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Small-data active learning for the inverse design of spinodoid architected materials

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Abstract

Architected materials offer unprecedented opportunities for tailoring mechanical performance, yet their design remains challenging due to the complex, nonlinear relationship between mesostructure and effective properties. In this contribution, we present an efficient, data-driven framework for the inverse design of architected materials, demonstrated using spinodoid architected materials. Because high-fidelity experimental characterization – particularly for fatigue-related properties – is prohibitively expensive, the workflow is specifically developed to operate effectively in a small-data regime. The proposed approach integrates computational augmentation with probabilistic learning and optimization. The framework proceeds iteratively: (1) mesostructures are encoded through statistical descriptors, (2) effective mechanical properties are obtained from numerical simulations, (3) a Gaussian-process surrogate is constructed to represent the structure–property linkage together with its uncertainty, (4) Bayesian optimization proposes promising new descriptor sets that are likely to improve performance or reduce uncertainty, and (5) corresponding candidate mesostructures are reconstructed. These steps are repeated until a convergence criterion is satisfied, such as a reduction in predictive uncertainty or the identification of mesostructures with favorable properties. Spinodoid architected materials serve as a representative and practically relevant test case. Their continuous, self-supporting morphologies make them attractive for multifunctional and fatigue-resistant designs. By augmenting a small initial dataset with in silico–generated spinodoid structures and their simulated effective properties, the framework progressively refines the structure–property linkage. This enables both the prediction of material behavior and the guided exploration of new regions in the design space that may yield improved performance.

Keywords:

Inverse design Architected materials Bayesian optimization Small-data regime Spinodoid