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# Generation and application of multivariate polynomial quadrature rules

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**Abstract**

The search for multivariate quadrature rules of minimal size with a specified polynomial accuracy has been the topic of many years of research. Finding such a rule allows accurate integration of moments, which play a central role in many aspects of scientific computing with complex models. The contribution of this paper is twofold. First, we provide novel mathematical analysis of the polynomial quadrature problem that provides a lower bound for the minimal possible number of nodes in a polynomial rule with specified accuracy. We give concrete but simplistic multivariate examples where a minimal quadrature rule can be designed that achieves this lower bound, along with situations that showcase when it is not possible to achieve this lower bound. Our second contribution is the formulation of an algorithm that is able to efficiently generate multivariate quadrature rules with positive weights on non-tensorial domains. Our tests show success of this procedure in up to 20 dimensions. We test our method on applications to dimension reduction and chemical kinetics problems, including comparisons against popular alternatives such as sparse grids, Monte Carlo and quasi Monte Carlo sequences, and Stroud rules. The quadrature rules computed in this paper outperform these alternatives in almost all scenarios.


*Keywords:* Multivariate integration; Moment-matching quadrature; Uncertainty quantification; Dimension reduction; Bayesian inference

## 1. Introduction

Let $D \subset \mathbb{R}^d$ be a domain with nonempty interior. Given a finite, positive measure $\mu$ on $D$ and a $\mu$-measurable function $f : D \to \mathbb{R}$, our main goal is computation of

$$\int_D f(x)\mathrm{d}\mu(x)$$

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The need to evaluate such integrals arise in many areas, including finance, stochastic programming, robust design and uncertainty quantification. Typically these integrals are approximated numerically by quadrature rules of the form

$$\int_D f(x)\mathrm{d}\mu(x) \approx \sum_{m=1}^{M} w_m f(x_m) \tag{1}$$

Examples of common quadrature rules for high-dimensional integration are Monte Carlo and quasi Monte Carlo methods [1–4], and Smolyak integration rules [5–7]. Quadrature rules are typically designed and constructed in deference to some notion of approximation optimality. The particular approximation optimality that we seek in this paper is based on polynomial approximation.

Our goal is to find a set of quadrature nodes $x_j \in D$, $j = 1, \ldots, M$, and a corresponding set of weights $w_j \in \mathbb{R}$ such that

$$\sum_{j=1}^{M} w_j p\left(x_j\right) = \int_D p(x)\mathrm{d}\mu(x), \qquad p \in P_\Lambda, \tag{2}$$

where $\Lambda \subset \mathbb{N}_0^d$ is a multi-index set of size $N$, and $P_\Lambda$ is an $N$-dimensional polynomial space defined by $\Lambda$. (We make this precise later.) $P_\Lambda$ can be a relatively "standard" space, such as the space of all $d$-variate polynomials up to a given finite degree, or more exotic spaces such as those defined by $\ell^p$ balls in index space, or hyperbolic cross spaces.

In this paper we will present a method for numerically generating polynomial based cubature rules. This paper provides two major contributions to the existing literature. Firstly we provide a lower bound on the number points that make up a polynomial quadrature rule satisfying (2). Our analysis is straightforward, but to the authors knowledge this is the first reported bound of its kind. Our second contribution is a numerical method for generating quadrature rules that are exact for a set of arbitrary polynomial moments. Our method has the following features:

- Positive quadrature rules are generated. (I.e., $w_m > 0$ for all $m$.)
- The algorithm applies to any measure $\mu$ for which moments are computable. Many existing quadrature methods only apply to tensor-product measures; for non-tensorial integrals this requires construction of mappings to transform integrals over non-tensorial domains to integrals over tensorial domains. Our method can construct quadrature rules for measures with, for example, non-linear dependence between variables, without the use of mappings or transformations.
- Analytical or sample-based moments may be used. In some settings it may be possible to compute moments of a measure exactly, but in other settings only samples from the measure are available. For example, one may wish to integrate a function using Markov Chain Monte Carlo-generated samples from a posterior of a Bayesian inference problem.
- A quadrature that is faithful to arbitrary sets of moments may be generated. Many quadrature methods are exact for certain polynomial spaces, for example total-degree or sparse grid spaces. However, some functions may be more accurately represented by alternative polynomial spaces, such as hyperbolic cross spaces. In these situations it may be more prudent to construct rules that can match a customized set of moments.
- Efficient integration of ridge functions is possible. Some high-dimensional functions can be represented by a small number of linear combinations of the input variables. In this case it is more efficient to integrate these functions over this lower-dimensional coordinate space. Such a dimension-reducing transformation typically induces a new measure on a non-tensorial space of lower-dimensional variables. For example, a high-dimensional uniform probability measure on a hypercube may be transformed into a non-uniform measure on a zonotope (a multivariate polygon).

Our algorithm falls into the class of moment-matching methods. There have been some recent attempts at generating quadrature using moment matching via optimization approaches. These methods frequently either start with a small candidate set and add points until moments are matched [8], or start with a large set of candidate points and reduce them until no more points can be removed without numerically violating the moment conditions [9–11]. These approaches sometimes go by other names, such as scenario generation or scenario reduction methods. Our numerical strategy is novel and our results show that it is rather effective, but we do not ameliorate persistent bottlenecks in computing multivariate quadrature rules: The difficulty of computing high-degree quadrature rules scales commensurately with the dimension of the polynomial space, and this dimension can generally grow