Machine learning accelerated design of architectured materials for tailored mechanics

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Introduction

Novel material design is based on tuning the composition and shaping the topology of the material. While the composition has been extensively discussed and applied, the topology and internal architecture of the material is not yet properly addressed. Designing architectured materials with tailored physical properties is a promising paradigm in the advancement of material landscape.

Architecting the material brings excellent possibilities while posing challenges when it comes to designing the architecture for a set of objective functions. While classical optimization techniques would demand extensive computational resources, the ability of machine learning algorithms seems to be promising. Multi-objective Bayesian optimization is among such algorithms that enables discovering the optimal designs and architecture of the material [1].

Considering the nature of the Bayesian optimization, this approach is equally applicable for multiphysics in which the objectives are from several fields such as mechanics and magnetism (coupling the equations of elasticity and Maxwell) and corresponding coupling material properties.

Additionally, the absence of limit for the number of objectives makes it possible to grasp the full anisotropy of the physics, and include several material properties (from the corresponding symmetry class) in the optimization machinery. Obviously in order to produce the required input data, the material architecture is to be generated in an automated fashion. Common options are truss-based lattices, TPMS (triply periodic minimal surface) lattices, spinodoid metamaterials [2], and Bezier-curve based geometries.

Auxetic architectures with enhanced fatigue life

To showcase the underlying idea, the application of multi-objective Bayesian optimization is presented here for architectures generated by Bézier curve (Figure 1) addressing two objective functions [3]. The objectives are selected to be the negative Poisson's ratio (auxetic response) and low-cycle fatigue life. The former is captured based on homogenization for elasticity, while the latter is determined based on elastoplastic homogenization incorporated with the critical distance theory [4].
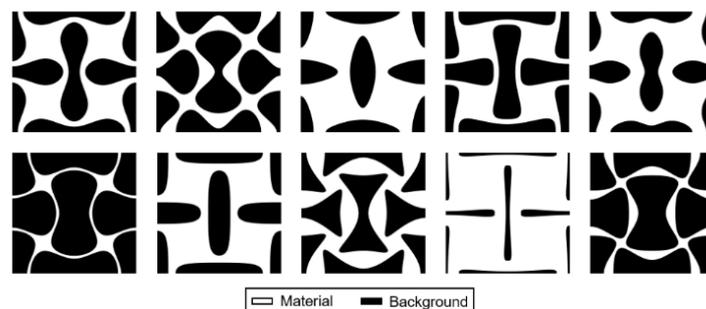

Figure 1: Diverse range of architecture materials based on Bezier curves (taken from [3])

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The results of multi-objective Bayesian optimization are demonstrated in Figure 2, in which the conventional auxetic lattices and selected optimized auxetic architectures are presented. The Pareto front obtained can be used efficiently for identifying the optimal design that balances both criteria, i.e. auxetic performance and fatigue life.
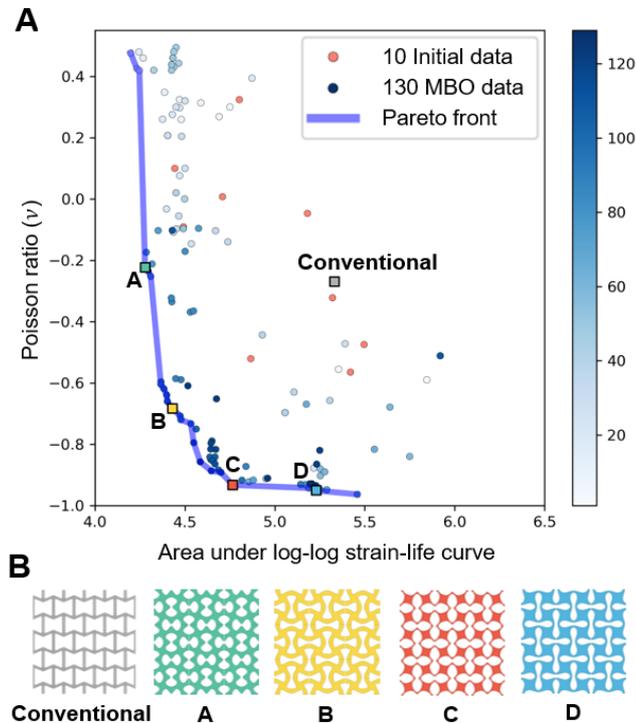

Figure 2: Results of multi-objective Bayesian optimization (MBO). (A) The scatterplot of MBO results, conventional auxetic lattices and selected optimized auxetic architectures for two different objects. (taken from [3]) (B) Conventional auxetic architectures and four optimized auxetic structure geometries. (taken from [3])

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