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NOTE ON ZEIFMAN'S BOUNDS ON THE RATE OF CONVERGENCE FOR BIRTH–DEATH PROCESSES

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Abstract

It is shown that the method of deriving bounds on the rate of convergence for birth–death processes developed by Zeifman can be effectively applied to stochastic models of chemical reactions.

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1. Introduction: a bound due to Zeifman

This note is concerned with some practical applications of the method of bounding the convergence rate of birth–death processes developed by Zeifman, singly and with Granovsky [1]–[3], [7], [8]. Let $X(t),\ t \geq 0$, be a nonhomogeneous birth–death process taking values in a finite set $\mathcal{S} = \{0, 1, \ldots, N\},\ N \geq 1$, with birth rates $\{\lambda_n(t)\}$ and death rates $\{\mu_n(t)\},\ n \in \mathcal{S}$. Put $\lambda_N(t) \equiv \mu_0(t) \equiv 0$; it is assumed that all other transition rates are nonnegative, locally integrable functions on $[0, \infty)$. For probability vectors $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$, define $\boldsymbol{p}_1(t) = \boldsymbol{p}_1\boldsymbol{P}(0, t)$ and $\boldsymbol{p}_2(t) = \boldsymbol{p}_2\boldsymbol{P}(0, t)$, where $\boldsymbol{P}(s, t),\ 0 \leq s \leq t$, is the transition probability matrix of $X(t)$. Set

$$a(t) = \min_{0 \leq n < N} (\lambda_n(t) + \mu_{n+1}(t) - \lambda_{n+1}(t) - \mu_n(t)).$$

The results of [8] imply the following statement.

Proposition 1. *If* $\int_0^\infty a(t)\,\mathrm{d}t = +\infty$, *then, when* $0 \leq s \leq t$,

$$\|\boldsymbol{p}_2(t) - \boldsymbol{p}_1(t)\| \leq 4N \exp\left(-\int_s^t a(u)\,\mathrm{d}u\right)\|\boldsymbol{p}_2(s) - \boldsymbol{p}_1(s)\|, \tag{1}$$

where $\|\cdot\|$ *denotes the absolute entry sum for vectors.*

The bound (1) gives an estimate of the 'mixing rate' for $X(t)$. If the chain is time-homogeneous, then (1) provides a bound on the rate of convergence to stationarity. This inequality can also be used in combination with sensitivity bounds to assess the stability of $X(t)$ under perturbations; see [4] and references cited therein.

It turns out that the condition of Proposition 1 is naturally satisfied for certain birth–death-type stochastic models of reversible chemical reactions; see [6] for background on stochastic modeling in chemical kinetics. This allows us to obtain simple bounds which relate the rate of convergence to the parameters of the model. We give some examples in the next section.

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2. Application to stochastic models of chemical reactions

Convergence bounds, such as (1), can provide important information about the behaviour of the chemical system under study. For reactions at a constant temperature, it is often desirable to know when the reaction becomes close to the state of chemical equilibrium. Since this state corresponds to the stationary state of the stochastic model, we can use convergence bounds to assess the duration of the nonequilibrium phase. In the case of varying rates, we may be interested in knowing when the dependence of the state probability distribution on the initial distribution becomes negligible; again, we may use convergence bounds to answer this question. The above-mentioned combination of sensitivity bounds and convergence bounds (see Section 1) allows us to estimate the sensitivity of the system to changes in the reaction rates; this may be necessary because, as a rule, there is some uncertainty about the numerical values for the rates, which are derived from experimental data.

In this section we apply the bound (1) to the four stochastic models of chemical reactions discussed in [5]. We suppose that the rate constants for the reactions, $k_1(t)$ and $k_2(t)$, may vary with t (such variations can be caused by quasi-equilibrium temperature changes in the reaction compartment). It is natural to assume that $\inf_{t\geq 0} k_1(t) > 0$ and $\inf_{t\geq 0} k_2(t) > 0$; this assumption implies that Proposition 1 holds for the models considered.

Example 1. (*The reaction* $A + B \rightleftharpoons C$.) Suppose that the reaction takes place in a closed compartment of volume V. Let α, β and γ be the respective initial numbers of molecules of the species A, B and C; we assume that $\alpha \geq \beta$. Suppose that at time t the system contains n_1, n_2 and n_3 molecules of A, B and C respectively. If $n_1, n_2 > 0$, then, for the reaction $A + B \to C$, the probability that a single reaction event occurs in the time interval $(t, t + \Delta t)$ equals $(k_1(t)/V)n_1 n_2 \Delta t + o(\Delta t)$; if $n_3 > 0$, then, for the reaction $C \to A + B$, the probability is $k_2(t)n_3\Delta t + o(\Delta t)$. It is easily seen that

$$n_1 = \alpha + \gamma - n_3, \qquad n_2 = \beta + \gamma - n_3, \qquad 0 \leq n_3 \leq \beta + \gamma.$$

Thus, the changes in the number of molecules of C may be described by a birth–death process taking values in $\{0, 1, \ldots, N\}$, where $N = \beta + \gamma$; the transition rates are given by

$$\lambda_n(t) = \frac{k_1(t)}{V}(\alpha + \gamma - n)(\beta + \gamma - n),$$
$$\mu_n(t) = k_2(t)n.$$

We obtain that

$$a(t) = \frac{k_1(t)}{V}(\alpha - \beta + 1) + k_2(t).$$

In the following examples, $\alpha, \beta, \gamma, \delta$ denote nonnegative integers such that $\alpha \geq \beta$ and $\delta \geq \gamma$; for further details, see [5] and references cited therein.

Example 2. (*The reaction* $A + B \rightleftharpoons C + D$.) The corresponding stochastic model is a birth–death process over $\{0, 1, \ldots, N\}$, where $N = \beta + \gamma$; the birth and death rates are given by

$$\lambda_n(t) = \frac{k_1(t)}{V}(\alpha + \gamma - n)(\beta + \gamma - n),$$
$$\mu_n(t) = \frac{k_2(t)}{V}n(n + \delta - \gamma).$$

We obtain that

$$a(t) = \begin{cases} \dfrac{k_1(t)}{V}(\alpha - \beta + 1) + \dfrac{k_2(t)}{V}(\delta - \gamma + 2N - 1), & k_1(t) \geq k_2(t), \\ \dfrac{k_1(t)}{V}(\alpha + \beta + 2\gamma - 1) + \dfrac{k_2(t)}{V}(\delta - \gamma + 1), & k_1(t) \leq k_2(t). \end{cases}$$

Example 3. (*The reaction* $A + B \rightleftharpoons 2C$.) The continuous-time Markov chain which models this reaction takes values in $\{0, 2, 4, \ldots, M\}$, where $M = 2\beta + \gamma$ and γ is assumed to be even. Only transitions $n \to n \pm 2$ are possible; denoting the transition rates for forward and backward jumps by $\hat{\lambda}_n(t)$ and $\hat{\mu}_n(t)$ respectively, we set

$$\hat{\lambda}_n(t) = \frac{1}{4}\frac{k_1(t)}{V}(2\alpha + \gamma - n)(2\beta + \gamma - n),$$
$$\hat{\mu}_n(t) = \frac{1}{2}\frac{k_2(t)}{V}n(n-1).$$

It is easily seen that the reaction may be described by the process $2X(t)$, where $X(t)$ is a birth–death process over $\{0, 1, \ldots, M/2\}$ with transition rates given by

$$\lambda_n(t) = \frac{1}{4}\frac{k_1(t)}{V}(2\alpha + \gamma - 2n)(2\beta + \gamma - 2n),$$
$$\mu_n(t) = \frac{k_2(t)}{V}n(2n-1).$$

For $X(t)$, we obtain that

$$\begin{cases} \dfrac{k_1(t)}{V}(\alpha - \beta + 1) + \dfrac{k_2(t)}{V}(2M - 3), & k_1(t) \geq 2k_2(t), \\ \dfrac{k_1(t)}{V}(\alpha + \beta + \gamma - 1) + \dfrac{k_2(t)}{V}, & k_1(t) \leq 2k_2(t). \end{cases}$$

Example 4. (*The reaction* $A \rightleftharpoons 2C$.) The corresponding model is a continuous-time Markov chain taking values in $\{0, 2, 4, \ldots, M\}$, where $M = 2\alpha + \gamma$ (γ is even). The transition rates (for jumps of size 2) are given by

$$\hat{\lambda}_n(t) = \frac{1}{2}k_1(t)(2\alpha + \gamma - n),$$
$$\hat{\mu}_n(t) = \frac{1}{2}\frac{k_2(t)}{V}n(n-1).$$

This reaction may be described by the process $2X(t)$, where $X(t)$ is a birth–death process over $\{0, 1, \ldots, M/2\}$ with transition rates given by

$$\lambda_n(t) = \frac{1}{2}k_1(t)(2\alpha + \gamma - 2n),$$
$$\mu_n(t) = \frac{k_2(t)}{V}n(2n-1).$$

For $X(t)$, we obtain that

$$a(t) = k_1(t) + \frac{k_2(t)}{V}.$$

Remark 1. For the reactions in Examples 1–4, in a similar way to the above, we can obtain convergence bounds in the cases where $k_1(t) \equiv 0$ or $k_2(t) \equiv 0$ (irreversible reactions).

Suppose now that $X(t)$ is time-homogeneous, so that $k_1(t) \equiv k_1$, $k_2(t) \equiv k_2$, $\lambda_n(t) \equiv \lambda_n$, $\mu_n(t) \equiv \mu_n$ and $a(t) \equiv a$. The quantity a is a lower bound on the decay parameter of $X(t)$; the latter, as is well known, equals the spectral gap of the generator. If $a > 0$, then

$$b := \max_{0 \le n < N} (\lambda_n + \mu_{n+1} - \lambda_{n+1} - \mu_n)$$

is an upper bound on the decay parameter [8]. It is interesting to note that in Example 2 we have $a = b$ if $k_1 = k_2$. Thus, in this case, Zeifman's estimates give exactly the decay parameter; the upper and lower bounds on the decay parameter are especially sharp if k_1 is near k_2. In Example 3, we have $a = b$ if $k_1 = 2k_2$.

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