Stochastic Simulations for DREAM4

Thomas Schaffter & Daniel Marbach

June 18, 2009

1 ODE model (DREAM3)

$$\frac{dx_i}{dt} = F_i^{RNA}(\boldsymbol{x}, \boldsymbol{y}) = m_i \cdot f_i(\mathbf{y}) - \lambda_i^{RNA} \cdot x_i \quad (1)$$

$$\frac{dy_i}{dt} = F_i^{Prot}(\boldsymbol{x}, \boldsymbol{y}) = r_i \cdot x_i - \lambda_i^{Prot} \cdot y_i \quad (2)$$

where m_i is the maximum transcription rate, r_i the translation rate, λ_i^{RNA} and $\lambda_i^{\mathrm{Prot}}$ are the mRNA and protein degradation rates, and $f_i(\cdot)$ is the so-called input function of gene i. The input function computes the *relative activation* of the gene, which is between 0 (the gene is shut off) and 1 (the gene is maximally activated), given the transcription-factor (TF) concentrations $\mathbf{y}$.

2 SDE model (DREAM4)

$$\frac{dx_i}{dt} = F_i^{RNA}(\boldsymbol{x}, \boldsymbol{y}) + \sigma_i^{RNA} \cdot \eta_i \quad (3)$$

$$\frac{dy_i}{dt} = F_i^{Prot}(\boldsymbol{x}, \boldsymbol{y}) + \sigma_i^{Prot} \cdot \zeta_i \quad (4)$$

where each η_i and ζ_i is an independent Gaussian white noise with zero mean and unit variance. σ_i^{RNA} and σ_i^{Prot} represent the amplitude (standard deviation) of the noise.

3 Numerical simulation of SDEs

For notational simplicity, we consider here only a single equation and not a system of equations. Equations (3) and (4) are of the following, general form (note that we use the Stratonovich scheme)

$$dX_t = F(X_t)dt + G(X_t)dW_t \quad (5)$$

$$dX_t = \underline{F}(X_t)dt + G(X_t) \circ dW_t \quad (6)$$

$$\underline{F} = F - \frac{1}{2}G'G \quad (7)$$

where dW_t is a Wiener process. The Itô scheme is defined by (5) and the equivalent Stratonovich scheme is given by (6) and (7).[1,5] In (3) and (4) the amplitude of the noise $G(X_t)$ is a constant σ_i.

We propose to use the Milstein scheme for the numerical integration, which is better than the basic Euler-Marumaya method, but still easy to implement.[1,3,5,6] Given $X(n) = X_n$, the value at the next discrete time point X_{n+h} is approximated by

$$\begin{aligned} X_{n+h} &= X_n + \underline{F}(X_n)h + G(X_n)\Delta W_n + \frac{1}{2}G'(X_n)G(X_n)[\Delta W_n]^2 && (8) \\ \Delta W_n &= [W_{t+h} - W_t] \sim \sqrt{h}\mathcal{N}(0,1) && (9) \end{aligned}$$

where h is the step size.

References

[1] P.M. Burrage, *Runge-Kutta methods for stochastic differential equations*, (1999).

[2] H. Gilsing and T. Shardlow, *SDELab: A package for solving stochastic differential equations in MATLAB*, Journal of Computational and Applied Mathematics **205** (2007), no. 2, 1002–1018.

[3] D.J. Higham, *An algorithmic introduction to numerical simulation of stochastic differential equations*, SIAM review (2001), 525–546.

[4] P.E. Kloeden, E. Platen, and H. Schurz, *Numerical solution of SDE through computer experiments*, Springer, 1994.

[5] H. Lamba, *Stepsize control for the Milstein scheme using first-exit-times.*

[6] Umberto Picchini, *Sde toolbox: Simulation and estimation of stochastic differential equations with matlab.*