Physics-informed Neural Networks for parameter estimation in cardiac mechanics ⋆

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1. INTRODUCTION

Medical imaging represents a relevant tool for diagnosing heart diseases. Different techniques are available, such as echocardiography, magnetic resonance imaging, computed tomography scans, and nuclear medicine. These are associated with an increasing space-time resolution, which may capture crucial details for the clinical decision-making process. However, the more detailed ones might have contraindications for some patients. For this reason, numerous research efforts are directed toward developing new mathematical methods to process those images (especially the most accessible ones) and extract meaningful indications. Deep Learning methods have been very successful in this area (Hernandez et al., 2020) by providing tools for the automatic segmentation of geometry and structural defects (resulting, e.g., from myocardial infarction) and for the computation of clinical biomarkers (such as cardiac motion and strains). Nevertheless, Deep Learning methods generally require large datasets for the training phase, which are not always available.

The knowledge of the physical laws governing the myocardial motion may balance this lack of data, enabling the training of the so-called physics-informed neural networks (PINNs) introduced in Raissi et al. (2019). PINNs consist of interconnected neurons, whose parameters are trained by minimizing the mismatch between the output and the available noisy data, together with additional terms encoding the partial differential equation (PDE) and the boundary conditions characterizing the physical phenomenon.

Compared to standard model personalization strategies (Chabiniok et al., 2016) based on iterative schemes requiring the numerical approximation of the forward and the adjoint problems at each iteration, PINNs enable the simultaneous numerical estimation of both the displacement and the parameters of interest. This is achieved by automatic differentiation, which provides a flexible and computationally inexpensive tool to evaluate the PDE residual and the boundary conditions in their strong form.

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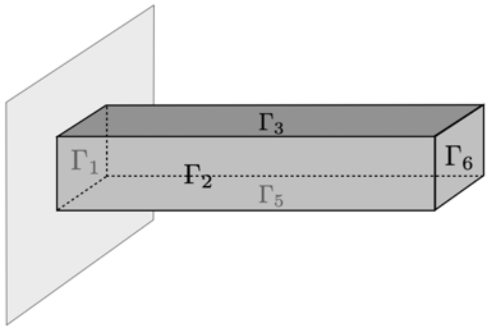

Fig. 1. Undeformed geometry of a parallelepiped with a fixed base.

In this framework, promising proofs of concept have been already presented in Zhang et al. (2020) and Nguyen-Thanh et al. (2020).

In this work, we study the feasibility of using PINNs in estimating parameters of interest for a 3D mechanical problem starting from scattered measurements of the displacement. We also focus on the effects of the density of data and the associated level of noise on the accuracy of the estimation.

2. MATHEMATICAL MODELS AND METHODS

We consider a quasi-static non-linear elastic problem to model the deformation of a parallelepiped with a fixed base (see Fig. 1) and different boundary conditions. We analyze traction, compression, and shear scenarios.

The mechanical problem for the undeformed configuration reads as follows:

$$\begin{cases} -\nabla \cdot \boldsymbol{\mathcal{P}}(\mathbf{d}) = 0 \quad \text{in } (0, L) \times (0, W) \times (0, W), \\ + \text{ B.C.}, \end{cases} \tag{1}$$

where $\mathbf{d} = \mathbf{d}(\mathbf{x})$ is the displacement, L and W define the dimensions of the parallelepiped, and $\boldsymbol{\mathcal{P}}$ is the first Piola-Kirchhoff stress tensor. Additional boundary conditions are considered for the three different scenarios (traction, compression, and shear). After introducing a hyperelastic energy $\mathcal{W} = \mathcal{W}(\boldsymbol{\mathcal{F}})$, the first Piola-Kirchhoff stress tensor $\boldsymbol{\mathcal{P}}$ can be computed as:

$$\boldsymbol{\mathcal{P}} = \frac{\partial \mathcal{W}}{\partial \boldsymbol{\mathcal{F}}} \ .$$

Among the several constitutive laws available for cardiac mechanics (Quarteroni et al., 2019), we use the following quasi-incompressible Neo-Hookean hyperelastic energy:

$$\mathcal{W} = \frac{\mu}{2}(\mathcal{J}^{-2/3}\mathrm{tr}(\boldsymbol{\mathcal{C}}) - 3) + \frac{\lambda}{4}\left((\mathcal{J}-1)^2 + \log^2(\mathcal{J})\right)$$

where $\mathcal{J} = \det(\boldsymbol{\mathcal{F}})$ is the determinant of the deformation tensor, $\boldsymbol{\mathcal{C}} = \boldsymbol{\mathcal{F}}^T\boldsymbol{\mathcal{F}}$ is the right Cauchy-Green tensor and, finally, μ and λ are the mechanical parameters (shear and bulk modulus, respectively). We construct in silico datasets by solving Eq. (1) with the Finite Element Method, by employing the Dolfin Python library (Logg et al., 2012). We sample the displacement in different locations of the computational domain, and we possibly add Gaussian noise to the pointwise values:

$$\mathbf{d}_{\mathrm{i}}^{\mathrm{obs}} = \mathbf{d}(\mathbf{x}_{\mathrm{i}}; \mu_{\mathrm{ex}}) + \epsilon_{\mathrm{i}} \qquad \epsilon_{\mathrm{i,j}} \sim \mathcal{N}(0, \sigma^2),$$

where μ_{ex} is the exact value of the parameter to be estimated. Indeed, we adopt PINNs to find the unknown parameter $\mu \subset \mathcal{P} \subset \mathbb{R}$ by solving a statistical learning problem in which the numerical solution of Eq. (1) is approximated by means of a fully-connected Neural Network $\mathcal{NN}$, formed by a set of neurons distributed over different layers. Moreover, $\mathcal{NN}$ is characterized by a set of parameters $\mathbf{W}$, namely weights and biases, which are tuned during the optimization process by solving the following PDE-constrained optimal control problem:

$$\begin{cases} \min\limits_{\mu,\mathbf{W}} & (\mathcal{J}_{\mathrm{fit}}(\mathbf{W}) + \mathcal{J}_{\mathrm{phys}}(\mu, \mathbf{W})) \\ \text{s.t.} & \mathbf{d}(\mathbf{x}) = \mathcal{NN}(\mathbf{x}; \mathbf{W}). \end{cases}$$

We minimize the loss function composed of the weighted sum of different components leveraging data and physics. Specifically, the mismatch between the output of the $\mathcal{NN}$ and the available N_{obs} noisy observations is measured through the following component of the loss function:

$$\mathcal{J}_{\mathrm{fit}}(\mathbf{W}) = \frac{\omega_{\mathrm{fit}}}{N_{\mathrm{obs}}} \sum_{i=1}^{N_{\mathrm{obs}}} \|\mathcal{NN}(\mathbf{x}_{\mathrm{i}}; \mathbf{W}) - \mathbf{d}_{\mathrm{i}}^{\mathrm{obs}}\|^2.$$

Here, $\omega_{\mathrm{fit}} > 0$ is an additional hyperparameter that weights the contribution of the available data with respect to the information coming from the physical model. The latter is encoded in $\mathcal{J}_{\mathrm{phys}}$, which is made by several terms containing the residuals of the PDE and boundary conditions, expressed in the strong form:

$$\mathcal{J}_{\mathrm{phys}}(\mu, \mathbf{W}) = \omega_{\mathrm{phys}} R_{\mathrm{phys}}(\mathbf{d}; \mu, \mathbf{W}) + \sum_{i=1}^{N_{\mathrm{bc}}} \omega_{\mathrm{bc}}^i B_{\mathrm{phys}}^i(\mathbf{d}; \mu, \mathbf{W}),$$

with scalar hyperparameters ω_{phys} and ω_{bc}^i, $i \in 1, \ldots, N_{\mathrm{bc}}$, that leverage the contributions of the mathematical model. In particular, $\mathcal{J}_{\mathrm{phys}}$ contains a regularization term R_{phys} formed by the norm of the PDE residual:

$$R_{\mathrm{phys}}(\mathbf{d}; \mu, \mathbf{W}) = \frac{1}{N_{\mathrm{c}}} \sum_{i=1}^{N_{\mathrm{c}}} \| - \nabla \cdot \boldsymbol{\mathcal{P}}(\mathcal{NN}(\mathbf{x}_{\mathrm{i}}^c; \mathbf{W}))\|^2,$$

which is averaged over the set of collocation points $\{\mathbf{x}_{\mathrm{i}}^c\}$, $i = 1, \ldots, N_{\mathrm{c}}$.

The training of $\mathcal{NN}$ parameters, along with the estimation of the unknown parameter μ, is attained by combining the first-order ADAM optimizer (Kingma and Ba, 2014) with the second-order BFGS optimizer. Specifically, we develop a multistage training strategy that allows robustly performing data fitting and parameter estimation over a wide range of initial guesses for the $\mathcal{NN}$ parameters $\mathbf{W}$.

3. DISCUSSION

We studied the ability of PINNs to estimate the solution of Eq. (1) and the unknown parameter μ for different benchmark test cases based on a 3D non-linear elastic problem. We investigated the performances of PINNs in different setups, showing the dependence of the accuracy in parameter estimation with respect to the level of noise and density of measures. Hyperparameters may be suitably tuned by properly weighting the different components of the loss function to handle large noise and low data regimes.

PINNs have proven to be a powerful and flexible tool for solving the parameter estimation problem in this context. This will potentially lead to the clinical exploitation of PINNs. Nevertheless, finding an automatic optimal tuning of the various hyperparameters in the algorithm remains an open challenge.

REFERENCES

Chabiniok, R., Wang, V.Y., Hadjicharalambous, M., Asner, L., Lee, J., Sermesant, M., Kuhl, E., Young, A.A., Moireau, P., Nash, M.P., Chapelle, D., and Nordsletten, D.A. (2016). Multiphysics and multiscale modelling, data-model fusion and integration of organ physiology in the clinic: ventricular cardiac mechanics. *Interface Focus*, 6(2), 20150083.

Hernandez, K.A.L., Rienmüller, T., Baumgartner, D., and Baumgartner, C. (2020). Deep learning in spatiotemporal cardiac imaging: A review of methodologies and clinical usability. *Computers in Biology and Medicine*, 104200.

Kingma, D.P. and Ba, J. (2014). Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*.

Logg, A., Mardal, K.A., and Wells, G. (2012). *Automated solution of differential equations by the finite element method: The FEniCS book*, volume 84. Springer Science & Business Media.

Nguyen-Thanh, V.M., Zhuang, X., and Rabczuk, T. (2020). A deep energy method for finite deformation hyperelasticity. *European Journal of Mechanics-A/Solids*, 80, 103874.

Quarteroni, A., Dede', L., Manzoni, A., and Vergara, C. (2019). *Mathematical Modelling of the Human Cardiovascular System: Data, Numerical Approximation, Clinical Applications.* Cambridge Monographs on Applied and Computational Mathematics. Cambridge University Press.

Raissi, M., Perdikaris, P., and Karniadakis, G.E. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics*, 378, 686–707.

Zhang, E., Yin, M., and Karniadakis, G.E. (2020). Physics-informed neural networks for nonhomogeneous material identification in elasticity imaging. *arXiv preprint arXiv:2009.04525*.