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A predictive deep-learning approach for homogenization of auxetic kirigami metamaterials with randomly oriented cuts

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This paper describes a data-driven approach to predict mechanical properties of auxetic kirigami metamaterials with randomly oriented cuts. The finite element method (FEM) was used to generate datasets, the convolutional neural network (CNN) was introduced to train these data, and an implicit mapping between the input orientations of cuts and the output Young's modulus and Poisson's ratio of the kirigami sheets was established. With this input–output relationship in hand, a quick estimation of auxetic behavior of kirigami metamaterials is straightforward. Our examples indicate that if the distributions of training and test datasets are close to each other, a good prediction is achievable. Our efforts provide a fast and reliable way to evaluate the homogenized properties of mechanical metamaterials with various microstructures, and thus accelerate the design of mechanical metamaterials for diverse applications.

Keywords: Deep-learning; mechanical metamaterials; kirigami; homogenization; finite element.

1. Introduction

Metamaterials are man-made materials that exhibit unusual or exceptional properties originating from arrangement of unit cells rather than their chemical composition. Metamaterials have been evolved from magnetic, optical, thermal, acoustic, to more recent nonlinear and mechanical metamaterials, whose behaviors are dictated by deformation, stress and motion.[1–3] As one of the unique types of mechanical metamaterials, kirigami metamaterials have attracted increasing attention recently

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because of their ease of manufacturing by cutting and folding, yet achieving unprecedented properties such as auxeticity, large stretchability, tunable surface friction, shape-morphing and programmable pattern formation.[4–8]

Thus far, the vast majority of kirigami metamaterials explored have periodic cuts. Kirigami metamaterials with regular and periodic cuts have a few degrees of freedoms, and their mechanical behavior can be captured by studying a unit cell and imposing periodic boundary conditions. Nevertheless, more exciting applications of kirigami metamaterials with non-periodic or random cuts result in kirigami sheets with more design variables and larger design dimensions. One intriguing application of kirigami sheets with random or non-periodic cuts is the shape-morphing or shape matching kirigami, a topic addressed very recently.[9–11] Designing cut patterns of a sheet and ensuring that the sheet deform or deploy from two-dimensional (2D) plane to any prescribed 3D surface set in the core of these shape-morphing structures design. Augmented design variables are needed for this sophisticated problem and the resultant kirigami design is definitely non-periodic or random.[9–11]

A quick estimation of mechanical properties of kirigami metamaterials with random cuts would accelerate design of these shape-morphing kirigami. In this aspect, help is resorted to homogenization, a concept and methodology widely used to investigate the behaviors of materials with various microstructures. Homogenization of kirigami sheets with random cuts was studied experimentally and numerically by Grima *et al.*[12] They constructed a class of perforated systems having randomly oriented cuts and investigated how Poisson's ratio and modulus of such systems are affected by randomness or disorder in cut orientation. From Grima's experimental results, the mean values of Poisson's ratio as well as modulus are biased and increase monotonically as order of randomness of cut orientations increased from dmax $= 0^\circ$ to dmax $= 25^\circ$, where dmax denotes the maximum magnitude of rotation for a particular system. We speculate that this arises from limited test data. An in-depth investigation of homogenization of this kirigami metamaterials is thus needed for better understanding of its mechanical behavior.

Conventional way of homogenization of materials with complex microstructures is implemented by choosing a representative unit cell, prescribing periodic boundary conditions, and then performing numerical simulations. Equivalent properties of the same unit are calculated by omitting detailed microstructures. When the parameters of microstructures vary, the whole simulation process repeats until the homogenized properties are obtained. This conventional process of homogenization is tedious and time-consuming. It is appealing to develop a quick and reliable way for homogenization of materials with complicated microstructures. Here, we describe a deep-learning approach for prediction of mechanical properties of auxetic kirigami metamaterials with randomly oriented cuts. The convolutional neural network (CNN) was adopted for data training and validation, and the datasets were generated by using finite element method. Our results indicate that the deep-learning algorithm can be used as a reliable and accurate method for quick prediction of auxetic kirigami metamaterials, in particularly when both the training datasets and the test datasets are randomly distributed but fall into similar distributions. Analogous deep-learning approaches have been used to evaluate properties of mechanical metamaterials, but not to kirigami metamaterials.[13–16]

2. Data Generation and Deep-learning Algorithm

Figure 1 shows the unit cell of a kirigami material sheet considered in this paper. The unit cell shown in Fig. 1(a) is a 1.21 mm $\times$ 1.21 mm square with periodic boundary conditions enforced, while the unit cell shown in Fig. 1(b) is a 3.63 mm $\times$ 3.63 mm square. The kirigami cuts considered in this paper are rectangle-shaped slits with dimensions 1 mm $\times$ 0.01 mm. The dimensions of all slits are fixed in simulation but the orientations vary randomly. Figure 1(a) contains a unit cell of cuts with four random orientations, denoted by θ_1, θ_2, θ_3, θ_4, while Fig. 1(b) gives another case with total 36 random cuts whose orientations are marked by θ_1, θ_2,...,θ_{36}. The materials used here are assumed to be linear isotropic with Young's modulus 3.2 MPa and Poisson's ratio 0.49. The commercial software, ABAQUS/Standard, is used for FEM simulation. Plane stress element (CPS3) was used and the unit cells in Figs. 1(a) and 1(b) were discretized by 1350 and 12,130 elements, respectively. To model the random cuts in Fig. 1, a Python code was programmed to construct the model and the orientation of each slit was set randomly. Intersection of any two slits is avoided. To prepare the datasets for the following CNN training and prediction, all together 10,000 FEM simulations were carried out. Among them, 8000 datasets were chosen for training and the remain 2000 datasets were used for test.

Figure 2 depicts the CNN algorithm for this study. The CNN model consists of two convolutional (CONV) layers and three fully connected (FC) layers. Using the model in Fig. 1(b) as a typical example, orientations of 36 random cuts are chosen as input data to the CNN, and the homogenized Young's modulus and Poisson's ratio are obtained as output data. Convolution of the input data is performed in the CONV layers, and features of the input data are extracted to form feature maps, which are then mapped to the output data by the FC layers. The CONV layers 1 and 2 have 16 and 32 filters, respectively. The FC layers 1, 2 and 3 include 512, 64 and 2 neurons, respectively. Rectified Linear Unit (ReLU) was adopted as the activation functions in all CONV layers and FC layers 1 and 2 as indicated in Fig. 2. We train the network using the Adam optimizer.

3. Result and Discussions

Regarding the material used for simulation (rubber with modulus 3.2 MPa taken from Ref. 12), the porosity of cuts (2.7%), and the randomness of orientation ($\pm 25°$), all the simulated data for Poisson's ratio falls into range $[-0.867, -0.744]$ with mean value -0.812 and standard deviation 0.016, while the calculated moduli are in the range [0.106 MPa, 0.17 MPa] with mean value 0.13 MPa and standard deviation 8.5×10^{-3} Mpa.

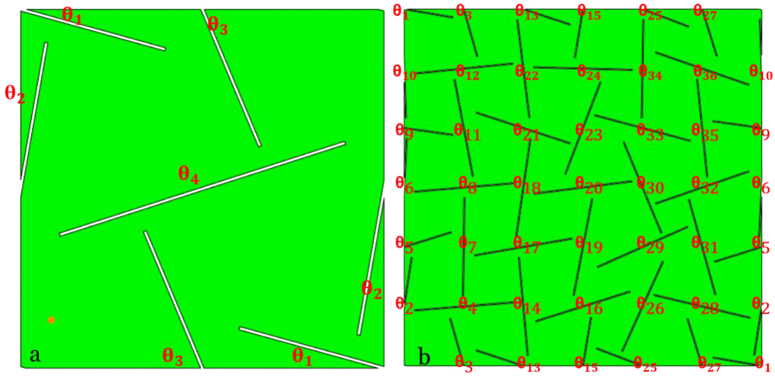

Fig. 1. (Color online) The unit cell FEM model of auxetic kirigami metamaterials sheet with randomly oriented cuts. All the cuts are rectangle-shaped with fixed length 1 mm and width 0.01 mm, while the orientation of each cut is random in the range $-25°$ $-25°$. (a) A 1.21 mm $\times$ 1.21 mm square unit cell contains four random cuts. (b) A 3.63 mm $\times$ 3.63 mm square unit cell with 36 random cuts.

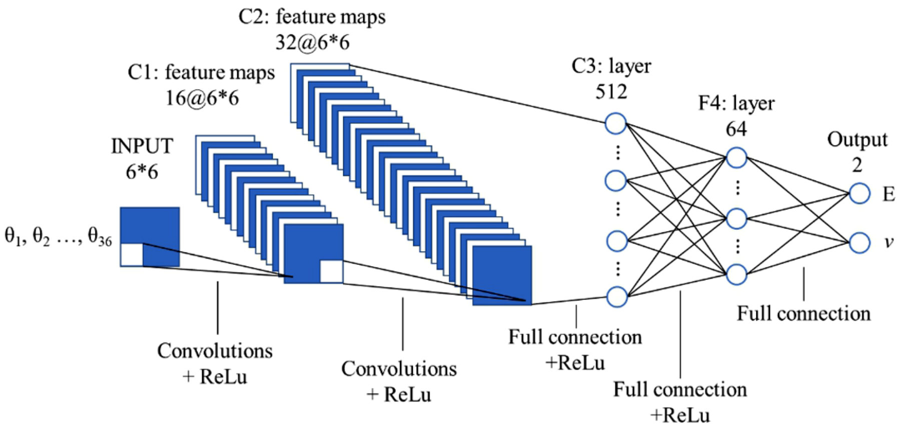

Fig. 2. The CNN model used for mechanical properties prediction of a kirigami metamaterial. The orientations of the random cuts are chosen as input variables (using the model in Fig. 1(b) as an example) and Young's modulus and Poisson's ratio are estimated as output variables.

Figure 3(a) plots the convergence history during the training and learning process. The black curve shows the convergence of Young's modulus, while the red line is the history of Poisson's ratio. In Fig. 3(a), the average error is defined as the deviation between the predicted value and the simulation value. Figures 3(b) and 3(c) plot the comparison of calculated (vertical axis) and predicted (horizontal axis) Poisson's ratios and Young's modulus, respectively. The red lines in Figs. 3(b) and 3(c) denote the straight line, $y = x$, and an excellent prediction is achieved when all data points collapse into the straight line. The results of Fig. 3 are obtained when the distributions of the training and test datasets coincide, i.e. all in $[-0.867, -0.744]$ for Poisson's ratio and [0.106 MPa, 0.17 MPa] for Young's modulus.

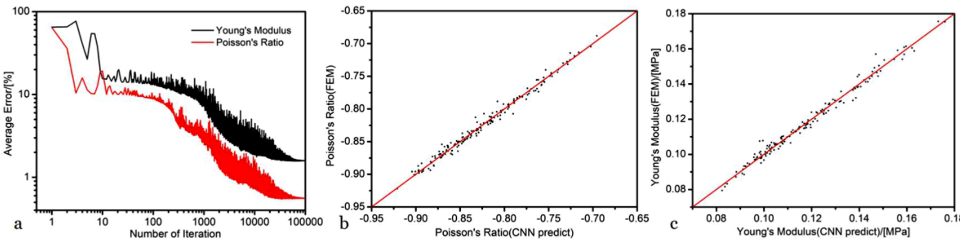

Fig. 3. (Color online) The convergence history (a) and performance of prediction of Poisson's ratio (b) and Young's modulus (c) of a kirigami metamaterial unit cell with four randomly oriented cuts. The straight red lines in (b) and (c) imply that the predicted values coincide with the unseen test data. Collapsing of the points into the near neighborhood of the straight line demonstrates excellent prediction capability of the proposed approach.

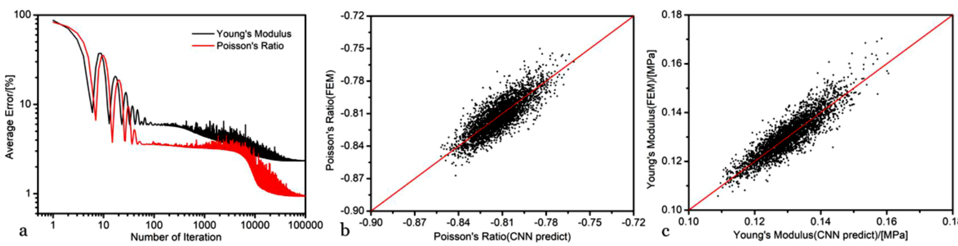

Fig. 4. (Color online) Convergence history and prediction of the model in Fig. 1(b) with 36 random cuts. The same distributions training and test datasets were utilized.

Figure 4 presents the similar results when the unit cell considered is that in Fig. 1(b) and the number of random cuts is increased to 36. The overall trend in Fig. 4 is the same as that in Fig. 3, but the calculated versus the predicted data deviate more or less from the linear red line, as shown in Figs. 4(b) and 4(c). This implies that for the simple standard CNN algorithm adopted here, it is possible that more datasets are needed to improved the performance of CNN. Figures 3 and 4 demonstrate that good prediction of CNN for mechanical properties of kirigami metamaterials is attained when the distributions of both training and test data fall into the similar distribution.

4. Summary

We describe a predictive deep-learning approach for fast and reliable homogenization of auxetic kirigami metamaterials with randomly oriented cuts. The datasets for training and test were generated by using finite element simulations. The CNN was adopted as the deep-learning algorithm. The orientations of random cuts were used as input variables, while the homogenized Young's modulus and Poisson's ratio were chosen as output variables, and an implicit mapping between input and output was obtained. With this input–output relationship in hand, a fast prediction of mechanical properties of kirigami metamaterials is straightforward and the accuracy is checked by comparing predicted data with unseen test data. Good prediction of CNN is guaranteed when the training and test datasets fall into similar range of distribution.

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