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LAW OF LARGE NUMBERS IN THE SUPREMUM NORM FOR A CHEMICAL REACTION WITH DIFFUSION[1]

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A space-time jump Markov process, modeling a chemical reaction with diffusion, is compared in the supremum norm to the usual model, the solution to a partial differential equation. Conditions are given which imply the deviation converges in probability to 0 uniformly on bounded time intervals. Estimates reflecting underlying large deviation behavior are obtained.

1. Introduction. In Arnold and Theodosopulu (1980) a stochastic model of a chemical reaction with diffusion was constructed and compared with the usual deterministic model, the solution of a partial differential equation. This model has been studied further by Kotelenez [(1982a), (1982b), (1986a), (1986b), (1987), (1988)]. The model, a space-time jump Markov process, is constructed by dividing $[0, 1]^q$ into N^q congruent cells of volume N^{-q} and modeling the concentration within a cell by a density-dependent birth and death process rescaled by l^{-1}, where l is a parameter proportional to the initial number of particles in a cell [see Kurtz (1971) or Ethier and Kurtz (1986)]. Also, particles diffuse symmetrically to neighboring cells with a jump rate proportional to N^2. This couples the cell reactors and extends the model of Kurtz (1971) to the spatially inhomogeneous case.

In Kotelenez (1986a), for a linear reaction (branching random walks) with $q = 1$, it was shown that $N^2/l \to 0$ is sufficient to prove a law of large numbers in $L_2([0, 1])$. In Blount [(1987), (1991)] this was improved by only requiring $l \to \infty$ as $N \to \infty$. In Kotelenez (1988), for a nonlinear reaction, a law of large numbers was shown to hold in a space of distributions rather than $L_2([0, 1]^q)$. In this paper we prove the law of large numbers holds in the supremum norm for any dimension q if $\log N/l \to 0$ as $N \to \infty$. The reaction may be linear or nonlinear. We believe our result is necessary as well as sufficient but have not proved this. However, we do give a nontrivial example, Example 4.19, which suggests the conditions are necessary. We obtain an estimate, (4.18), which reflects underlying large deviation behavior.

For simplicity we prove the result for $q = 1$ with periodic boundary conditions but remark at the end of the proof on the minor notational changes needed for extending the result to $q > 1$.

References to related work may be found in the papers of Kotelenez. We have only stated previous results that compare directly with this paper.

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Note that within a proof we may use the same symbol for different constants that depend on the same parameters so long as these are not N or l. Theorems, lemmas and numbered equations are considered on the same numbering system.

2. The deterministic model. Let $R(x) = b(x) - d(x) = \sum_{i=0}^{m} c_i x^i$ be a polynomial for $x \in \mathbf{R}$, with $c_m < 0$ and $b(x)$, $d(x)$ being polynomials of degree less than or equal to m with nonnegative coefficients. Assume $d(0) = 0$. For one reactant in the unit interval with periodic boundary conditions the concentration is given by $\psi(t, r)$, where, for $r \in [0, 1]$ and $t \geq 0$,

$$\begin{aligned} &\frac{\partial}{\partial t}\psi(t,r) = \Delta\psi(t,r) + R(\psi(t,r)), \\ (2.1)\qquad &\psi(t,0) = \psi(t,1), \\ &0 \leq \psi(0,r) < \rho < \infty. \end{aligned}$$

Δ denotes the Laplacian. Let $\psi(t) = \psi(t, \cdot)$ and note that $R(x) < 0$ for all large x. We assume ρ large enough so that $R(x) < 0$ for $x > \rho$ and that $\psi(0) \in C^3([0, 1])$, functions on $[0, 1]$ with three continuous derivatives and norm given by $\sum_{i=0}^{3} \|\psi^{(i)}\|_\infty$ where $\|\cdot\|_\infty$ denotes the supremum norm. In Kotelenez (1986b) it is shown that (2.1) has a unique mild solution in $C([0, \infty); C^3([0, 1]))$ and that $0 \leq \psi(t) < \rho$ for all $t > 0$.

Let H^N denote the real-valued step functions on $[0, 1]$ that are constant on the intervals $[kN^{-1}, (k+1)N^{-1})$, $0 \leq k \leq N-1$, where $N \geq 1$ is an integer; we extend functions in H^N to be periodic with period 1. For $f \in H^N$, let

$$\nabla_N^{\pm} f(r) = N(f(r \pm N^{-1}) - f(r))$$

and

$$\begin{aligned} \Delta_N f(r) &= -\nabla_N^{+}\nabla_N^{-} f(r) \\ &= -\nabla_N^{-}\nabla_N^{+} f(r) = N^2\left[f(r+N^{-1}) - 2f(r) + f(r-N^{-1})\right]. \end{aligned}$$

Rather than work directly with ψ, we use a spatially discretized version given by the solution of the differential equation

$$\begin{aligned} &\frac{\partial\psi^N(t,r)}{\partial t} = \Delta_N\psi^N(t,r) + R(\psi^N(t,r)), \\ (2.2)\quad &\psi^N(t,0) = \psi^N(t,1), \\ &\psi^N(0,r) = N\int_{kN^{-1}}^{(k+1)N^{-1}} \psi(0,u)\,du \quad \text{for } r \in [kN^{-1}, (k+1)N^{-1}). \end{aligned}$$

Set $\psi^N(t) = \psi^N(t, \cdot)$. From Kotelenez (1986b), we have

$$(2.3)\qquad 0 \leq \psi^N(t) < \rho \quad \text{for all } t$$

and

$$(2.4)\qquad \sup_{[0,T]} \|\psi^N(t) - \psi(t)\|_\infty \leq C(T, R, \psi(0))N^{-1} \quad \text{for } T > 0.$$

If N is an odd integer with $0 \le m \le N-1$ and m even, let $\varphi_{0,N} \equiv 1$ and define $\varphi_{m,N}(r) = \sqrt{2}\cos(\pi mkN^{-1})$ and $\psi_{m,N}(r) = \sqrt{2}\sin(\pi mkN^{-1})$ for $r \in [kN^{-1},(k+1)N^{-1})$. $\{\varphi_{m,N}, \psi_{m,N}\}$ are eigenvectors of Δ_N with eigenvalues defined by $-\beta_{m,N} = -2N^2(1-\cos(\pi mN^{-1})) \le 0$. For $f, g \in H^N$, the $L^2([0,1])$ inner product is given by $\langle f, g\rangle = \sum_{k=0}^{N-1} f(kN^{-1})g(kN^{-1})N^{-1}$. $\{\varphi_{m,N}, \psi_{m,N}\}$ form an orthonormal basis for $(H^N, \langle\cdot,\cdot\rangle)$. If N is even, we need the additional eigenfunction $\varphi_{N,N}(r) = \cos \pi k$ for $r \in [kN^{-1}, (k+1)N^{-1})$.

Let $T_N(t) = \exp(\Delta_N t)$ denote the semigroup on H^N generated by Δ_N. If $f \in H^N$, we have

$$T_N(t) f = \sum e^{-\beta_{m,N}t}\big(\langle f, \varphi_{m,N}\rangle \varphi_{m,N} + \langle f, \psi_{m,N}\rangle \psi_{m,N}\big). \tag{2.5}$$

Also note that for $f, g \in H^N$,

$$\langle \nabla_N^+ f, g\rangle = \langle f, \nabla_N^- g\rangle, \qquad T_N(t)\Delta_N f = \Delta_N T_N(t) f,$$

and Δ_N, $T_N(t)$ are self-adjoint on $(H^N, \langle\cdot,\cdot\rangle)$.

3. The stochastic model. Given $N \ge 1$ and a parameter $l > 0$, let

$$n(t) = (n_0(t), \dots, n_{N-1}(t))$$

denote the jump Markov process with integer-valued components and transition rates given by

$$\begin{aligned} (n_k, n_{k+1}) &\to (n_k - 1, n_{k+1} + 1) \quad \text{at rate } N^2 n_k,\\ (n_{k-1}, n_k) &\to (n_{k-1} + 1, n_k - 1) \quad \text{at rate } N^2 n_k,\\ n_k &\to n_k + 1 \quad \text{at rate } lb(n_k l^{-1}),\\ n_k &\to n_k - 1 \quad \text{at rate } ld(n_k l^{-1}). \end{aligned} \tag{3.1}$$

Here we set $n_N = n_0$ and $n_{-1} = n_{N-1}$ and b and d are the polynomials used to define (2.1). We view $n_k(t)$ as the number of particles in the kth cell at time t, where the cells are arranged on the unit circle. The last two jump rates reflect births or deaths in a cell and the first two reflect coupling of cells through diffusion. Particles diffuse on the circle according to simple random walks with jump rate $2N^2$ and particles are produced or removed within cells. Our subsequent assumptions will imply that l is proportional to the initial number of particles in each cell and that initially there are of order Nl particles distributed on the circle. We take $n(t)$ to be right-continuous with left limits and defined on some probability space.

Let $F_t^{N,l}$ denote the completion of the σ-algebra $\sigma(n(s): s \le t)$ and let $\delta n(t) = n(t) - n(t-)$ denote the jump at time t. If τ is an $F_t^{N,l}$ stopping time such that

$$\sup_{[0,T]} \sup_k I_{\{\tau > 0\}} n_k(t \wedge \tau) \le M(T, N, l) < \infty$$

for all $T > 0$, then as in Blount (1991) or Kotelenez (1988) we have:

3.2 LEMMA. *The following are $F_t^{N,l}$ martingales*:

(a)
$$n_k(t\wedge\tau) - N^2\int_0^{t\wedge\tau}(n_{k-1}(s) - 2n_k(s) + n_{k+1}(s))\,ds - \int_0^{t\wedge\tau} lR\big(n_k(s)l^{-1}\big)\,ds.$$

(b)
$$\sum_{s\le t\wedge\tau}(\delta n_k(s))^2 - N^2\int_0^{t\wedge\tau}(n_{k-1}(s) + 2n_k(s) + n_{k+1}(s))\,ds - \int_0^{t\wedge\tau} l\big(b\big(n_k(s)l^{-1}\big) + d\big(n_k(s)l^{-1}\big)\big)\,ds.$$

(c)
$$\sum_{s\le t\wedge\tau}(\delta n_{k+1}(s))(\delta n_k(s)) + N^2\int_0^{t\wedge\tau}(n_{k+1}(s) + n_k(s))\,ds.$$

Now we define the stochastic analogue of (2.1). Let

$$X^N(t,r) = n_k(t)l^{-1} \quad \text{for } r\in[kN^{-1},(k+1)N^{-1}).$$

$X^N(t,r)$ depends on N and l [as does $n(t)$], but we suppress the l in the superscript. Now let $X^N(t) = X^N(t,\cdot)$, and note that X^N is an H^N-valued Markov process. Using Lemma 3.2(a), we can write

$$X^N(t) = X^N(0) + \int_0^t \Delta_N X^N(s)\,ds + \int_0^t R(X^N(s))\,ds + Z^N(t), \tag{3.3}$$

where $Z^N(t\wedge\tau)$ is an $F_t^{N,l}$ martingale with values in H^N for τ as in Lemma 3.2.

4. The law of large numbers. In this section we prove the following result.

4.1 THEOREM. *Assume*:

(i) $\|X^N(0) - \psi(0)\|_\infty \to 0$ *in probability.*
(ii) $l = l(N)$ *satisfies* $\log N/l \to 0$ *as* $N\to\infty$.

Then $\sup_{[0,T]}\|X^N(t) - \psi(t)\|_\infty \to 0$ *in probability for any* $T>0$.

Before giving the proof we need some preliminary results and discussion.

4.2 LEMMA. $T_N(t)$ *is a positive contraction semigroup on* $(H^N, \|\cdot\|_\infty)$.

PROOF. If f is constant, then $T_N(t)f = f$, since $\Delta_N f = 0$. If $f\ge 0$, then $(2N^2+\Delta_N)f\ge 0$. Thus $T_N(t)f = \exp(-2N^2t)\exp[(2N^2+\Delta_N)t]f \ge 0$. These two facts imply the result. □

4.3 LEMMA. *Let* $f = NI_{[k/N,(k+1)/N)}$. *Then*

$$\left\langle (\nabla_N^+ T_N(t) f)^2 + (\nabla_N^- T_N(t) f)^2 + (T_N(t) f)^2, 1 \right\rangle \le h_N(t),$$

where $\int_0^t h_N(s)\,ds \le CN + t$.

PROOF. Using the observations at the end of Section 2, we have

$$\begin{aligned}
&\left\langle (\nabla_N^\pm T_N(t) f)^2, 1 \right\rangle \\
&\quad = -\langle T_N(2t) f, \Delta_N f \rangle \\
&\quad = \sum_m \left[\langle f, \varphi_{m,N} \rangle^2 + \langle f, \psi_{m,N} \rangle^2 \right] e^{-2\beta_{m,N} t} \beta_{m,N} \\
&\quad = \sum_m \left(\varphi_{m,N}^2(kN^{-1}) + \psi_{m,N}^2(kN^{-1}) \right) e^{-2\beta_{m,N} t} \beta_{m,N} \\
&\quad \le 2 \sum_m e^{-2\beta_{m,N} t} \beta_{m,N}.
\end{aligned}$$

Similarly $\langle (T_N(t) f)^2, 1 \rangle \le 1 + 2\Sigma_{m>0} e^{-2\beta_{m,N} t}$. The result then holds for $h_N(t) = 1 + 4\Sigma_{m>0} e^{-2\beta_{m,N} t}(\beta_{m,N} + 1)$, since $\beta_{0,N} = 0$ and $\beta_{m,N} > cm^2$ for $m > 0$ and $c > 0$, where c is independent of m and N. □

4.4 LEMMA. *Let* $m(t)$ *be a bounded martingale of finite variation defined on* $[t_0, t_1]$ *with* $m(t_0) = 0$ *and satisfying*:

(i) m *is right-continuous with left limits*.
(ii) $|\delta m(t)| \le 1$ *for* $t_0 \le t \le t_1$.
(iii) $\Sigma_{t_0 \le s \le t} (\delta m(s))^2 - \int_{t_0}^t g(s)\,ds$ *is a mean* 0 *martingale with* $0 \le g(s) \le h(s)$, *where* $h(s)$ *is a bounded deterministic function and* $g(s)$ *is* $F_t^{N,l}$ *adapted. Then* $E \exp(m(t_1)) \le \exp(\frac{3}{2}\int_{t_0}^{t_1} h(s)\,ds)$.

PROOF. Let $f(x) = e^x$ and note $0 \le f''(x+y) = f(x) f(y) \le 3 f(x)$ if $|y| \le 1$. Using change of variables for functions of bounded variation we have, for $t_0 \le t \le t_1$,

$$\begin{aligned}
f(m(t)) &= 1 + \int_{t_0}^t f'(m(s-))\,dm(s) \\
&\quad + \sum_{t_0 \le s \le t} \left[f(m(s)) - f(m(s-)) - f'(m(s-))\,\delta m(s) \right] \\
&\le 1 + \int_{t_0}^t f'(m(s-))\,dm(s) + \tfrac{3}{2} \sum_{t_0 \le s \le t} f(m(s-))(\delta m(s))^2,
\end{aligned}$$

by Taylor's theorem, (ii) and our observations at the start of the proof. Note that $\int_{t_0}^r f'(m(s-))\,dm(s)$ has mean 0 and after applying (iii) and taking expectations, we have $Ef(m(t)) \le 1 + \frac{3}{2}\int_{t_0}^t Ef(m(s)) h(s)\,ds$. The result then follows from Gronwall's inequality. □

Since $0 \le \psi(t) < \rho$ for all $t \ge 0$ and we are assuming $\|X^N(0) - \psi(0)\|_\infty \to 0$ in probability, we may, by conditioning on $\|X^N(0)\|_\infty < \rho$ if necessary, assume without loss of generality that

$$0 \le X^N(0) < \rho \quad \text{for all } N. \tag{4.5}$$

Also, by (2.4) it suffices to consider $\sup_{[0,T]}\|X^N(t) - \psi^N(t)\|_\infty$. Let $\tau = \inf\{t\colon \|X^N(t) - \psi^N(t)\|_\infty > \varepsilon_0\}$ for fixed $\varepsilon_0 \in (0,1]$ and define

$$\begin{aligned} \overline{X}^N(t) &= X^N(t\wedge\tau) \quad \text{for } 0 \le t \le \tau < \infty \text{ or } 0 \le t < \tau = \infty, \\ \overline{X}^N(t) &= X^N(t\wedge\tau) + \int_{t\wedge\tau}^t \Delta_N \overline{X}^N(s)\,ds \\ &\quad + \int_{t\wedge\tau}^t R(\overline{X}^N(s))\,ds \quad \text{for } \tau<t<\infty. \end{aligned} \tag{4.6}$$

$\overline{X}^N$ is obtained by running X^N until time τ and then running it deterministically afterwards (if $\tau < \infty$). We have

$$\begin{aligned} P&\Big[\sup_{[0,T]}\|X^N(t) - \psi^N(t)\|_\infty > \varepsilon_0\Big] \\ &\le P\Big[\sup_{[0,T]}\|X^N(t\wedge\tau) - \psi^N(t\wedge\tau)\|_\infty \ge \varepsilon_0\Big] \\ &\le P\Big[\sup_{[0,T]}\|\overline{X}^N(t) - \psi^N(t)\|_\infty \ge \varepsilon_0\Big], \end{aligned}$$

so we may consider $\sup_{[0,T]}\|\overline{X}^N(t) - \psi^N(t)\|_\infty$. We have

$$\overline{X}^N(t) = X^N(0) + \int_0^t \Delta_N \overline{X}^N(s)\,ds + \int_0^t R(\overline{X}^N(s))\,ds + Z^N(t\wedge\tau). \tag{4.7}$$

By our definitions, the jumps for X^N and $\overline{X}^N$ satisfy

$$\|\delta\overline{X}^N(t)\|_\infty = \|\delta X^N(t\wedge\tau)\|_\infty \le l^{-1}.$$

Since $0 \le \psi^N(t) < \rho$ for $t \ge 0$ and $l \to \infty$, we may assume that

$$0 \le X^N(t\wedge\tau) < \rho + 1 \quad \text{for } t \ge 0. \tag{4.8}$$

Using variation of constants we have that for $\tau < \infty$ and $t > \tau$,

$$\overline{X}^N(t) = T_N(t-\tau)X^N(\tau) + \int_\tau^t T_N(t-s)R(\overline{X}^N(s))\,ds.$$

By Lemma 4.2 and the definition of R, this shows we may also assume

$$0 \le \overline{X}^N(t) < \rho + 1 \quad \text{for } t \ge 0. \tag{4.9}$$

Using variation of constants we have

$$\begin{aligned} \overline{X}^N(t) - \psi^N(t) &= T_N(t)(X^N(0) - \psi^N(0)) \\ &\quad + \int_0^t T_N(t-s)\big(R(\overline{X}^N(s)) - R(\psi^N(s))\big)\,ds + Y^N(t), \end{aligned}$$

where $Y^N(t) = \int_0^t T_N(t-s)\,dZ^N(s\wedge\tau)$. Note that each $Z^N(s\wedge\tau, kN^{-1})$,

$0 \le k \le N-1$, is of bounded variation in s and T_N may be viewed as a continuous $N \times N$ matrix-valued function. Thus $Y^N(t, kN^{-1})$, $0 \le k \le N-1$, is defined as a Stieltjes integral. Using Lemma 4.2, (2.3) and (4.9), we have

$$\|\bar{X}^N(t) - \psi^N(t)\|_\infty$$
$$\le \|X^N(0) - \psi^N(0)\|_\infty + K\int_0^t \|\bar{X}^N(s) - \psi^N(s)\|_\infty\, ds + \|Y^N(t)\|_\infty,$$

where K depends on ρ and the coefficients of $R(x)$. By our previous discussion and Gronwall's inequality, Theorem 4.1 will follow from the following result.

4.10 LEMMA. $\sup_{[0,T]}\|Y^N(t)\|_\infty \to 0$ *in probability if* $\log N/l \to 0$ *as* $N \to \infty$.

PROOF. Fix $\bar{t} \in (0, T]$ and $k \in \{0, 1, \dots, N-1\}$ and let $f = NI_{[k/N,(k+1)/N)}$. Let $\bar{m}(t) = \langle \int_0^t T_N(\bar{t} - s)\, dZ^N(s \wedge \tau), f\rangle$ for $0 \le t \le \bar{t}$. Note that $\bar{m}$ is a mean 0 martingale on $0 \le t \le \bar{t}$ and $\bar{m}(\bar{t}) = Y^N(\bar{t}, kN^{-1})$ since $\langle g, f\rangle = g(kN^{-1})$ for $g \in H^N$. Basic computations using Lemma 3.2 show that, for $\psi \in H^N$,

$$(4.11)\qquad \begin{aligned} &\sum_{s \le t} (\delta\langle Z^N(s\wedge\tau), \varphi\rangle)^2 \\ &\quad -(Nl)^{-1}\int_0^{t\wedge\tau}\Big[\big\langle X^N(s), (\nabla_N^+\varphi)^2 + (\nabla_N^-\varphi)^2\big\rangle \\ &\qquad + \big\langle b(X^N(s)) + d(X^N(s)), \varphi^2\big\rangle\Big]\, ds \end{aligned}$$

is a mean 0 martingale. Thus, for $0 \le t \le \bar{t}$,

$$(4.12)\qquad \begin{aligned} &\sum_{s\le t} (\delta\bar{m}(s))^2 \\ &-(Nl)^{-1}\int_0^{t\wedge\tau}\big\langle X^N(s), (\nabla_N^+ T_N(\bar{t}-s)f)^2 + (\nabla_N^- T_N(\bar{t}-s)f)^2\big\rangle\, ds \\ &-(Nl)^{-1}\int_0^{t\wedge\tau}\big\langle b(X^N(s)) + d(X^N(s)), (T_N(\bar{t}-s)f)^2\big\rangle\, ds \end{aligned}$$

is a mean 0 martingale. Note that $|\delta\bar{m}(s)| \le l^{-1}$. For $\theta \in [0,1]$, let $m(t) = \theta l\bar{m}(t)$. Then $|\delta m(t)| \le 1$ and by Lemma 4.3, (4.8) and Lemma 4.4, we have

$$E\exp(\theta l\bar{m}(\bar{t})) \le \exp\big[c(\rho)\theta^2 l(1 + \bar{t}N^{-1})\big].$$

Since $\bar{t} \le T$, we may assume $\bar{t}/N \le 1$. Thus, for $\varepsilon > 0$, we have

$$\begin{aligned} P\big(Y^N(\bar{t}, kN^{-1}) > \varepsilon\big) &= P\big(\theta l Y^N(\bar{t}, kN^{-1}) > \theta l\varepsilon\big) \\ &\le E\exp\big(\theta l Y^N(\bar{t}, kN^{-1})\big)\exp(-\theta l\varepsilon) \\ &\le \exp\big[\theta l(c(\rho)\theta - \varepsilon)\big]. \end{aligned}$$

Thus we can choose θ so that

$$P\big[Y^N(\bar{t}, kN^{-1}) > \varepsilon\big] \le e^{-a\varepsilon^2 l} \quad \text{for } a = a(\rho) > 0,$$

independently of N, l, k and $\bar{t}$. The same holds for $P[-Y^N(\bar{t}, kN^{-1}) > \varepsilon]$. Thus, for $0 < t \le T$ and $k \in \{0, 1, \dots, N-1\}$, we have

$$P\big[|Y^N(t, kN^{-1})| > \varepsilon\big] \le 2e^{-a\varepsilon^2 l}.$$

Since $\|Y^N(t)\|_\infty = \sup_k |Y^N(t, kN^{-1})|$ and $Y^N(0) = 0$, we have

$$P\big[\|Y^N(t)\|_\infty > \varepsilon\big] \le 2Ne^{-a\varepsilon^2 l} \tag{4.13}$$

for $0 \le t \le T$ and $a = a(\rho) > 0$. We now show that (4.13) holds with $\|Y^N(t)\|_\infty$ replaced by $\sup_{[0,T]}\|Y^N(t)\|_\infty$ and N (on the right) replaced by N^3. We have $Y^N(t) = \int_0^t \Delta_N Y^N(s)\,ds + Z^N(t \wedge \tau)$. Thus for $nTN^{-2} \le t \le (n+1)TN^{-2}$ and $0 \le n \le N^2 - 1$, we have

$$Y^N(t) = Y^N(nTN^{-2}) + \int_{nTN^{-2}}^t \Delta_N Y^N(s)\,ds + \tilde{m}(t),$$

where $\tilde{m}(t) = Z^N(t \wedge \tau) - Z^N(nTN^{-2} \wedge \tau)$ for $nTN^{-2} \le t \le (n+1)TN^{-2}$. Taking norms and using the definition of Δ_N gives

$$\|Y^N(t)\|_\infty \le \|Y^N(nTN^{-2})\|_\infty + 4N^2 \int_{nTN^{-2}}^t \|Y^N(s)\|_\infty\,ds + \|\tilde{m}(t)\|_\infty.$$

Applying Gronwall's inequality shows

$$\begin{aligned} &\sup_{[nTN^{-2},(n+1)TN^{-2}]} \|Y^N(t)\|_\infty \\ &\quad \le \Big(\|Y^N(nTN^{-2})\|_\infty + \sup_{[nTN^{-2},(n+1)TN^{-2}]} \|\tilde{m}(t)\|_\infty\Big) e^{4T}. \end{aligned} \tag{4.14}$$

Fix $k \in \{0, 1, \dots, N-1\}$ and $\theta \in [0,1]$ and let $m(t) = \theta l \tilde{m}(t, kN^{-1})$. By Lemma 3.2(b) and the fact that $\delta Z^N(t, kN^{-1}) = \delta X^N(t, kN^{-1}) = l^{-1}\delta n_k(t)$,

$$\begin{aligned} \sum_{nTN^{-2} \le s \le t} (\delta m(s))^2 - \theta^2 l N^2 \int_{nTN^{-2}\wedge\tau}^{t\wedge\tau} \big[X^N(s,(k-1)N^{-1}) + 2X^N(s, kN^{-1}) \\ + X^N(s,(k+1)N^{-1})\big]\,ds \\ - \theta^2 l \int_{nTN^{-2}\wedge\tau}^{t\wedge\tau} \big[b(X^N(s,kN^{-1})) + d(X^N(s,kN^{-1}))\big]\,ds \end{aligned}$$

is a mean 0 martingale for $nTN^{-2} \le t \le (n+1)TN^{-2}$. Also $|\delta m(t)| \le 1$. By Lemma 4.4 and (4.8), we have

$$E\exp\big[m((n+1)TN^{-2})\big] \le \exp(c(\rho)\theta^2 lT).$$

Thus, applying Doob's inequality, we have

$$\begin{aligned} P\Big[\sup_{[nTN^{-2},(n+1)TN^{-2}]} \tilde{m}(t, kN^{-1}) \ge \varepsilon\Big] &\le E\exp\big[m((n+1)TN^{-2})\big]\exp(-\theta l\varepsilon) \\ &\le \exp(\theta l(c(\rho)T\theta - \varepsilon)) \\ &\le e^{-a\varepsilon^2 l} \quad \text{where } a = a(\rho, T) > 0. \end{aligned}$$

The same holds for $-\tilde{m}(t, k/N)$. But this shows

$$P\left[\sup_{[nTN^{-2},(n+1)TN^{-2}]} \|\tilde{m}(t)\|_\infty > \varepsilon\right] \le 2Ne^{-a\varepsilon^2 l}. \tag{4.15}$$

By (4.13), (4.14) and (4.15) we have

$$P\left[e^{-4T} \sup_{[nTN^{-2},(n+1)TN^{-2}]} \|Y^N(t)\|_\infty > \varepsilon\right] \le 4Ne^{-a\varepsilon^2 l}. \tag{4.16}$$

We also have

$$P\left[e^{-4T} \sup_{[0,T]} \|Y^N(t)\|_\infty > \varepsilon\right] \le \sum_{n=0}^{N^2-1} P\left[e^{-4T} \sup_{[nTN^{-2},(n+1)TN^{-2}]} \|Y^N(t)\|_\infty > \varepsilon\right].$$

By (4.16) this implies

$$P\left[e^{-4T} \sup_{[0,T]} \|Y^N(t)\|_\infty > \varepsilon\right] \le 4N^3 e^{-a\varepsilon^2 l}, \tag{4.17}$$

where $a = a(\rho, T) > 0$. And we have $\sup_{[0,T]}\|Y^N(t)\|_\infty$ converges to 0 in probability if $\log N/l \to 0$ as $N \to \infty$. This completes the proof of the lemma and Theorem 4.1. □

REMARK. Our result is easily extended to the q-dimensional hypercube, $[0, 1]^q$. In this case $[0, 1]^q$ is divided into N^q disjoint congruent cells of volume N^{-q}. Particles jump to each neighboring cell at rate N^2, or total rate $2qN^2$. Δ_N is given by

$$\Delta_N f(r_1, \dots, r_q) = \sum_{i=1}^{q} -\nabla_{N,i}^{+}\nabla_{N,i}^{-} f(r_1, \dots, r_q),$$

where

$$\nabla_{N,i}^{\pm} f(r_1, \dots, r_q) = N\left[f\left(r_1, \dots, r_i \pm N^{-1}, \dots, r_q\right) - f(r_1, \dots, r_q)\right].$$

Δ_N has N^q bounded eigenvectors formed by taking products of the one-dimensional eigenvectors.

Our final estimate, (4.17), now becomes

$$P\left[e^{-4T} \sup_{[0,T]} \|Y^N(t)\|_\infty > \varepsilon\right] \le 4N^{q+2} e^{-a\varepsilon^2 l}, \tag{4.18}$$

where the N^q arises from taking the supremum over all cells, as in (4.13) and (4.15). An important fact is that replacing N by N^q in Lemma 4.3 causes no change since this N^q is cancelled by replacing N^{-1} by N^{-q} in (4.12). Our result would also hold as well for reflecting boundary conditions. For a linear reaction one need only replace ρ by ρ_T.

Finally, we note that the idea of defining the martingale

$$\overline{m}(t) = \left\langle \int_0^t T_N(\bar{t} - s)\, dZ^N(s \wedge \tau), NI_{[k/N,(k+1)/N)} \right\rangle$$

to obtain information about $Y(\bar{t}, kN^{-1}) = \overline{m}(\bar{t})$ was used to bound the moments of X^N in Kotelenez (1988), but we have refined it here by bounding the moment generating function of $Y(\bar{t}, kN^{-1})$.

4.19 EXAMPLE. Assume the initial cell numbers $\{n_k(0): 0 \le k \le N-1\}$ are independent Poisson random variables, each with mean l. Also assume there is no reaction, only diffusion; that is, $b(x) = d(x) \equiv 0$. Then $X^N(t)$ has a stationary distribution with $\{lX^N(t, kN^{-1}): 0 \le k \le N-1\}$ being independent and mean l Poisson random variables for each $t \ge 0$. In this case, $\psi(t, r) \equiv 1$. Given $\varepsilon > 0$,

$$\begin{aligned} &P(\|X^N(0) - \psi(0)\|_\infty \ge \varepsilon) \\ &\quad \le \sum_{k=0}^{N-1} P(n_k(0) \ge l(1+\varepsilon)) + P(n_k(0) \le l(1-\varepsilon)) \\ &\quad = NP(n_1(0) \ge l(1+\varepsilon)) + NP(n_1(0) \le l(1-\varepsilon)) \\ &\quad \le 2N \exp[\theta l(\theta - \varepsilon)] \end{aligned}$$

for $\theta > 0$, after applying Markov's inequality and using the moment generating function of $n_1(0)$. Setting $\theta = \varepsilon/2$ shows that $\|X^N(0) - \psi(0)\|_\infty \to 0$ in probability if $\log N/l \to 0$ as $N \to \infty$. Thus, by Theorem 4.1, $\sup_{[0,T]}\|X^N(t) - \psi(t)\|_\infty \to 0$ in probability if $\log N/l \to 0$ as $N \to \infty$.

This can also be proved by an elementary argument as in Blount (1987). Conversely, we now show that if $N \to \infty$ and $\limsup(l/\log N) < \infty$, then one can choose $\varepsilon > 0$ such that

$$\limsup P\big[\|X^N(t) - \psi(t)\|_\infty \ge \varepsilon\big] \to 1 \quad \text{as } N \to \infty$$

for each fixed t. This will show that requiring $\log N/l \to 0$ as $N \to \infty$ is necessary for this special case.

By stationarity it suffices to consider $t = 0$. Let A_k be the event $\{n_k(0) \ge l(1+\varepsilon)\}$. Then

$$\begin{aligned} &1 - P(\|X^N(0) - \psi(0)\|_\infty \ge \varepsilon) \\ &\quad \le 1 - P\left(\bigcup_0^{N-1} A_k\right) = (1 - P(A_1))^N \le \exp(-NP(A_1)). \end{aligned} \tag{4.20}$$

Let $[\cdot]$ denote the greatest integer function. Then

$$\begin{aligned} NP(A_1) &\ge NP(n_1(0) = [l(1+\varepsilon)] + 1) \\ &\ge Ne^{-l} l^{l(1+\varepsilon)} / ([l(1+\varepsilon)] + 1)! \\ &\ge cNe^{-l} l^{l(1+\varepsilon)} e^{l(1+\varepsilon)} / \big(l^{1/2}(l(1+\varepsilon) + 1)^{l(1+\varepsilon)+1}\big), \end{aligned}$$

where we have applied Stirling's formula and $c = c(l)$ is bounded away from 0 for all large l. Thus,

$$\begin{aligned} NP(A_1) &\ge cNe^{\varepsilon l} / \big(l^{3/2}(1 + \varepsilon + l^{-1})^{l(1+\varepsilon+l^{-1})}\big) \\ &\ge cNl^{-3/2} \exp(-l(\varepsilon^2 + 2\varepsilon l^{-1} + l^{-1} + l^{-2})), \end{aligned}$$

where we have used $(1+x)^{-1} \geq e^{-x}$ for $x \geq 0$. If $\limsup(l/\log N) < \infty$, we can choose ε so that $\limsup NP(A_1) = \infty$. By (4.20), this implies $\limsup P(\|X^N(0) - \psi(0)\|_\infty \geq \varepsilon) = 1$.

Note that in this example one can obtain convergence by holding N fixed and letting $l \to \infty$ arbitrarily. However, this is because $\psi(t)$ is spatially homogeneous. If $\Delta\psi \not\equiv 0$, then letting $N \to \infty$ is necessary.

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