

Examples and Computation of Finite-Time Properties of Continuous-Time Markov Chains

Thursday, October 30, 2008
12:05 PM

Examples: 1) Birth-death processes

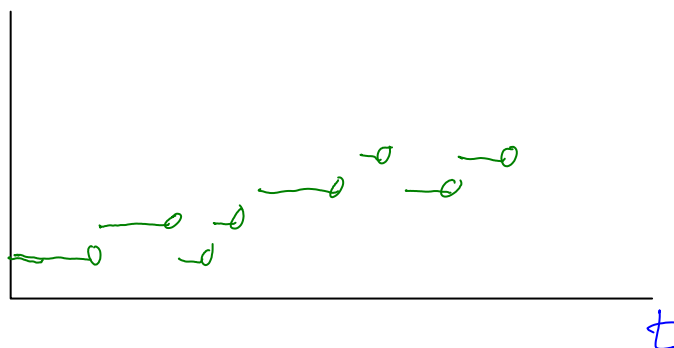
Tri-diagonal A

$$A_{i,j+1} = \lambda_i$$

$$A_{i,j-1} = \mu_i$$

$$A_{i,i} = -\lambda_i - \mu_i$$

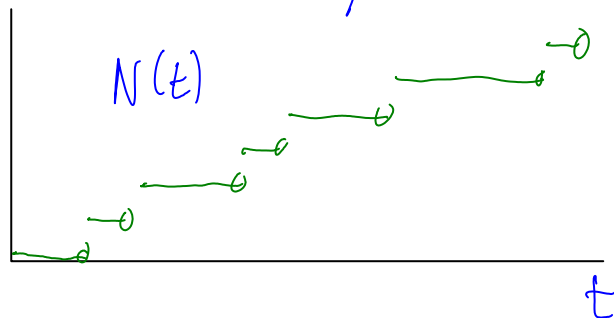
$$A_{i,j} = 0 \text{ for } |i-j| \geq 2$$



Many classical examples are special cases of birth-death processes:

a) Poisson counting process (arrivals, occurrence of random events)

$$\lambda_i = \lambda, \quad \mu_i = 0$$



b) Queueing models (k servers, queue can be unbounded)

$$\lambda_i = \lambda$$

$$\mu_i = \begin{cases} i\mu & \text{for } 0 \leq i < k \\ k\mu & \text{for } i \geq k \end{cases}$$

↑
single-server
rate

c) Population models

Various modeling possibilities

$$\lambda_i = \lambda_i \quad \text{or} \quad \lambda_i = \lambda i^2$$

$$\mu_i = \mu_i \quad \text{or} \quad \mu_i = \mu \frac{i^2}{K}$$

Compare logistic growth deterministic model:

$$\frac{dx}{dt} = \lambda x \left(1 - \frac{x}{K}\right)$$

↑ natural birth rate ↑ carrying capacity

But here we actually do encounter a possible problem with the technical conditions underlying the well-posedness of birth-death processes

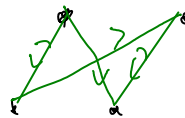
If we were to choose a birth-death process with

$$\lambda_i = \lambda i^2, \quad \mu_i = \frac{\mu i^2}{K}$$

violates the technical condition stated in [Karlin and Taylor Ch. 4, p. 135](#) which can happen when both the birth and death rates grow as the state value becomes large. Usually this is easily fixed by taking a more realistic model, such as slowing down the birth rate at large population values.

2) Finite-state processes without linear ordering

- atomic state transitions in atomic physics
- conformational changes in biomolecules
- climactic transitions



3) Biochemical networks

See the slides from last time.

How do we encode the list of reactions/processes into a transition rate matrix in a continuous-time Markov chain? Consider the heat shock model.

There are 9 basic molecules that are considered in that network, and they are labelled by mathematician as S_1 through S_9 . Then the state of the system is described by giving the number of each type of molecule present in the system.

$$\mathbb{X}(t) = (X_1(t), X_2(t), \dots, X_9(t))$$

where $X_j(t)$ is # molecules of type j .

Note that the individual $X_i(t)$ are by themselves not typically Markov chains because their values at earlier times can create delayed reactions on themselves through loops in the reaction network. On the other hand the vector of all these individual populations $\mathbb{X}(t)$ is generally very well modeled by a continuous time Markov chain, provided all relevant chemical species and environmental variables are taken into account.

How would we represent the process $\emptyset \rightarrow S_8$ in the transition rate matrix?

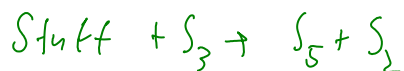
State $\mathbb{I} = (x_1, x_2, \dots, x_9)$

$$A_{\mathbb{I}\mathbb{J}} = 4.00 \times 10^0 \quad \text{for } \mathbb{J} = (x_1, x_2, \dots, x_8+1, x_9)$$

$$S_2 \rightarrow S_3$$

$$A_{\mathbb{I}\mathbb{J}} = 7.00 \times 10^{-1} x_2 \quad \text{for } \mathbb{J} = (x_1, x_2-1, x_3+1, x_4, \dots, x_9)$$

and $x_2 \geq 1$



$$A_{\mathbb{I}\mathbb{J}} = 6.3 \times 10^{-3} x_3 \quad \text{for } \mathbb{J} = (x_1, x_2+1, x_3-1, x_4, x_5+1, \dots, x_9)$$

The real challenge is how to simulate these continuous-time Markov chains in high dimensions.

Statistical computations for Continuous-Time Markov Chains

Let's first look at finite-time statistics. We'll generally consider time-homogenous continuous-time Markov chains. So then we are given a transition rate matrix A and an initial probability distribution $\vec{\phi}$

How do we calculate $P(t)$

where $P(t) = \{P_{ij}(t)\}$

$$P_{ij}(t) = P(\mathbb{X}(t) = j \mid \mathbb{X}(0) = i)$$

Again we derive this by knowing how it behaves infinitesimally through the Chapman-Kolmogorov equation

$$P_{ij}(t+s) = \sum_{k \in S} P_{ik}(t) P_{kj}(s)$$

Now we will use this together with our infinitesimal description for the evolution of the probability transition function

$$P_{ij}(t + \Delta t) = \sum_{k \in S} P_{ik}(\Delta t) P_{kj}(t)$$

$$P_{ik}(\Delta t) = \delta_{ik} + A_{ik} \Delta t + o_{ik}(\Delta t)$$

$$\left(\lim_{\Delta t \rightarrow 0} \frac{o_{ik}(\Delta t)}{\Delta t} \rightarrow 0 \right)$$

$$P_{ij}(t + \Delta t) \approx \sum_{k \in S} \left(\delta_{ik} + A_{ik} \Delta t + o_{ik}(\Delta t) \right) P_{kj}(t)$$

$$= P_{ij}(t) + \Delta t \sum_{k \in S} A_{ik} P_{kj}(t) + \sum_{k \in S} o_{ik}(\Delta t) P_{kj}(t)$$

$$\frac{P_{ij}(t + \Delta t) - P_{ij}(t)}{\Delta t} = \sum_{k \in S} A_{ik} P_{kj}(t) + \sum_{k \in S} \frac{o_{ik}(\Delta t)}{\Delta t} P_{kj}(t)$$

↪ goes to zero as $\Delta t \rightarrow 0$.

One has to be a bit careful about the error term because each term clearly goes to zero, but does the infinite sum also converge to zero? Here it's not so difficult to show because the $|P_{kj}(t)| \leq 1$

$$\text{and } \sum_{k \in S} \frac{o_{ik}(\Delta t)}{\Delta t} = - \frac{\bar{o}_i(\Delta t)}{\Delta t} \rightarrow 0 \quad \text{Karlin + Taylor Vol. I, II}$$

and use dominated convergence thm.

$$\frac{dP_{ij}(t)}{dt} = \sum_{k \in S} A_{ik} P_{kj}(t)$$

$$\frac{dP}{dt}(t) = A P(t) \quad \text{Kolmogorov Backward Equation}$$

$$P(t=0) = I$$

$$P(t=0) = I$$

There is also the **Kolmogorov forward equation**

$$\frac{dP(t)}{dt} = P(t) A$$

$$P(t=0) = I$$

This is derived in the same way as the Kolmogorov backward equation, starting from the Chapman-Kolmogorov equation, but now one sets up the calculation:

$$P_{ij}(t+\Delta t) = \sum_{k \in S} P_{ik}(t) P_{kj}(\Delta t)$$

It turns out that in the infinite-state case, the Kolmogorov backward equation is valid under wider conditions than the Kolmogorov forward equation.

Both equations, when they are well-defined have the same solution:

$$P(t) = e^{At} = \sum_{j=0}^{\infty} \frac{(At)^j}{j!}$$

This is well-defined and convergent certainly for finite-state matrices.

Practical ways to compute matrix exponentials for finite-state matrices:

- change basis to diagonalize the matrix

$$A = C D C^{-1}$$

↖ diagonal or Jordan

$$A^j = C D^j C^{-1}$$

$$e^{At} = C e^{Dt} C^{-1}$$

$$D = \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_m \end{pmatrix} \quad e^{Dt} = \begin{pmatrix} e^{\lambda_1 t} & & 0 \\ & e^{\lambda_2 t} & \\ 0 & & \ddots \\ & & & e^{\lambda_m t} \end{pmatrix}$$

"Nineteen Dubious Ways to Compute the Exponential of a Matrix, Twenty-Five Years Later," Clive Moler, Charles van Loan, SIAM Review

45, p. 3 (2003).

↓
MATLAB inventor

For the infinite state case, matrix exponentials are not so useful for computation and typically it's better just to work directly with the differential equations.

The Kolmogorov forward and backward equation give identical solutions for the probability transition function but each has a separate natural use when discussing other statistical properties of the continuous-time Markov chain.

Applied Math Days this weekend:

<http://appliedmathdays.math.rpi.edu>