ABSTRACT

Title of Dissertation: ANALYZING INVERSE DESIGN PROBLEMS FROM A TOPOLOGICAL PERSPECTIVE

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Inverse design (ID) problems are inverse problems that aim to rapidly retrieve the subset of valid designs having the desired performances and properties under the given conditions. In practice, this can be solved by training generative models to approximate and sample the posterior distributions of designs. However, little has been done to understand their mechanisms and limitations from a theoretical perspective. This dissertation leverages theoretical tools from general and differential topology to answer these three questions of inverse design: what does a set of valid designs look like? How helpful are the data-driven generative models for retrieving the desired designs from this set? What topological properties affect the subset of desired designs?

The dissertation proceeds by dismantling inverse (design) problems into two major subjects: that is, the representing and probing of a given set of valid designs (or data), and the retrieval of the desired designs (or data) from this given set. It draws inspiration from topology and geometry to investigate them and makes the main contributions below:

1. Chapter 3 details a novel representation learning method called *Least Volume*, which has properties similar to nonlinear PCA for representing datasets. It can minimize the representation's dimension automatically and, as shown in Chapter 4, conducts contrastive learning when applied to labeled datasets.

2. Two conditional generative models are developed to generate performant 2-D airfoils and 3-D heat sinks in Chapter 5 and 6 respectively. They can produce realistic designs to warm-start further optimization, with the relevant chapters detailing their acceleration effects.

3. Lastly, Chapter 7 describes how to use Least volume to solve high-dimensional inverse problems efficiently. Specifically, using examples from physic system identification, the chapter uncovers the correlation between the inverse problem's uncertainty and its intrinsic dimensions.