Mechanical Engineering Doctoral Defense

Data-Augmented Structure-Property Mapping for Accelerating Computational Design of Advanced Material Systems

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abstract

Advanced material systems refer to materials that are comprised of multiple traditional constituents but complex microstructure morphologies, which lead to their superior properties over conventional materials. This dissertation is motivated by the grand challenge in accelerating the design of advanced material systems through systematic optimization with respect to material microstructures or processing settings. While optimization techniques have mature applications to a large range of engineering systems, their application to material design meets unique challenges due to the high dimensionality of microstructures and the high costs in computing process-structure-property (PSP) mappings. The key to addressing these challenges is the learning of material representations and predictive PSP mappings while managing a small data acquisition budget. This dissertation thus focuses on developing learning mechanisms that leverage context-specific meta-data and physics-based theories. Two research tasks will be conducted: In the first, we develop a statistical generative model that learns to characterize high-dimensional microstructure samples using low-dimensional features. We improve the data efficiency of a variational autoencoder by introducing a morphology loss to the training. We demonstrate that the resultant microstructure generator is morphology-aware when trained on a small set of material samples, and can effectively constrain the microstructure space during material design. In the second task, we investigate an active learning mechanism where new samples are acquired based on their violation to a theory-driven constraint on the physics-based model. We demonstrate using a topology optimization case that while data acquisition through the physics-based model is often expensive (e.g., obtaining microstructures through simulation or optimization processes), the evaluation of the constraint can be far more affordable (e.g., checking whether a solution is optimal or equilibrium). We show that this theory-driven learning algorithm can lead to much improved learning efficiency and generalization performance when such constraints can be derived. The outcomes of this research is a better understanding of how physics knowledge about material systems can be integrated into machine learning frameworks, in order to achieve more cost-effective and reliable learning of material representations and predictive models, which are essential to accelerated computational material design.

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