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Data Driven Constitutive identification

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1. Introduction

How to extract strain-stress couples for an elastic material from a collection of non-homogenous full field measurements corresponding to different loading conditions?

2. Data-driven truss solver

The method of Kirchdoerfer & Ortiz (**Kirchdoerfer & Ortiz 2016**) for data-driven simulation seeks to assign to each truss element of the computational domain two states, a state being a strain-stress couple. Considering both mechanical equilibrium (of stress) and compatibility conditions (for strains) as non-questionnable, the mechanical state of a given element \mathbf{e} consists of a strain-stress $(\boldsymbol{\epsilon}_e, \boldsymbol{\sigma}_e)$ pair which exactly satisfies the above constraints. The second state associated to \mathbf{e} , denoted $(\boldsymbol{\epsilon}_{ie}^*, \boldsymbol{\sigma}_{ie}^*)$ is called the material state and is extracted from a collection of admissible material states for the specific material being simulated: $(\boldsymbol{\epsilon}_i^*, \boldsymbol{\sigma}_i^*)$, where $i \in \mathbf{1} : N^*$. The index $ie \in \mathbf{1} : N^*$ specifies the material state of element \mathbf{e} .

The proposed solver seeks, for every element, a mechanical and a material state as close to each other as possible and such that the former satisfies mechanical equilibrium and compatibility conditions. This is formally expressed as:

$$\text{solution} = \arg \min_{\boldsymbol{\epsilon}_e, \boldsymbol{\sigma}_e, ie} \frac{1}{2} \sum_e w_e \|(\boldsymbol{\epsilon}_e - \boldsymbol{\epsilon}_{ie}^*, \boldsymbol{\sigma}_e - \boldsymbol{\sigma}_{ie}^*)\|_C^2, \quad (1)$$

subject to:

$$\boldsymbol{\epsilon}_e = \sum_j \mathbf{B}_{ej} \mathbf{u}_j, \quad (2)$$

and:

$$\sum_e w_e \mathbf{B}_{ej} \boldsymbol{\sigma}_e = \mathbf{f}_j. \quad (3)$$

In the above equations, $\|(\boldsymbol{\epsilon}, \boldsymbol{\sigma})\|_C$ is some energetic norm, the matrix \mathbf{B}_{ej} encodes the connectivity and geometry of the truss, and w_e denotes the volume of the truss bar \mathbf{e} . Furthermore, \mathbf{u}_j and \mathbf{f}_j represent respectively the displacement and the force applied to the truss nodes. **Figure 1** illustrates the main ideas behind the method. For the particular choice:

For the particular choice:

$$\|(\epsilon_e, \sigma_e)\|_C^2 = C_e \epsilon_e^2 + C_e^{-1} \sigma_e^2, \quad (4)$$

the authors propose an efficient algorithm to solve this problem of combinatorial complexity. The constant (possibly defined element-wise) C_e is the only parameter of the method and can be interpreted as a modulus associated to the mismatch of the mechanical and material states.

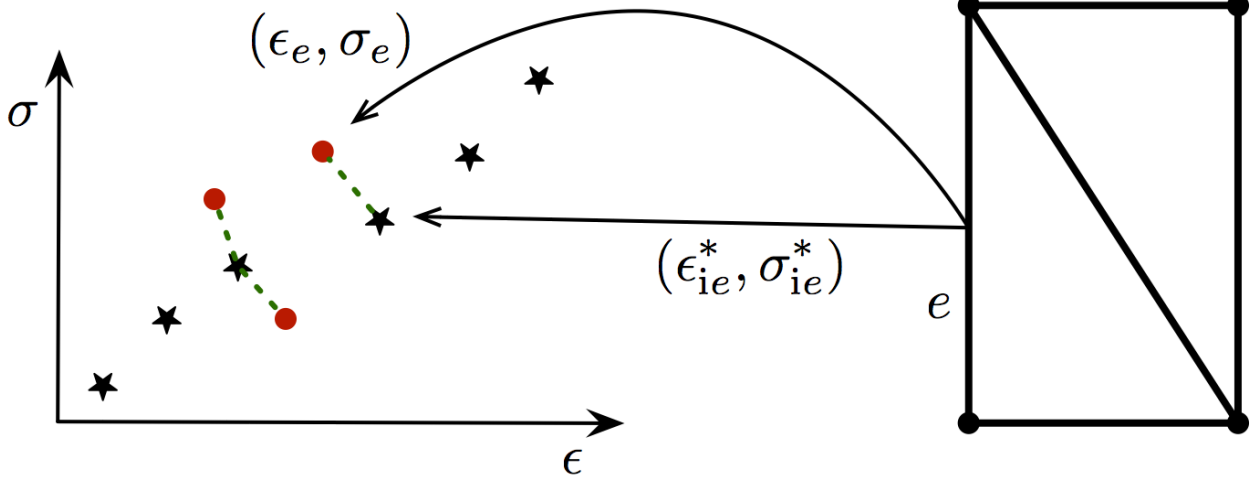


Figure 1:

Illustration of the two states (ϵ_e, σ_e) and $(\epsilon_{ie}^*, \sigma_{ie}^*)$ associated to a truss element e . The dashed line represents the energetic mismatch between the two states. On the left we see that the mapping \mathbf{ie} between elements and material states can assign the same particular material state to two different elements.

3. Data-driven identification

Let us now consider a slightly different problem related to material behavior identification. We assume that we have a large database of measurements made on real truss structures subject to different loading conditions, but where all truss elements have the same material behavior, and for each data item, indexed by \mathbf{X} , we have access to the following quantities:

- The truss geometry and connectivity, encoded as a matrix $B_{ej}^{\mathbf{X}}$,
- The nodal displacements $u_j^{\mathbf{X}}$,
- The applied forces $f_j^{\mathbf{X}}$,
- The prescribed nodal displacements.

The problem of identifying the material behavior of the truss elements now reduces to the determination of a finite number N^* of material states : $(\epsilon_i^*, \sigma_i^*)$, where $i \in 1 : N^*$, common to all the data items (thus independent of \mathbf{X}), and such that:

1. for each data item \mathbf{X} we can compute the mechanical stress $\sigma_e^{\mathbf{X}}$ of each element e which satisfies mechanical equilibrium for \mathbf{X} ,
2. for each data item, we can assign a material state $(\epsilon_{ie^{\mathbf{X}}}^*, \sigma_{ie^{\mathbf{X}}}^*)$ to each element e which is close to the mechanical state $(\epsilon_e^{\mathbf{X}}, \sigma_e^{\mathbf{X}})$ according to some energetic norm.

The above problem can be formulated as follows:

$$\text{solution} = \arg \min_{\sigma_e^{\mathbf{X}}, \epsilon_i^*, \sigma_i^*, ie^{\mathbf{X}}} \frac{1}{2} \sum_{\mathbf{X}} \sum_e w_e^{\mathbf{X}} \|(\epsilon_e^{\mathbf{X}} - \epsilon_{ie^{\mathbf{X}}}^*, \sigma_e^{\mathbf{X}} - \sigma_{ie^{\mathbf{X}}}^*)\|_C^2, \quad (5)$$

subject to:

$$\sum_e w_e^{\mathbf{X}} B_{ej}^{\mathbf{X}} \sigma_e^{\mathbf{X}} = f_j^{\mathbf{X}} \quad \forall \mathbf{X}. \quad (6)$$

Unlike the data-driven solver of Kirchdoerfer et al., we see that the mechanical strain $\epsilon_e^{\mathbf{X}}$ is not an unknown of the problem since it can be computed as $\epsilon_e^{\mathbf{X}} = \sum_j B_{ej}^{\mathbf{X}} u_j^{\mathbf{X}}$. This problem might seem quite difficult to solve, but we will show that it can be simplified a great deal. Let us first substitute the expression of the energetic norm in **Equation 5** and introduce a set of Lagrange multipliers $\eta_j^{\mathbf{X}}$ to enforce the equilibrium constraint. Assuming that the material state mapping $ie^{\mathbf{X}}$ is known, we obtain the following stationary problem:

$$\delta \left(\frac{1}{2} \sum_{\mathbf{X}} \sum_e \left(w_e^{\mathbf{X}} C_e^{\mathbf{X}} (\epsilon_e^{\mathbf{X}} - \epsilon_{ie^{\mathbf{X}}}^*)^2 + w_e^{\mathbf{X}} C_e^{\mathbf{X}-1} (\sigma_e^{\mathbf{X}} - \sigma_{ie^{\mathbf{X}}}^*)^2 - 2 \sum_j (w_e^{\mathbf{X}} B_{ej}^{\mathbf{X}} \sigma_e^{\mathbf{X}} - f_j^{\mathbf{X}}) \cdot \eta_j^{\mathbf{X}} \right) \right) = 0 \quad (7)$$

Taking all possible variations yields the following set of equations:

$$\delta \epsilon_i^* \Rightarrow \sum_{\mathbf{X}} \sum_{ie=i} w_e^{\mathbf{X}} C_e^{\mathbf{X}} (\epsilon_e^{\mathbf{X}} - \epsilon_{ie^{\mathbf{X}}}^*) = 0 \quad \forall i \quad (8)$$

$$\delta \sigma_i^* \Rightarrow \sum_{\mathbf{X}} \sum_{ie=i} w_e^{\mathbf{X}} C_e^{\mathbf{X}-1} (\sigma_e^{\mathbf{X}} - \sigma_{ie^{\mathbf{X}}}^*) = 0 \quad \forall i \quad (9)$$

$$\delta \sigma_e^{\mathbf{X}} \Rightarrow w_e^{\mathbf{X}} C_e^{\mathbf{X}-1} (\sigma_e^{\mathbf{X}} - \sigma_{ie^{\mathbf{X}}}^*) - \sum_j w_e^{\mathbf{X}} B_{ej}^{\mathbf{X}} \eta_j^{\mathbf{X}} = 0 \quad \forall e, \mathbf{X} \quad (10)$$

$$\delta \eta_j^{\mathbf{X}} \Rightarrow \sum_e (w_e^{\mathbf{X}} B_{ej}^{\mathbf{X}} \sigma_e^{\mathbf{X}} - f_j^{\mathbf{X}}) = 0 \quad \forall j, \mathbf{X} \quad (11)$$

Equation 8 simply states that each material strain ϵ_i^* is some weighted average of the mechanical strain of the elements that share this specific material strain. Since all the mechanical strains $\epsilon_e^{\mathbf{X}}$ are known, all the ϵ_i^* can be computed a priori through some kmeans-like algorithm (**MacQueen 1967; Lloyd 1982**). One should notice that this also yields the state mapping $ie^{\mathbf{X}}$.

Similarly **Equation 9** states that each material stress σ_i^* is some weighted average of the mechanical stress of the elements that share this specific material stress.

Finally the combination of **Equation 10** and **Equation 11** yields:

$$\sum_k \sum_e w_e^X C_e^X B_{ej}^X B_{ek}^X \eta_k^X = f_j^X - \sum_e w_e^X B_{ej}^X \sigma_{ie^X}^* \quad \forall j, X. \quad (12)$$

This equation simply states that for any data item X , the mechanical imbalance between the applied forces f_j^X and the internal material stresses $\sigma_{ie^X}^*$ can be explained through virtual nodal displacements η_j^X considering a pseudo-stiffness C_e^X for the truss elements.

4. Solution procedure

In the framework of a big-data approach, the number of different data items is likely to be very important, thereby preventing the simultaneous coupled solution of **Equation 8**, **Equation 9** and **Equation 12**. Indeed although these equations are linear the size of the system to solve could become very important since one has to determine simultaneously the virtual nodal displacement η_j^X for each node of each data item and the set for all material states $(\epsilon_i^*, \sigma_i^*)$. We therefore propose the following decoupled solution procedure:

1. From the known mechanical strains ϵ_e^X , compute the material strains ϵ_i^* and the state mapping ie^X using a kmeans-like algorithm.
2. Initialize the material stresses σ_i^* to zero or according to some a priori knowledge of the material behavior.
3. For all data items, compute the virtual nodal displacements η_j^X from **Equation 12**.
4. Update the value of the material stresses σ_i^* using **Equation 9**.
5. Iterate steps 3 and 4 until convergence of the material stresses.

Preliminary tests show that for large data sets this algorithm converges very fast, and the limiting step actually is the k-means quantization of the strains.

5. Comments

- Similarly to the data driven solver, the data driven identification proposed above entails only few parameters: the number N of material states to be identified and the pseudo-stiffness C_e^X . It should be noted that this parameter need not be the same for the different truss elements and data items and could therefore depend both on e and X . This could provide some additional flexibility in the method or be used as a tool to weight the data according to some a priori confidence level.
- Furthermore, one could also consider a different value of C_e^X for the determination of ϵ_i^* and σ_i^* .
- Even for non-linear material behaviors, the identification procedure is linear (except for the k-means).
- The iteration steps (3-4) are not too expensive for several reasons. 1-since the state mapping ie^X is fixed the averaging of the mechanical stresses to compute the material stresses does not involve any expensive search procedure. 2-The matrices appearing in **Equation 12** are constant through the iterations. They can therefore be factorized a priori leaving only inexpensive back-substitutes to perform during the iterations.
- The success of the proposed methods relies on several ingredients. First, the richness of the experimental data over all data items X (i.e. the extent of u_j^X and f_j^X) ensures the identification of the material behavior over a wide range of strains ϵ_i^* . Second the richness of the individual data items (i.e. the range of ϵ_i^X for a given X), which couples the through the mechanical equilibrium the different material and mechanical states.
- This identification procedure follows a path very close to the one of the data-driven solver. If the former is to provide the material behavior to the latter, this proximity is somewhat intellectually interesting.

6. Numerical results

In this section, we apply the above methodology to the identification of the mechanical behavior of truss elements exhibiting a non linear strain-stress relation. We use a synthetic data set generated by applying different loading conditions to the 2D truss structure depicted in **Figure 2**. This structure is made of 249 nodes and 657 bar elements with a nonlinear strain-stress behavior of the form: $\sigma = K(\epsilon + \epsilon^3)$. A total of $N^X = 50$ different loading scenarios involving traction, compression and shear along x and y have been simulated. Some representative deformed configuration are depicted in XXX.

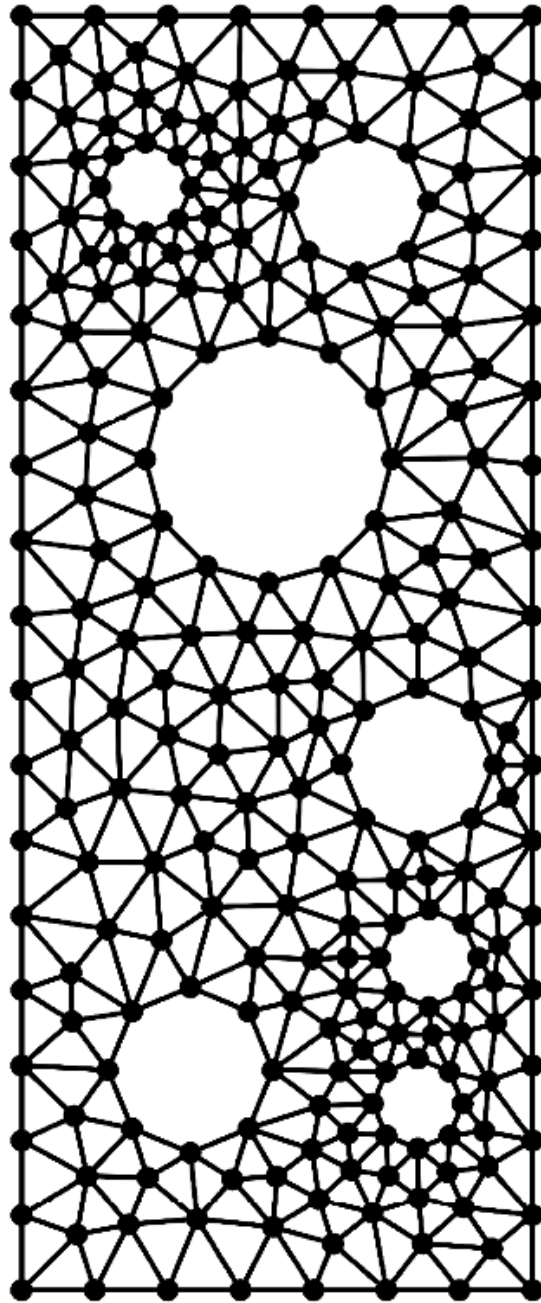


Figure 2:

Undeformed truss structure used for the generation of manufactured data. The structure comprises 249 nodes and 657 nonlinear bar elements.

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