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Improving direct physical properties prediction of heterogeneous materials from imaging data via convolutional neural network and a morphology-aware generative model

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ABSTRACT

Direct prediction of material properties from microstructures through statistical models has shown to be a potential approach to accelerating computational material design with large design spaces. However, statistical modeling of highly nonlinear mappings defined on high-dimensional microstructure spaces is known to be data-demanding. Thus, the added value of such predictive models diminishes in common cases where material samples (in forms of 2D or 3D microstructures) become costly to acquire either experimentally or computationally. To this end, we propose a generative machine learning model that creates an arbitrary amount of artificial material samples with negligible computation cost, when trained on only a limited amount of authentic samples. The key contribution of this work is the introduction of a morphology constraint to the training of the generative model, that enforces the resultant artificial material samples to have the same morphology distribution as the authentic ones. We show empirically that the proposed model creates artificial samples that better match with the authentic ones in material property distributions than those generated from a state-of-the-art Markov Random Field model, and thus is more effective at improving the prediction performance of a predictive structure-property model.

1. Introduction

Direct prediction of material properties through predictive models has attracted interests from both material and data science communities. Predictive models have the potential to mimic highly nonlinear physics-based mappings, thus reducing dependencies on numerical simulations or experiments during material design, and enabling tractable discovery of novel yet complex material systems [1–3]. Nonetheless, the construction of predictive models for nonlinear functions, such as material structure-property mappings, is known to be data-demanding, especially when the inputs, e.g., material microstructures represented as 2D or 3D images, are high-dimensional [4]. Thus, the added value of predictive models quickly diminishes as the acquisition cost increases for material samples. We investigate in this paper a computational approach to generate artificial material samples with negligible cost, by exploiting the fact that all samples within one material system share similar morphology. More concretely, we define morphology as a style vector quantified from a microstructure sample, and propose a generative model that learns from a small set of authentic samples, and creates an arbitrary amount of artificial samples that share the same distribution of morphologies as the authentic ones.

The key contribution of the paper is the introduction of a morphology constraint on the generative model that significantly improves the morphological consistency between the artificial and authentic samples from benchmark generative models. To demonstrate the utility of the proposed model, we run a case study on the prediction of the Young's modulus, the diffusion coefficient and the permeability coefficient of sandstone microstructures. We show that the generated artificial samples from the proposed model can improve the prediction performance more effectively than those from a state-of-the-art Markov Random Field (MRF) model.

As an overview, the proposed model follows the architecture of a variational autoencoder [5] that learns to encode material microstructures into a lower-dimensional latent space and to decode samples from the latent space back into microstructures. Both the encoder and the decoder are composed of feed-forward convolutional neural networks for extracting and generating local morphological patterns, and are jointly trained to minimize the discrepancy between the artificial

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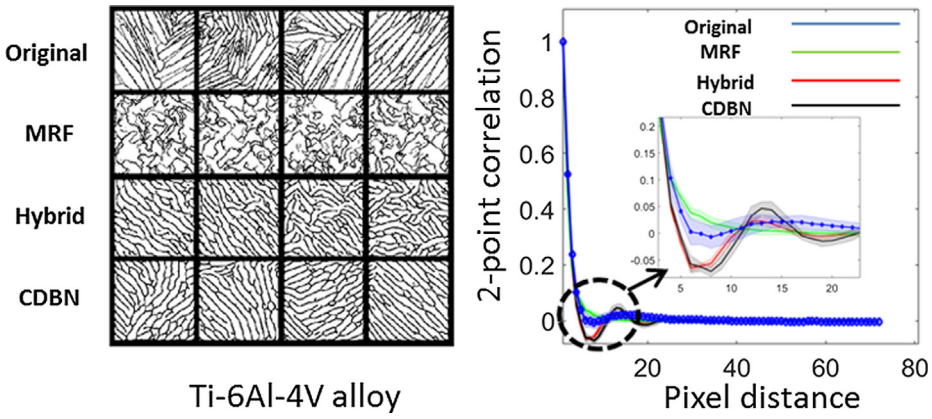

Fig. 1. Comparison of two-point correlation functions among four sets of images. From left to right: Authentic microstructure samples, samples generated by a Markov random field model [35], samples generated by a hybrid model with deep belief network and Markov random field [43], and samples generated by a deep belief network [42]. Better matching in the discretized 2-point correlation space does not indicate better microstructure generations.

and authentic samples. The target morphology is quantified from the authentic samples by an auxiliary network. The idea of quantifying material morphology through a deep network is inspired by the style transfer technique originally developed for image synthesis [6].

The rest of the paper is structured as follows: In Section 2 we review related work on material representations and reconstruction, based on which we delineate the novelty of this paper. We then introduce background knowledge on variational autoencoder and style transfer. Section 3 elaborates on the details of the proposed model. Section 4 presents a case study on the prediction of sandstone properties, where we demonstrate the superior performance of the proposed model against the benchmarks, in both microstructure generation, and the resultant property prediction accuracy. In Section 5 we summarize findings from the case study and propose potential future directions. Section 6 concludes the paper.

2. Background

2.1. Data science challenges in computational materials science

Incorporating data science into material discovery [1] and design [7] faces unique challenges with high dimensionality of material representations and the lack of material data due to high acquisition costs. We review existing work that address these challenges to some extent.

2.1.1. Challenge 1: Mechanisms for understanding material representations

A common approach to addressing the issue of high dimensionality is to seek for a representation, i.e., an encoder-decoder pair, for a material system: The encoder transforms microstructures to their reduced representations, and the decoder generates (i.e., reconstructs) them back from their representations. A good encoder-decoder pair should both achieve significant dimension reduction, and good matching between the data distribution (i.e., the distribution of authentic samples) and the model distribution (i.e., the distribution defined by the decoder). This is often feasible for material systems with consistent and quantifiable morphologies among their samples, as reviewed below.

Existing encoders for material representations can be categorized as physical and statistical, some of which have led to accelerated design of various material systems [8–12]. Among all, **physical encoders** characterize microstructures using composition (e.g., the percentage of each material constituent) [13,14], dispersion (e.g., inclusions' spatial relation, pair correlation,the ranked neighbor distance [15–20]), and geometry features (e.g., the radius/size distribution, roundness, eccentricity, and aspect ratio of elements of the microstructure [17,15,8,21–25]). Among **statistical encoders** are the N-point correlation functions [26,18,8,21,22]. Torquato et al. [27,28,8] show that the microstructure of heterogeneous materials can be characterized statistically via various types of N-point correlation functions [29,30]. Similar descriptors include lineal path function [31] and statistics calculated based on the frequency domain using fast Fourier transformation [32,33]. Another type of statistical encoders are **random fields** [34–36], which define joint probability functions on the space of microstructures. Typical probability models include Gaussian random fields [37,38,8] which treats binary microstructure images as level sets, and Markov random fields, where each pixel of the microstructure is assumed to be drawn from a probability function conditioned on its neighbouring pixels [35].

Decoding of representations, i.e., generation of microstructure through existing physical and statistical representations, involves optimization in the microstructure space: For physical representations and N-point correlation functions, a microstructure is searched to minimize its difference from the target descriptors. For random fields, the generation can be done by maximizing the joint probability through Markov chain Monte Carlo simulations [35,36]. While it is shown that material generation through these representations is feasible [18,22,8,11], the computational costs for the optimization through gradient [32,11] and non-gradient [28,39–41] methods are often high.

In addition to the difficulties in decoding, the existing encoders are not universally applicable, especially to material systems with complex morphology. More specifically, matching in the representation space does not guarantee the match in the microstructure space. An example can be found in Fig. 1, where we compare two-point correlation functions of Ti64 alloy samples and three sets of artificial images (see details from [35,42,43]). The visually more plausible set has worse match to the target with respect to the Euclidean distance in the discretized 2-point correlation space.

These existing difficulties lead to the need for new mechanisms to define material representations. We propose four metrics for evaluating the utility of a material representation: interpretability, dimensionality, expressiveness, and generation cost: Physical descriptors and correlation functions are designed to be interpretable and relatively low dimensional, yet may not be expressive enough to capture complex morphologies and requires optimization during generation; random fields are relatively expressive (and some permit fast generation [35]), but are often high-dimensional and less interpretable. Both categories of representations are material specific, i.e., new representations need to be manually identified for new material systems. Cang et al. [42] proposed to learn statistical generative models from microstructures to automatically derive expressive, low dimensional representations that enables fast microstructure generation. They showed that a particular type of generative model, called Convolutional Deep Belief Network (CDBN) [44], can produce reasonable microstructures for material systems with complex morphologies, by extracting morphology patterns at different length scales from samples, and decode an arrangement of these patterns (the hidden activation of the network) back into a microstructure. Nonetheless, CDBNs are trained layer-by-layer, and thus require additional material-dependent parameter tuning to achieve plausible generations.