Cross approximation of the solution of the Fokker-Planck equation

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Abbreviations

- **ODE** — ordinary differential equation
- **SDE** — stochastic differential equation
- **FPE** — Fokker-Planck equation
- **PDF** — probability density function
- **FFT** — fast Fourier transform

Outline

Stochastic differential equation

Consider stochastic differential equation (**SDE**)

$$d\boldsymbol{x} = \boldsymbol{f}(\boldsymbol{x}, t)\, dt + S(\boldsymbol{x}, t)\, d\boldsymbol{\beta},$$

$$\boldsymbol{x} = \boldsymbol{x}(t) \in \mathbb{R}^d, \quad \boldsymbol{f} \in \mathbb{R}^d, \quad S \in \mathbb{R}^{d \times d}, \quad \boldsymbol{\beta} \in \mathbb{R}^d$$

where t is time, $\boldsymbol{x} = \boldsymbol{x}(t)$ is a d-dimensional spatial variable and $\boldsymbol{\beta}$ is a Brownian motion ($d\boldsymbol{\beta}\, d\boldsymbol{\beta}^\top = Qdt$).

We are interested in the evolution of the probability density function (**PDF**) $\rho(\boldsymbol{x}, t)$ of the spatial variable $\boldsymbol{x}(t)$

$$\boldsymbol{x}(0) \sim \rho_0(\boldsymbol{x}), \quad \boldsymbol{x}(t) \sim \rho(\boldsymbol{x}) = ?$$

Fokker-Planck equation

It can be shown that PDF is the solution of the related Fokker-Planck equation (**FPE**)

$$\frac{\partial \rho(\boldsymbol{x},t)}{\partial t} = -\sum_{i=1}^{d} \frac{\partial}{\partial x_i} \left[\boldsymbol{f}_i(\boldsymbol{x},t)\rho(\boldsymbol{x},t)\right] + \sum_{i=1}^{d}\sum_{j=1}^{d} \frac{\partial}{\partial x_i}\frac{\partial}{\partial x_j}\left[D_{ij}(\boldsymbol{x},t)\rho(\boldsymbol{x},t)\right],$$

where $D = \frac{1}{2} SQS^\top$ is the diffusion tensor and $\rho(\boldsymbol{x},0) = \rho_0(\boldsymbol{x})$.

Model problem

Let assume for simplicity that

$$S(x,t) \equiv I, \quad Q \equiv 2I \quad \rightarrow \quad D(x,t) \equiv I,$$

where I is an $d \times d$ identity matrix.

Then equations look like

SDE: $d\boldsymbol{x} = \boldsymbol{f}(\boldsymbol{x},t)\,dt + d\boldsymbol{\beta}, \quad x(0) = x_0,$

FPE: $\frac{\partial \rho}{\partial t} = \Delta\rho - div\left[\boldsymbol{f}(\boldsymbol{x},t)\rho\right], \quad \rho(x,0) = \rho_0(x),$

and our value of interest is PDF $\rho(\boldsymbol{x},t)$ at time t ($t > 0$) on some discrete spatial grid.

Outline

Operator splitting technique

For ODE

$$\frac{\partial \boldsymbol{u}}{\partial t} = (A + B)\boldsymbol{u}, \quad \boldsymbol{u}(0) = \boldsymbol{u}_0,$$

with d-dimensional ($d > 1$) variable $\boldsymbol{u}$ at time $t = h$ we have

$$\boldsymbol{u} = e^{h(A+B)}\boldsymbol{u}_0,$$

$$e^{h(A+B)} = I + h(A + B) + \frac{h^2}{2}A^2 + \frac{h^2}{2}B^2 + \frac{h^2}{2}AB + \frac{h^2}{2}BA + o(h^2).$$

Some splitting techniques:

- $e^{h(A+B)} \approx e^{hA}e^{hB}$ - nonsymmetric splitting (1th order)
- $e^{h(A+B)} \approx \frac{1}{2}e^{hA}e^{hB} + \frac{1}{2}e^{hB}e^{hA}$ - symmetric splitting (2th order)
- $e^{h(A+B)} \approx e^{\frac{h}{2}A}e^{hB}e^{\frac{h}{2}A}$ - symmetric Strang splitting (2th order)

Stability condition: $\frac{A+A^\top}{2}$ and $\frac{B+B^\top}{2}$ are negative definite.

Splitting of Fokker-Planck equation

To solve FPE $\frac{\partial \rho}{\partial t} = \Delta \rho - div\left[\boldsymbol{f}(\boldsymbol{x}, t)\rho\right], \quad \rho(x, 0) = \rho_0(x)$,
we consider uniform time mesh with $m + 1$ points $t_k = hk$ ($k = 0, 1, \ldots, m$) and apply 1th order splitting scheme on time step k.

Equation 1 (EQ1):

$$\frac{\partial v}{\partial t} = \Delta v, \quad v_k = \rho_k = \rho(\boldsymbol{x}(t_k), t_k).$$

Equation 2 (EQ2):

$$\frac{\partial w}{\partial t} = -div\left[f(\boldsymbol{x}, t)w\right], \quad w_k = v_{k+1}.$$

Then we can approximate solution on the $(k + 1)$th step as

$$\rho_{k+1} = w_{k+1}, \quad k = 0, 1, \ldots, m - 1.$$

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Solution of EQ1

To solve EQ1 on the time step k

$$\frac{\partial v}{\partial t} = \Delta v, \quad v_k = \rho_k = \rho(\boldsymbol{x}(t_k), t_k), \quad v_{k+1} = ?,$$

we descritize operator on some spatial grid

$$\Delta = I \otimes I \otimes \ldots \otimes D + \ldots + D \otimes I \otimes \ldots \otimes I,$$

where D is a one dimensional differential matrix,

and then we calculate the matrix exponent

$$v_{k+1} = e^{h\Delta} v_k = e^h \left(e^D \otimes \ldots \otimes e^D \right) v_k.$$

Solution of EQ2

To solve EQ2 on the time step k

$$\frac{\partial w}{\partial t} = -div\left[f(\boldsymbol{x}, t)w\right], \quad w_k = v_{k+1}, \quad w_{k+1} = ?,$$

we use the fact that it looks like equation for PDF w of solution of the ODE without noise

$$d\boldsymbol{x} = \boldsymbol{f}(\boldsymbol{x}, t)\, dt.$$

It can be shown that its PDF on the spatial trajectories $w(\boldsymbol{x}(t), t)$ is the solution of the following $d+1$ dimensional system

$$\begin{cases} \frac{\partial \boldsymbol{x}}{\partial t} = \boldsymbol{f}(\boldsymbol{x}, t) \\ \frac{\partial \log w}{\partial t} = -tr\left(\frac{\partial f(\boldsymbol{x}, t)}{\partial \boldsymbol{x}}\right) \end{cases}.$$

Solution of EQ2

The system

$$\begin{cases} \frac{\partial \boldsymbol{x}}{\partial t} = \boldsymbol{f}(\boldsymbol{x}, t) \\ \frac{\partial \log w}{\partial t} = -tr\left(\frac{\partial f(\boldsymbol{x}, t)}{\partial \boldsymbol{x}}\right) \end{cases},$$

with known $\boldsymbol{x}_k$ and w_k can be solved by a standard ODE solver for the time $t_{k+1} = (k+1)h$.

Suppose that $\boldsymbol{x}_k$ is some point of selected spatial grid, and therefore w_k is the value for this point.

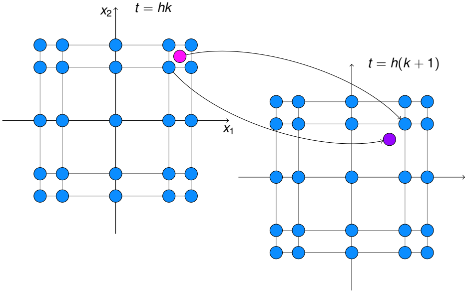
But the solution for w_{k+1} will be defined on $\boldsymbol{x}_{k+1}$, not on on the original spatial grid point $\boldsymbol{x}_k$, and hence we should interpolate obtained values from the solution of the system to original grid.

Outline

Discretization scheme

$$t_k = hk, \quad x^{ch}_{i_1,i_2,\ldots,i_d} = \begin{bmatrix} L_1 \cdot \cos \frac{i_1 \pi}{n_1} \\ L_2 \cdot \cos \frac{i_2 \pi}{n_2} \\ \ldots \\ L_d \cdot \cos \frac{i_d \pi}{n_d} \end{bmatrix}$$

$$k = 0, 1, \ldots, m,$$
$$i_j = 0, 1, \ldots, n_j,$$
$$j = 1, 2, \ldots, d.$$



We use uniform time mesh with $m + 1$ points and Chebyshev spatial grid with $(n+1)^d$ points.

Solution of EQ1 on the grid

$$\frac{\partial v}{\partial t} = \Delta v,$$
$$v_k = \rho_k, \quad v_{k+1} = ?,$$

$$v_{k+1} = e^h \left(e^D \otimes \ldots \otimes e^D \right) v_k.$$

As a one dimensional differential matrix $D \in \mathbb{R}^{n \times n}$ we use Chebyshev second order differential matrix

$$D[i,j] = \begin{cases} \frac{2n^2+1}{6}, & i = 0,\ j = 0, \\ -\frac{2n^2+1}{6}, & i = n,\ j = n, \\ -\frac{x_j}{2(1-x_j^2)}, & i = j,\ 1 \leq j < n, \\ \frac{c_i}{c_j} \frac{(-1)^{i+j}}{x_i - x_j}, & \text{otherwise}, \end{cases} \qquad c_i = \begin{cases} 2, & i = 0, \\ 1, & 1 \leq i < n, \\ 2, & i = n, \end{cases}$$

where x_i and x_j are the corresponding points of the Chebyshev grid.

Solution of EQ2 on the grid

$$\frac{\partial w}{\partial t} = -div\left[f(\boldsymbol{x},t)w\right], \qquad \begin{cases} \frac{\partial \boldsymbol{x}}{\partial t} = \boldsymbol{f}(\boldsymbol{x},t) \\ \frac{\partial \log w}{\partial t} = -tr\left(\frac{\partial f(\boldsymbol{x},t)}{\partial \boldsymbol{x}}\right) \end{cases},$$

$$w_k = v_{k+1}, \quad w_{k+1} = ?,$$

Suppose that $\boldsymbol{x}_k$ is some point of Chebyshev grid x^{ch} and $w_k = w_k(\boldsymbol{x}_k)$ is known.

If $(\boldsymbol{x}_{k+1}, w_{k+1})$ is solution of the system, then w_{k+1} is the value of w in $\boldsymbol{x}_{k+1}$ point (it is not a grid point!), and to coninue the iterative process for the next time step, we should perform interpolation

$$\overline{w_{k+1}} = E_{\boldsymbol{x}_{k+1}\to\boldsymbol{x}_k}[w_{k+1}]$$

Multidimensional Chebyshev interpolation

PDF w_{k+1} on time step $k+1$ on the spatial grid x^{ch} can be considered as a function of d variables

$$w_{k+1} = w_{k+1}(\boldsymbol{x}), \quad \boldsymbol{x} = (x_1, x_2, \ldots, x_d)^\top .$$

Multidimensional Chebyshev interpolation formula

$$w_{k+1} \approx \widehat{w_{k+1}} = \sum_{j_1=1}^{n_1} \sum_{j_2=1}^{n_2} \ldots \sum_{j_d=1}^{n_d} a_{j_1 j_2 \ldots j_d} T_{j_1}(x_1) T_{j_2}(x_2) \ldots T_{j_d}(x_d),$$

where T is a Chebyshev polynomial of the first kind

$$T_0(x) = 1, \quad T_1(x) = x, \quad T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), \quad n = 1, 2, \ldots .$$

Multidimensional Chebyshev interpolation

Interpolation coefficients can be considered as elements of a tensor

$$\mathscr{A} = \{a_{j_1 j_2 \dots j_d};\ 1 \le j_1 \le n_1,\ 1 \le j_2 \le n_2,\ \dots,\ 1 \le j_d \le n_d\}.$$

For construction of the tensor $\mathscr{A}$ we have to set equality in the interpolation nodes

$$\widehat{w_{k+1}}(x_{1,j_1}, x_{2,j_2}, \dots, x_{d,j_d}) = w_{k+1}(x_{1,j_1}, x_{2,j_2}, \dots, x_{d,j_d}),$$

$$j_1 = 1, \dots, n_1, \quad j_2 = 1, \dots, n_2, \quad \dots, \quad j_d = 1, \dots, n_d.$$

The corresponding values of w_{k+1} on the spatial grid points may be collected in a tensor $\mathscr{W}_{k+1}$

$$\mathscr{W}_{k+1} = \{w_{k+1}(x_{1,j_1}, x_{2,j_2}, \dots, x_{d,j_d});\ 1 \le j_1 \le n_1,\ \dots,\ 1 \le j_d \le n_d\}$$

Interpolation in the Tensor Train format

We can calculate any element $(j_1, j_2, \ldots, j_d)$ of the $\mathscr{W}_{k+1}$ throw solution of the system of ODEs.

It seems promising to use the multidimensional TT-cross method to construct approximation of this tensor in the TT-format.

$$\mathscr{W}(j_1, j_2, \ldots, j_d) \approx \mathscr{G}_1(j_1)\mathscr{G}_2(j_2)\ldots\mathscr{G}_d(j_d),$$

We can obtain tensor of interpolation coefficients by fast Fourier transform (**FFT**) of each kernel

$$\mathscr{G}_k(j_k) \xrightarrow{\text{FFT}} \mathscr{G}'_k(j_k),$$

$$\mathscr{A}(j_1, j_2, \ldots, j_d) \approx \mathscr{G}'_1(j_1)\mathscr{G}'_2(j_2)\ldots\mathscr{G}'_d(j_d).$$

Interpolation in the Tensor Train format

If we know tensor of interpolation coefficients in TT format:

$$\mathscr{A}(j_1, j_2, \ldots, j_d) \approx \mathscr{G}'_1(j_1)\mathscr{G}'_2(j_2)\ldots\mathscr{G}'_d(j_d),$$

then we can perform a fast calculation of the w at any spatial point $\boldsymbol{z} = [z_1, \ldots, z_d]^\top$

$$w(\boldsymbol{z}) \approx \sum_{j_1=1}^{n_1} \mathscr{G}'_1(j_1) T_{j_1}(z_1) \sum_{j_2=1}^{n_2} \mathscr{G}'_2(j_2) T_{j_2}(z_2) \ldots \sum_{j_d=1}^{n_d} \mathscr{G}'_d(j_d) T_{j_d}(z_d).$$

Summary (schematic algorithm)

For the time step $k+1$ with known interpolation coefficients $\mathscr{A}_k^{(int)}$ of solution ρ_k on the time step k we perform the following

1. Solve spatial part of EQ2

$$\frac{\partial \boldsymbol{x}}{\partial t} = \boldsymbol{f}(\boldsymbol{x}, t) \quad \boldsymbol{x}_{k+1} = x^{ch}, \quad \widehat{\boldsymbol{x}_k} = ?,$$

2. Interpolate ρ_k to $\widehat{\boldsymbol{x}_k}$ using $\mathscr{A}_k^{(int)}$

$$\overline{\rho_k} = E_{x^{ch} \to \widehat{\boldsymbol{x}_k}}[\rho_k],$$

3. Solve EQ1 $v_{k+1} = e^h \left(e^D \otimes \ldots \otimes e^D\right) \overline{\rho_k}$.
4. Solve PDF part of EQ2

$$\frac{\partial \log w}{\partial t} = -tr\left(\frac{\partial f(\boldsymbol{x}, t)}{\partial \boldsymbol{x}}\right), \quad w_k = v_{k+1}, \quad w_{k+1} = ?,$$

5. Set ρ_{k+1} values on the Chebyshev grid as w_{k+1}
6. Construct interpolation coefficients $\mathscr{A}_{k+1}^{(int)}$ for ρ_{k+1}

Thanks for your attention!