Quasistationary Distributions for Continuous-Time Markov Chains

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Quasi-Stationary Behaviour

Sample Path of B–D Chemical Process with $\alpha = 100$, $k_1 = 1$, $k_{-1} = 1$, $k_2 = 1$
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).
Recall . . .

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 $i + 1$. 
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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 $\lambda_i, \mu_i > 0, \ \forall i \in C$. We also assume that $\lambda_0 = 0$. 

Definitions

A distribution \( a = (a_i, \ i \in C) \) is a QSD over \( C \) if

\[
P_a(X(t) = j | X(t) \in C) = a_j,
\]

independently of \( t \).
Definitions

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  independently of $t$.

- A distribution $b = (b_i, \ i \in C)$ is a LCD over $C$ if for all $i, j \in C$,
  \[ \lim_{t \to \infty} P(X(t) = j | X(t) \in C, X(0) = i) = b_j. \]
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- A LCD must be quasistationary, but a QSD need not be limiting conditional.
A $\mu$-invariant measure (over $C$) for $P$ is a collection of numbers $m = (m_i, \ i \in C)$ which, for some $\mu > 0$, satisfy

$$\sum_{i \in C} m_ip_{ij}(t) = e^{-\mu t} m_j, \quad j \in C, \ t \geq 0.$$
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A $\mu$-invariant measure (over $C$) for $Q$ is a collection of numbers $m = (m_i, i \in C)$ which, for some $\mu > 0$, satisfy

$$\sum_{i \in C} m_i q_{ij} = -\mu m_j, \quad j \in C.$$
The Chemical Reaction

\[ A + X \xleftarrow{k_1} \xrightarrow{k_{-1}} 2X \]

\[ X \xrightarrow{k_2} B \]

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.
The Chemical Reaction

\[
\begin{align*}
A + X & \xrightarrow[k_1]{k_{-1}} 2X \\
X & \xrightarrow[k_2]{k_{-1}} B
\end{align*}
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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

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

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

Infinite state space - more difficult as Perron-Frobenius theory no longer applies.
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Again, the QSDs are given by $m$ such that

$$mP_C(t) = e^{-\nu t}m.$$
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- Again, the QSDs are given by $m$ such that
  $$mP_C(t) = e^{-\nu t}m.$$  
- The LCD (if it exists) is given by $m$ such that
  $$mP_C(t) = e^{-\lambda_C t}m.$$
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- Again, the QSDs are given by $m$ such that
  \[ mP_C(t) = e^{-\nu t}m. \]
- The LCD (if it exists) is given by $m$ such that
  \[ mP_C(t) = e^{-\lambda_C t}m. \]
- However these expressions involve $P$ and $\lambda_C$, which are not known and difficult/impossible to find analytically.
A solution $m$ to $mQ_C = -\mu m$ also satisfies $mP_C(t) = e^{-\mu t} m$ (and is therefore a QSD) iff

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

has only the trivial solution for some (all) $\kappa < \mu$. 
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- Conditions do not depend explicitly on $P$ or $\lambda_C$.
- Do depend on having a particular $\mu, m$ to check.
Infinite State Space

If \( m \) is a \textit{finite} \( \mu \)-invariant measure for \( Q \) (i.e. \( \sum m_i < \infty \)), then

\[
\mu = \sum_{i \in \mathcal{C}} m_i q_{ij}
\]

is necessary and sufficient for \( m \) to be a QSD.
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This allows us to find all finite \( \mu \)-invariant measures for \( Q \), and we can then check which of these are QSDs using the previous result.
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When finding \( \mu \)-invariant measures for \( Q \), we can now eliminate \( \mu \) explicitly from the system we need to solve, however this renders the system

\[ \sum_{i \in C} m_i q_{ij} = -\mu(m)m_j, \quad j \in C \]

non-linear in \( m \).
If the equations

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

have only the trivial solution for some (all) $\kappa > 0$, then all finite $\mu$-invariant measures for $Q$ are also $\mu$-invariant for $P$ and are therefore QSDs.
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If this condition holds, all we have to do is find a $\mu$-invariant measure for $Q$ and this is a QSD.
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have only the trivial solution for some (all) $\kappa > 0$, then all finite $\mu$-invariant measures for $Q$ are also $\mu$-invariant for $P$ and are therefore QSDs.

- If this condition holds, all we have to do is find a $\mu$-invariant measure for $Q$ and this is a QSD.
- But we want it to be $\lambda_C$-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 $D < \infty$ then there is a unique QSD which is the LCD.
- If $D = \infty$ then either
  - $\lambda_n = 0$ and there are no QSDs, or
  - $\lambda_n > 0$ and there is a one-parameter family of QSDs, one of which is the LCD.

Here

\[ D = \sum_{n=1}^{\infty} \frac{1}{\mu_n \pi_n} \sum_{m=n}^{\infty} \pi_m, \quad \pi_n = \frac{\lambda_1 \cdots \lambda_{n-1}}{\mu_2 \cdots \mu_n}. \]
The Chemical Reaction

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

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

So, let’s replace

$D$ diverges (converges)

in van Doorn’s result with

the Reuter FE condition holds (fails)
**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 \( \mu \)-invariant measure; it is in fact \( \lambda_C \)-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 \( \mu \)-invariant measures (QSDs), \( 0 < \mu \leq \lambda_C \), of which the \( \lambda_C \)-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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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 $n \to \infty$?
Truncation Approximation

We know that \( \lambda^{(n)} \downarrow \lambda_C \) as \( n \to \infty \).
Truncation Approximation

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- But under what conditions does $m^{(n)}$ ‘converge’, in some sense?
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Truncation Approximation

- We know that $\lambda^{(n)} \downarrow \lambda_C$ as $n \to \infty$.
- But under what conditions does $m^{(n)}$ ‘converge’, in some sense?
- If $m^{(n)}$ converges, does it converge to $m$?
- We know:
  - Works for the Birth-Death Process.
  - Works for the subcritical Markov Branching Process.
Another Chemical Reaction

\[ A + X \xrightarrow{k_1} 2X \]
\[ 2X \xrightarrow{k_2} B \]

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

Sample Path of B-D Chemical Process with $\alpha = 100$, $k_1 = 1$, $k_{-1} = 1$, $k_2 = 1$