An Analogy of Approximation Methods

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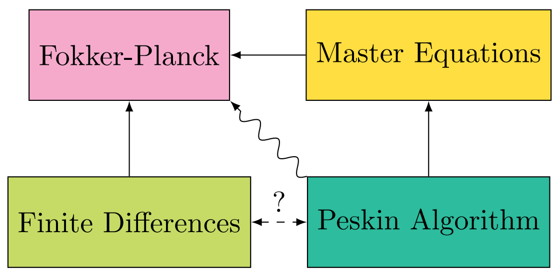

Figure 1: Approximation methods and their relationships to the Fokker-Planck equation.

The probability density $u(x,t)$ evolves according to the Fokker-Planck equation

$$\partial_t u(x,t) = \partial_x \left(u(x,t)\phi'(x) + \partial_x u(x,t) \right) \tag{1}$$

where $\phi(x)$ is the potential energy [2]. In one spatial dimension, this is a simple convection-diffusion equation.

1 Finite Differences

First we will write an explicit finite difference scheme for (1). We assume we work on the closed domain $[0,1] \times [0,t_F]$. Note that we must use a finite time interval, but t_F can be made as large as desired. We denote the uniform spacings by h and s for space and time, respectively. Then the mesh points are

$$(x_j = jh, t_n = ns),\ j = 0,1,2\dots,J,\ n = 0,1,2,\dots,$$

and $h = 1/J$. We use the notation

$$U_j^n \approx u(x_j, t_n)$$

to mean the approximations of the solution at the mesh points.

The left side of (1) is approximated using a forward difference for the time derivative:

$$\frac{U_j^{n+1} - U_j^n}{s} \approx \frac{\partial u(x_j,t_n)}{\partial t}. \tag{2}$$

Next will we derive the approximation for the right side of (1). We rewrite this as

$$\partial_x(u\phi') + u_{xx} = \partial_x(u\phi' + u_x).$$

Rather than expanding the first term using the product rule, we follow [1] and write

$$U^n_{j+1/2}\left(\frac{\phi_{j+1}-\phi_j}{h}\right) \approx \left[u(x,t)\frac{d\phi(x)}{dx}\right]^n_{j+1/2}$$

and similarly for j replaced with $j-1$. Subtracting these two and dividing by h, we obtain

$$\frac{1}{h^2}\left[U^n_{j+1/2}\Delta_j\phi - U^n_{j-1/2}\Delta_{j-1}\phi\right] \approx \partial_x\left(u(x_j,t_n)\phi'(x_j)\right)$$

where $\Delta_j\phi = \phi_{j+1}-\phi_j$ and $\Delta_{j-1}\phi = \phi_j - \phi_{j-1}$. This approach requires the computation of $u(x,t)$ for values of x half-way between space steps. An alternative is to use

$$\frac{1}{2}\left(U^n_{j+1}+U^n_j\right) \approx U^n_{j+1/2}$$

and similarly for j replaced with $j-1$. Making these approximations, we arrive at

$$\frac{1}{2h^2}\left[(U^n_{j+1}+U^n_j)\Delta_j\phi + (U^n_j+U^n_{j-1})\Delta_{j-1}\phi\right] \approx \partial_x(u\phi'). \tag{3}$$

For the second term of the right side, we use a centered second difference:

$$\frac{1}{h^2}\left[U^n_{j+1}-2U^n_j+U^n_{j-1}\right] \approx u_{xx}. \tag{4}$$

Now adding (3) and (4) we obtain the full approximation for the right side of (1). Since this scheme is explicit, we can solve for U^{n+1}_j easily:

$$U^{n+1}_j = U^n_j + \frac{s}{2h^2}\left[U^n_{j+1}(\Delta_j\phi+2) + U^n_j(\Delta_j\phi+\Delta_{j-1}\phi-4) + U^n_{j-1}(\Delta_{j-1}\phi+2)\right] \tag{5}$$

2 Master Equations

We now try to derive the same set of equations by considering a spatially discrete jump process. At any spacial point j, the change in the probability of that point being occupied in time can be described as *Flux In - Flux Out*. Using $F_{j+1/2}$ to denote the forward jump from x_j to x_{j+1} and $B_{j+1/2}$ to denote a backward jump from x_{j+1} to x_j, we can write

$$\frac{dU_j}{dt} = \left[F_{j-1/2}U_{j-1} + B_{j+1/2}U_{j+1}\right] - \left[F_{j+1/2}U_j + B_{j-1/2}U_j\right]. \tag{6}$$

We define $F_{j+1/2}$ and $B_{j+1/2}$ according to [1]:

$$F_{j+1/2} = \frac{1}{h^2}\frac{\Delta_j\phi}{\exp(\Delta_j\phi)-1},$$
$$B_{j+1/2} = \frac{1}{h^2}\frac{-\Delta_j\phi}{\exp(-\Delta_j\phi)-1}.$$

We can compute the Taylor expansion of these to find

$$\begin{aligned} F_{j+1/2} &\approx \frac{1-\Delta_j\phi/2 + O\left((\Delta_j\phi)^2\right)}{h^2}, \\ B_{j+1/2} &\approx \frac{1+\Delta_j\phi/2 + O\left((\Delta_j\phi)^2\right)}{h^2}. \end{aligned} \tag{7}$$

Now substituting (7) into (6), we find

References

[1] K. W. Morton and D. F. Mayers. *Numerical solution of partial differential equations.* Cambridge University Press, 2005.

[2] H. WANG, C. S. PESKIN, and T. C. ELSTON. A robust numerical algorithm for studying biomolecular transport processes. *Journal of Theoretical Biology*, 221(4):491–511, 2003.