} = \sum_{e'} (I_{ee'} - M_{ee'}) w_{e'} (I_{e'a} - M_{e'a}) \quad \forall e, a, \tag{17}$$

the material database $\{(\mathscr{E}_i, \mathscr{S}_i)\}_{i=1\ldots N_{\mathscr{D}}}$ can be eliminated from loss function expression (9):

$$\mathscr{F}(\boldsymbol{\sigma}_e, P_{ei}) = \frac{1}{2} \sum_{e',a'} H_{e'a'} \boldsymbol{\epsilon}_{e'} : \mathbb{C} : \boldsymbol{\epsilon}_{a'} + \frac{1}{2} \sum_{e',a'} H_{e'a'} \boldsymbol{\sigma}_{e'} : \mathbb{C}^{-1} : \boldsymbol{\sigma}_{a'}. \tag{18}$$

In the above expression, the matrix $H_{e,a}$ implicitly depends on the pairing P_{ei}. For a given pairing defined through P_{ei}, the mechanical stress field $\boldsymbol{\sigma}_e$ is the solution of the following problem:

$$\boldsymbol{\sigma}_e = \arg\min \sum_{e'a'} H_{e'a'} \boldsymbol{\sigma}_{e'} : \mathbb{C}^{-1} : \boldsymbol{\sigma}_{a'}, \tag{19}$$

with

$$\sum_{e'} \mathbf{D}_{ke'} \cdot \boldsymbol{\sigma}_{e'} = \mathbf{f}_k \quad \forall k \in 1 \dots n. \tag{20}$$

In order to initialize this alternated minimization strategy the simplest method is to start from a preliminary pairing P_{ei} which can be obtained by computing a k-means [13] clustering of the available mechanical states data. A possible strategy for computing the DDI solution through alternated minimization is thus:

(1) Estimate the mechanical stress $\boldsymbol{\sigma}_e$ in any reasonable way.
(2) Initialize P_{ei} through a w_e-weighted k-means clustering in the $\mathbb{C}$-norm applied to the mechanical states $(\boldsymbol{\epsilon}_e, \boldsymbol{\sigma}_e)$.
(3) Update the mechanical stress $\boldsymbol{\sigma}_e$ through Equations (19), (20).
(4) Update the material database through Equations (12), (13).
(5) Update the pairing P_{ei} through Equation (10).
(6) Iterate 3–5 until convergence.

The use of k-means at the initialization stage is not fortuitous since steps 4–5 actually correspond to a weighted k-means iteration applied to the current estimate of mechanical states $(\boldsymbol{\epsilon}_e, \boldsymbol{\sigma}_e)$. For elastic behaviors, as $\boldsymbol{\sigma}_e$ is a function of $\boldsymbol{\epsilon}_e$, it is reasonable to assume that the pairing P_{ei} can be determined a priori from the strain data only. The solution strategy becomes:

(1) Initialize P_{ei} through a w_e-weighted k-means clustering in the $\mathbb{C}$-norm applied to the mechanical strain $\boldsymbol{\epsilon}_e$.
(2) Compute the mechanical stress $\boldsymbol{\sigma}_e$ through Equations (19), (20).
(3) Compute the material database through Equations (12), (13).

In case the experimental data consists of different loading scenarios applied to one or several samples, all the above analysis remains valid provided that the indices corresponding to quadrature points (e.g. e) and nodes (e.g. k in Equation (1)) are extended. They should no longer be limited to a single computational mesh but become indices over all meshes at all times. The number of unknowns might however become very large and dedicated iterative methods should be used to solve Equations (19), (20).

3. Analysis

3.1. *Some properties of P, M, H*

In this section we discuss some properties of the matrices defined in the previous section and establish some results used in latter sections. We introduce the following vectors:

$$v_e^{(i)} = 1 \quad \text{if } e \in \Omega_i, \quad i \in 1 \dots N_{\mathscr{D}} \tag{21}$$

$$= 0 \text{ otherwise,} \tag{22}$$

and

$$u_a^{(i)} = \frac{w_a}{W_i} \quad \text{if } a \in \Omega_i, \quad i \in 1 \dots N_{\mathscr{D}} \tag{23}$$

$$= 0 \text{ otherwise.} \tag{24}$$

For each cluster Ω_i, $v_e^{(i)}$ is constant over the cluster and corresponds to the ith column of P_{ei}. It is also a right eigenvector of M_{ea}. The vector $u_a^{(i)}$ corresponds to the normalized weights of the cluster. As the intersection of the different clusters is empty the vectors $v_e^{(i)}$ (resp. $u_a^{(i)}$) are orthogonal to each other. The matrix $I_{ea} - M_{ea}$ introduced in Section 2 can be rewritten as:

$$I_{ea} - M_{ea} = I_{ea} - \sum_{i'}^{N_{\mathscr{D}}} v_e^{(i')} u_a^{(i')} \quad \forall e, a, \tag{25}$$

and appears therefore as a deflation of the Identity. Its has $N_{\mathscr{D}}$ zero right-eigenvalues and $v_e^{(i)}$ are the eigenvectors associated to the zero eigenvalues; the other right-eigenvalues are 1. The matrix H_{ea} also introduced in Section 2 has therefore $N_{\mathscr{D}}$ zero eigenvalues and is not strictly positive definite. The vectors $v_e^{(i)}$ (or equivalently the columns of P_{ei}) provide an orthogonal basis for its nullspace. We can further define the two semi-norms:

$$\|(\boldsymbol{\epsilon}_{e'})_{e'}\|^2_{H\mathbb{C}} = \sum_{e',a'} H_{e'a'}\boldsymbol{\epsilon}_{e'} : \mathbb{C} : \boldsymbol{\epsilon}_{a'}, \tag{26}$$

$$\|(\boldsymbol{\sigma}_{e'})_{e'}\|^2_{H\mathbb{C}^{-1}} = \sum_{e',a'} H_{e'a'}\boldsymbol{\sigma}_{e'} : \mathbb{C}^{-1} : \boldsymbol{\sigma}_{a'}, \tag{27}$$

from which we get a compact expression of the DDI loss function as:

$$\mathscr{F}(\boldsymbol{\sigma}_e, P) = \tfrac{1}{2}\|(\boldsymbol{\epsilon}_{e'})_{e'}\|^2_{H\mathbb{C}} + \tfrac{1}{2}\|(\boldsymbol{\sigma}_{e'})_{e'}\|^2_{H\mathbb{C}^{-1}}. \tag{28}$$

3.2. *On the true stresses*

In this section we derive, for a given clustering, two intuitively obvious results concerning the stress field in the case of purely elastic material behaviors. If the local stress is a function $\hat{\boldsymbol{\sigma}}(\boldsymbol{\epsilon})$ of the local strain only, the following first order approximation of the stress at the cluster average strain can be assumed:

$$\hat{\boldsymbol{\sigma}}(\boldsymbol{\epsilon}_e) = \hat{\boldsymbol{\sigma}}_e = \hat{\boldsymbol{\sigma}}(\boldsymbol{\epsilon}_e^*) + \left.\frac{\partial\hat{\boldsymbol{\sigma}}}{\partial\boldsymbol{\epsilon}}\right|_{\boldsymbol{\epsilon}=\boldsymbol{\epsilon}_e^*} : (\boldsymbol{\epsilon}_e - \boldsymbol{\epsilon}_e^*) \quad \forall e. \tag{29}$$

We furthermore assume that the largest eigenvalue of $\partial\hat{\boldsymbol{\sigma}}/\partial\boldsymbol{\epsilon}|_{\boldsymbol{\epsilon}=\boldsymbol{\mathscr{E}}_i}$ can be bounded by a constant K. By taking the cluster average of the above and since all starred quantities are constant per cluster and equal to the w_e-weighted cluster average of the corresponding un-starred quantities we have:

$$\hat{\boldsymbol{\sigma}}(\boldsymbol{\mathscr{E}}_i) = \frac{1}{W_i}\sum_{e'\in\Omega_i} w_{e'}\hat{\boldsymbol{\sigma}}_{e'} \quad \forall i. \tag{30}$$

It is therefore consistent to define the true material stress database entry $\hat{\boldsymbol{\mathscr{S}}}_i$ either as the constitutive equation applied to the corresponding material strain database entry $\boldsymbol{\mathscr{E}}_i$ or as the cluster average of the true stress field $\hat{\boldsymbol{\sigma}}_e$.

$$\hat{\boldsymbol{\mathscr{S}}}_i = \hat{\boldsymbol{\sigma}}(\boldsymbol{\mathscr{E}}_i) = \frac{1}{W_i}\sum_{e'\in\Omega_i} w_{e'}\hat{\boldsymbol{\sigma}}_{e'} \quad \forall i. \tag{31}$$

The true material stress field $\hat{\boldsymbol{\sigma}}_e^*$ is then defined as:

$$\hat{\boldsymbol{\sigma}}_e^* = \sum_{i'} P_{ei'}\hat{\boldsymbol{\mathscr{S}}}_{i'} \quad \forall e, \tag{32}$$

which yields the following bound:

$$\|(\hat{\boldsymbol{\sigma}}_{e'})_{e'}\|^2_{H\mathbb{C}^{-1}} \leq \frac{K^2}{\lambda_{\mathbb{C}}^2}\|(\boldsymbol{\epsilon}_{e'})_{e'}\|^2_{H\mathbb{C}}, \tag{33}$$

where $\lambda_{\mathbb{C}}$ is the smallest eigenvalue of $\mathbb{C}$.

3.3. *Existence and uniqueness of the solution*

Due to the combinatorial nature of the problem addressed by DDI, multiple solutions corresponding to local minima exist. In the context of the alternated minimization scheme introduced in Section 2.2 we discuss in this section the uniqueness of solutions to Equations (19), (20) upon stagnation of the alternated minimization, when P_{ei} is fixed.

Since the mechanical equilibrium problem described through Equation (1) is statically indeterminate, several statically admissible stress fields exists, which are potential DDI solutions. The difference between any two of those potential solutions lies in the nullspace of $\mathbf{D}_{je}$. If multiple solutions exist, they must all satisfy mechanical equilibrium and yield the same loss function value. Since H_{ea} is positive semi-definite, uniqueness is achieved when the intersection of the nullspace of $\mathbf{D}_{je}$ and the nullspace of $H_{ea}\mathbb{C}^{-1}$ reduces to the origin. This result can also be easily derived from the stationarity conditions of Equations (19), (20).

Since the nullspace of H_{ea} is of dimension N_D, the nullspace of $H_{ea}\mathbb{C}^{-1}$ grows proportionally to $N_{\mathscr{D}}$. There is therefore a limit to the size of the database beyond which the solution ceases to be unique. The actual maximal value of $N_{\mathscr{D}}$ is however difficult to compute since it strongly depends on the clustering details. In the limit case of $N_{\mathscr{D}} = m$ clusters, each associated to a single quadrature point, the matrix H_{ea} actually becomes all zeros and the nullspace of $H_{ea}\mathbb{C}^{-1}$ is the entire stress space.

It is convenient to investigate the nullspace of $\mathbf{D}_{je}$ through the columns of P_{ei} as they provide a basis of the nullspace of H_{ea}. We consider the following operator:

$$\mathbf{S}_{ki} = \sum_{e'} \mathbf{D}_{ke'} P_{e'i} \quad \forall k, i. \tag{34}$$

For a given pairing, Equations (19), (20) have a unique solution if and only if the nullspace of $\mathbf{S}_{ki}$ is of dimension zero, or equivalently if all its singular values are non-zero. In this form we see that the uniqueness does not explicitly depend on $\mathbb{C}$ but only indirectly through the clustering it generates. The operator $\mathbf{S}_{ki}$ defined above can be interpreted as the equilibrium matrix condensed over the clusters, meaning that all stress values within the same cluster are constrained to be equal. The DDI solution is therefore unique if and only if there is no stress field that is at the same time self-balanced (i.e. in the nullspace of $\mathbf{D}_{je}$) and constant per cluster (i.e. in the nullspace of $H_{ea}\mathbb{C}^{-1}$).

3.4. *Stress identification error*

In this section, we discuss the capacity of the DDI to correctly approximate the true (unknown) stress field and in the case of elastic behavior we provide a bound for the error on the mechanical stress field defined as:

$$E_{\boldsymbol{\sigma}}^2 = \sum_{e'} \|(\boldsymbol{\sigma}_{e'} - \hat{\boldsymbol{\sigma}}_{e'})\|_2^2 = \|(\boldsymbol{\sigma}_{e'} - \hat{\boldsymbol{\sigma}}_{e'})_{e'}\|_2^2. \tag{35}$$

Since both $\boldsymbol{\sigma}_e$ and $\hat{\boldsymbol{\sigma}}_e$ are statically admissible stress fields, their difference belongs to the nullspace of $\mathbf{D}_{ke}$. As Equation (27) defines a semi-norm, it satisfies the triangular identity which yields:

$$\|(\boldsymbol{\sigma}_{e'})_{e'}\|_{H\mathbb{C}^{-1}} + \|(\hat{\boldsymbol{\sigma}}_{e'})_{e'}\|_{H\mathbb{C}^{-1}} \geq \|(\boldsymbol{\sigma}_{e'} - \hat{\boldsymbol{\sigma}}_{e'})_{e'}\|_{H\mathbb{C}^{-1}} \geq \lambda \|(\boldsymbol{\sigma}_{e'} - \hat{\boldsymbol{\sigma}}_{e'})_{e'}\|_2,$$

where λ^2 is the smallest eigenvalue of $H_{ea}\mathbb{C}^{-1}$ over the nullspace of $\mathbf{D}_{ke}$. Under the uniqueness assumptions discussed in the previous section, the nullspaces of $H_{ea}\mathbb{C}^{-1}$ and $\mathbf{D}_{ke}$ only intersect at the origin, making λ strictly positive. The bound on $E_{\boldsymbol{\sigma}}$ reads:

$$E_{\boldsymbol{\sigma}} = \|(\boldsymbol{\sigma}_{e'} - \hat{\boldsymbol{\sigma}}_{e'})_{e'}\|_2 \leq \frac{1}{\lambda}(\|(\boldsymbol{\sigma}_{e'})_{e'}\|_{H\mathbb{C}^{-1}} + \|(\hat{\boldsymbol{\sigma}}_{e'})_{e'}\|_{H\mathbb{C}^{-1}}). \tag{36}$$

This can be further particularized in the case of elastic material behavior as:

$$E_{\boldsymbol{\sigma}} = \|(\boldsymbol{\sigma}_{e'} - \hat{\boldsymbol{\sigma}}_{e'})_{e'}\|_2 \leq \frac{1}{\lambda}\left(\|(\boldsymbol{\sigma}_{e'})_{e'}\|_{H\mathbb{C}^{-1}} + \frac{K}{\lambda_{\mathbb{C}}}\|(\boldsymbol{\epsilon}_{e'})_{e'}\|_{H\mathbb{C}}\right). \tag{37}$$

In the above Equations (36), (37) the $1/\lambda$ factor shows that when the problem degenerates and λ goes to zero, the proposed error bounds actually diverge. For a finite value of λ:

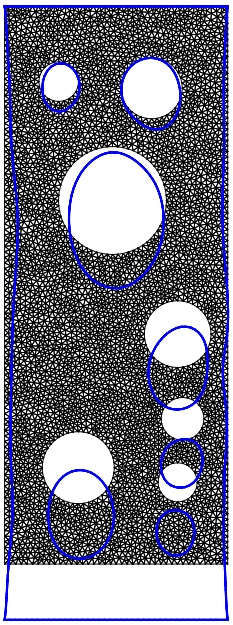

Figure 1. Computational mesh used for generating the synthetic data and performing the DDI. The bold lines represent the contour of the deformed configuration.

- In the case of anelastic material behavior, Equation (36) suggests that the stress estimate is good as long as the stress $\hat{\boldsymbol{\sigma}}_e$ does not deviate too much from its mean value within each cluster. This should for example be the case for elastoplastic material behaviors subject to monotonous loadings. An enhanced constitutive space that accounts for strain, stress and their increment over a small time interval has been used in the work of Vinel et al. [9] to promote this idea.
- In the case of an elastic material behavior, Equation (37) shows that the error on the estimated stress field should decrease with the DDI loss function.

3.5. *Numerical test*

In this section, we illustrate quantitatively and discuss the previous results with synthetic data. The data is generated by computing the finite element response of a sample depicted in Figure 1 subject to a 10% strain in the vertical direction assuming infinitesimal strain and plane stress. The FE mesh comprises 4866 nodes and 9204 elements. The material is assumed to be incompressible, with the following strain–stress relation:

$$\hat{\boldsymbol{\sigma}}(\boldsymbol{\epsilon}) = -p\mathbf{I} + 2G(1 + \alpha\,\mathrm{dev}(\boldsymbol{\epsilon}) : \mathrm{dev}(\boldsymbol{\epsilon}))\mathrm{dev}(\boldsymbol{\epsilon}), \tag{38}$$

where $\mathrm{dev}(\boldsymbol{\epsilon})$ is the deviatoric part of $\boldsymbol{\epsilon}$. The parameter α controls the nonlinear response and is arbitrarily selected as $\alpha = 3$. In part of the following analysis, the noise influence is considered. The noisy dataset is generated by adding to the displacement field a random zero mean perturbation with a uniform distribution. The maximum pointwise amplitude of this perturbation is half of the smallest nonzero vertical nodal displacement on the mesh. This specific choice perturbs the problem just enough to observe the influence of the parameter $N_{\mathscr{D}}$. By default, all presented results refer to the dataset without noise.

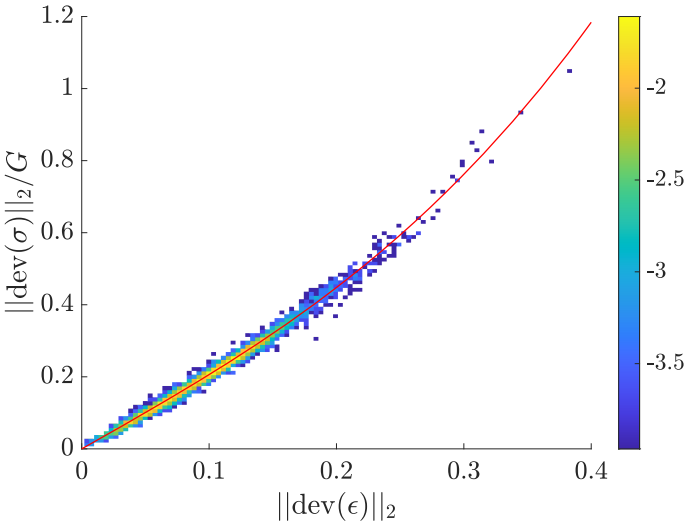

Figure 2. Comparison of the estimated mechanical stress with the constitutive model (plain line) in the $\mathrm{dev}(\boldsymbol{\epsilon}) - \mathrm{dev}(\boldsymbol{\sigma})$ space. The colorscale represents the logarithm of the density of mechanical states.

For the DDI, we selected the parameter $\mathbb{C}$ as:

$$\mathbb{C} = \left.\frac{\partial \hat{\boldsymbol{\sigma}}}{\partial \boldsymbol{\epsilon}}\right|_{\boldsymbol{\epsilon}=\mathbf{0}},$$

and w_e are set to the mesh quadrature weights. The DDI is carried out for different values of $N_{\mathscr{D}}$ ranging from 10 to 1000. For each value of $N_{\mathscr{D}}$, the pairing matrix P_{ei} is computed a priori from a w_e-weighted k-means clustering performed on the strain only.

The largest $N_{\mathscr{D}}$ value for which the uniqueness criterion is satisfied is $N_{\mathscr{D}} = 370$, yielding an average cluster size of 24.9. This criterion can be evaluated solely based on the clustering. The actual DDI solution can then be computed using any appropriate minimization technique.

The estimated DDI mechanical stress is shown in Figure 2. The density of states is plotted in the $\mathrm{dev}(\boldsymbol{\epsilon}) - \mathrm{dev}(\boldsymbol{\sigma})$ space providing a simple visualization where the color scale represents the logarithm of the mechanical state density. The underlying constitutive model is represented by the continuous line. We observe a good agreement between the DDI predictions and constitutive model used to generate the data. As can be expected, the agreement is better where the density of states is higher. In Figure 3 we compare the identified material database with the material model. Database points associated to clusters of less than 4 mechanical states are represented with +. Less dispersion is observed for the material database as it averages the error of each cluster. The analysis of this increased accuracy and the derivation of an improved error estimator is however beyond the scope of the present work.

In Figure 4 the relative error of DDI-estimated mechanical stress is depicted as a function of $N_{\mathscr{D}}$ along with its estimated value from Equation (37),when the uniqueness condition holds. When computing the error estimator we selected K as twice the largest eigenvalue of $\mathbb{C}$. The actual error on the estimated stress scales like $\sim N_{\mathscr{D}}^{-0.3}$, eventually reaching a value of about 5%. On the other hand, the error estimator decreases much faster: $\sim N_{\mathscr{D}}^{-0.5}$ but its convergence is eventually limited as the uniqueness criterion is no longer satisfied for large $N_{\mathscr{D}}$. The estimated relative error is nevertheless more than one order of magnitude larger than the actual value. This

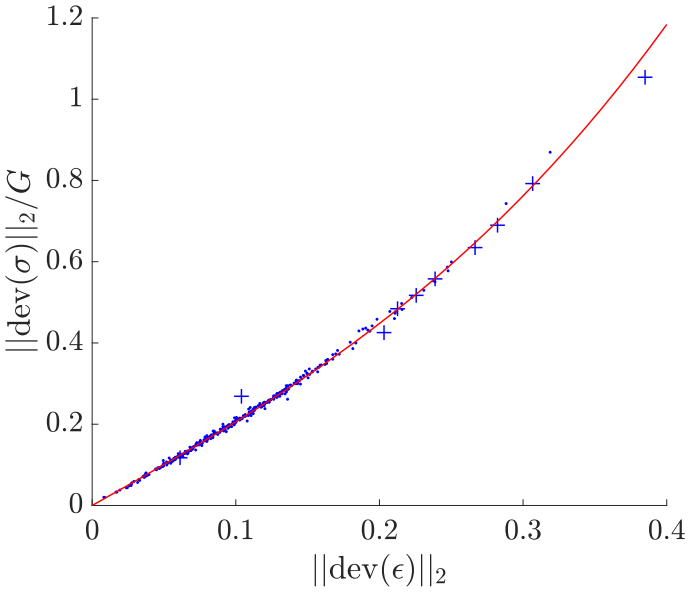

Figure 3. Comparison of the identified material database (symbols) with the constitutive model (solid line) in the dev($\boldsymbol{\epsilon}$) – dev($\boldsymbol{\sigma}$) space. The points associated to clusters of less than 4 elements are depicted using + symbols.

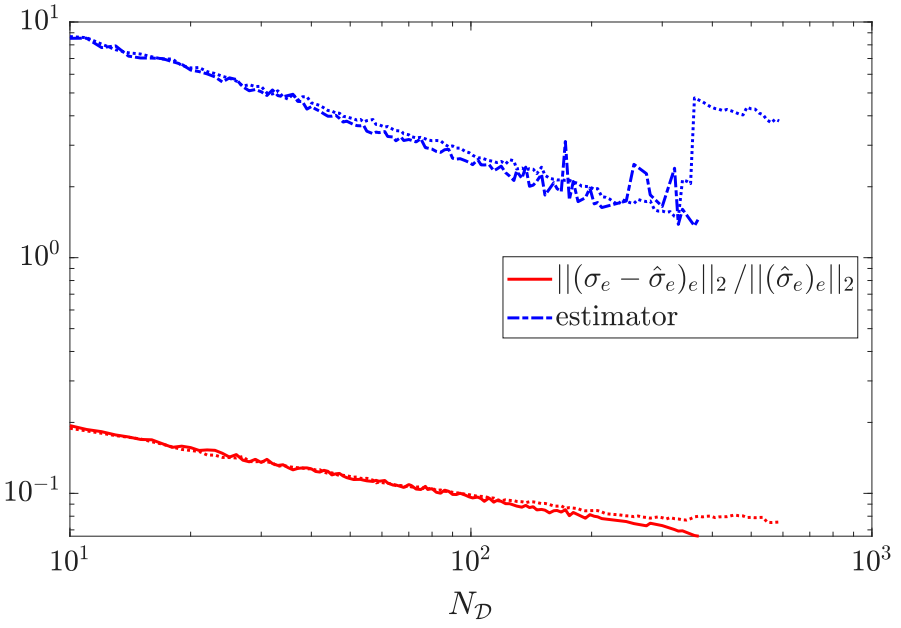

Figure 4. Comparison of the relative error on the estimated stress with its estimate derived from Equation (37) as a function of the material database size $N_{\mathscr{D}}$. The dotted lines correspond to the same quantities computed using the noisy dataset.

is no surprise in view of the rather conservative bounds provided by the triangular inequality and the eigenvalue identities used in its derivation.

The dotted lines in Figure 4 represent the same quantities, but computed from the noisy dataset. As the DDI uses a clustering to estimate the mechanical stress, it is not surprising that the noise is averaged out for small database sizes. Both datasets yield the same result. As the database size increases smaller clusters emerge and the influence of noise becomes visible. At some point, the error on the predicted stress tends to stagnate or increase slightly. The error estimator seem however capable of detecting this. Another remarkable feature is that the DDI problem seem to degenerate for larger $N_{\mathscr{D}}$ in the case of a noisy dataset. This retardation is probably related to the fact that the noise arbitrarily perturbs the clustering making the alignment of the nullspaces of $H_{ea}\mathbb{C}^{-1}$ and $\mathbf{D}_{je}$ more difficult. This also suggests that other clustering techniques might improve the performance of the method.

4. Conclusions and perspectives

In this paper we have presented a clear mathematical formulation of the DDI method. In particular this reformulation exposes that, unlike DDCM, the minimization problem at hand is not a mixed integer quadratic programming problem since both the pairing matrix P and the material database are unknown. The convergence of the alternated minimization heuristics is therefore still an open issue.

For a given pairing or upon convergence (i.e. stagnation of the minimization heuristic) it is possible to assess the uniqueness of the solution through an eigenvalue analysis for which we have provided a simple interpretation. The DDI solution is unique only if it is impossible to build a self balanced material stress field. This criterion is independent of the value of the metric parameter $\mathbb{C}$ and provides a way of selecting an appropriate database size $N_{\mathscr{D}}$. Furthermore, when the uniqueness criterion holds, it is possible to derive a simple error bound on the identified mechanical stress in the case of elastic behaviors.

These results have been tested on synthetic data where the convergence with respect to the size of the material database has been observed. This convergence is stopped for large database for which the solution ceases to be unique. The too fine clustering does not provide enough regularization to the stress estimation problem.

The development of uniqueness and convergence criteria opens the door to the optimization of several aspects of the method.

- Having a better characterization of the degeneracy of the DDI regularization allows for the development of additional regularization terms on the mechanical stress to allow, for a fixed data set, the identification of larger material databases.
- In the current formulation, the clustering only aims at making compact clusters. The proposed error bound and the uniqueness criteria show that there is actually a tight connection between the pairing matrix P_{ei} and the equilibrium operator $\mathbf{D}_{ke}$. This suggests that it might be possible to drive the clustering to postpone degeneracy and improve the error bound, for example by maximizing λ^2, the smallest eigenvalue of $H_{ea}\mathbb{C}^{-1}$ over the nullspace of $\mathbf{D}_{ke}$.
- The same idea can also be applied to the design of a loading path and sample geometries through topology optimization.
- In the case of non elastic materials, the proposed error bound suggests that it is possible to have good stress estimates as long as the real (unknown) stress within each cluster does not deviate much from its mean. This can be achieved by introducing a clustering based on the strain history on or other a priori knowledge to extend the scope of the present analysis.

Declarations

Declaration of interests

The authors do not work for, advise, own shares in, or receive funds from any organization that could benefit from this article, and have declared no affiliations other than their research organizations.

References

[1] S. Avril, M. Bonnet, A.-S. Bretelle, et al., "Overview of identification methods of mechanical parameters based on full-field measurements", *Exp. Mech.* **48** (2008), no. 4, pp. 381–402.

[2] A. Benady, E. Baranger and L. Chamoin, "NN-mCRE: a modified constitutive relation error framework for unsupervised learning of nonlinear state laws with physics-augmented neural networks", *Int. J. Numer. Methods Eng.* **125** (2024), no. 8, article no. e7439.

[3] M. Flaschel, S. Kumar and L. De Lorenzis, "Unsupervised discovery of interpretable hyperelastic constitutive laws", *Comput. Methods Appl. Mech. Eng.* **381** (2021), article no. 113852.

[4] P. Thakolkaran, A. Joshi, Y. Zheng, M. Flaschel, L. De Lorenzis and S. Kumar, "NN-EUCLID: deep-learning hyperelasticity without stress data", *J. Mech. Phys. Solids* **169** (2022), article no. 105076.

[5] F. As'ad, P. Avery and C. Farhat, "A mechanics-informed artificial neural network approach in data-driven constitutive modeling", *Int. J. Numer. Methods Eng.* **123** (2022), no. 12, pp. 2738–2759.

[6] T. Kirchdoerfer and M. Ortiz, "Data-driven computational mechanics", *Comput. Methods Appl. Mech. Eng.* **304** (2016), pp. 81–101.

[7] A. Leygue, M. Coret, J. Rethore, L. Stainier and E. Verron, "Data-based derivation of material response", *Comput. Methods Appl. Mech. Eng.* **331** (2018), pp. 184–196.

[8] M. Dalemat, M. Coret, A. Leygue and E. Verron, "Measuring stress field without constitutive equation", *Mech. Mater.* **136** (2019), article no. 103087.

[9] A. Vinel, R. Seghir, J. Berthe, G. Portemont and J. Réthoré, "Experimental characterization of material strain-rate dependence based on full-field data-driven identification", *Int. J. Impact Eng.* **194** (2024), article no. 105083.

[10] M. Dalémat, M. Coret, A. Leygue and E. Verron, "Robustness of the data-driven identification algorithm with incomplete input data", *J. Theor. Comput. Appl. Mech.* (2024), article no. 12590.

[11] L. Costecalde, A. Leygue, M. Coret and E. Verron, "Data-driven identification of hyperelastic models by measuring the strain energy density field", *Rubber Chem. Technol.* **96** (2023), no. 4, pp. 443–454.

[12] Y. Kanno, "Mixed-integer programming formulation of a data-driven solver in computational elasticity", *Opt. Lett.* **13** (2019), no. 7, pp. 1505–1514.

[13] S. Lloyd, "Least squares quantization in PCM", *IEEE Trans. Inform. Theory* **28** (1982), no. 2, pp. 129–137.