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Data-Efficient Design of Multistable, Robust Structures for Additive Manufacturing Using Bayesian Optimization

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Abstract

Additive manufacturing (AM) enables the fabrication of complex, highly customized geometries. However, the design and fabrication of structures with advanced functionalities, such as multistability and fail-safe mechanism, remain challenging due to the significant time and costs required for high-fidelity simulations and iterative prototyping. In this study, we investigate the application of Bayesian Optimization (BO), an advanced machine learning framework, to accelerate the discovery of optimal AM-compatible designs with such advanced properties.

BO uses a probabilistic surrogate to strategically balances the exploration of design space with few test designs and the exploitation of design space near current best-performing designs, thereby reducing the number of design simulations needed. While existing studies have demonstrated the potential of BO in AM, most have focused on static or simple designs. Here, we target multistable structures that can reconfigure among multiple stable states in response to external conditions. Since mechanical performance (e.g., strength) is configuration-dependent, our goal is to identify high-performing designs while ensuring that strength in all stable configurations exceeds a prescribed threshold for structural robustness.

1 Introduction

Additive manufacturing (AM) enables complex, customized geometries which provide ad-vanced behaviors including multistability and fail-safe responses. In particular, this study focuses on multistable structures which can reconfigure on demand and adapt to changing external conditions. Their performance (e.g., strength) depends on the active stable configu-ration, and designs must remain robust across all stable states while meeting AM constraints (e.g., minimum features, anisotropy). Finding such designs by brute-force exploration often requires a large number of high-fidelity and time-costly simulations.

We address this challenge with Bayesian Optimization (BO), a state-of-the-art machine learning framework that replaces direct evaluations of costly objectives and constraints with a probabilistic surrogate and selects new designs via an acquisition function that balances exploration and exploitation [1, 2]. While there have been recent studies applying BO to AM, these existing studies have mainly focused on static or simple behaviors [3, 4, 5, 6]. We target the harder setting of configuration-dependent robustness in multistable systems.

The main contributions of this study are as follows:

- Problem formulation: A constrained, multi-configuration AM design problem that encodes robustness across all stable states.
- BO framework: A Gaussian process surrogate-based BO approach applied to multistable design optimization.
- Numerical study: Empirical results on simulation data showing faster discovery of high-strength multistable designs than grid or random search under the same evaluation budget.

2 Methodology

2.1 Problem formulation

Selecting the best design from a vast set of feasible alternatives requires optimization to ensure that manufacturing quality meets the desired objectives. The main challenge is the highly complex and nonlinear relationship between the design parameters X and the objective function $f(X)$. Evaluating this relationship often requires expensive experimental procedures such as physics-based simulations and high-cost physical validations.

Formally, the design optimization problem can be expressed as:

$$X^* = \arg\max_{X \in \mathcal{X}} f(X), \tag{1}$$

where $f(x)$ is computationally expensive and time-consuming to evaluate. In practice, experimental-based optimization typically follows the workflow illustrated in Fig. 1. Candidate designs are repeatedly sampled and evaluated from the design space until the all evaluation budget is used. The design that achieves the highest observed objective value is then selected as the final solution.

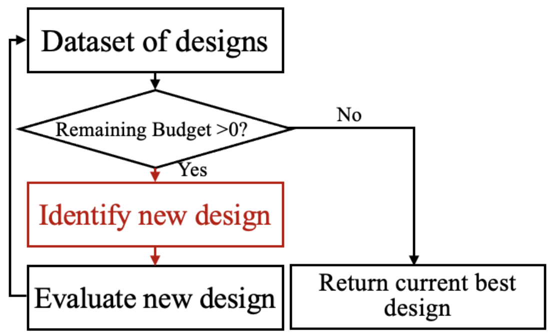

Figure 1: Experimental-based workflow for manufacturing design optimization.

In literature [7], two approaches are commonly used: grid search and random search. Grid search is essentially a full factorial design method, in which all candidate designs are systematically evaluated across the parameter space. By contrast, random search is simpler and selects design samples randomly from the feasible design pool. However, several significant disadvantages arise with these methods: 1) Both approaches require a large number of evaluations to identify an optimal design, which is often impractical in AM due to the high cost of simulations and prototyping. 2) In manufacturing design, uncertainties are frequently present, and neither grid search nor random search is capable of effectively addressing these uncertainties.

2.2 Design informed Bayesian optimization

To address these challenges, we propose a Bayesian optimization (BO) [8] for pre-manufacturing design optimization. BO has two main components: a surrogate model and an acquisition function.

Directly evaluating the objective function $f(X)$ is time consuming. To work around this, BO replaces it with a probabilistic surrogate model $f'(X)$, which is cheap to evaluate. This surrogate model enables the optimization algorithm to make informed predictions about unexplored regions of the design space while quantifying the uncertainty associated with those predictions.

One of the most widely used surrogate models in BO is the Gaussian Process (GP). A GP is a non-parametric Bayesian model that defines a prior distribution over functions. Given a set of observed designs and their objective values, the GP posterior yields both the mean prediction (expected objective value) and the variance (uncertainty estimate) at any candidate design point. This allows the optimization process to strategically trade off between exploration (sampling uncertain regions) and exploitation (sampling regions with high predicted objective values). Thus, GP is widely used as surrogate model for BO in pre-manufacturing design optimization [9]. Formally, a GP is defined as:

$$f'(X) \sim GP(\mu(X), k(X, X')), \tag{2}$$

where $\mu(X)$ is the mean function and $k(X, X')$ is the covariance kernel function. The choice of kernel, such as the Radial Basis Function (RBF), determines the smoothness and correlation structure of the modeled objective function.

While the surrogate model provides probabilistic predictions of the objective function, we also need a principled way to decide where to sample next in the design space. This is conducted by the acquisition function $a(X)$. The acquisition function is designed to be cheap to evaluate and optimize. Its purpose is to balance the trade-off between:

- Exploration: sampling regions of the design space where the surrogate model's uncertainty is high, which helps discover potentially better designs that have not been evaluated yet.
- Exploitation: sampling regions where the surrogate model predicts a high objective value, focusing resources on refining the best-known designs.

By optimizing the acquisition function at each iteration, Bayesian Optimization adaptively selects the next candidate design to evaluate, ensuring efficient use of the limited evaluation budget.

A commonly used acquisition function is Expected Improvement (EI). The key idea of EI is to measure the expected gain in performance relative to the current best observation (design). For a candidate design point X, the EI is defined as:

$$EI(X) = \mathrm{E}[max(f(X) - f(X^+), 0)], \tag{3}$$

where $f(X^+)$ is the current best design.

Algorithm 1 Bayesian Optimization with GP Surrogate and EI Acquisition

Require: Initial design $\mathcal{D}_0 = \{(X_i, f(X_i))\}_{i=1}^{n}$; search design space $\mathcal{X}$; evaluation budget T; GP prior $GP \sim (\mu(\cdot), k(\cdot))$; acquisition $a(\cdot)$ (e.g., EI)

Fit a Gaussian Process (GP) on $\mathcal{D}_0$
for $t = n + 1$ **to** T **do**
    Using the current GP, compute predictive mean $\mu(X)$ and std. $\sigma(X)$ for $X \in \mathcal{X}$
    Select next design by maximizing the acquisition:

$$X_t \in \arg\max_{X \in \mathcal{X}} a(X; \mu(X), \sigma(X), \mathcal{D}_{t-1})$$

    Evaluate the objective: $y_t \leftarrow f(X_t)$
    Augment the data: $\mathcal{D}_t \leftarrow \mathcal{D}_{t-1} \cup \{(X_t, y_t)\}$
    Update (refit) the GP on $\mathcal{D}_t$
end for

The detail of BO algorithm is shown in Algorithm 1. Each iteration, fit (or update) a surrogate model (GP) to approximate $f(X)$ and optimize an acquisition function $a(X)$ to choose the next candidate, evaluate f, and update the dataset. This loop concentrates evaluations on promising, informative regions of the design space.

3 Simulation study

In this section, we conduct a simulation study to evaluate BO on a synthetic, multimodal objective to illustrate its sample efficiency under limited budgets.

We first set a test objective function for the simulation study:

$$f_{\text{simulation}}(X) = 1.4 \exp\left(-0.5 \left(\frac{X - 1.1}{0.18}\right)^2\right) + 0.12 \sin(7X). \tag{4}$$

defining on the domain $\mathcal{X} = [0, 2]$. Our goal is to maximize this objective function. Both grid search and random search are compared as benchmark methods. For grid search, A uniform grid of 100 equally spaced samples was evaluated across the domain. Similarly, for random search, 100 samples were drawn at random from the domain.

For BO, we initialized the search with three evaluations at the domain boundaries and center, i.e., $x = \{0, 1, 2\}$. A GP surrogate model with a Matern kernel was used, and the EI criterion was employed as the acquisition function. At each iteration, the maximizer of EI was evaluated and added to the GP.

The result is shown in Fig. 2, we can see all three methods identified the similar maximizer of $f_{simulation}$. In this process, BO only uses 8 evaluations, which is much less than grid search and random search, showing its effectiveness in optimizing an unknown complex function.

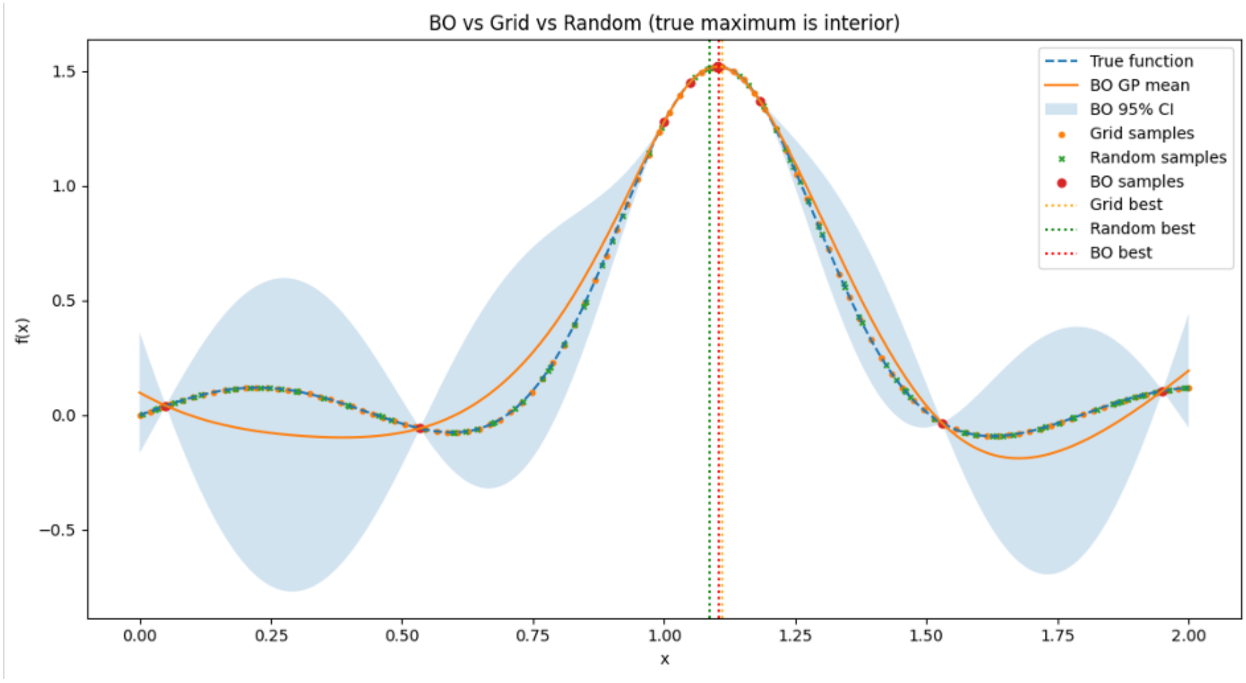

Figure 2: Simulation study of BO vs. Grid search vs. Random search

4 Case study

To further demonstrate the effectiveness of BO in pre-manufacturing design optimization, we present a real-world case study involving the design of a bistable beam structure [10]. Fig. 3 illustrates a bistable beam structure we consider in this study. A bistable structure is a system that can stably exist in two distinct configurations, separated by a significant energy barrier. Transition between these two states requires an external force to overcome the barrier; once this threshold is reached, the structure snaps into the alternative stable configuration, typically without the need for continuous energy input.

In this study, we denote the displacement of the beam as d and the corresponding

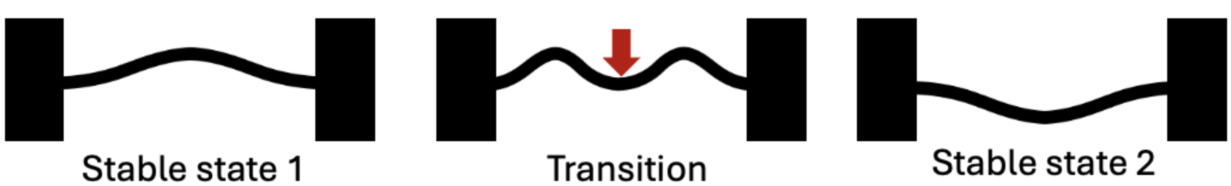

Figure 3: Illustration of a bistable beam structure considered in this study

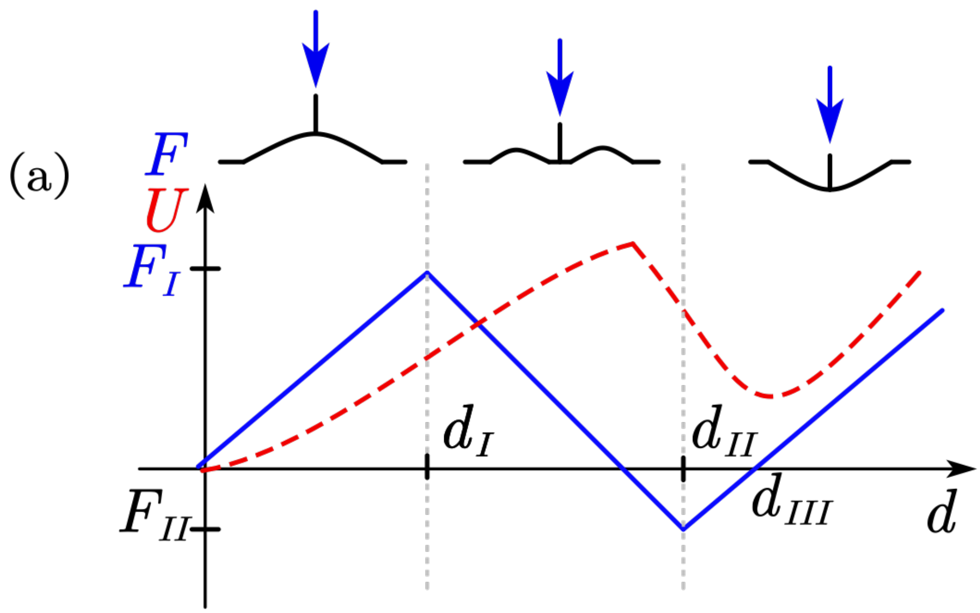

Figure 4: Displacements vs. force in bistable structures

applied force as F, The force–displacement relationship for a given design X can be expressed as $F = f_d(X)$. A schematic illustration of this relationship is provided in Fig. 4.

The bistable beam structure is parameterized by four geometric variables, as summarized in Table 1. We seek an optimal bistable beam design that maximizes the difference

Table 1: Definitions of Parameters

Symbol	**Description**
X_{l_1}	Span length (mm) – horizontal distance between supports.
X_h	Arch height (mm) – vertical rise at the beam's center.
X_{t_1}	Beam section area (mm^2) – area of the cross-section.
X_{b_1}	Beam width (mm) – out-of-plane cross-sectional width.
Ex	Elastic modulus (MPa)
Iz	Moment of inertia of section (mm^4)

between the maximum and minimum forces in the force–displacement curve.

$$J(X) = \max_{d \in \mathcal{D}} f_d(X) - \min_{d \in \mathcal{D}} f_d(X). \tag{5}$$

We employ Finite Element Analysis (FEA) simulations to evaluate candidate designs. ANSYS Mechanical is a widely used FEA platform for simulating structural behavior under diverse conditions such as stress, deformation, and thermal loads. Its ability to handle a broad range of materials and complex physics makes it indispensable in engineering fields including aerospace, automotive, and civil engineering. In this study, simulations are performed using ANSYS Mechanical APDL (ANSYS Parametric Design Language). The three

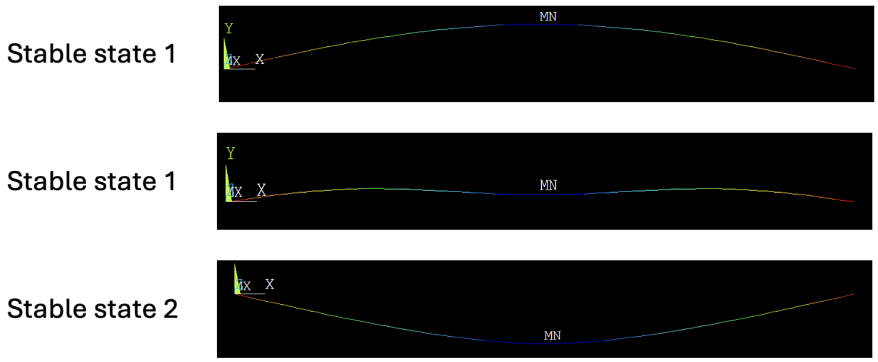

Figure 5: Beam states in simulator

structural states of the simulated beam are illustrated in Fig. 5.

In the simulation, a curved aluminum beam is analyzed to investigate the snapping mechanism as load is gradually applied. For a bistable curved beam, stable equilibria are identified by tracing the load–displacement curve. By incrementally applying displacement at the beam's midpoint and recording the corresponding reaction load, the curve reveals two distinct branches, each representing a stable equilibrium configuration. The sudden snap-through transition between these branches indicates an unstable region. Throughout this process, the maximum and minimum forces $(\max_{d\in\mathcal{D}} f_d(X), \min_{d\in\mathcal{D}} f_d(X))$, as well as the associated displacement values, are captured. These results provide critical insights into the beam's nonlinear response and its bistable characteristics.

Similar to the simulation study, BO is implemented with a GP surrogate model using a Matern kernel. The EI criterion serves as the acquisition function. For comparison, grid search and random search with 100 evaluations each are included as benchmarks. The optimization results are presented in Fig. 6.

As shown in the figure, BO converges to the optimal design with the fewest evaluations. In contrast, both grid search and random search fail to identify an appropriate design that maximizes the force difference, even when a larger number of evaluations are performed. This highlights BO's efficiency and adaptivity in exploring complex design spaces where evaluations are expensive.

5 Conclusion

This study presented a GP–EI Bayesian optimization (BO) framework for pre-manufacturing design of AM-compatible, multistable structures. BO efficiently targets informative designs, reducing the number of expensive evaluations needed compared with grid and random

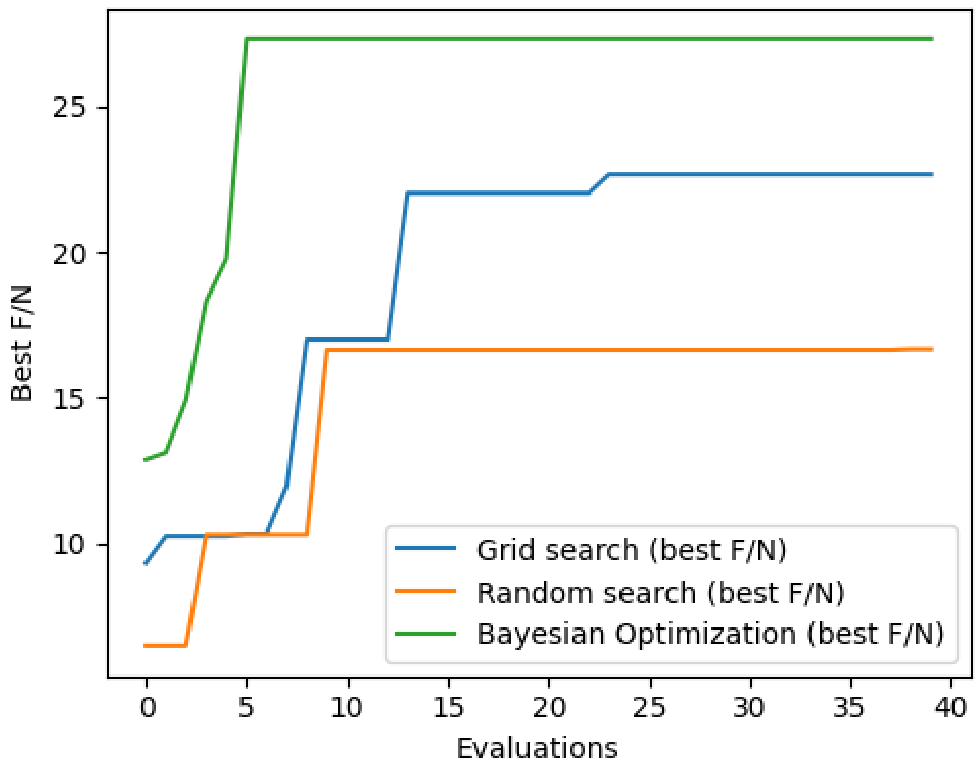

Figure 6: Convergence of Best Observations (Bayesian Optimization vs. Grid search vs. Random search) for Bistable structure experiments

search. In both simulation and case studies, BO identified the optimum with far fewer evaluations than existing methods. The approach naturally accommodates configuration-dependent objectives and robustness constraints. Limitations include scalability to high-dimensional spaces and challenging acquisition maximization. Future work will explore multi-objective/constrained BO, batch evaluations, and physics-informed kernels to further improve reliability and speed.

6 Acknowledgment

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