An Introduction to Discrete–Event Simulation

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IMA Workshop, May 12, 2008

Markov Jump Processes

Goal: Compute $u^*(t) = (u^*(t,x) : x \in S)$,
where $u^*(t,x) = E_x f(X(t))$

Method: Solve

$$\begin{aligned} u'(t) &= Qu(t) \\ \text{s/t} \quad u(0) &= f \end{aligned}$$

Classical method for establishing existence/uniqueness:

$$u_n^*(t,x) = E_x f(X(t)) I(J(t) \le n)$$

$$\begin{aligned} u_n^*(t,x) &= f(x)e^{-\lambda(x)t} \\ &\quad + \sum_{y \neq x} \int_0^t \lambda(x) e^{-\lambda(x)s} \cdot \frac{Q(x,y)}{\lambda(x)} u_{n-1}^*(t-s,y)\,ds \end{aligned}$$

Now, let $n \to \infty$.

Note: Jump time out of x determined by single exponential rv

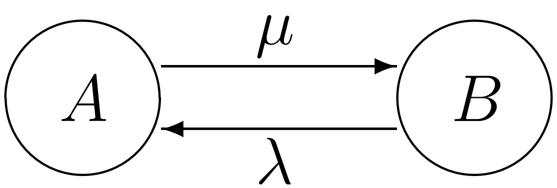
Classical method for simulating Markov jump processes:

1. $n \leftarrow 0$, $T \leftarrow 0$
2. Generate $\eta \sim \text{Exp}(\lambda(X(T)))$
3. Generate Y from p.m.f. $\dfrac{Q(X(T),\ \cdot)}{\lambda(X(T))}$
4. $T \leftarrow T + \eta$
5. $X(T) \leftarrow Y$ and go to 2.

(aka Gillespie algorithm... but goes back to early days of Markov jump processes)

Competing Exponentials

e.g. N independently evolving individuals



$X(t) =$ # of type A individuals at time t

$X = (X(t) : t \geq 0)$ is a birth–death process with rates $\lambda(x) = \lambda x$ and $\mu(x) = (N - x)\mu$.

Simulation: One exponential

vs

N competing exponentials

Competing exponentials can be more efficient when :

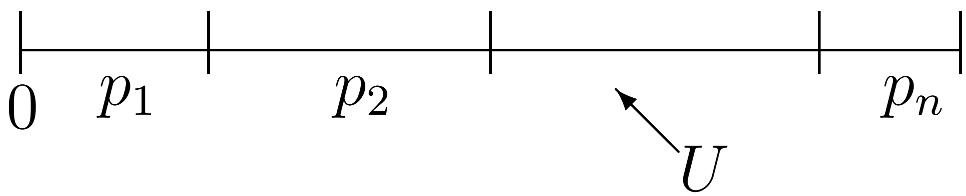
- one uses an efficient data structure to store FES
- "Classical method" is slow because:

$$\left(\frac{Q(X(T_n), y)}{\lambda(X(T_n))} : y \in S \right)$$

must be dynamically computed and/or

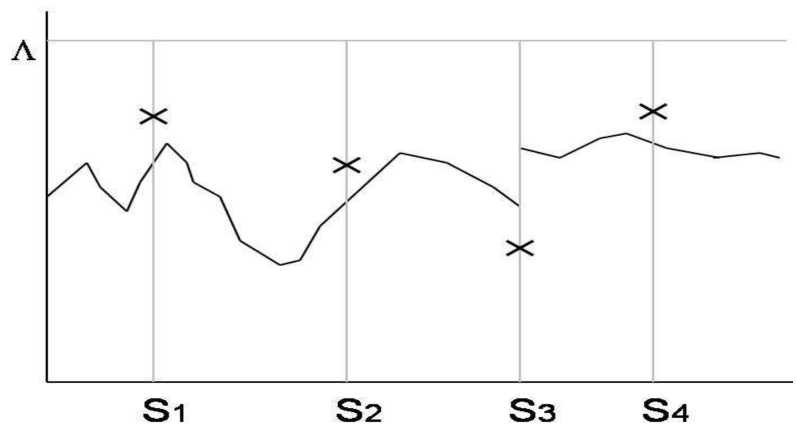
$$\left(\frac{Q(X(T_n), y)}{\lambda(X(T_n))} : y \in S \right)$$

is non–sparse



Thinning

- $X = (X(t) : t \geq 0)$ Markov jump process with time–dependent rate matrix $Q(t)$
- Assume $\Lambda = \sup\{\lambda(t,x) : x \in S, t \geq 0\} < \infty$



- Generate points $S_1, S_2, \ldots$ according to a Poisson process with rate Λ
- Accept with prob. $\lambda(S_i, X(T))/\Lambda$
- At transition epoch, generate next state according to p.m.f. $(Q(S_i, X(T), y)/\lambda(S_i, X(T)) : y \in S)$

I. Discrete–Time Conversion

$Y = (Y_n : n \geq 0)$ embedded DTMC

To estimate $\alpha = Eg(X(t) : t \geq 0)$, note that

$$\alpha = EW$$

where $W = E[g(X(t) : t \geq 0)|Y]$.

e.g. $g(X(t) : t \geq 0) = \inf\{t \geq 0 : X(t) \in A\}$

$$W = \sum_{i=0}^{\tau_A - 1} 1/\lambda(Y_i)$$

$$\text{var } W \leq \text{var } g(X)$$

II. Antithetics

$X = (X(t) : t \geq 0)$ birth–death process

$$\begin{aligned} X_1(t) &= X(0) + N_+\left(\int_0^t \lambda(X_1(s))ds\right) - N_-\left(\int_0^t \mu(X_1(s))ds\right) \\ X_2(t) &= X(0) + N_-\left(\int_0^t \lambda(X_2(s))ds\right) - N_+\left(\int_0^t \mu(X_2(s))ds\right) \end{aligned}$$

If $g(X)$ ($\triangleq g(X(t) : t \geq 0)$) is monotone in N_+, N_-, then

$$\operatorname{var}\left(\frac{g(X_1) + g(X_2)}{2}\right) < \operatorname{var} g(X).$$

III. Control Variates

Suppose we can compute $E\beta$. Then $\alpha = Eg(X)$ can be estimated via

$$g(X) - \lambda(\beta - E\beta).$$

Optimal λ^* (to reduce variance maximally) is

$$\lambda^* = \frac{\text{cov}(g(X), \beta)}{\text{var}\beta}$$

For any Markov jump process and function $f : [0, \infty) \times S \to R$,

$$M(t) \triangleq f(t, X(t)) - \int_0^t \left[\frac{\partial f(s, X(s))}{\partial s} + (Q(s) f_s)(X(s)) \right] ds$$

is a martingale, so

$$E_x M(t) = f(0, x).$$

If we wish to compute $E_x g(X(t))$, note that if we choose $\widetilde{f}$ as the solution to

$$\begin{aligned} \frac{\partial \widetilde{f}}{\partial s} &= Q\widetilde{f} \\ \text{s/t } \widetilde{f}(0) &= g, \end{aligned}$$

then $\dfrac{\partial \widetilde{f}(t-s, X(s))}{\partial s} + (Q\widetilde{f}_{t-s})(X(s)) = 0$ and we conclude that

$$E[\widetilde{f}(0, X(t)) - \widetilde{f}(t, x)] = 0$$

i.e. $g(X(t)) - \widetilde{f}(t, x)$ is a control

Schlögl Model

$$R_0 \underset{3}{\overset{1}{\rightleftarrows}} R \qquad R_2 + 2R \underset{1}{\overset{3}{\rightleftarrows}} 3R$$

$X_n(t) =$ # molecules at time t of a substance R in a volume n

X_n is a birth–death process with birth–death rates:

$$\begin{aligned} \widetilde{\lambda}_n(x) &= n(1 + 3x(x - 1/n)) \\ \widetilde{\mu}_n(x) &= n(3x + x(x - 1/n)(x - 2/n)) \end{aligned}$$

$$n^{-3/4}X_n(n^{1/2}t) - n^{1/4} \Rightarrow Z(t)$$

where

$$dZ(t) = -Z(t)^3 dt + 2\sqrt{2}dB(t)$$

In place of $\widetilde{f}(s, x) = E_x g(X(s))$, use

$$\widetilde{f}_{\text{approx}}(s, x) = \widetilde{E}_{n^{-3/4}x - n^{1/4}} g(n^{1/4} + n^{3/4}Z(n^{-1/2}t))$$

IV. Sensitivity Analysis

Goal: Compute $\alpha = Eg(X_1) - Eg(X_2)$

X_i: birth–death with birth rates $(\lambda_i(x) : x \geq 0)$ and death rates $(\mu_i(x) : x \geq 1)$.

$$\text{e.g.} \quad \begin{aligned} \lambda_1(x) &= \lambda(\theta, x) \\ \lambda_2(x) &= \lambda(\theta + h, x) \end{aligned}$$

$$X_i(t) = X_i(0) + N_+\left(\int_0^t \lambda_i(X_i(s))ds\right) - N_-\left(\int_0^t \mu(X_i(s))ds\right)$$

same N_+, N_-

Use of change–of–measure

P_λ: probability under which N evolves as a Poisson process with rate λ

$$
\begin{aligned}
P_{\lambda_2}(\tau_1 \in dt_1, \ldots, \tau_n \in dt_n) &= \prod_{i=1}^{n} \lambda_2 e^{-\lambda_2 t_i} dt_i \\
&= \prod_{i=1}^{n} \left(\frac{\lambda_2}{\lambda_1}\right) e^{-(\lambda_2-\lambda_1)t_i} \lambda_1 e^{-\lambda_1 t_i} dt_i \\
&= E_{\lambda_1} I(\tau_1 \in dt_1, \ldots, \tau_n \in dt_n) L_n
\end{aligned}
$$

$$
L_n = \exp\left(-(\lambda_2 - \lambda_1)T_n + \int_{[0,T_n]} (\log \lambda_2 - \log \lambda_1) N(ds)\right)
$$

More generally:

P_i: X evolves according to

$$X(t) = X(0) + N_+\left(\int_0^t \lambda_i(X(s))ds\right) - N_-\left(\int_0^t \mu(X(s))ds\right)$$

$$\begin{aligned} P_2(A) &= E_1 I(A) L(t) \\ L(t) &= \exp\Big(-\int_0^t \left(\lambda_2(X(s)) - \lambda_1(X(s))\right) ds \\ &\quad + \int_{[0,t]} \left(\log(\lambda_2(X(s-))) - \log(\lambda_1(X(s-)))\right) N_+(ds)\Big) \end{aligned}$$

For sensitivity analysis:

$$\lambda_2(x) = \lambda(h, x)$$

$$\begin{aligned} \frac{d}{dh} E_h g(X) &= E_0 g(X) \frac{d}{dh} L(h,t) \Big|_{h=0} \\ &= E_0 g(X) \left[\int_{[0,t]} \frac{\lambda'(0, X(s-))}{\lambda(0, X(s-))} N_+(ds) - \int_0^t \lambda'(0, X(s)) ds \right] \end{aligned}$$

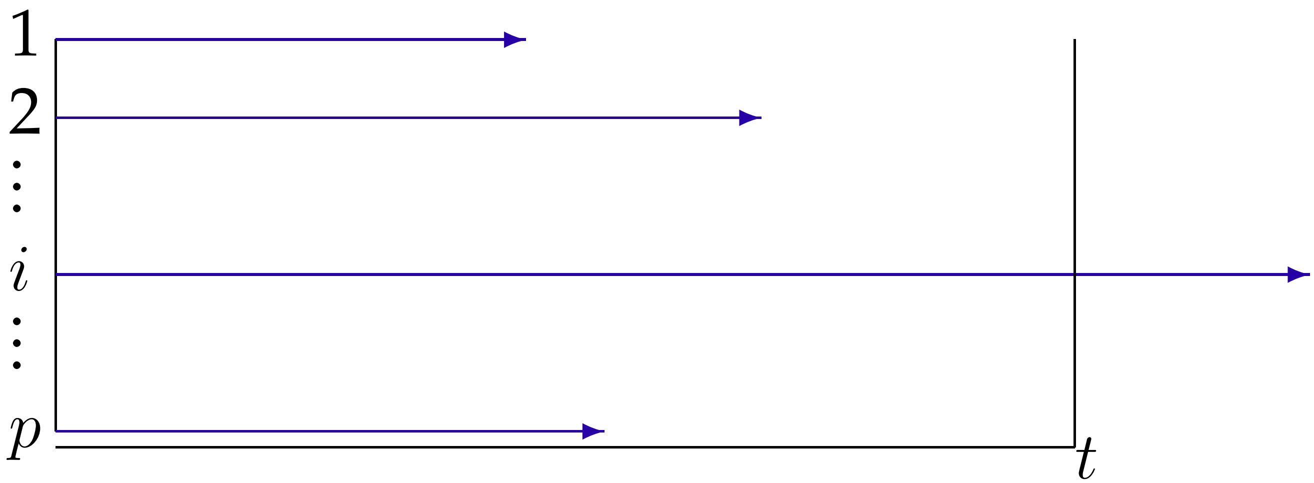
For rare–event simulation,

$$P_2(A) = E_1 I(A) L(t)$$

Choose λ_1 to simulate more rare reactions.

Massively Parallel Simulations

- Start same computation independently on many processors



- If one terminates computation at t, slowly running simulations are excluded from final estimate

  Bias!

Conclusions

- Review of discrete–event simulation and modeling
- Simulation of Markov jump processes
- Basic variance reduction techniques