MS43040: Project E
Physics-consistent stress-strain modeling of elastic materials

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1 Motivation

Hyperelasticity refers to the property of materials that exhibit significant elasticity, meaning they can undergo large deformations when subjected to stress and then return to their original shape once the stress is removed. Materials that exhibit hyperelasticity include rubber, polymers (e.g., nylon, polyethylene, and Teflon) and biological tissues (e.g., skin, cardiac muscles, and brain tissue). Hyperelastic materials differ from linear elastic materials in that their stress-strain relationships are nonlinear. Unlike linear elasticity where the stress and strain are directly proportional according to Hooke's Law, the relationship between stress and strain can be much more complex and nonlinear for hyperelastic materials (see Figure 1).

More specifically, the stress-strain relation, i.e., **constitutive model**, of a hyperelastic material is modeled as following.

- Let $\boldsymbol{F}$ denote the deformation gradient. $\boldsymbol{F}$ is a 3×3 matrix with positive determinant and represents the strain state of a deformed material. Note that $\boldsymbol{F} = \boldsymbol{I}$ denotes the underformed state.
- For a given $\boldsymbol{F}$, the strain energy density of the material is given by a nonlinear function $W(\boldsymbol{F})$.
- The stress state of the material is represented by the first Piola–Kirchhoff stress tensor $\boldsymbol{P}$ and given by:

$$P_{ij}(\boldsymbol{F}) = \frac{\partial W(\boldsymbol{F})}{\partial F_{ij}}, \qquad \text{with} \quad i, j = 1, 2, 3. \tag{1}$$

- The model then boils down to finding an appropriate nonlinear function for the energy density $W(\boldsymbol{F})$.

Neural networks provide a data-driven approach to learn hyperelastic constitutive models by capturing complex nonlinearities present in the material behavior. Through training on pairs of input (e.g., strain) and output (e.g., energy or stress) data, neural networks can learn intricate patterns and relationships, offering flexibility in modeling various hyperelastic materials and loading conditions without relying on predefined equations. They automatically extract relevant features from the data, adapt to different material types and conditions, and can be integrated into experimental setups (e.g., Figure 1) or simulation frameworks to enhance efficiency and accuracy, making them valuable tools for predicting the behavior of hyperelastic materials.

2 Problem

Here, we will develop strategy to represent the strain energy density $W(\boldsymbol{F})$ using a NN as a function of $\boldsymbol{F}$. However, naively fitting a NN to some given data and learning the constitutive model is not sufficient. Such a constitutive model must strictly satisfy certain constraints for the stress-strain response to be physically and thermodynamically valid.

Here, we consider three such constraints. We will then devise a neural network (NN) architecture to approximate an unknown material's strain energy density (i.e., its constitutive model) while being physically consistent with these constraints.

(C1): The strain energy density W should be independent of the coordinate axes. Therefore, instead of considering W as a function of $\boldsymbol{F}$, we consider W as a function of coordinate invariants of $\boldsymbol{F}$. For the scope of this project, we consider:

$$\text{Strain energy density: } W(I_1, J), \quad \text{with} \quad I_1(\boldsymbol{F}) = \mathrm{tr}(\boldsymbol{F}^T\boldsymbol{F}) \text{ and } J(\boldsymbol{F}) = \det(\boldsymbol{F}). \tag{2}$$

Notably, $I_1(\boldsymbol{F})$ and $J(\boldsymbol{F})$ are independent of the coordinate axes chosen for $\boldsymbol{F}$.

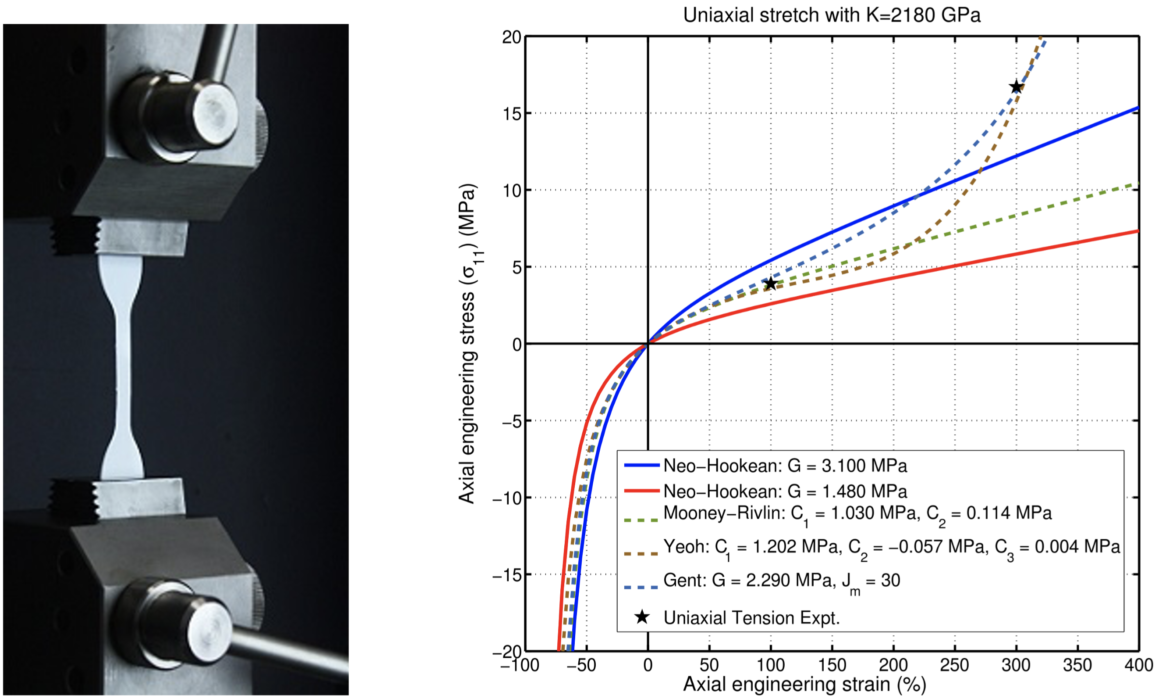

Image credit: https://www.veryst.com/services/testing/material-test-library/uniaxial-tension-testing)

(Image credit: Bbanerje, *Stress-strain relations for hyperelastic materials under uniaxial stretch,* 2010)

Figure 1: Exemplar constitutive models (right) for hyperelastic materials under uniaxial stretch. These models are calibrated using stress-strain data obtained from experimental mechanical testing (left).

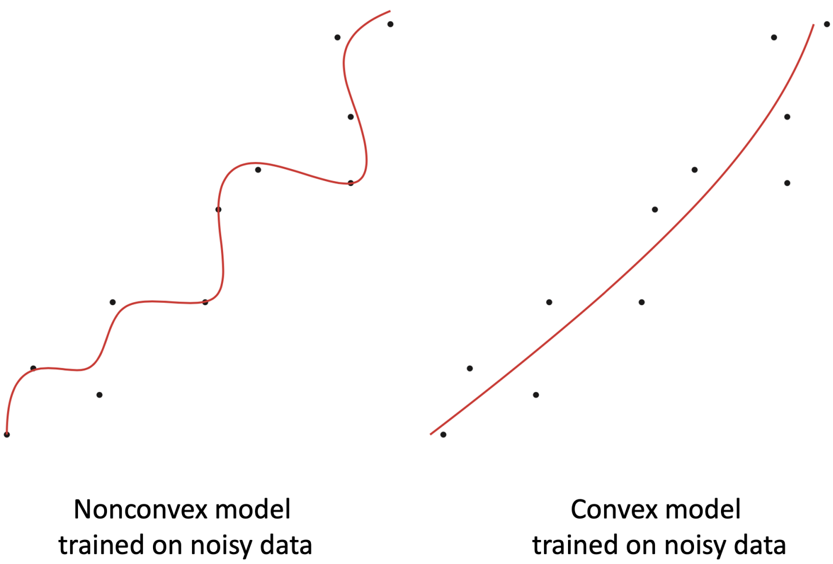

Figure 2: Examples of nonconvex vs. convex models trained on noisy data. Images adapted from Ref. [2].

(C2): The strain energy density $W(\boldsymbol{F}) \equiv W(I_1, J)$ must be convex with respect to the invariants I_1 and J. This implies that the material at any point has positive stiffness and that the energy and stress should increase as the deformation increases (i.e., it should become harder to deform the material as the strain levels increase).

A conventional NN may not result in a convex output, especially when the data is noisy (see Figure 2). Therefore, we will devise a special type of neural network architecture called "**Input-Convex Neural Networks**" (ICNN) [1, 2, 3] whose outputs are always guaranteed to be convex with respect to its inputs.

Specifically, Thakolkaran et al. [1] showed that a conventional feed-forward neural network can be made convex (i.e., converted into an ICNN) with the following two adaptations to its architecture:

- The weight matrices of the hidden layers should only contain non-negative entries.
- The activation functions should be convex and non-decreasing.

(C3): The strain energy density W should be a smooth function (at least twice continuously differentiable) such that stiffness (which is the second derivative, i.e., $\partial^2 W / \partial \boldsymbol{F}^2$) is continuous. This implies that there are no sharp changes or kinks in the overall material response.

3 Data description

The data you are offered to develop, test, and analyze your machine learning model are provided in two files: `energy_train.csv` and `energy_test.csv`. You may only use the data from `test_data.csv` only for testing; not for training.

The training data contains observations from three different mechanical tests (200 rows each, 600 rows total) – namely, uniaxial tension, shear, and biaxial tension. The test data contains 200 observations from simultaneous uniaxial tension and shear (along different directions as in the training data).

Both data files contain 10 columns each as described below.

- `Fij` with `i,j=1,2,3`: respective components of the deformation gradient $\boldsymbol{F}$.
- `W`: an unknown hyperelastic material's strain energy density W corresponding to the deformation gradient $\boldsymbol{F}$ in the same row.

4 Tasks

The final objective of the project is to develop a NN-based constitutive model of the unknown hyperelastic material. The NN must take as input the deformation gradient as a 3×3 matrix and outputs the strain energy density W.

To achieve this objective, the following sub-tasks can be identified:

- Develop a naive NN that maps $\boldsymbol{F}$ to W without concerning any constraints. Interpret the quality of energy predictions.
- Compute and interpret the quality of stress tensors for the test data by differentiating your NN. This can be done using PyTorch functions: `torch.autograd.grad()` (see documentation: [LINK]) or `.backward()` (see documentation: [LINK]).
- Improve your NN architecture* and results by including the constraint (C1).
- Improve your NN architecture* and results by including the constraint (C2) and (C3).
- Offer your perspective on shortcomings and routes to improve the model accuracy.

* PyTorch supports defining custom NN hidden layers that are later compatible with `torch.nn.Sequential()`; see documentation [LINK].

References

[1] Brandon Amos, Lei Xu, and J. Zico Kolter. Input convex neural networks, 2016.

[2] Faisal As'ad, Philip Avery, and Charbel Farhat. A mechanics-informed artificial neural network approach in data-driven constitutive modeling. *International Journal for Numerical Methods in Engineering*, 123(12):2738–2759, March 2022.

[3] Prakash Thakolkaran, Akshay Joshi, Yiwen Zheng, Moritz Flaschel, Laura De Lorenzis, and Siddhant Kumar. Nn-euclid: Deep-learning hyperelasticity without stress data. *Journal of the Mechanics and Physics of Solids*, 169:105076, December 2022.