Constraint Active Search for Experimental Design

Bolong Cheng, Gustavo Malkomes, Michael McCourt

Simulation and Optimization

Using numerical simulation to study the impact of design decisions prior to manufacturing has become a common strategy to reduce the cost of finding an effective design. We often work in the following settings.

- Multiple competing objective metrics
- Limited compute resources/time-consuming computation

Idea: Bayesian optimization (BO) is a sample efficient algorithm for effectively searching the optimal design parameters, especially under compute/time restrictions.

Limitation: Results from Bayesian optimization often lack interpretability, unable to provide any insight of the varying designs on the resulting metrics. This prevents wider adoption of BO in engineering applications.

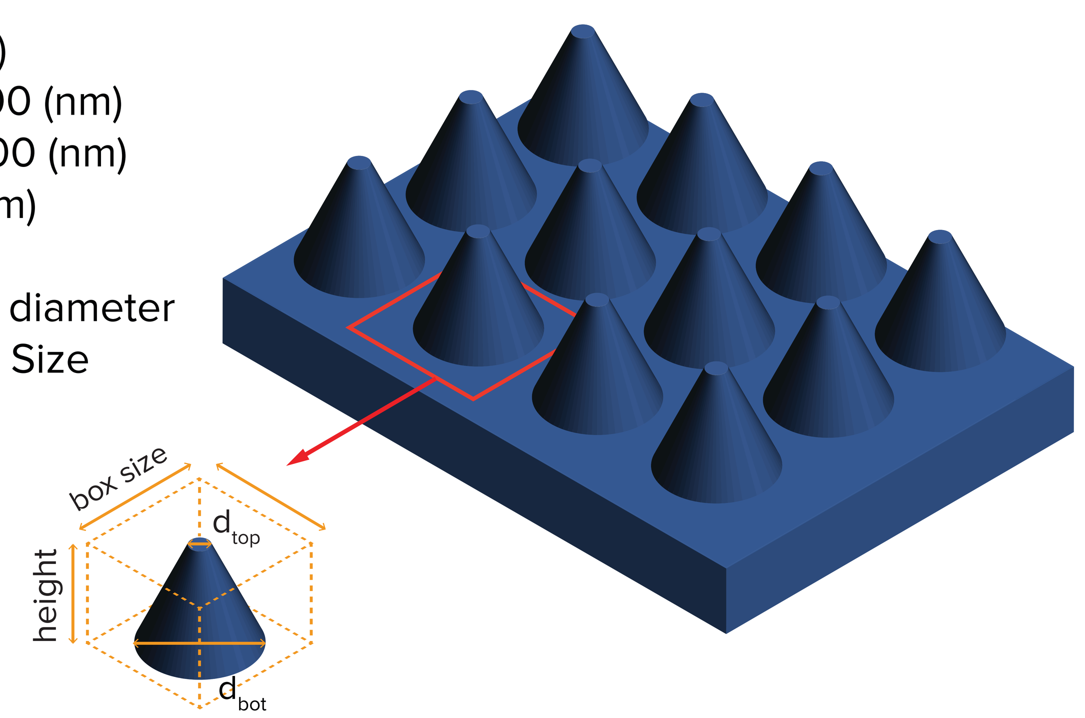
Example: Nanofabrication

We want to fabricate an omnidirectional antireflective glass surface. In particular, we are searching for the Pareto optimal design choices that minimize reflectance at two angles of incidence.

$$\min_{\mathbf{x}\in\mathcal{X}} R_{\text{normal}}(\mathbf{x}), \min_{\mathbf{x}\in\mathcal{X}} R_{\text{oblique}}(\mathbf{x})$$

Height: 1 - 800 (nm)
Bot diameter: 1 - 400 (nm)
Top diameter: 1 - 400 (nm)
Box size: 1 - 400 (nm)

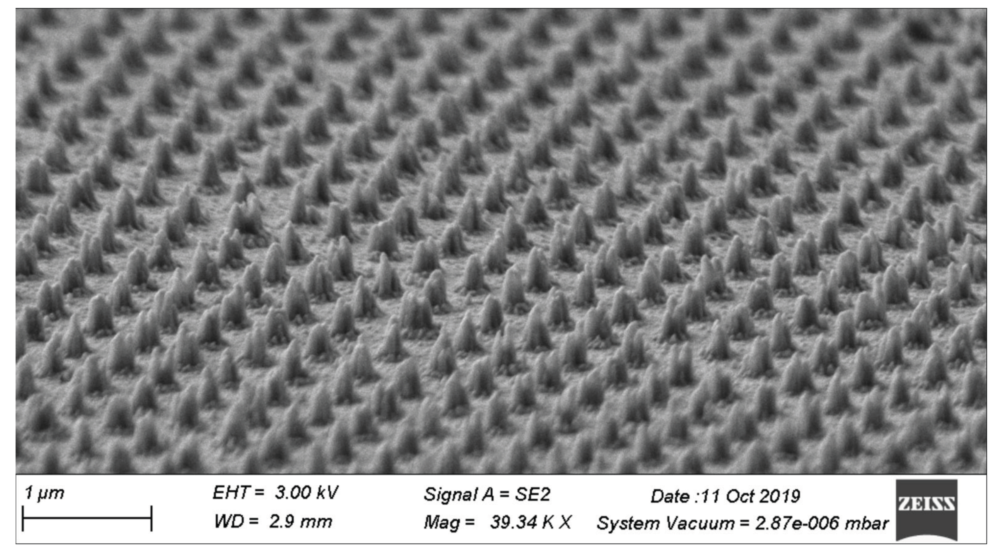
Bot diameter ≥ Top diameter
Bot diameter ≤ Box Size



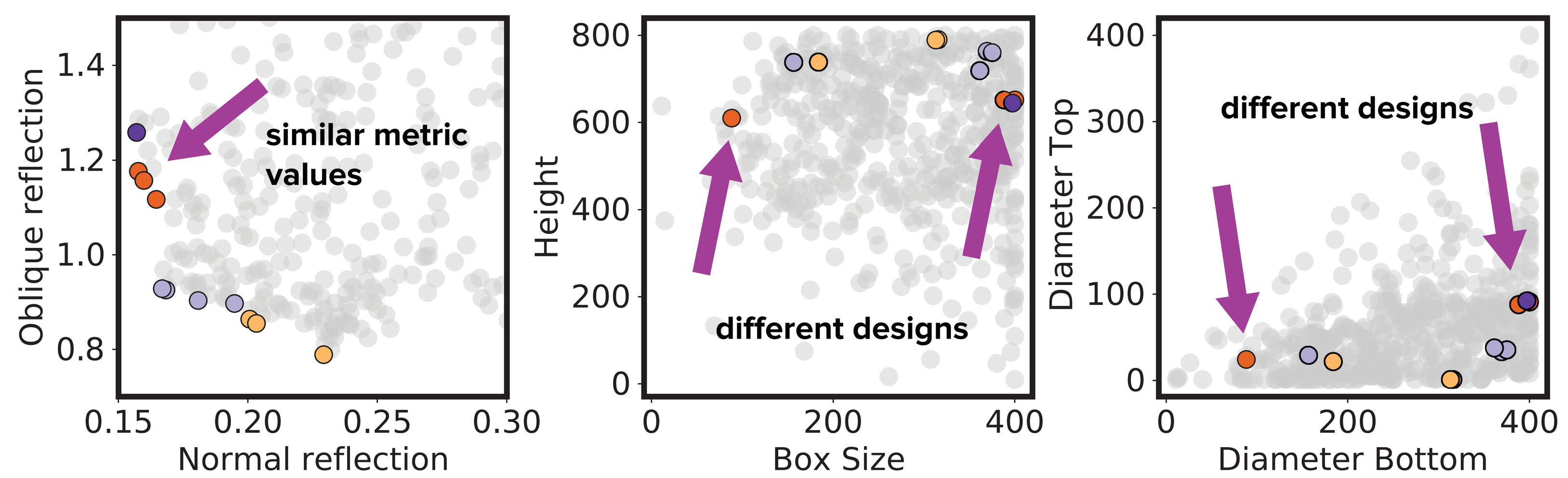
Sajad Haghanifar, Michael McCourt, Bolong Cheng, Jeffrey Wuenschell, Paul Ohodnicki, and Paul Leu. Discovering high-performance broadband and broad angle antireflection surfaces by machine learning. Optica, 7(7), 2020.
Shali Jiang, Gustavo Malkomes, Geoff Converse, Alyssa Shofner, Benjamin Moseley, Roman Garnett. Efficient nonmyopic active search. Proceedings of the 34th International Conference on Machine Learning, PMLR 70:1714-1723, 2017.

Shortcoming of Optimization

The fabrication outcome does not exactly match the simulation due to limited precision of the equipment. Even if we knew the true Pareto frontier during simulation, the manufactured result would not be optimal.



Problem: Small differences in the *metric space* can be associated with drastically different designs in *parameter space*.

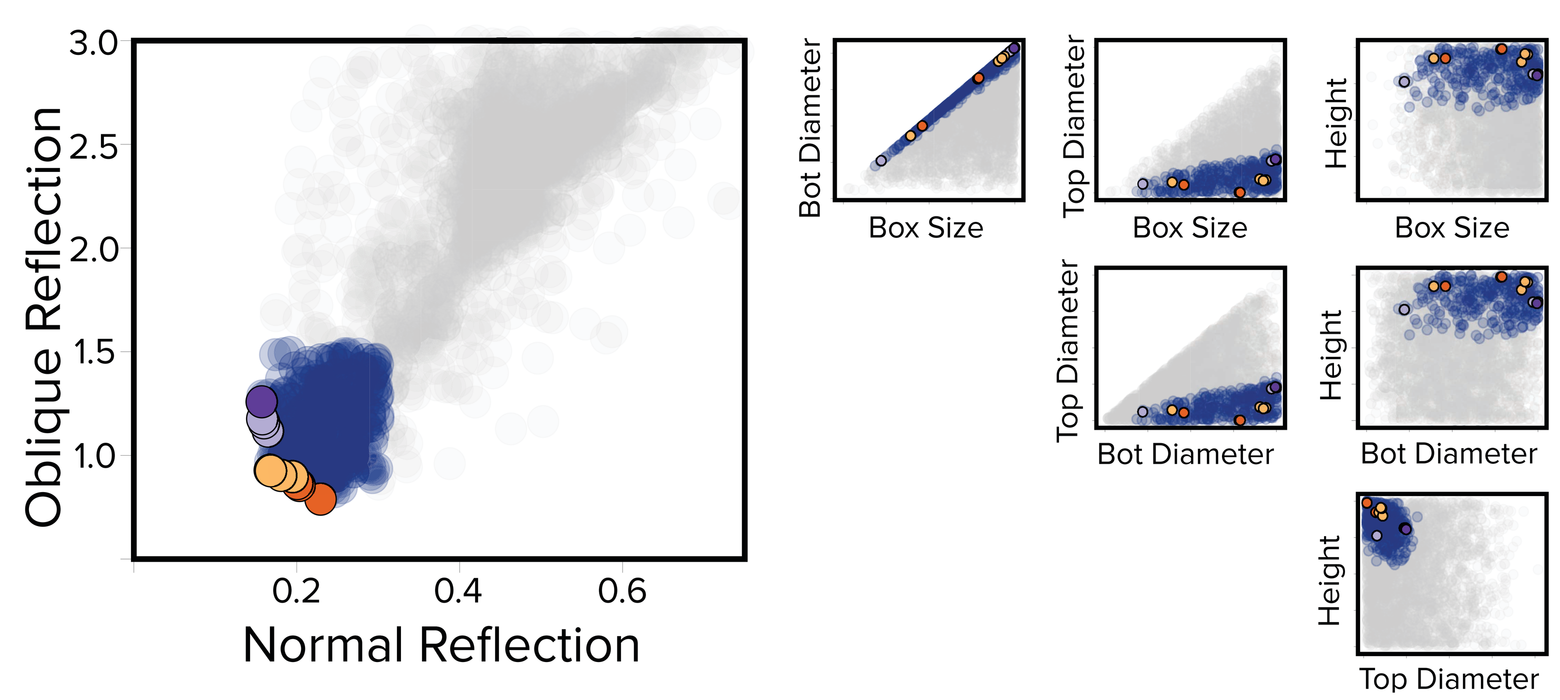


Opportunity: Address the problem in the parameter space.

Alternative to the Pareto Frontier

We propose constraint search as an alternative to multiobjective optimization for finding effective designs. We solicit constraints for each metric of interest; these serve as minimum performance thresholds.

$$\text{Find } : \{\mathbf{x} : R_{\text{normal}}(\mathbf{x}) \leq \tau_{\text{normal}}, R_{\text{oblique}}(\mathbf{x}) \leq \tau_{\text{oblique}}\}$$



Constraint Active Search

We prefer the constraint search formulation for the following reasons.

- An efficient constraint search would find more actionable design information for the actual manufacturing, to account for limitations in the fabrication process.
- The use of constraints on objectives as performance thresholds naturally fits into engineering applications. These thresholds are interpretable, even by people not involved in the design process.
- Noise distribution of a design objective is not required *a priori*, unlike a robust optimization formulation where the noise distribution should be explicitly defined.
- An efficient constraint search runs independently of the number of objectives, unlike a multiobjective optimization which becomes more difficult as the number of objectives grows.

Related Works and Open Challenges

Our proposed constraint search fomulation shares elements with strategies from numerous fields.

- **Multiobjective optimization**, but we are interested in more than maximizing the hypervolume.
- **Robust optimization**, but we also want to reveal the structure of input space of desirable outcomes

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- **Active search**, but we also want to explore the constraint-satisfying parameter space rather than simply maximizing the number of positive outcomes.

Open Challenges

- Reducing the required number of design evaluations. The figures above are the result of 10,000 design evaluations, which is impractical when using actual simulation (rather than a surrogate model).
- Designing a utility function that can quantify the desire to effectively explore the constraint-satisfying region of the design space.

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