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A low-rank approach to the computation of path integrals

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ABSTRACT

We present a method for solving the reaction–diffusion equation with general potential in free space. It is based on the approximation of the Feynman–Kac formula by a sequence of convolutions on sequentially diminishing grids. For computation of the convolutions we propose a fast algorithm based on the low-rank approximation of the Hankel matrices. The algorithm has complexity of $\mathcal{O}(nrM\log M + nr^2M)$ flops and requires $\mathcal{O}(Mr)$ floating-point numbers in memory, where n is the dimension of the integral, $r \ll n$, and M is the mesh size in one dimension. The presented technique can be generalized to the higher-order diffusion processes.

1. Introduction

Path integrals [1–3] play a dominant role in description of a wide range of problems in physics and mathematics. They are a universal and powerful tool for condensed matter and high-energy physics, theory of stochastic processes and parabolic differential equations, financial mathematics, quantum chemistry and many others. Different theoretical and numerical approaches have been developed for their computation, such as the perturbation theory [4], the stationary phase approximation [5,6], the functional renormalization group [7,8], various Monte Carlo [9] and sparse grids methods [10,11]. The interested reader can find particular details in the original reviews and books [12–14].

In this paper we focus on the one-dimensional reaction–diffusion equation with initial distribution $f(x) : \mathbb{R} \to \mathbb{R}^+$ and a constant diffusion coefficient σ

$$\begin{cases} \dfrac{\partial}{\partial t}u(x,t) = \sigma \dfrac{\partial^2}{\partial x^2}u(x,t) - V(x,t)u(x,t), \\ u(x,0) = f(x) \end{cases} \qquad t \in [0,T], \quad x \in \mathbb{R}. \tag{1}$$

This equation may be treated in terms of a Brownian particle motion [15–17], where the solution $u(x,t) : \mathbb{R} \times [0,T] \to \mathbb{R}^+$ is the density distribution of the particles. The potential (or the dissipation rate) $V(x,t)$ is bounded from below. We do not consider the drift term $\rho \frac{\partial}{\partial x}u(x,t)$ because it can be easily excluded by a substitution $u(x,t) \to \tilde{u}(x,t)e^{-\rho x}$ [18].

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The solution of (1) can be expressed by the Feynman–Kac formula [18–20]

$$u(x,T) = \int\limits_{\mathcal{C}\{x,0;T\}} f(\xi(T)) e^{-\int_0^T V(\xi(\tau),T-\tau)d\tau} \mathcal{D}_\xi, \tag{2}$$

where the integration is done over the set $\mathcal{C}\{x,0;T\}$ of all continuous paths $\xi(T):[0,T]\to\mathbb{R}$ from the Banach space $\Xi([0,T],\mathbb{R})$ starting at $\xi(0)=x$ and stopping at arbitrary endpoints at time T. $\mathcal{D}_\xi$ is the Wiener measure, and $\xi(t)$ is the Wiener process [21,22]. One of the advantages of the formulation (2) is that it can be directly applied for the unbounded domain without any additional (artificial) boundary conditions.

Path integral (2) corresponding to the Wiener process is typically approximated by a *finite* multidimensional integral with the Gaussian measure (details are given in Section 2.1). The main drawback is that this integral is a high-dimensional one and its computation requires a special treatment. Several approaches have been developed to compute the multidimensional integrals efficiently. The sparse grid method [23,24] has been applied to the computation of path integrals in [25], but only for dimensions up to ~ 100, which is not enough in some applications. The main disadvantage of the Monte Carlo simulation is that it does not allow to achieve a high accuracy [26,27] for some cases (highly oscillatory functions, functions of sum of all arguments).

The multidimensional *integrand* can be represented numerically as a multidimensional array (*a tensor*), which contains values of a multivariate function on a fine uniform grid. For the last decades several approaches have been developed to efficiently work with tensors. They are based on the idea of *separation of variables* [28–31] firstly introduced in [32,33]. It allows to present a tensor in the *low-rank* or *low-parametric* format [34–36], where the number of parameters used for the approximation is almost linear (with respect to dimensionality). To construct such decompositions numerically the very efficient algorithms have been developed recently: two-dimensional *incomplete cross approximation*[1] for the skeleton decomposition, three-dimensional cross approximation [37] for the Tucker format [38–41] in 3D, *tt-cross* [42] approximation for the tensor train decomposition [43,44], which can be also considered as a particular case of the hierarchical Tucker format [45–47] for higher dimensional case. For certain classes of functions commonly used in the computational physics (multiparticle Schrödinger operator [48–53], functions of a discrete elliptic operator [54–59], Yukawa, Helmholtz and Newton potentials [60–63], etc.) there exist low-parametric representations in separated formats and explicit algorithms [64,65] to obtain and effectively work with them (especially *quantized tensor train* (QTT) format [66–73]). In many cases it is very effective to compute the multidimensional integrals [74] using separated representations [75], particularly for multidimensional convolutions [76–79] and highly oscillatory functions [80].

Our approach presented here is based on the *low-rank approximation* of matrices used in an essentially different manner. We formulate the Feynman–Kac formula as an iterative sequence of convolutions defined on grids of diminishing sizes. This is done in Section 3.2. To reduce the complexity of this computation, in Section 3.3 we find a *low-rank* basis set by applying the *cross approximation* (see Appendix A) to a matrix constructed from the values of a one-dimensional function on a very large grid. That gives reduction of computational time and memory requirements, resulting in fast and efficient algorithm presented in Section 3.4. The numerical examples are considered in Section 4. The most interesting part is that we are able to treat non-periodic potentials without any artificial boundary conditions (Section 4.3).

2. Problem statement

2.1. Time discretization

Equation (2) corresponds to the Wiener process. A standard way to discretize the path integral is to break the time range $[0,T]$ into n intervals by points

$$\tau_k = k\cdot\delta t, \qquad 0\le k\le n, \qquad n:\ \tau_n = T.$$

The average path of a Brownian particle $\xi(\tau_k)$ after k steps is defined as

$$\xi^{(k)} = \xi(\tau_k) = x + \xi_1 + \xi_2 + \ldots + \xi_k,$$

where every random step ξ_i, $1\le i\le k$, is independently taken from a normal distribution $\mathcal{N}(0,2\sigma\delta t)$ with zero *mean* and *variance* equal to $2\sigma\delta t$. By definition, $\xi^{(0)}=x$.

Application of a suitable quadrature rule on the uniform grid (i.e., trapezoidal or Simpson rules) with the weights $\{w_i\}_{i=0}^n$ to the time integration in (2) gives

$$\Lambda(T) = \int\limits_0^T V(\xi(\tau),T-\tau)d\tau \approx \sum_{i=0}^n w_i V_i^{(n)}\delta t, \qquad V_i^{(n)} \equiv V(\xi(\tau_i),\tau_{n-i}), \tag{3}$$

[1] Because the low-rank representation of large matrices based on the adaptive cross approximation is directly related to the manuscript we summarize the basics of the method in Appendix A.