Thermodynamically consistent constitutive modeling of isotropic hyperelasticity based on artificial neural networks

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Herein, a neural network-based constitutive model for isotropic hyperelastic solids which makes use of a physically motivated dimensionality reduction into the invariant space is presented. In order to automatically fulfill thermodynamic consistency, gradients of the network with respect to the input quantities are considered within a customized training loop. The proposed approach is exemplarily applied to the finite element simulation of two three-dimensional samples, while only data collected from pure two-dimensional virtual experiments are needed for the model calibration before.

1 Introduction

The classical constitutive modeling and calibration in continuum solid mechanics based on experimental or synthetic data is still challenging and time consuming in many cases. Due to this, a variety of data-driven approaches which circumvent this task and can handle even noisy data are currently developed [2, 5]. Likewise, artificial neural networks (ANNs) are a possibility to automate constitutive modeling by approximating stress-strain relations. Within the training of ANNs, thermodynamic consistency can be ensured by choosing a suitable network architecture and loss function [3, 4, 6]. In this contribution, an ANN-based model for isotropic hyperelasticity is considered. A gradient-based training process is applied for the calibration.

2 Modeling framework based on artificial neural networks

Isotropic hyperelasticity In the case of hyperelasticity, the symmetric 2nd Piola-Kirchhoff stress tensor \( \mathbf{T} \) is given by \( \mathbf{T} = 2\partial_C \psi \). Therein, \( \psi \) denotes the Helmholtz free energy density and \( \mathbf{C} := \mathbf{F}^T \cdot \mathbf{F} \) is the right Cauchy-Green deformation tensor following from the deformation gradient \( \mathbf{F} \). If the constitutive response is furthermore restricted to the case of isotropy, \( \psi \) can be described in terms of the three deformation type principal invariants \( I_i \) with \( \alpha \in \{1, 2, 3\} \). By using the chain rule, the relationship \( \mathbf{T} = \sum_{\alpha} f_\alpha \mathbf{G}^\alpha \) for the calculation of the stress tensor can be achieved, where the so called stress coefficients are given by \( f_\alpha := 2 \partial_{I_i} \psi \) and the tensor generators follow to \( \mathbf{G}^\alpha := \partial_C I_\alpha \).

Data processing From now on, it is assumed that a denoised data set consisting of tuples \( \mathcal{D}_i := (\mathbf{C}, \mathbf{T}) \) which are related to an unknown hyperelastic isotropic constitutive law is given. In order to predict the stress \( \mathbf{T} \) for a given state of deformation \( \mathbf{C} \) with high accuracy while keeping the number of neurons as few as possible, a dimensionality reduction of the input and output variables is necessary, respectively. Thus, following the work of Shen et al. [6], where the principle invariants are chosen as input values, a lower-dimensional data tuple \( \mathcal{D}_i^{\text{red}} := (\mathbf{I}, \mathbf{T}) \) is derived for each \( \mathcal{D}_i \) by

\[
\begin{align*}
\mathbf{I}_1 &= \text{tr} \mathbf{C}, \quad \mathbf{I}_2 = \frac{1}{2} \left( \text{tr}^2 \mathbf{C} - \text{tr} \mathbf{C}^2 \right), \quad \mathbf{I}_3 = \det \mathbf{C} \quad \text{and} \quad \mathbf{I}^\alpha(\mathbf{C}) &= \arg \min_{\boldsymbol{\xi} \in \mathbb{R}^{3 \times 1}} \left\| \mathbf{T}^\alpha(\mathbf{C}) - \sum_{\alpha=1}^3 \xi_\alpha \mathbf{G}^\alpha(\mathbf{C}) \right\|^2. (1)
\end{align*}
\]

In contrast to the principal invariants \( \mathbf{I} = (\mathbf{I}_1, \mathbf{I}_2, \mathbf{I}_3) \in \mathbb{R}^{3 \times 1} \), an analytical expression for the free energy function \( \psi \) is generally unknown. Thus, the previously introduced stress coefficients \( \mathbf{I}^\alpha = (I_1^\alpha, I_2^\alpha, I_3^\alpha) \in \mathbb{R}^{3 \times 1} \) have to be calculated from the linear least squares method given in the equation above.

Model formulation and training process In order to fulfill the 2nd law of thermodynamics a priori, the ANN is now chosen as input values, a lower-dimensional data tuple

\[
\mathbf{I} = (I_1, I_2, I_3) \in \mathbb{R}^{3 \times 1}, \quad \mathbf{T} \rightarrow \mathbf{I}^\alpha, \quad \psi^\text{ANN} : \mathbb{R}^{3 \times 1} \rightarrow \mathbb{R}, \quad \mathbf{I} \rightarrow \mathbf{I}^\alpha, \quad \mathbf{I}^\alpha \rightarrow \mathbf{I}^\alpha, \quad \text{where the fractal symbol} \quad \mathbf{I}^\alpha \text{denotes a normalized value of} \quad \mathbf{I}^\alpha. \quad \text{The network architecture is restricted to only one hidden layer containing} \quad N \in \mathbb{N} \text{ neurons. Furthermore, the activation function is given by a hyperbolic tangent function and the output is chosen to be affine linear. Instead of using conventional training loops to determine the neural network’s weights by only inserting values of} \quad \psi \quad \text{in the loss function directly, a gradient-based approach is adopted. Hence, to avoid a numerical calculation of the free energy} \quad \psi \quad \text{for}
\]

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the training process, the loss function
\[ \mathcal{L} := \sum_{i=1}^{n} \left\| \frac{\partial \psi^{\text{ANN}}}{\partial \mathbf{u}}(\mathbf{u}) - \frac{1}{2} \mathbf{f}(\mathbf{u}) \right\| \quad \text{with} \quad \psi^{\text{ANN}}(i) := B + \sum_{\beta=1}^{N} W_{\beta} \tanh \left( \sum_{\gamma=1}^{3} W_{\beta \gamma} i_{\gamma} + b_{\beta} \right) \] (2)
which only takes into account the normalized derivative of the ANN-based model and the corresponding true values is defined.
Moreover, compared to the development of a neural network predicting the stress coefficients directly, this approach reduces the number of trainable parameters \( B, \mathbf{W}, \mathbf{w}, \mathbf{b} \) while the same number of neurons are included in the hidden layer. The reduced data set is randomly divided into training and test data to allow a generalization of the neural network to unknown data \((\mathbf{u}, \mathbf{f})\). An implementation of the described workflow is realized using Python and Tensorflow.

### 3 Numerical examples

Finally, to demonstrate the ability of the proposed ANN-based method, synthetic stress-strain data generated with a highly nonlinear Ogden-type constitutive model are chosen. To enable the training process of the constitutive ANN within a broad subset of the invariant space, the deformation states of the training dataset have to be as heterogeneous as possible. For this purpose, data collected from a finite element (FE) calculation in which a square specimen with several elliptical holes is loaded under uniaxial tension. To obtain perfect plane stress data which are preferable from an experimental viewpoint [1], the virtual experiment is performed in a two-dimensional setting. By using the proposed training process, the weights of a comparatively small network containing 8 neurons in the hidden layer are determined from the data set.

The constitutive ANN is implemented in the open source software FEniCS and verified by using two different three-dimensional validation load cases. At first, a cuboid containing several cylindrical holes is loaded up to 40% relative elongation into an uniaxial tension mode, cf. Fig. 1 (a). Secondly, a torsional sample with three cylindrical holes is loaded by specifying a distortion of 45°, cf. Fig. 1 (b). In order to assess the approximation quality of the trained ANN, the predicted local stress fields are compared to reference solutions generated with the original Ogden-type model. Regarding the relative stress errors \( |P_{K1} - P_{K1}^{\text{ANN}}| / \max |P_{K1}| \) with \( \mathbf{P} := \mathbf{T} \cdot \mathbf{F}^T \) denoting the 1st Piola-Kirchhoff stress tensor, rather low deviations below 1.5% could be achieved for both examples, cf. Fig. 1 (a), (b). Thus, the proposed method enables an accurate prediction of fully three-dimensional stress fields, although only two dimensional stress states were used for the training.

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