Quasistationary Distributions for Continuous-Time Markov Chains

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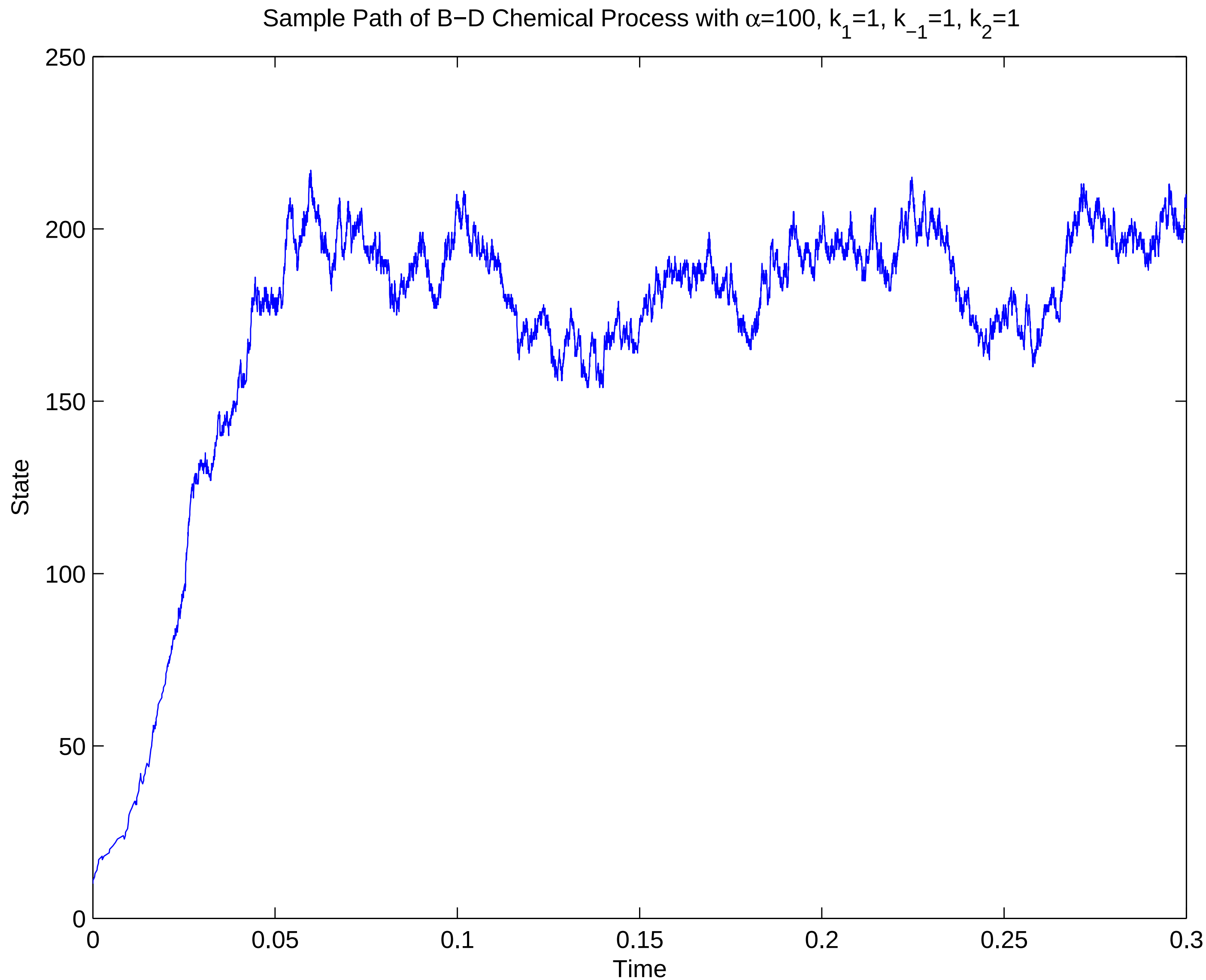
Quasi-Stationary Behaviour



We will:

- Briefly review some facts about continuous-time Markov chains (CTMCs).
- Look at this type of behaviour in the context of a chemical reaction.
- Look at the analytical tools available to describe this behaviour — quasistationary distributions (QSDs) and limiting conditional distributions (LCDs).
- Look at the tools available to establish the existence of QSDs.
- Briefly discuss numerical methods for establishing approximations to these QSDs.

Recall . . .

- A time-homogeneous CTMC $(X(t),\ t \geq 0)$ taking values in a countable set S ($\mathbb{Z}^+$) is completely described by its *transition function* $P(t) = (p_{ij}(t),\ i,j \in S,\ t \geq 0)$.
- In practice we know only the *transition rates* $(p'_{ij}(0+) = q_{ij},\ i,j \in S)$.
- If we know P, we can in principle answer any question about the behaviour of the chain. The challenge is to try and answer these questions in terms of Q.
- We will assume that the process is absorbed with probability one, and is therefore regular (non-explosive).

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A Birth-Death Process is a CTMC with the property that if the chain is in state i, transitions can only be made to state $i-1$ or $i+1$. The q-matrix has the form

$$q_{ij} = \begin{cases} \lambda_i & \text{if } j = i+1 \\ \mu_i & \text{if } j = i-1,\ i \geq 1 \\ -(\lambda_i + \mu_i) & \text{if } j = i \geq 1 \\ -\lambda_0 & \text{if } j = i = 0 \\ 0 & \text{otherwise} \end{cases}$$

where $\lambda_i, \mu_i > 0, \quad \forall i \in C$. We also assume that $\lambda_0 = 0$.

Definitions

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$$\mathbb{P}_a(X(t) = j | X(t) \in C) = a_j,$$

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- A LCD must be quasistationary, but a QSD need not be limiting conditional.

Definitions

- A μ-invariant measure (over C) for P is a collection of numbers $m = (m_i,\ i \in C)$ which, for some $\mu > 0$, satisfy

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- A μ-invariant measure (over C) for Q is a collection of numbers $m = (m_i,\ i \in C)$ which, for some $\mu > 0$, satisfy

$$\sum_{i \in C} m_i q_{ij} = -\mu m_j, \qquad j \in C.$$

The Chemical Reaction

$$\mathrm{A} + \mathrm{X} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 2\mathrm{X}$$

$$\mathrm{X} \xrightarrow{k_2} \mathrm{B}$$

- Model the number of molecules of X with a CTMC — a birth-death process on $S = \{0\} \cup C$, where zero is absorbing and C is an irreducible transient class.

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- Model the number of molecules of X with a CTMC — a birth-death process on $S = \{0\} \cup C$, where zero is absorbing and C is an irreducible transient class.
- The system can be either *closed* or *open* with respect to A & B. $C = \{1, 2, \ldots, N\}$ or $\{1, 2, \ldots\}$, respectively.

Finite State Space

- Finite state space - easy because of Perron-Frobenius theory.
- The unique QSD (and LCD) is given by m such that

$$mP_C(t) = e^{-\nu t}m.$$

- This is equivalent to

$$mQ_C = -\nu m$$

where $-\nu$ is the eigenvalue with maximal real part (it is real and negative).

The Decay Parameter

- The quantity

$$\lambda_C := \lim_{t \to \infty} \frac{-\log(p_{ij}(t))}{t}$$

exists and is independent of $i, j \in C$.

- Called the decay parameter because

$$p_{ij}(t) \leq M_{ij} e^{-\lambda_C t}, \qquad 0 < M_{ij} < \infty.$$

- Can show that for a μ-invariant measure for P over C to exist, it is necessary that $(0 <)\mu \leq \lambda_C$.

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- However these expressions involve P and λ_C, which are not known and difficult/impossible to find analytically.

Infinite State Space

A solution m to $mQ_C = -\mu m$ also satisfies $mP_C(t) = e^{-\mu t}m$ (and is therefore a QSD) iff

$$\sum_{i \in C} y_i q_{ij} = -\kappa y_j, \qquad 0 \le y_i \le m_i,$$

has only the trivial solution for some (all) $\kappa < \mu$.

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- Conditions do not depend explicitly on P or λ_C.
- Do depend on having a particular μ, m to check.

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If m is a *finite* μ-invariant measure for Q (i.e. $\sum m_i < \infty$), then

$$\mu = \sum_{i \in C} m_i q_{ij}$$

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- This allows us to find *all* finite μ-invariant measures for Q, and we can then check which of these are QSDs using the previous result.
- When finding μ-invariant measures for Q, we can now eliminate μ explicitly from the system we need to solve, however this renders the system

$$\sum_{i \in C} m_i q_{ij} = -\mu(m) m_j, \qquad j \in C$$

non-linear in m.

Infinite State Space

If the equations

$$\sum_{i \in C} y_i q_{ij} = \kappa y_j, \qquad y_i \geq 0, \ \sum_i y_i < \infty$$

have only the trivial solution for some (all) $\kappa > 0$, then all finite μ-invariant measures for Q are also μ-invariant for P and are therefore QSDs.

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- If this condition holds, all we have to do is find a μ-invariant measure for Q and this is a QSD.
- But we want it to be λ_C-invariant, so that we have the LCD.

Birth-Death Process

For a B-D process with which is absorbed with probability one, suppose the initial distribution has compact support. Then

- If $\mathcal{D} < \infty$ then there is a unique QSD which is the LCD.
- If $\mathcal{D} = \infty$ then either
  - $\lambda_C = 0$ and there are no QSDs, or
  - $\lambda_C > 0$ and there is a one-parameter family of QSDs, one of which is the LCD.

Here

$$\mathcal{D} = \sum_{n=1}^{\infty} \frac{1}{\mu_n \pi_n} \sum_{m=n}^{\infty} \pi_m, \qquad \pi_n = \frac{\lambda_1 \cdots \lambda_{n-1}}{\mu_2 \cdots \mu_n}.$$

The Chemical Reaction

- For the (B-D) chemical system, one can show that

$$\mathcal{D} = \sum_{n=1}^{\infty} \frac{n\Gamma(n+r)}{[nk_2 + n(n-1)\frac{k_{-1}}{2}](\alpha s)^{n-1}} \sum_{m=n}^{\infty} \frac{(\alpha s)^{m-1}}{m\Gamma(m+r)},$$

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  and that this is in fact finite.

- So there is a unique quasistationary distribution, which is limiting conditional.

A Connection

- It can be shown that for a Birth-Death process, the Reuter FE conditions hold iff $\mathcal{D} = \infty$.

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- It can be shown that for a Birth-Death process, the Reuter FE conditions hold iff $\mathcal{D} = \infty$.
- So, let's replace

$$\mathcal{D} \text{ diverges (converges)}$$

in van Doorns' result with

$$\text{the Reuter FE condition holds (fails)}$$

Infinite State Space

Conjecture: Suppose a process is absorbed with probability one, and that the initial distribution has compact support. Then

- If the Reuter FE conditions fail then there is only one μ-invariant measure; it is in fact λ_C-invariant and is therefore the LCD.
- If the Reuter FE conditions hold, either
  - $\lambda_C = 0$ and there are no QSDs (and no LCD), or
  - $\lambda_C > 0$ and there is a one-parameter family of μ-invariant measures (QSDs), $0 < \mu \leq \lambda_C$, of which the λ_C-invariant measure is the LCD.

Truncation Approximation

Having established the existence of a LCD, how do we go about approximating it, given that a closed form solution is almost never available?

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Having established the existence of a LCD, how do we go about approximating it, given that a closed form solution is almost never available?

Let $C^{(1)} \subset C^{(2)} \subset \cdots \subset C$ be a sequence of finite truncations of C. What happens to the solutions $m^{(n)}$ of

$$\sum_{i \in C^{(n)}} m_i^{(n)} q_{ij}^{(n)} = -\lambda^{(n)} m_j^{(n)}, \quad j \in C^{(n)},$$

where $-\lambda^{(n)}$ is the P-F maximal negative eigenvalue of $Q_{C^{(n)}}$, as $n \to \infty$?

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- But under what conditions does $m^{(n)}$ 'converge', in some sense?
- If $m^{(n)}$ converges, does it converge to m?
- Breyer & Hart (2000) give some sufficient conditions.
- We know:
  - Works for the Birth-Death Process.
  - Works for the subcritical Markov Branching Process.

Another Chemical Reaction

$$\mathrm{A} + \mathrm{X} \xrightarrow{k_1} 2\mathrm{X}$$

$$2\mathrm{X} \xrightarrow{k_2} \mathrm{B}$$

- This is not a Birth-Death process: it has jumps up of size 1, but jumps down of size 2.

The Quasi-Stationary Distribution