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A density-matching approach for optimization under uncertainty

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Abstract

Modern computers enable methods for design optimization that account for uncertainty in the system—so-called *optimization under uncertainty* (OUU). We propose a metric for OUU that measures the distance between a designer-specified probability density function of the system response (the *target*) and the system response's density function at a given design. We study an OUU formulation that minimizes this distance metric over all designs. We discretize the objective function with numerical quadrature, and we approximate the response density function with a Gaussian kernel density estimate. We offer heuristics for addressing issues that arise in this formulation, and we apply the approach to a CFD-based airfoil shape optimization problem. We qualitatively compare the density-matching approach to a multi-objective robust design optimization to gain insight into the method.

Keywords: Optimization under uncertainty; Design under uncertainty; Density-matching

1. Introduction

Modern computing power enables industrial-scale design optimization with high-fidelity numerical simulations of physical systems. Simulation-based design is found in aircraft [1], engine [2], automotive [3] and shipping [4] industries, among many others. To optimize, designers must precisely specify operating scenarios and manufactured production. Off-design operation and manufacturing tolerances are typically incorporated afterward. A more complete perspective on design optimization accounts for these uncertainties, e.g., by employing statistical performance metrics within the design optimization. This perspective leads to *optimization under uncertainty* (OUU).

The computational engineering literature is chock full of formulations and approaches for OUU. Allen and Maute [5] give an excellent overview that broadly categorizes these formulations as either *robust design optimization* (RBO) or *reliability-based design optimization* (RBDO). The essential idea behind RBO formulations is to

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simultaneously maximize a statistical measure of the system performance (e.g., the mean) while minimizing a statistical measure of system variability (e.g., the variance), thus improving robustness to variability in operating conditions. The optimization is often formulated with multiple objective functions (e.g., maximize mean and minimize variance), which leads to a Pareto front of solutions representing a trade-off between robustness and performance. Alternative formulations treat performance as the objective function and robustness as a constraint or vice versa. Some applications of RBO include the design of Formula One brake ducts [6], compressor blades [7], compression systems [8], airfoils [9], and structures [10]. The RBDO formulations seek designs that satisfy reliability criteria, such as maintaining a sufficiently small probability of failure, while minimizing a cost function of the design [11]. Estimating the failure probabilities within the optimization with randomized methods (e.g., Monte Carlo) can be prohibitively expensive for large-scale models; several methods exist for approximating regions of low failure probability [12]. Engineering examples of RBDO include transonic compressors [13], aeroelasticity [14], structures [5], and vehicle crash worthiness [15].

The statistical measures in the RDO and RBDO objective functions and constraints are typically low-order moments – e.g., mean and variance – or probabilities associated with the system response. The chosen statistical measures affect the optimal design, so they must be chosen carefully for each specific application.

In this paper, we propose an alternative OUU formulation. We assume the designer has described the desired system performance as a probability density function (pdf), which we call the *target pdf*, and we seek to minimize the distance between the design-dependent system response pdf and the target pdf. In other words, all criteria on the stochastic system's moments or failure probabilities are encoded in the target pdf. Mathematically, we treat the target pdf as given; it is not a tunable parameter. In any real-world scenario, this pass-the-buck attitude places tremendous responsibility on the designer to devise the perfect target pdf. We expect that a practical methodology including the proposed statistical measure will involve some back and forth between designer and optimizer to devise the most appropriate target pdf. Using a designer-specified response pdf has some precedent in the OUU literature. Rangavajhala and Mahadevan [16] assume a designer-specified pdf in their *optimum threshold design*, which finds thresholds that satisfy the given joint probability while allowing for preferences among multiple objectives.

Compared to other OUU formulations, density-matching is appropriate when the designer is able to specify her desiderata for the uncertain response as a pdf. The density-matching approach finds the design that best matches the designer's specified pdf, and there is no need to estimate the Pareto front of a multi-objective optimization (as in RDO) or minimize a failure probability (as in RBDO). Tolerated variability and failures are encoded in the target pdf.

We present a single-objective OUU formulation where the distance between target and response pdfs is the objective function. We explore some interesting properties of this optimization problem, namely how the objective's gradient behaves when the two pdfs are not sufficiently large on the same support (Section 2). We propose a consistent discretization of the objective function – based on numerical quadrature and kernel density estimation – that produces a continuous approximation well-suited for gradient-based optimization (Section 3). Our prior work uses histograms to approximate the response pdf, which leads to a less scalable optimization problem with integer variables [17]. There are some drawbacks to the density-matching formulation; we offer heuristics for addressing these drawbacks in Section 4. In Section 5, we test the formulation on an algebraic test problem and a shape optimization problem with the NACA0012 airfoil. In the latter case, we qualitatively compare the optimal designs to those generated by a multi-objective RDO strategy.

2. Mathematical formulation

Consider a function $f = f(s, \omega)$ that represents the response of a physical model with design variables $s \in \mathcal{S} \subseteq \mathbb{R}^n$ and random variables $\omega \in \Omega \subseteq \mathbb{R}^m$; the random variables represent the uncertainty in the physical system. The space $\mathcal{S}$ encodes the application-specific constraints on the design variables, e.g., bounds or linear inequality constraints. We assume that ω are defined on a probability space with sample space Ω and probability density function $p = p(\omega)$, which encode all available knowledge about the system's uncertainties.[1] We assume that f is scalar-valued, $f \in \mathcal{F} \subseteq \mathbb{R}$, and continuous in both s and ω. For a fixed $s \in \mathcal{S}$, let $q_s : \mathcal{F} \to \mathbb{R}_+$ be a probability density function of

[1] The final results depend on Ω and $p(\omega)$. If multiple probability density functions are consistent with the available information, then one should check the sensitivity of the results to perturbations in these quantities.