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Computational investigations of scrambled Faure sequences

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Abstract

The Faure sequence is one of the well-known quasi-random sequences used in quasi-Monte Carlo applications. In its original and most basic form, the Faure sequence suffers from correlations between different dimensions. These correlations result in poorly distributed two-dimensional projections. A standard solution to this problem is to use a randomly scrambled version of the Faure sequence. We analyze various scrambling methods and propose a new nonlinear scrambling method, which has similarities with inversive congruential methods for pseudo-random number generation. We demonstrate the usefulness of our scrambling by means of two-dimensional projections and integration problems.

Keywords: Faure sequence; Low-discrepancy sequences; (quasi)-Monte Carlo; Linear scrambling; Nonlinear scrambling

1. Introduction

The term ‘Monte Carlo (MC) method’ is often used to refer to a well-known family of stochastic algorithms and techniques for solving a wide variety of problems. It is well-known that the probabilistic error for these Monte Carlo methods converges as $\mathcal{O}(N^{-1/2})$ if information about regularity (or smoothness) is not used. Here, N is the number of sample points used. So-called ‘quasi-Monte Carlo (qMC) methods’ [21], based on deterministic point-sets or sequences, form an alternative to MC methods and lead to smaller approximation errors in many practical situations. While quasi-random numbers do improve the convergence of applications like numerical integration, it is by no means trivial to provide practical error estimates in qMC due to the fact that the only rigorous error bounds, provided via the Koksma–Hlawka inequality, are very hard to utilize. In fact, the common practice in MC of using a predetermined error criterion as a deterministic termination condition, is almost impossible to achieve in qMC without extra technology. In order to provide such dynamic error estimates for qMC methods, several researchers [27,23] proposed the use of Randomized qMC (RqMC) methods [14], where randomness can be brought to bear on quasi-random sequences through scrambling and other related randomization techniques [30,3]. One can rigorously show [16] that under relatively loose conditions each of the randomized qMC rules are statistically independent and thus can be used to form a traditional MC error estimate using confidence intervals based on the sample variance. The core of randomized qMC is a fast and effective algorithm to randomize (scramble) quasi-random sequences.

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When randomized qMC is used to estimate integration problems, the integration variance can depend strongly on the scrambling methods [24]. Much of the work dealing with scrambling methods has been aimed at ways of linear scrambling methods. In this paper, we take a close look at various scrambling methods and propose a nonlinear scrambling method for Faure sequences which we also compare with the linear scrambling methods. The nonlinear scrambling methods will focus on inversive scrambling. We compare these nonlinear scrambling methods with linear scrambling methods by two-dimensional projections, discrepancy and a set of test-integrals.

The organization of this paper is as follows: in Section 2, a brief introduction to the theory of constructing Faure sequences is given. In Section 3, we give an overview of different scrambling methods and we then introduce a nonlinear scrambling method in Section 4. Properties for the two-dimensional projections of this nonlinear scrambling method are presented in Section 5 and $\mathcal{L}^2$-discrepancy computations are reported in Section 6. Numerical integration results are given in Section 7 and conclusions follow in Section 8.

2. The Faure Sequence

Before we begin our discussion of the various scrambling methods for the Faure sequence, it behooves us to describe in detail the standard and widely accepted methods of Faure sequence generation. We start from the construction of another related "classical" quasi-random sequence, namely the Halton sequence.

2.1. Van der Corput and Halton sequences

Let $b \geq 2$ be an integer and n a non-negative integer with:

$$n = n_m b^m + \cdots + n_1 b + n_0$$

its b-adic representation. Then the nth term of the Van der Corput sequence is

$$\phi_b(\boldsymbol{n}) = \frac{n_0}{b} + \frac{n_1}{b^2} + \cdots + \frac{n_m}{b^m}.$$

Here $\phi_b(\boldsymbol{n})$ is the radical inverse function in base b and $\boldsymbol{n} = (n_0, n_1, \ldots, n_m)^T$ is the digit vector of the b-adic representation of n. The function $\phi_b(\cdot)$ simply reverses the digit expansion of n and places it to the right of the "decimal" point. The Van der Corput sequence in s dimensions, more commonly called the Halton sequence, is one of the most basic quasi-random sequences and its nth point can be written in the following form:

$$\boldsymbol{x}_n = (\phi_{b_1}(\boldsymbol{n}),\ \phi_{b_2}(\boldsymbol{n}), \ldots, \phi_{b_s}(\boldsymbol{n})), \tag{1}$$

where the bases $b_1, b_2, \ldots, b_s$ are pairwise coprime. Note that (1) is a special case of the more general form

$$\boldsymbol{x}_n = (\phi_{b_1}(C^{(1)}\boldsymbol{n}), \phi_{b_2}(C^{(2)}\boldsymbol{n}), \ldots, \phi_{b_s}(C^{(s)}\boldsymbol{n})), \tag{2}$$

where the $C^{(j)}$ are called "generator matrices". For the Halton sequence, each "generator matrix" $C^{(j)}$ for $j = 1, \ldots, s$ is the identity matrix.

2.2. Faure sequences

By cleverly constructing the generator matrices in (2), one can obtain other quasi-random sequences. Faure [7] sets $b_j = b$ for $j = 1, \ldots, s$ and uses powers of the upper triangular Pascal matrix modulo b for the generator matrices. The nth element of the Faure sequence is expressed as

$$\boldsymbol{x}_n = (\phi_b(P^0\boldsymbol{n}), \phi_b(P^1\boldsymbol{n}), \ldots, \phi_b(P^{s-1}\boldsymbol{n})),$$

where b is a prime number greater than or equal to the dimension s and P is the Pascal matrix modulo b whose (i, j)-element is equal to $\begin{pmatrix} j-1 \\ i-1 \end{pmatrix} \bmod b$. The matrix-vector products $P^j\boldsymbol{n}$ for $j = 0, \ldots, s-1$ are done in modulo b arithmetic. Fig. 1 illustrates a disadvantage of the original Faure sequence: the above construction leads to a sequence that has correlations between its individual coordinates. This leads among others to bad two-dimensional projections and also has its consequences when the sequence is used for numerical integration, as will be illustrated in Section 7.