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A New Quasi-Monte Carlo Technique Based on Nonnegative Least Squares and Approximate Fekete Points

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Abstract. The computation of integrals in higher dimensions and on general domains, when no explicit cubature rules are known, can be "easily" addressed by means of the quasi-Monte Carlo method. The method, simple in its formulation, becomes computationally inefficient when the space dimension is growing and the integration domain is particularly complex. In this paper we present two new approaches to the quasi-Monte Carlo method for cubature based on *nonnegative least squares* and *approximate Fekete points*. The main idea is to use less points and especially *good points* for solving the system of the moments. *Good points* are here intended as points with good interpolation properties, due to the strict connection between interpolation and cubature. Numerical experiments show that, in average, just a tenth of the points should be used mantaining the same approximation order of the quasi-Monte Carlo method. The method has been satisfactory applied to 2 and 3-dimensional problems on quite complex domains.

AMS subject classifications: 11K45, 41A45, 65D30, 65D32
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1. Introduction

Consider the problem of calculating the integral

$$I(f) = \int_\Omega f(x)dx, \quad \Omega \subset \mathbb{R}^d.$$

We know that if $\lambda_d(\Omega) < \infty$ (the d dimensional Lebesgue measure of Ω) we can turn Ω into a probability space with probability measure

$$\mathrm{d}\mu(x) = \frac{1}{\lambda_d(\Omega)}\mathrm{d}x.$$

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Then for $f \in L^1(\mu)$ we have

$$I(f) = \int_\Omega f(x)\mathrm{d}x = \lambda_d(\Omega) \int_\Omega f \mathrm{d}\mu(x) = \lambda_d(\Omega) E(f),$$

where $E(f)$ is the expected value of f.

The *Monte Carlo* (MC) method for numerical integration is obtained by taking N independent μ-distributed random samples $x_1, \ldots, x_N \in \Omega$ and, then approximating the integral as follows

$$I(f) \approx \lambda_d(\Omega) \frac{1}{N} \sum_{i=1}^{N} f(x_i) = I_N(f). \tag{1.1}$$

For the strong law of large numbers, as $N \to \infty$ we then know that the r.h.s. in (1.1) converges in the Lebesgue measure to the value of the integral.

Differently to the classical Monte Carlo method or Monte Carlo integration, which is based on sequences of pseudo-random numbers, a *quasi-Monte Carlo* (qMC) method is a method for numerical integration that uses the so-called *low-discrepancy sequences* (also known as *quasi-random sequences* or sub-random sequences). Well known low discrepancy sequences are *Halton* (also known as *Van de Corput-Halton*), *Hammersley* and the so-called (t, s)-sequences, such as the *Sobol* sequence. For the definition and properties of all these sequences we invite interested readers to refer to the book [15].

When dealing with a (quasi-)Monte Carlo method of integration we need to find a large number N of points in order to approximate the value of the integral. This means a lot of flops and storage, which become unpractical when the space dimension d grows. How can we avoid this?

In the paper we propose two techniques aimed to reduce the number of quasi-random nodes, while still keeping the same accuracy of the quasi-Monte Carlo approach. The new approaches are *"compressed cubature"* that we then apply to quite general domains in space dimensions $d = 2, 3$.

In the next section we introduce some useful results on low-discrepancy sequences and their use in cubature, then in Section 3 we describe the new approaches based on *nonnegative least squares* (NNLS) and *approximate Fekete points* (AFP). In Section 4 we provide an error analysis for the NNLS case that can be adapted to the case of the AFP when the *measure of stability*, ρ (cf. formula (4.4)), is not too big. In Section 5 we present some numerical tests supporting the validity of our new approaches. We also point out that all the algorithms have been implemented in Matlab for consistency with previous works done by collaborators at the CAA-research group for the construction of cubature formulas on various 2 and 3-dimensional domains (cf. e.g. [27, 30]). To conclude the Introduction, we observe that our approaches can be extended to any space dimension. The reason why we have confined ourselves to $d = 2, 3$ is mainly due to hardware limitations on which the numerical experiments have been performed.