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Neural Networks for Structural Optimisation of Mechanical Metamaterials

Stefan Bronder[1,*], **Stefan Diebels**[1], and **Anne Jung**[1]

[1] Saarland University, 66123 Saarbrücken

Mechanical metamaterials are man-made designer materials with unusual properties, which are derived from the microstructure rather than the base material. Thus, metamaterials are suitable for tailoring and structural optimisation to enhance certain properties. A widely known example for this class of materials are auxetics with a negative Poisson's ratio. In this work an auxetic unit cell is modified with an additional half strut.During the deformation this half strut will get into contact with the unit cell and provide additional stability. This leads to a higher plateau stress and consequently to a higher energy absorption capacity. To achieve the maximum energy absorption capacity, a structural optimisation is carried out. But an optimisation exclusively based on finite element simulations is computationally costly and takes a lot of time. Therefore, in this contribution neural networks are used as a tool to speed up the optimisation. Neural networks are one of many machine learning methods and are able to approximate any arbitrary function on a highly abstract level. So the stress-strain behaviour and its dependency from the geometry parameters of a type of microstructure can be learned by the neural network with only a few finite element simulations of varying geometry parameters. The modified auxetic structure is optimised with respect to the mass specific energy absorption capacity. As a result a qualitative trend for the optimal geometry parameters is obtained. However, the Poisson's ratio for this optimisation is close to zero.

1 Introduction

With dwindling resources and new technologies, the demand for new, specialised materials is ever increasing. Mechanical metamaterials provide a material class designable for certain applications and tailored to enhance certain properties. The microstructure rather than the base material is the property-defining factor [**?**], thereby making e.g. auxetics ideal for simulation-aided structural optimisation. Auxetics are a subclass of mechanical metamaterials with the characteristic of a negative Poisson's ratio. Hence, they show an increased impact resistance and energy absorption capacity, which makes them perfect for crash absorbers in e.g. cars or trains.

The optimisation with solely a finite element (FE) solver is highly time-consuming, since the simulations have to be carried out with a microstructural resolution. Therefore, a parameterised optimisation method combined with neural networks [**?**] as a powerful machine learning tool can be applied to significantly speed up the process. This contribution focuses on the generation of training data and application of neural networks to a modified auxetic structure. An re-entrant honeycomb, auxetic unit cell is supplemented by an additional half strut (Fig. **??**a) in the middle to provide increased stability after an initial deformation. The modified auxetic structure was optimised with respect to the mass specific energy absorption capacity.

2 Materials and methods

2.1 Training data generation

To provide the training data for the neural network, FE simulations of a parameterised model are carried out with the FE software ABAQUS®. A modified auxetic unit cell with the geometry parameters strut thickness, strut waist, re-entrant angle, overall unit cell size and length of the half strut (Fig. **??**a) is multiplied in all the space directions to create a macroscopic sample. This sample is then subjected to a simulated compression experiment between two rigid plates. The energy absorption capacity as well as the model's total mass, the stress-strain behaviour and the Poisson's ratio of the sample were extracted from the resulting database. An elastic-plastic material model based on tensile test data of selective laser melted Aluminum was chose for the simulations since samples will be manufactured this way after a successful optimisation.

So the training data of the neural network consist of the material parameters Young's modulus, density and Poisson's ratio (Fig. **??**c, table) of the base material, the five geometry parameters and the stress-strain behaviour.

2.2 Neural network

The neural network was implemented using TensorFlow®with the Keras API in Python®. A feed forward neural network was used with the goal to predict the stress-strain behaviour for a set of geometry parameters. A set of material and geometry parameters, by which one unit cell is specified, along with continuous strain values is used as input. The neural network

* Corresponding author: e-mail stefan.bronder@uni-saarland.de, phone +49 681 302 3648

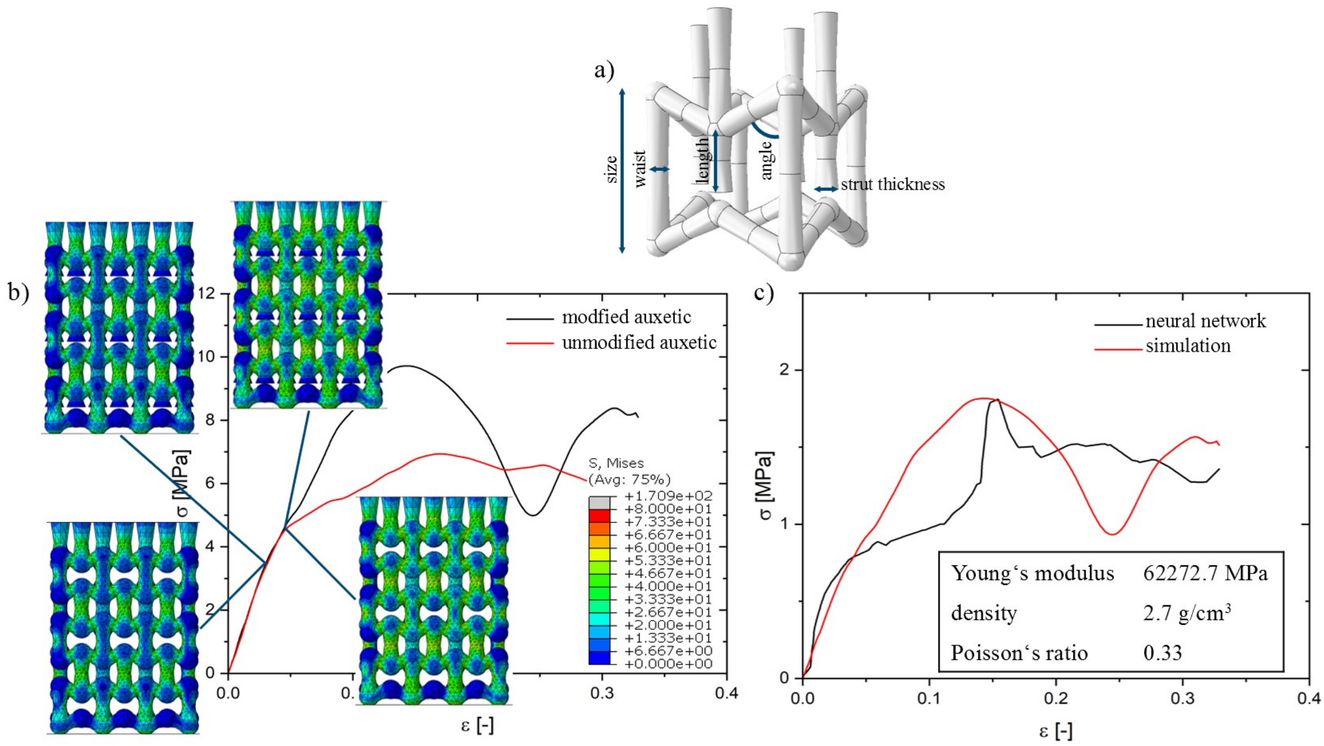

Fig. 1: a) modified auxetic unit cell with the five geometry parameters marked; b) Comparison of the stress-strain behaviour of the modified auxetics and pure auxetics; c) stress-strain diagram of a simulation and the prediction from the neural network for the validation data, the material data for the SLM Aluminum are listed in the table.

then approximates the mass specific stress value for each strain, resulting in the mass specific stress-strain diagram. The area beneath this curve is then calculated as the mass specific energy absorption capacity.

2.3 Optimisation

Finding the maximum energy absorption capacity while saving overall mass can be transferred to a minimisation problem by a surrogate model technique. A modification of the quasi-Newton minimiser of Broyden, Fletscher, Goldfarb and Shannon [**?**] is used to find the minimum of the fifth dimensional quadratic polynomial linking the geometry parameters to the mass specific energy absorption capacity. As a result new geometry parameters are derived for which the neural network can in turn approximate the stress-strain behaviour and thereby the energy absorption capacity. The surrogate polynomial can then be fitted accordingly and a new minimum can be found.

3 Results and discussion

The modified auxetics were able to achieve a higher energy absorption capacity due to the additional half strut. Upon reaching contact they maintained the stiffness for larger deformation and achieved a higher plastic collapse stress (Fig. **??**b). A neural network with 26 hidden layers and 100 neurons on each layer yields a reasonable well approximation of the stress-strain behaviour (Fig. **??**c) to do an optimisation. Even though there is some error to the neural network's prediction, the optimisation based on the neural network yields a qualitative trend for the geometry parameters. To maximise the energy absorption capacity should have a re-entrant angle between 68° and 72°, a small as possible unit cell size and thick struts with a waist. The downside of such a structure is a Poisson's ratio close to zero, so the auxetic effect almost vanishes. Therefore, the Poisson's ratio will be included as a second constraining factor in the future. Furthermore, the application of a thin, noncrystalline nickel coating [**?**] will be investigated to enhance the properties.

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