Computation of the diffusion equation path integrals via tensor train decomposition

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Let us consider a one-dimensional diffusion equation with the initial distribution $f(x) : \mathbb{R} \to \mathbb{R}$ and a constant diffusion coefficient σ

$$\begin{cases} \dfrac{\partial u(x,t)}{\partial t} = \sigma \, \dfrac{\partial^2 u(x,t)}{\partial x^2} - \nu(x,t) u(x,t), \\ u(x,0) = f(x). \end{cases}$$

This equation describes a Brownian particle motion, where $\nu(x,t) : \mathbb{R} \times [0,t] \to [0,\infty)$ means a probability density of annihilation of Brownian particles, $f(x)$, $\nu(x,t)$ are continuous and bounded for all x in their domain of definition.

According to the Feynman-Kac formula the solution of equation (2) is written in the path integral form

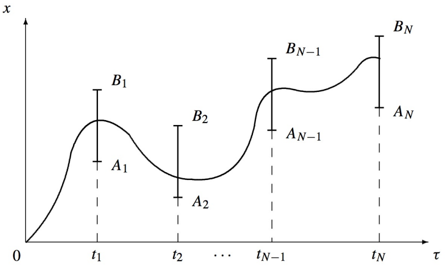
$$u(x,t) = \int_{\mathcal{C}\{x,0;t\}} \left[f(\xi(t)) \exp\left(- \int_0^t \nu(\xi(\tau), t-\tau) d\tau \right) \right] \mathcal{D}_\xi(\tau)$$

where the integration is done over a set of all possible trajectories starting at $\xi(0) = x$ with arbitrary endpoints at time t, $\mathcal{D}_\xi(\tau)$ is the Wiener measure and $\xi(t)$ is the Wiener process.

$$\int_{\mathcal{C}\{x,0;t\}} f(\xi(t))\mathcal{D}_\xi(\tau) \approx \int_{(n)} f(\xi^{(n)})\mathcal{D}_\xi^{(n)} =$$

$$= \int_{-\infty}^{\infty} d\xi_1 \frac{\exp\left(-\frac{\xi_1^2}{4\sigma\delta t}\right)}{\sqrt{4\pi\sigma\delta t}} \int_{-\infty}^{\infty} d\xi_2 \frac{\exp\left(-\frac{\xi_2^2}{4\sigma\delta t}\right)}{\sqrt{4\pi\sigma\delta t}} \times \dots$$

$$\dots \times \int_{-\infty}^{\infty} d\xi_n \frac{\exp\left(-\frac{(\xi_n)^2}{4\sigma\delta t}\right)}{\sqrt{4\pi\sigma\delta t}} f(x + \xi_1 + \dots + \xi_n)$$



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

$$\tau_k = k \cdot \delta t, \qquad 0 \le k \le n,$$

$$n : \tau_n = t.$$

Consider a particle on a one-dimensional infinite chain moving from the node i to node j with probability

$$W(ia - ja, \varepsilon) = \begin{cases} \frac{1}{2} & \text{if} \quad |i-j| = 1, \\ 0, & \text{otherwise} \end{cases} \qquad i, j \in \mathbb{Z}$$

After n steps

$$W(ia{-}ja, n\varepsilon) = \begin{cases} 0 & \text{if} \quad |i-j| > n \quad \text{or} \quad i-j+n \quad \text{is odd,} \\ \frac{1}{2^n}\binom{n}{\frac{n+i-j}{2}} & \text{if} \quad |i-j| \le n \quad \text{and} \quad i-j+n \quad \text{is even} \end{cases}$$

<u>The Brownian motion:</u>

– homogenious in space $(i-j)$

– homogenious in time

– isotropic $(i, j) \to (-i, -j)$

$$W(ia - ja, n) \to w(ia, n\varepsilon) = w_i(n)$$

$$w_i(n) = \begin{cases} 0 & \text{if} \quad |i| > n \quad \text{or} \qquad i+n \quad \text{is odd,} \\ \dfrac{1}{2^n}\dbinom{n}{\frac{n+i}{2}} & \text{if} \quad |i| \leq n \quad \text{and} \quad i+n \quad \text{is even} \end{cases} \tag{1}$$

$$\binom{n+1}{k} = \binom{n}{k} + \binom{n}{k-1} \tag{2}$$

$$w(x, t+\varepsilon) = \frac{1}{2}w(x+a, t) + \frac{1}{2}w(x-a, t) \tag{3}$$

$$x = ia, \qquad t = n\varepsilon \tag{4}$$

$$\frac{w(x,t+\varepsilon)-w(x,t)}{\varepsilon}=\frac{a^2}{2\varepsilon}\frac{w(x+a,t)-2w(x,t)+w(x-a,t)}{a^2} \tag{5}$$

$$\sigma=\frac{a^2}{2\varepsilon} \tag{6}$$

$$\frac{\partial}{\partial t}w(x,t)=\sigma\frac{\partial^2}{\partial x^2}w(x,t) \tag{7}$$

$$w(x,t)=\frac{1}{\sqrt{4\pi\sigma t}}\exp\left(-\frac{x^2}{4\sigma t}\right), \qquad f(x)=\delta(x) \tag{8}$$

$$w(x,t)=\frac{1}{\sqrt{4\pi\sigma t}}\int_{-\infty}^{\infty}f(y)\exp\left(-\frac{(x-y)^2}{4\sigma t}\right)dy \tag{9}$$

Exact solution:

$$u(x,t) = \int_{\mathcal{C}\{x,0;t\}} \left[f(\xi(t)) \exp\left(- \int_0^t \nu(\xi(\tau), t-\tau) d\tau \right) \right] \mathcal{D}_\xi(\tau)$$

corresponding discrete version:

$$u^{(n)}(x,t) = \int_{-\infty}^{\infty} \mathcal{D}_\xi^{(n)}\, f\left(\xi^{(n)}\right) \prod_{i=0}^{n} \exp\left(-\eta_i \nu(\xi^{(i)}, \tau_{n-i}) \delta t \right),$$

Time discretization in the exponent

$$\int_0^t \nu(\xi(\tau), t-\tau) d\tau \approx \sum_{i=0}^{n} \eta_i \nu(\xi^{(i)}, \tau_{n-i}) \delta t$$

Gaussian-weighted integral

$$\Phi_{\{\mu\}}[F] = \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \prod_{k=1}^{n} dx_k \exp(-\mu_k x_k^2) F(x_1, \dots, x_n)$$

can be approximated by the Gauss-Hermite quadrature with weights $\{\lambda_k(i_k)\}_{i_k=1}^{l_k}$ and nodes $\{p_k(i_k)\}_{i_k=1}^{l_k}$ in each dimension $1 \leq k \leq n$. $p_k(i_k)$ – roots of Hermite polynomial $H_{l_k}(x)$, $i_k = 1, 2, \dots, l_k$ $\lambda_k(i_k) = \frac{2^{l_k - 1} l_k! \sqrt{\pi}}{l_k^2 \left[H_{l_k - 1}(x_{i_k})\right]^2}$

$$\Phi_{\{\mu\}}[F] \approx \sum_{i_1, i_2, \dots i_n} \lambda_1(i_1)\lambda_2(i_2) \dots \lambda_n(i_n) F(p_1(i_1), p_2(i_2), \dots, p_n(i_n)).$$

Summation is done over a multidimensional mesh, which is a Kronecker product of one-dimensional meshes $\mathbf{p}_1 \otimes \mathbf{p}_2 \otimes \dots \otimes \mathbf{p}_n$.

The idea of separation of variables

$$F(x_1, x_2, \dots, x_n) \approx \sum_{\alpha=1}^{r} u_1(x_1, \alpha) u_2(x_2, \alpha) \dots u_n(x_n, \alpha). \tag{10}$$

Minimal number r in sum is called *separation rank*.

The advantage of the decomposition (10) may be clearly seen from the following equality

$$\Phi_{\{\mu\}}[f] \approx \sum_{\alpha=1}^{r} \int_{-\infty}^{\infty} u_1(x_1, \alpha) \exp(-\mu_1 x_1^2)\, dx_1 \dots \int_{-\infty}^{\infty} u(x_n, \alpha) \exp(-\mu_n x_n^2)\, dx_n$$

In case of $r \ll n$ the dimensionality of the problem is significantly reduced.

In discrete case, when the function is defined on the multidimensional mesh indexed by i_k, $1 \leq k \leq n$, the separated representation turns out to be *canonical decomposition* of tensor **F**

$$F(i_1, i_2, \dots, i_n) \approx \sum_{\alpha=1}^{r} U_1(i_1, \alpha) U_2(i_2, \alpha) \dots U_n(i_n, \alpha),$$

the number r is called *canonical rank*, $U_k(i_k, \alpha)$ are real or complex matrices of size $I_k \times r$.

The advantage: complexity of the problem is reduced from $\mathcal{O}(n^d)$ to $\mathcal{O}(rnd)$, where n is the mesh size, d - dimension, r – rank.

A tensor **F** is sad to be in the TT-format if its elements satisfy the relation

$$F(i_1, i_2, \ldots, i_n) = G_1(i_1) G_2(i_2) \ldots G_n(i_n),$$

$G_k(i_k)$ are $r_{k-1} \times r_k$ matrices for each fixed i_k, $r_0 = r_n = 1$. The numbers r_k are called *TT-ranks* The parameter-depended matrices $G_k(i_k)$ can be considered as three-dimensional tensors $G_k(\alpha_{k-1}, i_k, \alpha_k)$, where α_k vary from 1 to r_k.
For a given tensor and fixed ranks r_k there exists the best possible approximation in the TT-format.

$$\Phi_{\{\mu\}}[F] \approx S_1 S_2 \ldots S_n,$$

$$S_k = \sum_{i_k=1}^{I_k} G_k(i_k),$$

Python toolbox `ttpy`: `tt.cross()`, `tt.sum()`, `tt.multifuncrs()`, etc.
`https://github.com/oseledets/ttpy`
I.V. Oseledets, T. Saluev, S. Dolgov, and D. Savostyanov.

Test example:

$$V(x,t) = -\frac{1}{t+1} - \frac{1}{x^2+1} + \frac{4x^2}{(x^2+1)^2},$$

$$f(x) = \frac{1}{\pi}\frac{1}{x^2+1},$$

with exact solution

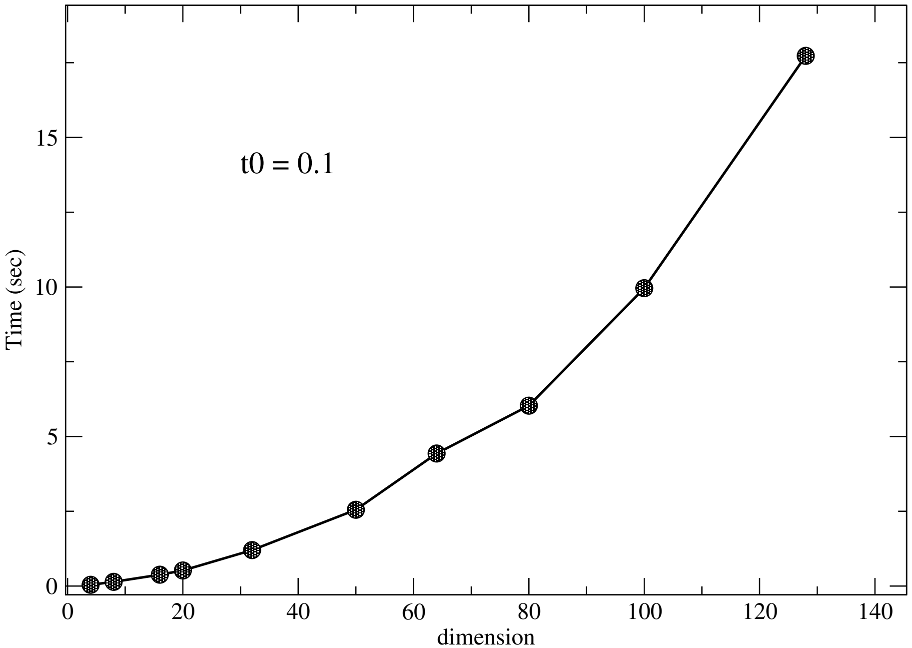
$$u_v(x,t) = \frac{1}{\pi}\frac{t+1}{x^2+1}.$$

Table : Path integral for $t_0 = 0.1$, $x_0 = 2.1$, cross accuracy $\varepsilon = 10^{-6}$, number of the mesh nodes $m = 10$

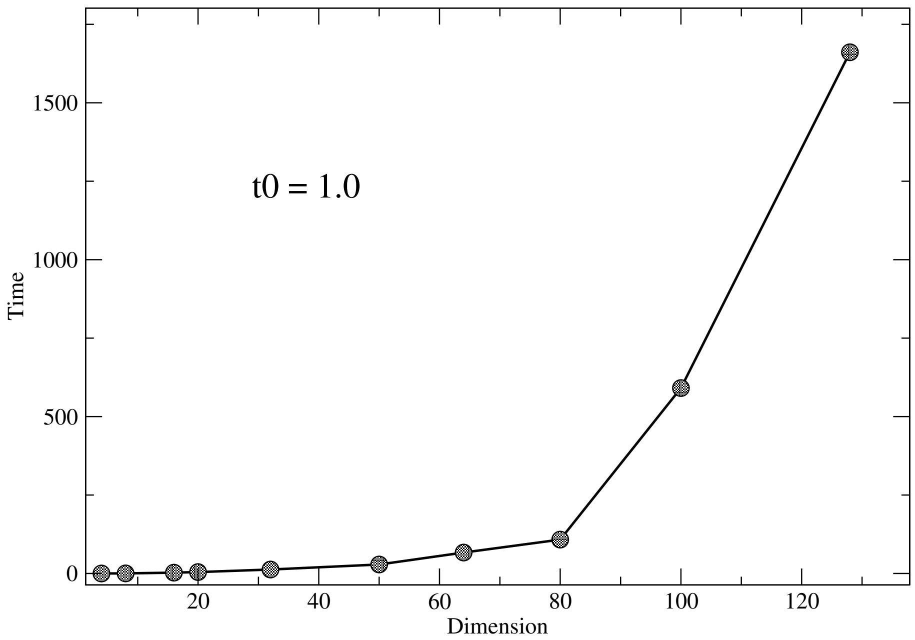
n	δt	Value	Rel. Error	T (sec.)	N calls
		0.06472105^{ex}			
128	$7.81 \cdot 10^{-4}$	0.06470589	$2.34 \cdot 10^{-4}$	17.73	1 100 600
100	$1.00 \cdot 10^{-3}$	0.06470165	$3.00 \cdot 10^{-4}$	9.96	884 740
80	$1.25 \cdot 10^{-3}$	0.06469680	$3.75 \cdot 10^{-4}$	6.03	701 150
64	$1.56 \cdot 10^{-3}$	0.06469074	$4.68 \cdot 10^{-4}$	4.43	571 660
50	$2.00 \cdot 10^{-3}$	0.06468227	$5.99 \cdot 10^{-4}$	2.55	440 480
32	$3.13 \cdot 10^{-3}$	0.06466049	$9.36 \cdot 10^{-4}$	1.20	273 680
20	$5.00 \cdot 10^{-3}$	0.06462425	$1.50 \cdot 10^{-3}$	0.52	171 510
16	$6.25 \cdot 10^{-3}$	0.06460014	$1.87 \cdot 10^{-3}$	0.38	130 520
8	$1.25 \cdot 10^{-2}$	0.06448006	$3.72 \cdot 10^{-3}$	0.14	49 510
4	$2.50 \cdot 10^{-2}$	0.06424237	$7.40 \cdot 10^{-3}$	0.04	11 930

Table : Path integral for $t_0 = 1.0$, $x_0 = 2.1$, cross accuracy $\varepsilon = 10^{-6}$, number of the mesh nodes $m = 10$

n	δt	Value	Rel. Error	T (sec.)	N calls
		0.11767463^{ex}			
128	$7.81 \cdot 10^{-3}$	0.11752589	$1.26 \cdot 10^{-3}$	1661	66 403 870
100	$1.00 \cdot 10^{-2}$	0.11748495	$1.61 \cdot 10^{-3}$	591	38 318 670
80	$1.25 \cdot 10^{-2}$	0.11743854	$2.01 \cdot 10^{-3}$	108	10 909 020
64	$1.56 \cdot 10^{-2}$	0.11738108	$2.49 \cdot 10^{-3}$	66.9	8 251 230
50	$2.00 \cdot 10^{-2}$	0.11730169	$3.17 \cdot 10^{-3}$	28.6	5 000 380
32	$3.13 \cdot 10^{-2}$	0.11710311	$4.86 \cdot 10^{-3}$	12.6	3 057 670
20	$5.00 \cdot 10^{-2}$	0.11678969	$7.52 \cdot 10^{-3}$	4.54	1 695 880
16	$6.25 \cdot 10^{-2}$	0.11659266	$9.19 \cdot 10^{-3}$	2.62	1 226 620
8	$1.25 \cdot 10^{-1}$	0.11573941	$1.64 \cdot 10^{-2}$	0.38	219 120
4	$2.50 \cdot 10^{-1}$	0.11451109	$2.69 \cdot 10^{-2}$	0.14	33 770



t0 = 0.1
Time (sec)
dimension
0
5
10
15
0
20
40
60
80
100
120
140


t0 = 1.0
Time
Dimension
0
500
1000
1500
20
40
60
80
100
120

Iteration of initial distribution

– Time evolution step Δt is fixed

$$u_{k+1}^{(n)}(x) = u^{(n)}(x, \Delta t) = \int_{-\infty}^{\infty} \mathcal{D}_{\xi}^{(n)}\, g_k\left(\xi^{(n)}\right) \prod_{i=0}^{n} \exp\left(-\eta_i \nu(\xi^{(i)}, \tau_{n-i})\delta t\right),$$

$$g_k(x) = u_k^{(n)}(x), \qquad g_0(x) = f(x)$$

1) linear growing of the definition domain $\sim n \max(|\sum_k \xi_k|)$
2)The error grows up proportional to the number of iterations $\varepsilon \cdot n$

Thank you for your attention!