Variational methods in material sciences: the data-driven approach

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SFB PDE Taming Complexity in Partial Differential Systems

PDE Afternoon

12/01/2022

Main sources

[1] S. Conti, S. Müller, and M. Ortiz. "Data-Driven Problems in Elasticity". In: *Archive for Rational Mechanics and Analysis* 229.1 (2018), pp. 79–123. DOI: 10.1007/s00205-017-1214-0.

[2] T. Kirchdoerfer and M. Ortiz. "Data-driven computational mechanics". In: *Computer Methods in Applied Mechanics and Engineering* 304 (June 2016), pp. 81–101. ISSN: 0045-7825. DOI: 10.1016/j.cma.2016.02.001.

Outline

1. Why the data-driven approach?
2. General data-driven setting
3. The case of linear elasticity
4. Existence for non-weakly closed data sets

Why the data-driven approach?

prototypical problem in materials sciences
two core elements

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two core elements

constitutive relations
provide “universal” equilibrium
and compatibility conditions

Material sciences problems

prototypical problem in materials sciences
two core elements

constitutive relations		empirical data
provide “universal” equilibrium and compatibility conditions	+	about the material, obtained through measurements

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minimum problems

An example: linear elasticity

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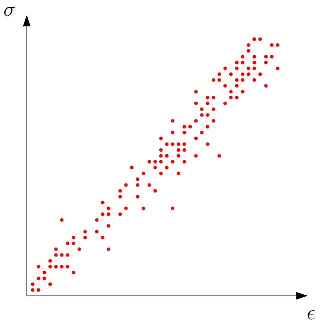

Empirical measurements

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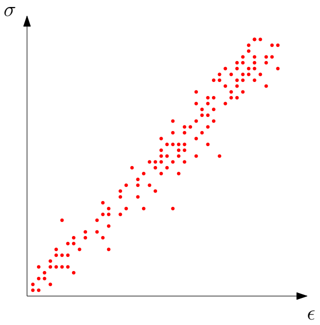

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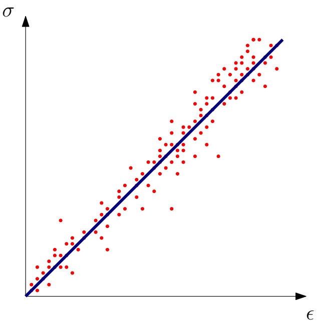

Hooke's law

$$\sigma = \epsilon$$

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$$\inf_{u \in u_0 + H_0^1} \left\{ I(u) := \frac{1}{4} \int_\Omega e(u)^2 \, dx + \text{ terms given by } f \text{ and B.C.} \right\}$$

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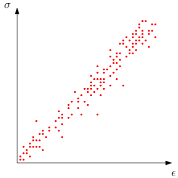

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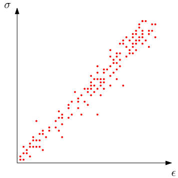

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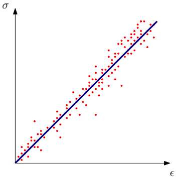

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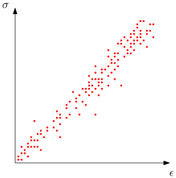

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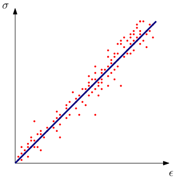

Hooke's law

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$$\Rightarrow \begin{cases} \operatorname{div}\sigma = \operatorname{div}\mathbb{C}\epsilon = f \\ \text{B.C.} \end{cases}$$

General data-driven setting

In a phase space

$$Z := L^2(\Omega; A) \times L^2(\Omega; A),$$

with A a suitable subspace of $\mathbb{R}^N$, we consider the two sets

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Given through local measurements $\mathcal{D}_{loc} \subset A$ as

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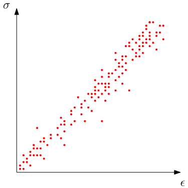

Data-driven solution

The data-driven approach sidesteps the empirical modelling, looking for functions which satisfy the constraint $\mathcal{E}$ and minimize the distance from the data-set $\mathcal{D}$, i.e. a data-driven solution is a minimizer of

$$\boxed{\inf_{z\in\mathcal{E}}\{d(z,\mathcal{D})\}} \qquad (MP)$$

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Problems:

- well-posedness
- existence of minimizers
- relation with the corresponding classical problem.

The case of linear elasticity

We give the example of a simple problem in the context of elasticity following the layout of the paper "*Data-Driven Problems in Elasticity*" by S. Conti, S. Müller and M. Ortiz [1].

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equipped with the following norm

$$\|z\| = \|(\epsilon, \sigma)\| = \left(\int_\Omega \left(\frac{1}{2}\mathbb{C}\epsilon \cdot \epsilon + \frac{1}{2}\mathbb{C}^{-1}\sigma \cdot \sigma\right) dx\right)^{1/2},$$

with $\mathbb{C} \in \mathcal{L}(\mathbb{R}^{n\times n}_{sym})$ a nominal elasticity tensor which is self adjoint and positive.

The state of the elastic body is described by the displacement field $u : \Omega \to \mathbb{R}^n$ whose compatibility and equilibrium laws are

$$\begin{cases} \epsilon(x) = \frac{1}{2}\left(\nabla u(x) + \nabla u^t(x)\right) & \text{in } \Omega \\ u(x) = g(x) & \text{on } \Gamma_D, \end{cases} \tag{1}$$

$$\begin{cases} \operatorname{div} \sigma(x) + f(x) = 0, & \text{in } \Omega \\ \sigma(x)\nu(x) = h(x), & \text{on } \Gamma_N. \end{cases} \tag{2}$$

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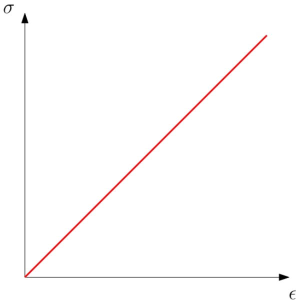
They are encoded in the set

$$\mathcal{E} = \{(\epsilon, \sigma) \in Z \mid \text{(1) and (2)}\}.$$

The data set corresponding to linear elasticity is

$$\mathcal{D} = \{(\epsilon, \sigma) \in Z \mid \sigma = \mathbb{C}\epsilon \text{ a.e } \},$$



Theorem (Existence. S. Conti, S. Müller, M. Ortiz. Theorem 2.2)

Let $\Omega \subset \mathbb{R}^n$ *be open, bounded and Lipschitz and let* $\mathcal{D}$ *and* $\mathcal{E}$ *as above. Let* Γ_D, Γ_N *be disjoint open subsets of* $\partial\Omega$ *such that* $\Gamma_D \neq \emptyset$*,* $\overline{\Gamma}_D \cup \overline{\Gamma}_N = \partial\Omega$ *and* $\mathcal{H}^{n-1}(\overline{\Gamma}_D \setminus \Gamma_N) = \mathcal{H}^{n-1}(\overline{\Gamma}_N \setminus \Gamma_D) = 0$*. Assume*

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Then, the data-Driven problem (MP) *admits a unique solution.*

Linear elasticity: existence

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Then, the data-Driven problem (MP) admits a unique solution. Moreover, such solution is "classical", i.e satisfies

$$\sigma = \mathbb{C}\epsilon.$$

Lemma

Given $Z = L^2(\Omega;\mathbb{R}^n) \times L^2(\Omega;\mathbb{R}^n)$ *and* $\mathcal{E} = \{(\epsilon,\sigma) \in Z : \text{(1) and (2)}\}$, *let*

$$\mathcal{D} = \{z \in Z \mid z(x) \in \mathcal{D}_{loc} \text{ a.e. in } \Omega\}, \quad \mathcal{D}_{loc} = \{(\epsilon,\sigma) \in (\mathbb{R}^{n\times n}_{sym})^2 \mid \sigma = \mathbb{C}\epsilon\}.$$

$$\mathcal{D}_j = \{z \in Z \mid z(x) \in \mathcal{D}_{loc,j} \text{ a.e. in } \Omega\}, \quad \mathcal{D}_{loc,j} \subset \mathbb{R}^{n\times n}_{sym} \times \mathbb{R}^{n\times n}_{sym}$$

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and assume

1. *(Fine approximation):* $\exists\ \rho_j \searrow 0$ *such that, for every* $\xi \in \mathcal{D}_{loc}$,
$$d(\xi, \mathcal{D}_{loc,j}) \leq \rho_j;$$
2. *(Uniform approximation):* $\exists\ t_j \searrow 0$ *such that, for every* $\xi \in \mathcal{D}_{loc,j}$,
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2. *(Uniform approximation):* $\exists\ t_j\searrow 0$ *such that, for every* $\xi\in\mathcal{D}_{loc,j}$,
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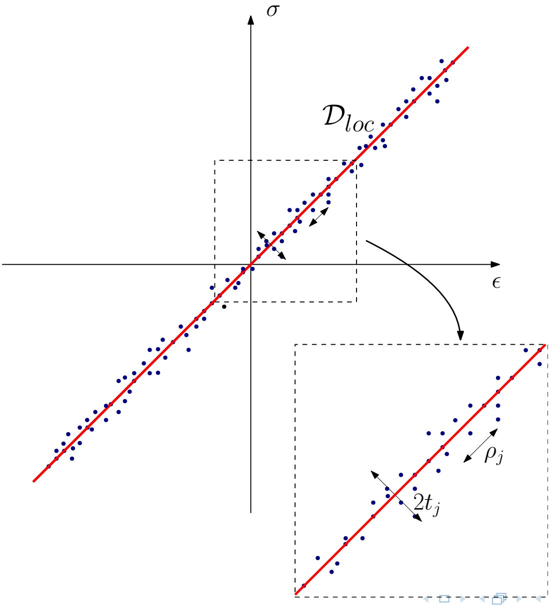
Then, $\mathcal{D} = M-\lim_j\mathcal{D}_j$.



σ
$\mathcal{D}_{loc}$
ϵ
ρ_j
$2t_j$

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Theorem (Existence for weakly closed data sets)

Let Z be a reflexive, separable Banach space and $\mathcal{E}, \mathcal{D}$ be weakly closed subsets of Z. If the equi-transversality condition holds, i.e. there exist constants $c > 0$ and $b \geq 0$ such that $\|y - z\| \geq c\,(\|y\| + \|z\|) - b$ for every $y \in \mathcal{D}$ and $z \in \mathcal{E}$, then the data-driven problem

$$S := \operatorname*{argmin}_{z \in Z}\{I_{\mathcal{E}}(z) + d^2(z, \mathcal{D})\} = \operatorname*{argmin}_{z \in \mathcal{E}}\{d^2(z, \mathcal{D})\}$$

admits solution.

Existence for non-weakly closed data sets

Definition ($\mathcal{D} \times \mathcal{E} = K_0(\Delta) - \lim_j (\mathcal{D}_j \times \mathcal{E})$)

Let $\mathcal{E}, \mathcal{D}, \mathcal{D}_j$ be subsets of Z and $F_j : Z \times Z \to \overline{\mathbb{R}}$, $F_j(y,z) = I_{\mathcal{D}_j \times \mathcal{E}} + \|y - z\|^2$. We say that $\mathcal{D} \times \mathcal{E}$ is the data-driven relaxation of the sequence $\mathcal{D}_j \times \mathcal{E}$ if:

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1. for every sequence $((y_j, z_j))_j \subset Z \times Z$ such that $F_j(y_j, z_j) \to 0$ there exists $z \in \mathcal{D} \cap \mathcal{E}$ such that $(z,z) = \Delta - \lim_j (y_j, z_j)$;

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Remark

This notion of data-driven relaxation refers only to the intersection $\mathcal{D} \cap \mathcal{E}$. Suitable for cases where the existence of a classical solution is known.

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If $\liminf F_j = 0$, *then we have existence of solutions.*
The interesting (and still open) problem is when the same is true if $\liminf F_j > 0$ *(or not a priori known)!!*

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- prove consistency without assuming that the $\liminf$ is zero (non linearity);
- when a solution exists even if the $\liminf$ is NOT zero (non linearity);
- Extend the results to the case of plasticity, where in addition to non linearity we also have dependence on time.

Thank you for your attention