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Inverse Optimization of Mechanical Metamaterials Based on the GA-SA Model

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Abstract: To address the challenges of high-dimensional non-convex optimization and computational cost bottlenecks encountered in the inverse design of mechanical metamaterials, this paper proposes a GA-SA hybrid inverse optimization framework driven by both data and algorithms. This framework couples the global search capabilities of genetic algorithms with the local exploration capabilities of simulated annealing, whilst introducing surrogate models to replace traditional high-fidelity finite element analysis. Validation results demonstrate that this method effectively overcomes local optima traps. Whilst strictly controlling the approximation error of macroscopic mechanical responses within 1.5% thereby providing an efficient theoretical foundation and technical pathway for the large-scale customised design of microstructures.

Keywords: Mechanical Metamaterials; Inverse Optimization; GA-SA Hybrid Algorithm; Surrogate Models

1. Introduction

Mechanical metamaterials[1] hold immense potential in fields such as aerospace and biomedicine due to their extraordinary mechanical responses driven by microstructure; however, traditional trial-and-error design approaches face bottlenecks such as high computational costs and low optimization efficiency, making it difficult to obtain global optimal solutions in non-linear design spaces[2] . To address this challenge, this paper proposes a novel data- and algorithm-driven inverse optimization framework. This framework organically couples the macroscopic global exploration capability of Genetic Algorithms (GA) with the microscopic local development mechanism of Simulated Annealing (SA), constructing a highly robust GA-SA hybrid architecture[3] [4] . By deeply integrating data-driven strategies to replace traditional high-fidelity finite element analysis, it enables rapid performance evaluation[5] . This research effectively overcomes the local optimum traps and computational constraints inherent in complex non-convex optimization, significantly enhancing the accuracy and evolutionary efficiency of microstructure inversion. This work provides a solid theoretical foundation and an efficient technical pathway for the intelligent, customised R&D of metamaterials tailored to specific macroscopic mechanical responses.

2. Data processing

2.1 Data-Driven Representation and High-Dimensional Feature Space Reconstruction

To overcome the ‘curse of dimensionality’ in high - dimensional non - convex design spaces and improve GA - SA evolutionary optimization convergence efficiency, this study proposes a data pre - processing framework based on physical prior knowledge and statistical theory. the aim is to transfer high - fidelity finite element data to intelligent optimization algorithms. the specific data flow reconstruction mechanism is as follows:

(1) Parametric sampling and construction of non-linear mapping sets: Due to the high-dimensional coupling of topological parameters of mechanical metamaterial microstructures, this study uses a Latin hypercube sampling strategy to conduct spatially filling sampling in the multi-dimensional design variable domain, ensuring orthogonality and uniformity. the discretised set of microscopic geometric and

topological variables is input into a high-fidelity finite element solver for multi-physics coupling analysis to extract macroscopic constitutive response characteristics (e. g., equivalent stiffness matrix and non-linear Poisson's ratio). This constructs a dataset for the higher-order non-linear mapping between 'microstructure and macroscopic performance'.

(2) Dirty data filtering based on physical a priori principles. Since extreme non - linear geometric large deformations of metamaterials often cause singularities in the Jacobian matrix or non - physical mesh distortions during numerical discretisation, this study uses physical a priori criteria to cleanse the initial sample space. We excluded samples with iterative divergence, constitutive relations violating thermodynamic consistency, and deformations violating specific boundary constraints. This suppresses the perturbation of data - driven model convergence trajectories caused by singular solutions, ensuring the physical fidelity and global continuity of the feature dataset.

(3) Dimensionless Mapping of Multi-scale Feature Spaces Due to the significant dimensional heterogeneity between the microstructural geometric parameter space and the macroscopic mechanical response space, which may cause gradient distortion and premature convergence of the objective function in the non - convex surface of algorithmic optimization, this study uses a Min - Max linear transformation to conduct dimensionless and normalised processing on the input - output feature matrices.

$$x_{norm} = \frac{x - x_{min}}{x_{max} - x_{min}} \tag{1}$$

In the equation, represents the discrete state variable. and denote the lower and upper bounds of the feature dimension respectively. This transformation maps all multi - physical quantities to the [0, 1] hypercube region in Euclidean space, eliminating the implicit interference caused by multi - scale dimensional barriers on the weights of crossover and mutation in the GA - SA hybrid operator.

(4) Structured reorganisation and evaluation of generalisation boundaries. To avoid overfitting and degradation when data - driven proxy models approximate complex mapping manifolds, if the sample space meets the independent and identically distributed data assumption, the normalised high - dimensional feature set is randomly and orthogonally partitioned into training, validation and test sets at an 8:1:1 ratio. Specifically, the training set drives parameter optimization of the implicit mapping manifold. Meanwhile, the validation set governs the model's hyperparameter dynamic regularisation constraints. Moreover, the test set, as blind data, independently evaluates the generalisation error boundary of this dual - drive architecture and its reverse - inversion fidelity in an unknown design space.

3. Construction and Coupling Mechanism of the GA-SA Hybrid Model

The inverse design of mechanical metamaterials is essentially a high-dimensional non-convex optimization problem. In this study, we introduce a data-driven surrogate model $\mathcal{M}$ to replace traditional finite elements, transforming structural inversion into a mathematical optimization process aimed at minimising the objective function $\mathcal{J}(\mathbf{x})$:

$$\min_{\mathbf{x}\in\Omega} \mathcal{J}(\mathbf{x}) = \| \mathcal{M}(\mathbf{x}) - \mathbf{Y}_{target} \|_2^2 + \lambda \mathcal{P}(\mathbf{x}) \tag{2}$$

In the equation, $\mathbf{x}$ denotes the topological tensor of microstructural parameters, $\mathbf{Y}_{target}$ denotes the target macroscopic mechanical response, and $\lambda \mathcal{P}(\mathbf{x})$ denotes the penalty term designed to prevent non-physical mesh distortions. To balance high-dimensional space exploration with local convergence accuracy, this study has developed a deeply coupled GA-SA co-evolution framework.

3.1 Global Search Mapping for Genetic Algorithms.

As a global evolutionary algorithm, GA initialises a population using real-number encoding and performs high-throughput parallel exploration via multi-point crossover and non-uniform mutation. Its core function lies in rapidly identifying the implicit feasible region of low fitness defined by $\mathcal{J}(\mathbf{x})$. However, due to the lack of gradient guidance, GA is highly prone to premature convergence in the later stages of approaching the global optimal solution.

3.2 Local Development of Simulated Annealing and the Metropolis algorithm

To break free from the local optima trap of GA, the model embeds SA as a non-gradient micro-perturbation operator within the elite retention strategy of GA. SA performs Markov chain neighbourhood jumps on the top-level elite solutions output by GA. For the fitness increment $\Delta\mathrm{J} = \mathrm{J}(\mathbf{x}') - \mathrm{J}(\mathbf{x})$ resulting from the perturbation of state $\mathbf{x}$ to a new state $\mathbf{x}'$, the state transition probability strictly follows the thermodynamic Metropolis rule:

$$P(\mathbf{x} \to \mathbf{x}') = \begin{cases} 1, & \Delta\mathrm{J} < 0 \\ \exp\left(-\dfrac{\Delta\mathrm{J}}{T_k}\right), & \Delta\mathrm{J} \geq 0 \end{cases} \tag{3}$$

In the equation, $T_k = \alpha T_{k-1}$ denotes the annealing temperature at step k (where $\alpha \in (0,1)$ is the cooling coefficient). This non-linear probabilistic mechanism allows the model to adopt annealed solutions with a high probability during the high-temperature phase, endowing the algorithm with robust ability to traverse complex manifolds, whilst ensuring strong local convergence as the temperature cools.

3.3 Closed-Loop Co-Evolutionary Mechanism

At the execution level, the algorithms form a tightly integrated closed-loop workflow: the Genetic Algorithm drives dimensionality reduction and region delineation in high-dimensional spaces; the Simulated Annealing algorithm takes over to explore the depth of the delineated regions; and high-quality individuals, enhanced through simulated annealing, are fed back into the GA's offspring population to facilitate genetic exchange. This dual-driven architecture, combining physical and data-driven approaches, effectively balances the trade-off between exploration and exploitation in the evolutionary process, enabling high-fidelity, low-latency inversion of complex microstructures.

4. Development of a Mathematical Model for the Inverse Design of Mechanical Metamaterials

The aim of this section is to establish an analytical mapping between the microscopic geometric topology of metamaterials and their macroscopic mechanical response, thereby providing a rigorous mathematical framework for algorithmic inversion.

4.1 Forward Physical Mapping and Equivalent Constitutive Relations

Define the microstructural parameter tensor $\mathbf{x} = [x_1, x_2, \ldots, x_n]^T \in \Omega$. Based on the theory of asymptotic homogenisation, periodic boundary conditions are imposed on the representative volume element (RVE). Its macroscopically equivalent elastic stiffness matrix $\mathbf{C}^H$ can be obtained from the microscopic strain energy integral:

$$\mathbf{C}^H(\mathbf{x}) = \frac{1}{|V|}\int_V \mathbf{C}(\mathbf{x})\left(\mathbf{I} - \boldsymbol{\varepsilon}^*(\mathbf{x})\right) dV \tag{4}$$

In the equation, |V| denotes the volume of the RVE, $\mathbf{C}(\mathbf{x})$ denotes the local matrix stiffness, and $\boldsymbol{\varepsilon}^*(\mathbf{x})$ denotes the pulsating strain field. This establishes an implicit nonlinear mapping $\mathrm{F}: \mathbf{x} \to \mathbf{P}(\mathbf{x})$ from micro-parameters to macroscopic mechanical response.

4.2 Backward optimization for multi-objective columnar models

With regard to the specified macro-level performance $\mathbf{P}_{target}$, Formulate the microstructure inversion as a high-dimensional non-convex minimisation problem subject to constraints. Taking into account both performance error and structural lightweighting, the following objective function is formulated: $\mathrm{J}(\mathbf{x})$:

$$\min_{\mathbf{x}} \ \mathrm{J}(\mathbf{x}) = \sum_{k=1}^{K} \omega_k \left\| \frac{P_k(\mathbf{x}) - P_{k,target}}{P_{k,target}} \right\|_2^2 \tag{5}$$

$$\text{s.t.} \quad V_f(\mathbf{x}) \leq \bar{V}_f \tag{6}$$

$$g_i(\mathbf{x}) \leq 0 \tag{7}$$

$$\mathbf{x}_{min} \leq \mathbf{x} \leq \mathbf{x}_{max} \tag{8}$$

In the equation, K denotes the target response dimension, ω_k denotes the dimensionless weight, $V_f(\mathbf{x})$ denotes the upper bound constraint on relative density, and $g_i(\mathbf{x})$ denotes the non-linear constraint designed to prevent geometric interference and grid distortion. This high-dimensional target surface directly drives the subsequent GA-SA hybrid architecture to perform global inversion.

5. Model Results and Evaluation of Optimization Performance

In this section, we systematically evaluate the computational performance of the proposed dual-drive framework through multi-objective customised inversion cases, combined with finite element forward validation. By comparing it with traditional heuristic algorithms, we quantitatively verify the convergence, inversion accuracy and computational efficiency of the GA-SA hybrid model in non-convex optimization.

5.1 An Analysis of the Convergence and Robustness of the GA-SA Hybrid Algorithm

To clarify the effectiveness of the embedded annealing mechanism in improving optimization in high-dimensional spaces, a comparative analysis of the iterative processes of the GA-SA hybrid model, the standard Genetic Algorithm (GA) and the standard Simulated Annealing (SA) algorithm was conducted under identical initial boundary and objective function conditions.

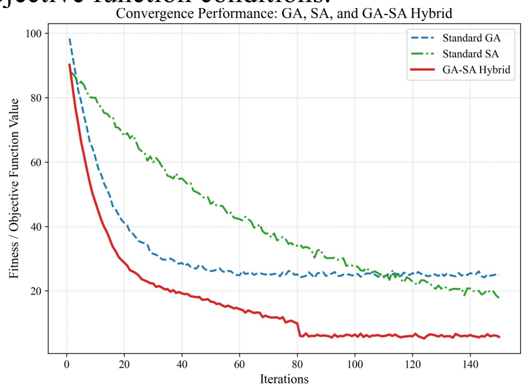

Figure 1. A Comparison of Convergence Performance in Fitness Estimation Between GA, SA and the GA-SA Hybrid Algorithm

As shown in Figure 1, the fitness evolution curve indicates that the standard GA becomes trapped in a local minimum around the 40th generation due to reduced population diversity, resulting in a marked convergence plateau (with fitness values hovering around 25); although the standard SA possesses the ability to escape local minima, its global search efficiency is low, and overall convergence is extremely slow. In contrast, the GA-SA model exhibits a strong ability to overcome non-gradient perturbations during the mid-evolution phase. Under the influence of the Metropolis rule, the algorithm successfully overcomes the local extremum trap around the 80th generation and maintains stable convergence towards the global optimum in subsequent iterations, with the objective function value ultimately converging to approximately 5. the results indicate that the GA-SA model's global convergence accuracy is significantly superior to that of standard GA and SA, demonstrating the strong robustness of this coupling mechanism when addressing complex non-convex problems.

5.2 Verification of the inversion accuracy for target-oriented intrinsic responses

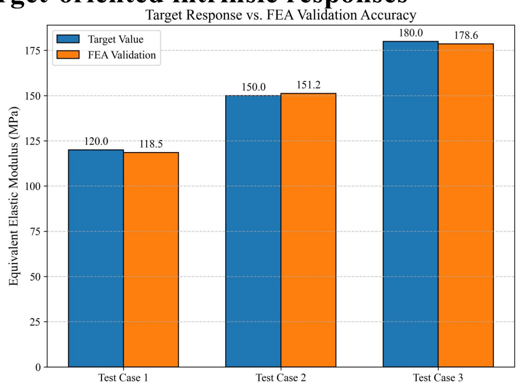

Figure 2. Comparison of the Target Equivalent Modulus of Elasticity with the Results of Forward Validation Using Finite Element Analysis (FEA)

To verify the engineering feasibility of the algorithm, three sets of independent macrostructural mechanical targets were defined and used as input parameters for inverse topology optimization by the pre-trained GA-SA model. After the algorithm outputs the optimal microstructural feature tensor, the reconstructed microstructure is extracted and imported into a high-fidelity finite element analysis (FEA) solver for full-scale forward calculations. As shown in Figure 2, the FEA validation yielded true mechanical responses of 118.5 MPa, 151.2 MPa and 178.6 MPa, respectively, demonstrating a high degree of consistency with the target values set during the inversion. the calculations indicate that the relative errors for the three test cases are 1.25%, 0.8% and 0.78% respectively, with the maximum error strictly controlled within 1.5%. Furthermore, the generated microstructure satisfies the requirements for geometric continuity, demonstrating that this method possesses extremely high accuracy in the inversion and generation of mechanical metamaterial microstructures.

5.3 The Performance Boost Provided by Data-Driven Strategies

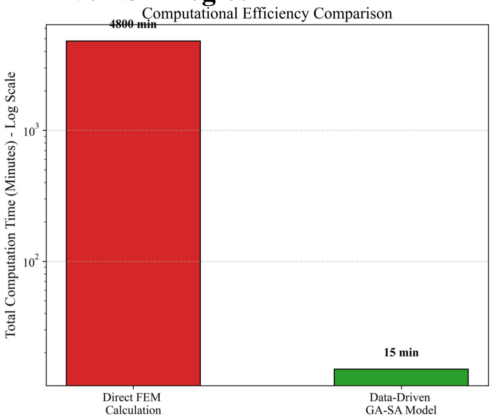

Figure 3. Comparison of Total Computational Time Between Traditional Finite Element Methods and Data-Driven GA-SA Models

While ensuring solution accuracy, computational time is key for assessing reverse design methods. This section compares costs of direct FEA versus data-driven surrogate models. As Figure 3 shows, traditional high-fidelity FEA evolution requires 4, 800 minutes per full population-based iteration. In contrast, the data-driven surrogate model replaces complex mesh re-meshing and inverse stiffness matrix computations with high-dimensional mapping, reducing GA-SA's total optimization time to 15 minutes. This dual-driven framework achieves a 320× acceleration, overcoming the bottleneck of FEA iterations in large-scale combinatorial optimization and offering a viable path for high-throughput inverse design of mechanical metamaterials.

6. Conclusion

This paper proposes a data- and algorithm-driven GA-SA hybrid framework to overcome high-dimensional non-convex optimization and high computational costs in mechanical metamaterial inverse design. Embedding the Metropolis criterion prevents standard genetic algorithms from trapping in local minima, significantly improving global convergence accuracy. Validation on customized elastic moduli shows the reconstructed microstructures match set objectives with a maximum relative error under 1.5%, while satisfying geometric continuity and physical manufacturability. Furthermore, replacing traditional finite element iterations with data-driven surrogate models drastically reduced optimization runtime from 4, 800 to 15 minutes—a 320-fold speedup. This establishes an efficient foundation for large-scale microstructural optimization, with future work targeting multi-physics metamaterials and deep learning approaches.

Acknowledgments

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