

CONDITIONAL FLOW MATCHING FOR ML-BASED INVERSE DESIGN PROBLEMS

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Abstract

Engineering design optimization problems such as structural and thermal topology optimization often rely on iterative solvers that can be computationally expensive. Machine learning-based inverse design methods provide an alternative approach by learning to generate optimal or near-optimal designs. With recent progress in generative models, several studies have explored their use for engineering design generation.

In this work, we study conditional flow matching as a generative model for engineering inverse design and compare it with two commonly used approaches: conditional diffusion models and conditional generative adversarial networks (cGANs). The models are trained on datasets generated using EngiBench, an engineering design platform that provides standardized benchmark problems and datasets. We evaluate the models on three benchmark problems: the Beam2D structural compliance problem, which focuses on designing structures that minimize compliance under given loads and boundary conditions; the HeatConduction2D problem, which aims to optimize material distribution for efficient heat conduction under prescribed thermal boundary conditions; and a photonics problem that seeks structures with desired electromagnetic responses.

The flow-matching and diffusion models share a similar conditional U-Net-style backbone that maps engineering conditions to image-like design fields, while the cGAN baseline provides an adversarial alternative with a different training and sampling paradigm. Each model generates designs conditioned on the problem boundary conditions.

We evaluate the generated designs using both standard computer science metrics and physics-based performance objectives. In addition, we compare the models in terms of training data requirements, generation cost, and training stability. Our results highlight practical trade-offs between these generative modeling approaches for engineering design tasks, providing insights into how diffusion, adversarial, and flow-based generative models behave in physics-driven design problems.