SB^3C2022
Summer Biomechanics, Bioengineering and Biotransport Conference
June 20-23, Eastern Shore, MD, USA

A NOVEL MACHINE LEARNING-BASED FRAMEWORK TO PREDICT THE ANISOTROPIC MECHANICAL PROPERTIES IN SOFT MATERIALS USING ANISOTROPIC INDENTATION

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INTRODUCTION

Characterizing the mechanical properties of soft tissues and biomaterials is of intense interest as changes in mechanical properties in these materials can be a sign of disease and abnormalities. Many biological materials are anisotropic due to the alignment of the fibers in their internal structure which increases the difficulty in characterization (1, 2).

Characterization of anisotropic mechanical properties in soft materials is challenging due to the difficulties that exist in the nature of biological material, applying and measuring the mechanical loads, and the need to combine the data from multiple experimental protocols (3). Indentation is widely used to determine the local mechanical properties of soft materials due to the ability to test samples in their native state without harvesting (4, 5). However, a single indentation experiment with a symmetric (conical or spherical) probe is not sufficient to estimate the anisotropic mechanical properties; the force-displacement data need to be combined with other experimental and computational techniques such as tracking 3D deformations and inverse finite element model fitting (3, 4, 5).

Here, we develop a machine learning (ML)-based framework to predict the local anisotropic mechanical properties of anisotropic soft materials using two orthogonal indentation protocols with a novel anisotropic indenter. We demonstrate the applicability of the proposed framework using the experimental data for chicken breast and develop a normalization process and workflow which makes the approach applicable for a wide range of anisotropic materials from micro to macro scale.

METHODS

Frozen chicken breasts were defrosted in air until they were able to be sliced into reproducible-sized slabs. The samples were cut to an average width and length of 25-40 mm and thickness of ~10 mm. Typical samples are shown in (Fig. 1a). Indentation experiments were performed with an anisotropic indenter made from a curved metal wire of major radius 3.5 mm and minor radius 0.5 mm at 0.1 mm/s to a maximum depth of 2 mm using an Instron EP1000 with 1N load cell (±1mN) (Fig. 1b). The maximum load was set between 0.15 N-0.3 N. The direction of fibers was determined visually for each sample. At each site, indentations were performed for two directions: 0-degree (the long axis of the indenter aligned with the fiber direction) and 90-degree. The indentation sites were chosen away from the sample edges to avoid the edge effects.

Finite element (FE) modeling (Abaqus) was used to generate a labeled dataset using the indentation simulation for different material property sets. The size of the sample is 40 by 30 mm with a thickness of 10 mm. Mesh convergence and optimization was performed. The elements were modeled as transversely isotropic material with values in Table 1. The whole process was automated.

We then extracted features for our ML model using the resultant normalized pair of force-displacement curves for each data point. For this purpose, each pair of curves was transformed to a feature vector which is constructed as follows: the range of the indentation for each pair of curves was split to a certain number of knots (the number of knots is a hyper-parameter that can be tuned to improve the performance of the model). The indentation value, the force corresponding to 0-degree alignment, and the force corresponding to 90-degree alignment were then extracted at each knot. These values were finally concatenated for all knots to construct the feature vector. To train the ML model, 80 percent of the dataset was used, and the remaining 20 percent was used for testing the model after shuffling. Linear regression, random forests, and fully connected neural networks were used to develop the ML models per aspect ratio, R. A max depth of 40 was used to build the random forests model. For the fully connected neural network model, we used 3 layers in which the first, second, and third layers had 20, 10, and 20 nodes respectively. Our activation function was ReLU.

RESULTS

A total of 37 sets of orthogonal indentations were completed on 17 different chicken samples. The average of the results for each indentation angle was then measured, and the results are shown in (Fig. 1c). The results of indentation experiments as well as FE simulation with two different property sets are shown in Fig. 1d (black: $E_1 = 20$, $E_2 = 10$, $G_{12} = G_{23} = 10$; blue: $E_1 = 30$, $E_2 = 5$, $G_{12} = 15$, $G_{23} = 2.5$; $\nu = 0.47$ for both and moduli in kPa) showing an obvious difference for the predicted force-displacement curves in 0-deg and 90-deg for anisotropic elastic constants in agreement with the experimental results.

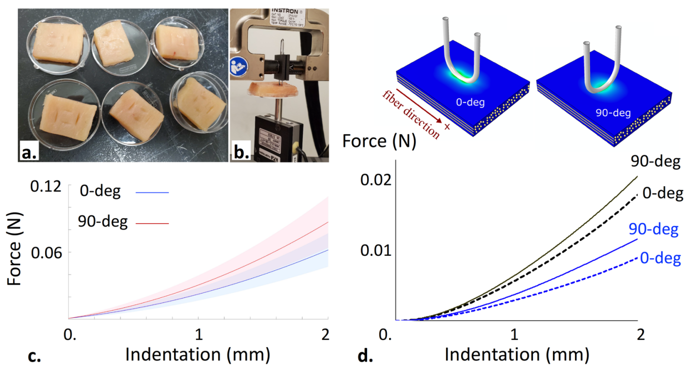

Figure 1: a) chicken breast samples post indentation. b) Experimental setup for indentation experiments. c) Average indentation results ± 1 SD with a shade of similar color for each direction. d) The results of FE simulation for two example material property sets, for 0- and 90- degree alignment (see text).

After validation of the FE model using the Hertz contact theory for a spherical indentation into an isotropic material, 3568 pairs of orthogonal force-displacement (F-d) curves were simulated for each combination of the material properties presented in Table 1. The values of the material properties are taken from the literature as representative of a broad range of biological tissues (3, 5, 6). The F-d data were normalized to remove the scale dependency by dividing the displacement by the maximum indentation, d_{max} and the force values by $d_{max}^{3/2}\sqrt{r}$ according to the Hertz contact rule where r is the smaller radius of the indenter.

Table 1: Transversely anisotropic material properties and indenter geometry values for grid generation with $E_1 > E_2 = E_3$.

parameter	values
$E_1\ (kPa)$	[1, 5, 10, 30, 50, 70, 90, 100]
$E_2 = E_3\ (kPa)$	[1, 5, 10, 30, 50, 70, 90, 100]
$\upsilon_{12} = \upsilon_{13}$	[0.3, 0.47]
υ_{23}	[0.3, 0.47]
$G_{12} = G_{13}\ (kPa)$	[0.1, 0.5, 1, 5, 10, 20, 30, 40]
G_{23}	$E_2/(2(1+\upsilon_{23}))$
R (large:small indenter radius ratio)	[3.25, 5, 7, 10]

The best overall performance achieved for the linear regression, random forests, and fully connected neural networks models are 0.63, 0.76, and 0.9 respectively. The performance of the ML framework in predicting the elastic constants for the training and test set using the fully connected neural networks for R=3.25 is presented in Fig. 2. The neural networks model shows the highest R^2 among all the ML techniques with the lowest overfitting meaning that it achieved the best performance. Random forests tended to over-fit the training set and the linear regression model achieved a very poor performance due to the complex pattern that exists between the dependent features and the response (elastic constants).

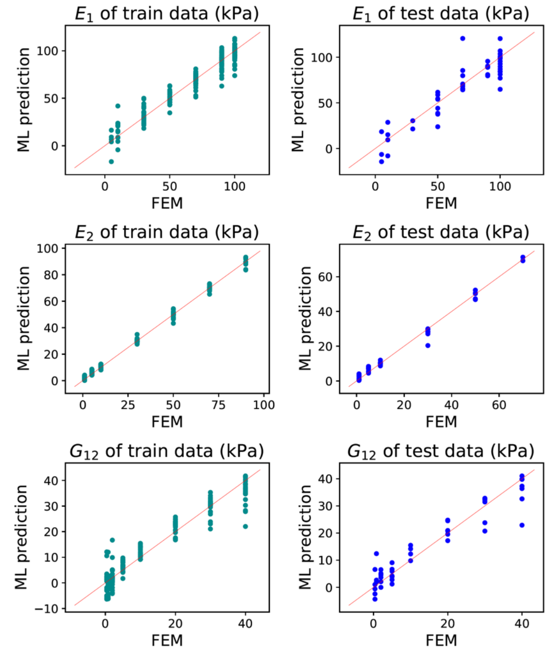

Figure 2: Predictions on the training and test sets using neural networks. R^2= 0.94 for the training set and R^2= 0.9 for the test set.

DISCUSSION

For an anisotropic material, indentation with an anisotropic indenter along and perpendicular to the preferred mechanical axis (i.e., fiber direction) will result in different force-indentation behavior. Here, we proposed a novel ML-based methodology to predict the anisotropic mechanical properties of biological material using the difference between the force-displacement curves resulting from two asymmetric orthogonal indentations parallel and perpendicular to the fiber directions. The main application of the proposed framework is to determine anisotropic properties for biological materials for which performing multiple experiments such as biaxial testing and shear testing is not straightforward (e.g., living cells, in situ tissues). We built a computationally effective model that can determine the anisotropic mechanical parameters for a given material in just a few seconds on a standard desktop computer by using just one set of two indentation test results as input. This result is more significant if we compare it with the average time for running a single forward FE simulation for a pair of indentations (more than half an hour on a standard computer). Solving the inverse problem and finding the properties using the force-displacement curves using the available techniques requires multiple simulations and an optimization protocol e.g., genetic algorithm taking many hours. The proposed framework has the potential to be a powerful tool for quickly determining the anisotropic properties of biological materials with application in disease diagnosis.

ACKNOWLEDGEMENTS

This work was supported by the NSF (CMMI 1761432) and ARMI BiofabUSA (T0137).

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