Project: Inverse-designed spinodoid metamaterials

Introduction

The spinodoid metamaterial (see ref. [1] and slides from lab session-4) is parameterized by 4 design parameters:

$$\boldsymbol{\Theta} = [\rho, \theta_1, \theta_2, \theta_3]. \tag{1}$$

While ρ determines the relative density of the metamaterials, $\{\theta_1, \theta_2, \theta_3\}$ control the structural anisotropy. Given a design vector $\boldsymbol{\Theta}$, you can use the provided MATLAB code `visualize_spinodoid.m` to visualize the corresponding spinodoid metamaterial as a .STL object.

We are interested in studying the anisotropic stiffness of spinodoid metamaterials. The anisotropic stiffness is represented by a 6×6 symmetric stiffness matrix of the form:

$$\mathbb{C} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ & C_{22} & C_{23} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & \text{sym.} & & & C_{55} & 0 \\ & & & & & C_{66} \end{bmatrix}. \tag{2}$$

The stiffness matrix contains 9 independent constants which can be vectorized as:

$$\boldsymbol{S} = [C_{11}, C_{12}, C_{13}, C_{22}, C_{23}, C_{33}, C_{44}, C_{55}, C_{66}]. \tag{3}$$

The stiffness matrix can be visualized as an elasticity surface where each point on the surface corresponds to the Young's modulus in that direction. Given a stiffness vector $\boldsymbol{S}$, you can use the provided MATLAB code `visualize_elasticity_3d.m` to visualize the elasticity surface. You are also provided the MATLAB code `visualize_elasticity_2d.m` to plot one or two elasticity surfaces (for comparison with each other) projected onto the $x - y$, $y - z$, and $z - x$ planes.

In the following parts, we will follow a step-by-step approach to inverse designing spinodoid metamaterials with machine learning. **The questions in each part are open-ended and only serve as a guideline.**

Part I: Theory

Describe – in your **own words** – a high-level summary of spinodoid metamaterials (including e.g., their design inspiration, sub-types, tunable anisotropic stiffness, benefits over other metamaterials, etc.). Use ref. [1] and slides from lab session-4 for reference. Limit: 200-300 words with 1-2 images.

Part II: Data exploration

You have been provided a dataset of thousands of spinodoid metamaterials. The dataset contains the design vectors $\boldsymbol{\Theta}$ and corresponding stiffness vectors $\boldsymbol{S}$. An important step before doing any machine learning is exploring, understanding, and visualizing the data. To get you started, you may include (but not limited to) the following points.

- Visualize the distribution of the each column of the dataset (both design parameters and stiffness properties) via histograms. **Optional** tip: you may look into the following function from the package `seaborn`. Link: https://seaborn.pydata.org/generated/seaborn.pairplot.html
- Visualize the percentage of designs in lamellar, columnar, or cubic categories.

- Visualize representative examples (both spinodoid design and stiffness vectors) for each category.

Discuss the steps taken and the resulting observations in your data exploration.

Tip: Look up Exercise-3A on how to use `pandas` to load data from a `.csv` file.

Part III: Forward modeling – structure-to-property prediction

Using the provided dataset, train a neural network model of **your choice** that takes in a design vector $\boldsymbol{\Theta}$ as input and accurately predicts the anisotropic stiffness in form of the stiffness vector $\boldsymbol{S}$.

Follow all the essential practices for neural network training that we covered in the lab sessions – including but not limited to:

- data normalization
- splitting the dataset into training and test data
- designing appropriate loss function
- tracking loss histories
- checking for underfitting/overfitting
- evaluating prediction accuracy on test data
- tuning the architecture with number of layers, layer widths, activation functions
- and more . . .

Discuss the data preprocessing steps, neural network model choices, training protocols, prediction performance, and improvements due to model tuning. Support your observations with quantitative results/plots. Clearly list all the model and training parameters in a table.

For reference, see ref. [1] and slides from lab session-4.

Tip: When implementing the codes, it is advised to use a very small subset of the data to allow for fast debugging. Once you are confident in your implementation, you may train the model on the whole dataset.

Tip: If the training time is significantly high, reduce the model complexity or use a small subset of the data.

Part IV: Inverse design – property-to-structure prediction

We are now interested in the inverse design – i.e., given a target anisotropic stiffness matrix, we aim to efficiently predict a spinodoid design that has the same target stiffness.

Using the provided dataset, train a neural network model of **your choice** that takes in a stiffness vector $\boldsymbol{S}$ (referred to as *target stiffness*) as input and predicts a design vector $\boldsymbol{\Theta}^*$ (referred to as *predicted design*). As discussed in the lab session, the predicted design may be very different from the *true design* $\boldsymbol{\Theta}$. For validation purpose, the stiffness of the *predicted design* may be reconstructed as $\boldsymbol{S}^*$ (referred to as *reconstructed stiffness*) such that $\boldsymbol{S}^* \approx \boldsymbol{S}$. Due to the multiplicity in the correct solutions (i.e., designs with similar stiffness), the loss function needs to be carefully chosen (refer to discussion from lab session-4).

Follow all the essential practices for neural network training that we covered in the lab sessions – including but not limited to:

- data normalization
- splitting the dataset into training and test data
- designing appropriate loss function
- tracking loss histories
- checking for underfitting/overfitting
- evaluating prediction accuracy on test data
- tuning the architecture with number of layers, layer widths, activation functions
- and more . . .

Discuss the data preprocessing steps, neural network model choices, training protocols, prediction performance, and improvements due to model tuning. Support your observations with quantitative results/plots. Clearly list all the model and training parameters in a table.

For reference, see ref. [1] and slides from lab session-4.

Note: The design parameters predicted by the inverse design neural network may slightly violate the bounds of the parameters. When evaluating accuracy on the test data, please correct these deviations before reconstructing the stiffness (as a post-processing step; not during training). For example, $\theta_1 = -0.01^\circ$ may be corrected to $\theta_1 = 0^\circ$.

Tip: When implementing the codes, it is advised to use a very small subset of the data to allow for fast debugging. Once you are confident in your implementation, you may train the model on the whole dataset.

Tip: If the training time is significantly high, reduce the model complexity or use a small subset of the data.

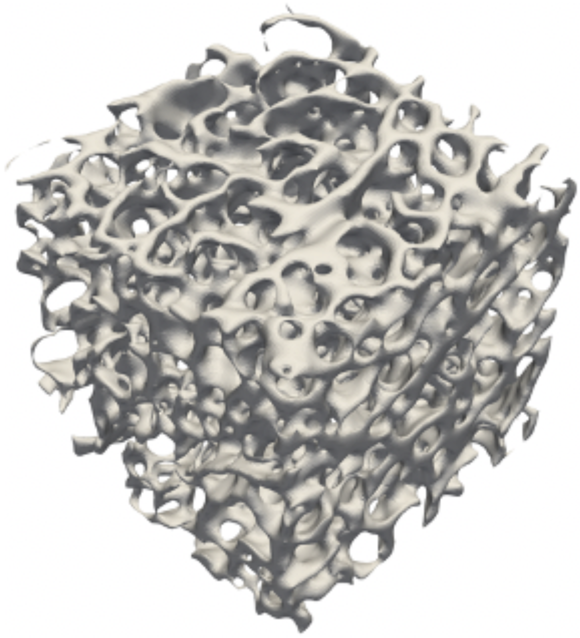

Figure 1: Example bone specimen.

Part V: Inverse design – match the anisotropic stiffness of a bone specimen

You are given the *target* anisotropic stiffness of a bone specimen (Figure 1):

$$\begin{bmatrix} C_{11}=0.390831 & C_{12}=0.058835 & C_{13}=0.061290 & & & \text{zeros} \\ & C_{22}=0.160911 & C_{23}=0.031779 & & & \\ & & C_{33}=0.155180 & & & \\ & & & C_{44}=0.039351 & & \\ & & & & C_{55}=0.081009 & \\ \text{sym.} & & & & & C_{66}=0.073581 \end{bmatrix} \tag{4}$$

Use the inverse design neural network to obtain and report the spinodoid design (in form of parameter vector $\mathbf{\Theta}$). Using the forward modeling neural network, *reconstruct* and report the stiffness of the spinodoid.

Do the target (bone) and reconstructed (spinodoid) stiffnesses match? Visualize the elasticity surface of both on the same plot. Visualize the inverse-designed spinodoid metamaterial.

Describe in less than 100 words what would be the motivation for inverse designing metamaterials to match the anisotropic stiffness of a bone specimen.

References

[1] S. Kumar, S. Tan, L. Zheng, and D. M. Kochmann, "Inverse-designed spinodoid metamaterials," *npj Computational Materials*, vol. 6, no. 1, Jun. 2020. [Online]. Available: https://doi.org/10.1038/s41524-020-0341-6