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**Geometric deep learning for computational mechanics. I: Anisotropic hyperelasticity.** (English) [Zbl 07337944](#)

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**Summary:** We present a machine learning approach that integrates geometric deep learning and Sobolev training to generate a family of finite strain anisotropic hyperelastic models that predict the homogenized responses of polycrystals previously unseen during the training. While hand-crafted hyperelasticity models often incorporate homogenized measures of microstructural attributes, such as the porosity or the averaged orientation of constituents, these measures may not adequately represent the topological structures of the attributes. We fill this knowledge gap by introducing the concept of the weighted graph as a new high-dimensional descriptor that represents topological information, such as the connectivity of anisotropic grains in an assemble. By leveraging a graph convolutional deep neural network in a hybrid machine learning architecture previously used in [*A. L. Frankel et al.*, “Predicting the mechanical response of oligocrystals with deep learning”, *Comput. Mater. Sci.* 169, Article ID 109099, 19 p. (2019; doi:10.1016/j.commatsci.2019.109099)], the artificial intelligence extracts low-dimensional features from the weighted graphs and subsequently learns the influence of these low-dimensional features on the resultant stored elastic energy functionals. To ensure smoothness and prevent unintentionally generating a non-convex stored energy functional, we adopt the Sobolev training method for neural networks such that a stress measure is obtained implicitly by taking directional derivatives of the trained energy functional. Results from numerical experiments suggest that Sobolev training is capable of generating a hyperelastic energy functional that predicts both the elastic energy and stress measures more accurately than the classical training that minimizes  $L_2$  norms. Verification exercises against unseen benchmark FFT simulations and phase-field fracture simulations that employ the geometric learning generated elastic energy functional are conducted to demonstrate the quality of the predictions.

**MSC:**

- 74 Mechanics of deformable solids
- 68 Computer science

**Keywords:**

geometric machine learning; graph; polycrystals; microstructures; anisotropic energy functional; phase-field fracture

**Software:**

[HYPLAS](#); [Keras](#); [MTEX](#); [Neper](#); [word2vec](#)

**Full Text:** [DOI](#)

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