An Efficient Randomized Approximation Algorithm for Volume Estimation and Design Centering

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1 Motivation

Design centering is a long-standing and central problem in systems engineering and model inference. It is concerned with determining design parameters of a system or model that guarantee operation within given specifications and are robust against random variations. While *design optimization* aims to determine the design that *best* fulfills (one aspect of) the specifications, *design centering* wants to find the design that meets the specifications most *robustly*. Traditionally, this problem has been considered in electronic circuit engineering [10], where a typical task is to determine the nominal values of electronic components (e.g., resistances, capacitances, etc.) such that the circuit fulfills some specifications and is robust against manufacturing tolerances in the components. Examples of specifications in electronic circuits are frequency response, harmonic distortion, energy consumption, and manufacturing cost. Recently, related ideas have also entered the field of synthetic biology with the aim of robustly designing novel synthetic biological circuits [3, 32]. Any criterion that can be verified for a given design can be used as a specification.

In order to be robust against perturbations, the specifications cannot be defined too narrowly. This implies that there are usually many designs that fulfill the specifications. The size or volume of the set of all these *feasible* designs is an intuitive measure for the robustness with which the specifications can be fulfilled. Robustness is therefore related to the probability that the design still fulfills the same specifications when the design parameters randomly vary, or the specifications fluctuate. Quantifying this robustness requires estimating the size or volume of the set of all feasible designs.

Volume estimation and design centering in the most general form only assume that a given design can be evaluated through a procedure (referred to as "oracle" [11]) that checks whether the design fulfills the specifications, or not. In this general setting, design centering and volume estimation are hard problems. Exhaustively determining the set of all feasible designs requires exponentially many design trials in the number of design parameters. Since typical systems or circuits have tens to hundreds of design parameters, testing all possible combinations is prohibitive. It is hence intuitive that exact solutions to design centering are NP-hard [20], i.e., they cannot be efficiently determined on a deterministic computer. Less intuitively, it is also NP-hard to determine the exact volume of a high-dimensional set using a deterministic algorithm [2, 15], even if the set is convex. Efficient approaches to design centering and volume estimation are hence always approximate. However, even though volume estimation is closely related to design centering, previous approximate approaches have considered them separately.

2 Prior work

We therefore separately review previous approaches to design centering and volume approximation.

2.1 Previous approaches to design centering

Previous approaches to design centering can be classified into geometrical and statistical approaches [21]. Geometrical approaches use simple geometric bodies to approximate the feasible region, which is usually assumed to be convex [22]. Examples of geometrical approaches include Simplical Approximation [7, 28], which approximates the boundary of the feasible region by adaptation of a convex polytope. Due to the curse of dimensionality, however, Simplical Approximation becomes unpractical in dimensions $n > 8$ [24, 14]. Suggested improvements to relax the convexity requirement instead assume differentiability of the specifications [29], which cannot be guaranteed in black-box problems. Another example of a geometrical approach is Ellipsoidal Approximation [1], which finds the ellipsoid of largest volume that still completely fits into the feasible region. All endpoints of the ellipsoidal axes and the center of the ellipsoid need to be feasible. While Ellipsoidal Approximation does not strictly require convexity of the feasible region, its approximation properties strongly depend on it. A third example of a geometrical approach is the polytope method [21], which also uses a convex polytope to approximate the feasible region, but then finds the design center by either inscribing the largest Hessian ellipsoid or by using a convex programming approach. The latter approach, however, requires an explicit probabilistic model of the variations in the design parameters, which is usually not available in practice.

Statistical approaches approximate the feasible region by Monte Carlo sampling. Since exhaustive sampling is not feasible in high dimensions, the key ingredient of statistical methods is to find a smart sampling proposal, and concentrate on informative regions. The methods then sample points from this proposal and evaluate the specifications for these points to decide if they are feasible. The ratio of feasible to infeasible points sampled then provides information about the robustness of a design [12]. Constraint adaptation by Differential Evolution (CADE) [25] is a classical statistical design centering method based on Differential Evolution [26]. It assumes the feasible region to be convex and starts from a population of initial points. To find those points, the specifications (constraints) are first relaxed and then tightened successively back to the original ones. After the original specifications are met, the mean of all points (which have to be feasible) is used as an approximation of the design center. Another representative statistical approach is the Advanced First-Order Second Moment (AFOSM) method [23]. It samples candidate points from L_p-balls in order to estimate the yield (i.e., the ratio of feasible to infeasible points) and approximate the feasible region. Which L_p-norm to use is directly related to the assumed statistical distribution of the random perturbations. The proposal L_p-balls are adapted to maximize their volume while still being completely contained within the feasible region. This therefore does not allow estimating the total volume of the feasible region. A third example of a statistical method is the Center of Gravity Method [24]. In each iteration, it computes the center of gravity of the feasible samples and of the infeasible samples. The design center is then moved toward the center of the feasible points and away from the center of the infeasible ones. The Momentum-Based Center of Gravity Method [27] extends this idea to include information from the past *two* iterations.

2.2 Previous approaches to volume estimation

Volume computation is an important problem in many areas, e.g. software engineering, computer graphics, economics, and statistics [19]. Deterministic methods for volume computation of convex polytopes use for example triangular methods or signed decomposition methods [5]. The former decompose the polytope into simplices whose volumes are easily computed and summed [5]. The latter decompose the polytope into signed simplices such that the signed sum of their volumes is the volume of the polytope [5]. However, it has been shown that deterministically computing the volume is NP-hard [9, 16, 15], even for convex bodies.

Using a randomized algorithm, the volume of a convex body can be approximated to arbitrary precision in polynomial time [8]. Over the years, Dyer, Frieze, and Kannan's breakthrough-algorithm (with a theoretical complexity of $\mathcal{O}^\star(n^{23})$ oracle calls) has been improved in a sequence of papers until Lovasz and Vempala's $\mathcal{O}^\star(n^4)$-algorithm[1].

3 Problem statement

We consider the design (or parameter) space to be $\mathbb{R}^n$, i.e., the n-dimensional vector space of real numbers. The region (subspace) of the parameter space that contains all parameter vectors for which the system meets or exceeds the specifications is called the *feasible region* $A \subset \mathbb{R}^n$. We denote the total volume of the feasible region by $\mathrm{vol}(A)$, defined as the integral of the uniform density

[1]the asterisk in the order notation indicates that logarithmic factors in n are omitted

over A. This volume is a natural measure for the total amount of feasible designs available and can be used to compare and choose between different designs or competing models [13]. Moreover, the overall shape and orientation of the feasible region contains information about correlations between design parameters, which can be exploited for model reduction and to guide experimental verification of a design.

Depending on the available side-information about the design specifications, different operational definitions of the *design center* $\mathbf{m} \in A$ exist, including the *nominal design center*, the *worst-case design center*, and the *process design center* [23]. For instance, in the example of manufacturing an electronic circuit from components with known manufacturing tolerances, the design center maximizes the production yield. Here, we follow the general statistical definition of the design center [18] and seek among all points (parameter vector) $\mathbf{x} \in A$ the design center $\mathbf{m} \in A$ that represents the mean of a probability distribution $q(\mathbf{x})$ of maximal volume covering the feasible region A with a given *target hitting probability* P. For convex feasible regions, using the uniform probability distribution over A and $P = 1$, the design center coincides with the geometric center of the feasible region, which historically inspired the terminology.

When encountering a new problem one usually has no knowledge of the shape of its feasible region and wants to estimate different properties of it. If we know that the region is convex, good methods for both design centering and volume approximations are known. In real-world problems, however, we usually cannot guarantee convexity of the feasible region, but still want to get approximations for its design center or its volume. For this, a more general framework is needed that does not make any assumptions about the feasible region and can ideally be used for a broad range of applications.

4 Contribution

Here, we jointly consider the problems of design centering and volume estimation in their most general form. We present an approximate statistical method that unites the two problems under the same framework. We also present an efficient computational algorithm, called L_p-Adaptation, for practical application of this new framework. Our contribution is hence twofold: a conceptual framework that unites design centering and robustness estimation, and a computationally efficient randomized approximation algorithm for it.

The proposed conceptual framework exposes several links and trade-offs between design centering and volume estimation. It is inspired by the observation that robust designs are a hallmark of biological systems, such as cell signaling networks, blood vasculature networks, and food chains [17]. Biological systems have to be robust against fluctuations, as otherwise they would likely not survive in a changing environment. It has been observed that the robustness of biological networks is related to the volume of the set of feasible parameters [6, 30]. This is the same definition of robustness we use for engineering systems. Nature has hence found a way of approximating both design centering and volume estimation through self-organization and natural selection. This succession of design alteration and design selection is akin to bio-inspired optimization algorithms, such as evolution strategies [4] and genetic algorithms [31], with the important difference that not optimization is the goal, but design centering and volume estimation. In our framework, design selection is hence done by checking whether the specifications are fulfilled. Feasible designs then undergo random alterations with the specific aim of exploring the space of all feasible designs as broadly and efficiently as possible.

Efficient and broad exploration of feasible designs is the core of the L_p-Adaptation algorithm. Following the biological inspiration, the algorithm is based on stochastic sampling of designs together with a consistent way of converting the explored samples to an estimate of the robustness and the design center. L_p-Adaptation is computationally efficient, reaching or outperforming the previous state of the art, as we show in this thesis. Most importantly, however, L_p-Adaptation is based on the joint consideration of the two problems and therefore relaxes the limiting assumptions previous approaches needed to make about either the convexity or smoothness of the set of feasible designs, or the correlations between parameters. L_p-Adaptation provides the first computationally efficient and versatile method for approximately solving general, oracle-based and non-convex design centering and volume estimation problems.

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