LARGE DEVIATION RESULTS FOR A CLASS OF MARKOV CHAINS ARISING FROM POPULATION GENETICS

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Let $\{X_n\}$ be a Markov chain on a bounded set in R^d with $E_x(X_1)=f_N(x)=x+\beta_Nh_N(x)$, where x_0 is a stable fixed point of $f_N(x)=x$, and $\operatorname{Cov}_x(X_1)\approx\sigma^2(x)/N$ in various senses. Let D be an open set containing x_0 , and assume $h_N(x)\to h(x)$ uniformly in D and either $\beta_N\equiv 1$ or $\beta_N\to 0$, $\beta_N\gg \sqrt{\log N/N}$. Then, assuming various regularity conditions and $X_0\in D$, the time the process takes to exit from D is logarithmically equivalent in probability to $e^{VN\beta_N}$, where V>0 is the solution of a variational problem of Freidlin–Wentzell type [if $\beta_N\to 0$ and d=1, $V=\inf\{2\int_x^\gamma \sigma^{-2}(u)|h(u)\,du|:y\in\partial D\}$]. These results apply to the Wright–Fisher model in population genetics, where $\{X_n\}$ represent gene frequencies and the average effect of forces such as selection and mutation are much stronger than effects due to finite population size.

1. Introduction and main results. The purpose here is to consider a class of Markov chains which are strongly attracted to a stable fixed point, and obtain results such as (i) the amount of time required to escape a fixed neighborhood of the stable fixed point, and (ii) the equilibrium probability that the process is found away from the fixed point. Specifically, for integers $N \ge 1$, let $\{X_n\}$ be a Markov chain on a bounded convex set Q in R^d such that

(1.1)
$$E_x(X_1) = f_N(x) = x + \beta_N h_N(x), \qquad h_N(x_0) = 0,$$

$$\operatorname{Cov}_x(X_1) \sim \sigma^2(x)/N \quad \text{as } N \to \infty,$$

in various senses [see (1.11) below]. Let D be a connected open set containing x_0 , and assume $h_N(x) \to h(x)$ uniformly in D. We also assume

$$|f_N(x) - x_0| \le (1 - \kappa \beta_N)|x - x_0|, \qquad \kappa > 0,$$

or a similar discrete Liapounov condition for $\{f_N\}$. Let $T_e = \min\{n: X_n \notin D\}$. Then, given sufficient regularity conditions on $\{X_n\}$, we show that there exist constants V>0 and $\omega_N\to 0$ such that

(1.2)
$$\lim_{N \to \infty} P_x \left(e^{N\beta_N (V - \omega_N)} \le T_e \le e^{N\beta_N (V + \omega_N)} \right) = 1, \quad \text{all } x \in D.$$

With additional conditions, we can also show

(1.3)
$$\log \mu_N(E) = -N\beta_N v(E)(1+o(1))$$
 as $N \to \infty$, $v(E) > 0$,

for open sets $E \subseteq Q$ such that $x_0 \notin \overline{E}$, where μ_N is the stationary distribution of

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 $\{X_n\}$. Two cases are considered, $\beta_N \to 0$ and $\beta_N \equiv 1$. If $\beta_N \to 0$ and the dimension d=1, the constants V and v(E) can be expressed in terms of integrals of h(x) and $\sigma^2(x)$. Our results for $\beta_N \to 0$ are extensions of results for solutions of the stochastic differential equation

(1.4)
$$dX_t = \varepsilon_N \sigma(X_t) dW_t + h(X_t) dt$$

with $1/\varepsilon_N^2$ in place of $N\beta_N$ in (1.2) and (1.3) [Freidlin and Wentzell (1984), Freidlin (1985) and Varadhan (1984); see also Kipnis and Newman (1985) and Day (1987)].

The conditions on $\{X_n\}$ given below simplify for Markov chains of the form

(1.5)
$$X_{n+1} \approx \frac{1}{N} \sum_{i=1}^{N} Y_{i,x}^{N}$$
, given $X_n = x$,

where $\{Y_{i,x}^N: 1 \le i \le N\}$ are i.i.d. random variables. Our motivating example is the Wright-Fisher model in population genetics, for which

(1.6)
$$X_{n+1} \approx \frac{B(N, f_N(x))}{N}, \text{ given } X_n = x,$$

where B(N, f) represents a multinomial random variable with frequencies $f \in \Delta^d$ for $\Delta^d = \{x \in R^d : x_i \geq 0, \sum x_i \leq 1\}$. Then X_n gives the joint frequencies of d+1 alleles in generation n, and (1.1) with $N\beta_N \to \infty$ models a situation in which the average effect of forces such as selection and mutation are significantly stronger than random effects due to the finite population size N. Nagylaki (1977) and Ewens (1979) are good general references for population genetics models.

If $N\beta_N \to \beta < \infty$ in (1.1), $\{X_n\}$ can be approximated by solutions of the stochastic differential equation

$$dX_t = \frac{1}{\sqrt{\beta}} \sigma(X_t) dW_t + h(X_t) dt, \qquad t \approx n\beta_N,$$

for bounded intervals of t [Trotter (1958) and Ethier and Kurtz (1986); see Ewens (1979) for biological examples]. If $N\beta_N \to \infty$, the deterministic forces act on a shorter time scale, and under additional assumptions

(1.7)
$$X_n \approx \varepsilon_N Y_t + Z_t, \quad t \approx n\beta_N, \quad \varepsilon_N = 1/\sqrt{N\beta_N},$$

where $\{Y_t\}$ is a mean-zero Gaussian process and $\{Z_t\}$ is a deterministic solution of Z'(t) = h(Z(t)) [Norman (1975) and Nagylaki (1986); see also Kurtz (1971, 1981), Barbour (1976, 1980) and Ethier and Kurtz (1986)]. The relation (1.7) suggests that $\{X_n\}$ spends most of its time near $\{Y_t\}$ in the time scale $t \approx n\beta_N$, but this is difficult to quantify since (1.7) is often only proven for $n\beta_N = O(1)$. Sawyer (1983) has a population genetics model in which an approximation of the form (1.7) for $n \gg N$ is crucial [note $1/\beta_N = o(N)$ in (1.7)], and for which $\{X_n\}$ remains near $\{Y_t\}$ for times of order $O(N^b)$ for all $b < \infty$. Barbour (1976) has similar conclusions for a continuous-time random walk model. An unpublished manuscript of Darden (1983) has large deviation results for the Wright-Fisher model with two alleles and heterotic selection.

Note that a Markov chain $\{X_n\}$ satisfying (1.1) can be written as

(1.8)
$$X_{n+1} \approx X_n + \beta_N \left(h_N(X_n) + \frac{1}{\beta_N} (X_{n+1} - f_N(X_n)) \right),$$

where $E_x(X_{n+1}|X_n) = f_N(X_n)$. Ventsel' (1976a, b, 1979, 1982) and Azencott and Ruget (1977) consider Markov chains of the form

(1.9)
$$Z_{n+1} \approx Z_n + \tau V_{Z_n} + o(\tau) \quad \text{as } \tau \to 0,$$

where, given $Z_n=z$, the term V_z has a fixed distribution μ_z independent of τ [see also Freidlin and Wentzell (1984), Chapter 5]. The models of Ventsel' (1979, 1982) are more general, but are still essentially of the form (1.9). Their arguments imply (1.2) with the scaling $1/\tau$ in place of $N\beta_N$, but are not sufficient to imply (1.2) for the Wright-Fisher model (1.6). Note that the scaling $N\beta_N$ appears in (1.2) for (1.8) rather than $1/\beta_N$, and $\beta_N\equiv 1$ is possible. Also, if $\beta_N\to 0$, the constant V in (1.2) turns out to be the same for (1.8) as for the approximating diffusion (1.4), while (1.9) generally leads to different formulas for V [Kushner (1982) and Freidlin and Wentzell (1984), Chapter 5, page 160]. In particular, Markov chain models with the same infinitesimal-variance diffusion approximations (1.4) can satisfy (1.2) with different large deviation constants V.

The proofs of our main results will essentially follow the outline of Ventsel' (1976a, b) and Freidlin and Wentzell (1984). However, new arguments for $\{X_n\}$ in (1.8) have to be introduced in many places, and the details of the dependence of the estimates on N and β_N are crucial. We proceed by linking certain tightness arguments (Propositions 3.1 and 3.2 below) with uniform upper and lower large deviation bounds (Propositions 4.1 and 4.2) for the Markov chains $\{X_n\}$. The arguments in Section 3 are the most novel from the point of view of large deviation theory, since the processes (1.8) do not have natural self-scaling properties. The proofs of our main results are given in Section 5. Section 2 is devoted to some preliminary lemmas.

We now state our main assumptions. Let $\{X_n\}$ be a Markov chain depending on a parameter N defined on a bounded convex set $Q\subseteq R^d$. Let D be a connected open subset of Q, and assume $D_{\delta}, D_{\eta}\subseteq Q$ for fixed $0<\delta<\eta$ where $D_{\varepsilon}=\{x\in R^d\colon |x-D|\leq \varepsilon\}$. In the following, doubly subscripted expressions such as $E_{x,\,t}(\Phi(X_1))$ and $\mathrm{Cov}_{x,\,t}(X_1)$ denote expectations and covariances with respect to the associated or Cramér-transformed distribution of X_1 , for example,

(1.10)
$$E_{x,t}(\Phi(X_1)) = \frac{E_x(\Phi(X_1)e^{tX_1})}{E_x(e^{tX_1})}.$$

Our basic assumptions for $\beta_N \to 0$ are

(1.11) (i)
$$f_N(x) = E_x(X_1) = x + \beta_N h_N(x)$$
, $h_N(x_0) = 0$, $x_0 \in D$.

(ii) For
$$\Sigma_N^2(x) = \text{Cov}_x(X_1)$$
, there exist $\varepsilon_0 > 0$, $C < \infty$ such that

$$0 < \frac{\varepsilon_0}{N} \le \Sigma_N^2(x) \le \frac{C}{N} < \infty$$
, all $x \in D_\eta$.

(iii) There exists $\omega > 0$ such that

$$\Sigma_{N,t}^2(x) = \text{Cov}_{x,t}(X_1) = \Sigma_N^2(x) + O\left(\frac{|t| + N\beta_N}{N^2}\right),$$

uniformly for $|t| \leq \omega N$ and $x \in D_n$.

(iv) $h_N(x) \to h(x)$ and $N\Sigma_N^2(x) \to \sigma^2(x)$ uniformly for $x \in D_\eta$, where $\sigma^2(x)$ and h(x) are continuously differentiable functions on the closed set D_η .

If $d \geq 2$, (1.11)(ii) means with respect to the natural ordering of Hermitian matrices; that is, it holds for the minimal and maximal eigenvalues of $\Sigma_N^2(x)$. By choosing smaller values of ω , ε_0 , and so forth, if need be, we can assume (1.11)(ii) holds for $\Sigma_{N,t}^2(x)$ for $|t| \leq \omega N$ and sufficiently large N. A crucial tool will be the use of the Legendre function

(1.12)
$$\lambda(N, x, u) = \sup_{t \in R^d} (tu - \log E_x(e^{tX_1})), \quad x, u \in D_{\eta},$$
$$= t(N, x, u)u - \log E_x(e^{t(N, x, u)X_1}),$$

which we assume is finite and uniquely attained for $N \ge 1$ and $x, u \in D_{\eta}$. Uniqueness follows from (1.11)(ii); a sufficient condition that the supremum be attained is

$$D_n \subset \operatorname{int}(\operatorname{conv.hull}(\operatorname{supp}(X_1))), \text{ given } X_0 = x \in D_n, N \ge 1$$

[see, e.g., Azencott and Ruget (1977)]. We also assume

(1.13)
$$\sup_{x, u \in D_n} |t(N, x, u)| \le C_3 N < \infty, \quad \text{all } N \ge 1,$$

which is a uniformity condition in N and x. In particular by (1.12) and (1.13) (recall that $X_n \in Q$ for a bounded set Q)

(1.14)
$$\sup_{x, u \in D_n} |\lambda(N, x, u)| \le C_4 N < \infty, \quad \text{all } N \ge 1.$$

In the Bernoulli case (1.6), conditions (1.11)(ii, iii), (1.13) and (1.14) hold whenever $f = f_N(x)$ is such that $f_i \geq \varepsilon > 0$ and $\sum_{i=1}^d f_i \leq 1 - \varepsilon$ for all $x \in D_\eta$ for some $\varepsilon > 0$. See the remarks at the end of the section. We also assume

$$(1.15) |f_N(x) - x_0| \le (1 - \kappa \beta_N) |x - x_0|, x \in D_n,$$

for some $\kappa > 0$. The condition (1.15) can be replaced by a more general Liapounov condition for $\{f_N\}$ in Theorems 1.1 and 1.2 below; see (3.4) in Section 3. If $\beta_N \to 0$, we assume that D is asymptotically stable for solutions of u' = h(u); that is,

(1.16)
$$u(0) \in D, \quad u'(t) = h(u(t)) \quad \text{for } 0 \le t \le L,$$
 implies $u(t) \in D, 0 \le t \le L.$

If $D = \{x: |x - x_0| < r\} \subseteq D_{\eta}$ for some r > 0, then (1.16) follows from (1.15) (see Lemma 5.3 in Section 5). If (1.16) fails but the other conditions still hold, (1.2)

and Theorems 1.1 and 1.2 below follow for initial values $X_0 \in B$ where B is the largest spherical neighborhood of x_0 contained in D.

We also need that for all $M < \infty$ there exists $C_M < \infty$ such that

$$(1.17) \left| \log E_x(e^{tX_1}) - \log E_y(e^{tX_1}) \right| \le C_M |t| |x - y|, |t| \le MN,$$

for $x, y \in D_{\eta}$. If (1.17) holds with $C_M|t|$ replaced by C_MMN for complex t, then (1.17) holds as stated by the Schwarz lemma. However, we only require (1.17) for real t. If $\{X_n\}$ is multinomial [i.e., (1.6)], (1.17) is equivalent to a uniform Lipschitz condition on $\{f_N(x)\}$. Finally, assume

(1.18)(i)
$$\lim_{N \to \infty} \frac{N\beta_N^2}{\log N} = \infty \quad \text{if } d = 1,$$

or

(1.18)(ii)
$$\lim_{N\to\infty} \frac{N\beta_N^2}{\log(N+q_N)} = \infty \quad \text{if } d \ge 2,$$

where

$$(1.19) q_N = \sup_{x \in D} E_x \left(e^{\lambda(N, x, X_1)} I(X_1 \in D_\delta) \right).$$

In general $q_N = O(N)$ if d=1, and $q_N = O(N^{d/2})$ for multinomial $\{X_n\}$ for $d \geq 1$ (see the remarks in Section 4 below). In these cases (1.18)(i, ii) are equivalent. Note that the conditional variance of the terms inside the large parentheses in (1.8) is proportional to $1/N\beta_N^2$, so that a condition like (1.18) may be essential.

For discrete trajectories $[u] = (u_n: 0 \le n \le T) \subseteq D_{\delta}$, define

$$S(N, T, [u]) = \sum_{n=0}^{T-1} \lambda(N, u_n, u_{n+1}),$$

$$V(N, x, y) = \inf\{S(N, T, [u]) : T \ge 1, [u] \subseteq D_\delta, u_0 = x, u_T = y\},$$

$$A_N(x) = \inf_{y \in D} V(N, x, y),$$

$$A_N = A_N(x_0),$$

for $\lambda(N, x, u)$ in (1.12). The function S is called the action of [u]; V(N, x, y) and $A_N(x)$ are the action potential and minimal action. The asymptotic behavior of V(N, x, y) for $\beta_N \to 0$ depends on

(1.21)
$$V(x, y) = \inf \left\{ \frac{1}{2} \int_{0}^{L} (u' - h(u), \sigma^{-2}(u)(u' - h(u))) dt : \\ L > 0, u(0) = x, u(L) = y, \{u(t)\} \subseteq D_{\delta} \right\}.$$

If d = 1, (1.21) can be evaluated in closed form, and is

$$V(x, y) = 2 \int_x^y \frac{|h(u)| du|}{\sigma^2(u)}.$$

If $d \ge 2$, we need a regularity condition on the boundary of D. Specifically, if $\beta_N \to 0$, we assume that for each $\gamma_0 \in \partial D$ such that

$$(1.22) V(x_0, y_0) = V = \inf_{y \in D^c} V(x_0, y),$$

there exists a right circular cone $C \subseteq Q$ with vertex y_0 , height h > 0 and interior angle $\alpha > 0$ such that $C \cap \overline{D} = \{y_0\}$. This condition is satisfied if the boundary ∂D is C^1 , and is sometimes described by saying that each solution $y_0 \in \partial D$ of (1.22) can be touched by a "well-sharpened pencil" from the outside of D. We suspect that our results are correct as long as each y_0 in (1.22) is a regular point for the Dirichlet problem in D, but we have not proven this. Theorems 1.1 and 1.2 below are false without some conditions on ∂D for $d \geq 2$.

Our main results are

THEOREM 1.1. Assume $\beta_N \to 0$. Then, under the above assumptions, there exist constants V > 0 and $\omega_N \to 0$ such that

(1.23)(i)
$$\lim_{N \to \infty} P_x \left(e^{N\beta_N(V - \omega_N)} \le T_e \le e^{N\beta_N(V + \omega_N)} \right) = 1$$

and

(1.23)(ii)
$$\lim_{N \to \infty} \frac{1}{N\beta_N} \log E_x(T_e) = V$$

for all $x \in D$, where V satisfies

(1.24)
$$\lim_{N \to \infty} \frac{A_N}{N\beta_N} = V = \inf_{y \in \partial D} V(x_0, y) > 0$$

for A_N in (1.20) and V(x, y) in (1.21).

If $\beta_N \equiv 1$, we assume instead of (1.11):

(i)
$$f_N(x) = E_x(X_1)$$
 satisfies $f_N(x_0) = x_0 \in D$.

(ii) For each $\omega < \infty$, there exists $C(\omega) < \infty$ such that

$$\Sigma_{N,t}^2(x) = \operatorname{Cov}_{x,t}(X_1) \le \frac{C(\omega)}{N},$$

uniformly for $|t| \leq \omega N$ and $x \in D$.

(iii)
$$\lim_{N\to\infty} f_N(x) = f(x)$$
 exists for all $x \in D$, where

(iv)
$$f: D \to D$$

We assume $\lambda(N, x, u)$ is defined and the supremum in (1.12) is uniquely attained for all $x \in D$ and $u \in Q$, and similarly (1.13)-(1.15) holds with $x, u \in D_{\eta}$

replaced by $x \in D$, $u \in Q$. We also assume

(1.26)
$$\lim_{N\to\infty} \frac{\lambda(N,x,u)}{N} = \lambda(x,u) \text{ exists for all } x\in D, u\in Q.$$

If $\{X_n\}$ are of the form (1.5) with $\{Y_{i,x}^N\}$ identically distributed in N, then $(1/N)\lambda(N,x,u)\equiv\lambda(x,u)$ and (1.26) holds automatically. When $\beta_N\equiv 1$, condition (1.16) is replaced by (1.25)(iv), and (1.17) is assumed to hold with " $C_M|t|$ " replaced by " C_MMN ." We also assume that (1.18) and (1.19) hold with q_N in (1.19) replaced by

(1.27)
$$q'_{N} = \sup_{x \in D} E_{x}(e^{\lambda(N, x, X_{1})}).$$

If $\beta_N \equiv 1$, the "well-sharpened pencil" condition is replaced by the weaker assumption that any solution y_0 of (1.22) is in the closure of the interior of the complement of D. Then we have

THEOREM 1.1. Assume $\beta_N \to 0$. Then, under the above assumptions, there exist constants V > 0 and $\omega_N \to 0$ such that

$$V = \lim_{N \to \infty} \frac{A_N}{N}$$

$$= \inf \left\{ \sum_{n=0}^{T-1} \lambda(u_n, u_{n+1}) \colon T \ge 1, \right.$$

$$u_0 = x_0, u_i \in D \ (0 \le i < T), u_T \in Q - D \right\}$$

for A_N in (1.20) and $\lambda(x, u)$ in (1.26).

As in Friedlin and Wentzell (1984), there is a corresponding result for stationary distributions. Let $E \subset Q$ be an open set such that $x_0 \notin \overline{E}$. Assume the hypotheses of either Theorem 1.1 or Theorem 1.2 with $D = Q - \overline{E}$ except that (i) (1.15) is required for all $x \in Q$, (ii) (1.16) or (1.25)(iv) need not be assumed, (iii) $\lambda(N, x, u)$ is defined and uniquely attained for $x, u \in Q$, with q_N in (1.18) and (1.19) replaced by

(1.29)
$$q_N'' = \sup_{x \in Q} E_x(e^{\lambda(N, x, X_1)}),$$

(iv) (1.25)(ii) is required for all $x \in Q$ for some $\omega > 0$ [in addition to either (1.11)(iii) or (1.25)(ii) as stated] and (v) for each N, the Markov chain $\{X_n\}$ is ergodic on some set $Q_N \subseteq Q$ with stationary distribution μ_N on Q_N . Then:

THEOREM 1.3. Assume $\beta_N \to 0$ or $\beta_N \equiv 1$. Then, as $N \to \infty$, under the above assumptions,

$$(1.30) \quad \log \mu_N(E) = -N\beta_N v(E)(1+o(1)), \qquad v(E) = \inf_{y \in E} V(x_0, y) > 0.$$

REMARKS. If $X_{n+1} \approx (1/N)\sum_{i=1}^{N} Y_{i,x}^{N}$ given $X_n = x$, where $\{Y_{i,x}^{N}\}$ are i.i.d. as in (1.5), then

$$\Sigma_{N,\,t}^2(x) = \frac{1}{N} \sigma_{N,\,t/N}^2(x),$$

where $\sigma_{N,s}^2(x) = \operatorname{Cov}_{x,s}(Y_i^N)$ is the covariance of Y_i^N with respect to the associated distribution of Y_i with weight e^{sY_i} . Since $Y_{i,x}^N \in Q$ are bounded, $\sigma_{N,s}^2(x) = \sigma_N^2(x) + O(|s|)$ uniformly in N and x. Hence, (1.11)(ii) holds if $\operatorname{Cov}_x(Y_i^N) \geq \varepsilon_0 > 0$, and (1.11)(iii) holds for arbitrary $\omega < \infty$. Assume

$$\lambda^{Y}(N, x, u) = \sup_{t \in R^{d}} \left(tu - \log E_{x}(e^{tY_{i}^{N}}) \right)$$
$$= t^{Y}(N, x, u)u - \log E_{x}(e^{t^{Y}(N, x, u)Y_{i}^{N}})$$

is defined and uniquely attained for $N \ge 1$ and $x, u \in D_{\eta}$. Then for $\lambda(N, x, u)$ in (1.12)

(1.31)
$$\lambda(N, x, u) = N\lambda^{Y}(N, x, u), \quad t(N, x, u) = Nt^{Y}(N, x, u).$$

If $\{Y_{i,x}^N\}$ are identically distributed in n as in the Bernoulli case (1.6), conditions (1.13) and (1.14) hold if $\sup\{|t^Y(1,x,u)|: x,u\in D_\eta\}<\infty$. In the Bernoulli case (1.6), (1.11)(ii, iii) and (1.13) and (1.14) are equivalent to $f_i\geq \varepsilon>0$ and $\sum_{i=1}^d f_i\leq 1-\varepsilon$ for $f=f_N(x)$ for all $x\in D_\eta$ (see the remarks in Section 4), and (1.17) is equivalent to a uniform Lipschitz condition on $\{f_N(x)\}$.

2. Some preliminary lemmas. The following lemmas are essential for Sections 3-5. The first lemma is a bound on the oscillation of $\{X_n\}$ with respect to associated distributions. Lemmas 2.3 and 2.4 are only needed if $\beta_N \to 0$.

LEMMA 2.1. There exist constants c > 0 and $\omega_0 > 0$ such that for $0 < r < \omega_0$,

$$(2.1) P_{x,\,t}\big(|X_1-E_{x,\,t}(X_1)|>r\big)\leq 2de^{-cNr^2}, x\in D_\eta,\,|t|\leq \omega_0N.$$

PROOF. For all $v \in \mathbb{R}^d$,

(2.2) $P_{x,t}(v(X_1 - E_{x,t}(X_1)) > r) \le \exp(-(\theta r - \phi_{x,t}(\theta v)))$, all $\theta > 0$, for

(2.3)
$$\phi_{r,t}(u) = \log E_{r,t}(e^{uX_1}) - uE_{r,t}(X_1).$$

Since $\phi_{x,t}(0) = \nabla_u \phi_{x,t}(0) = 0$, by Taylor's theorem

(2.4)
$$\begin{aligned} \phi_{x,t}(\theta v) &= \frac{1}{2}\theta^2 \left(v, \nabla^2 \phi_{x,t}(\gamma \theta v) v \right) \\ &= \frac{1}{2}\theta^2 \left(v, \Sigma_{N,t+\gamma \theta v}^2(x) v \right) \le \frac{1}{2}\theta^2 |v|^2 \frac{C}{N}, \qquad C < 1, \end{aligned}$$

by (1.11)(iii) if $|t + \gamma \theta v| \le \omega N$, where $0 < \gamma < 1$. Applying (2.4) and (2.2) with |v| = 1, $|t| \le \frac{1}{2}\omega N$ and $\theta = Nr/C$, where $0 < r < \omega/2$, and letting v range over unit coordinate vectors in \mathbb{R}^d , we obtain Lemma 2.1 with c = 1/(2Cd) and $\omega_0 = \omega/2$. \square

LEMMA 2.2. There exist constants $\alpha > 0$ and $C_2 < \infty$ such that for $x, z, x_i, z_i \in D_n$ and $N \ge 1$,

(i)
$$\lambda(N, x, z) \ge \alpha N |z - f_N(x)|^2,$$

(ii)
$$|\lambda(N, x_1, z_1) - \lambda(N, x_2, z_2)| \le C_2 N(|x_1 - x_2| + |z_1 - z_2|).$$

Proof. By (1.12)

(2.5)
$$\lambda(N, x, z) = \sup_{u \in R^d} (uz - \log E_x(e^{uX_1}))$$
$$\geq u(z - f_N(x)) - \phi_x(u), \qquad u = \gamma N(z - f_N(x)),$$

where $\phi_x = \phi_{x,0}$ in (2.3) and $\gamma > 0$ is sufficiently small so that $|u| < \omega N$ for all $x, z \in Q$ and $\gamma C \le 1$ for C in (2.4). Then $\phi_x(u) \le \frac{1}{2} \gamma^2 C N |z - f_N(x)|^2$ by (2.4), and Lemma 2.2(i) follows from (2.5) with $\alpha = \gamma/2$.

If $M_x(t) = E_x(e^{tX_1})$, then by (1.12)

$$|\lambda(N, x_1, z_1) - \lambda(N, x_2, z_2)|$$

$$= \left| \sup_{t} \left(tz_1 - \log M_{x_1}(t) \right) - \sup_{t} \left(tz_2 - \log M_{x_2}(t) \right) \right|$$

$$\leq MN|z_1 - z_2| + C_M MN|x_1 - x_2|$$

by (1.13) with $M=C_3$ and (1.17), which implies Lemma 2.2(ii). \Box

The next two results are more delicate, and assume $\beta_N \to 0$.

LEMMA 2.3. There exist constants $\omega_1 > 0$ and $C_9 < \infty$ such that if $x, z \in D_\delta$, $y \in D_n$, $|x-z| < \omega_1$, $|y-z| < \omega_1$ and $\beta_N < \omega_1$,

(i)
$$|t(N, y, z)| \le C_9 N(\beta_N + |y - z|),$$

(ii)
$$|\lambda(N, x, z) - \lambda(N, y, z)| \le C_9 N|x - y|(\beta_N + |x - z| + |y - z|).$$

PROOF. Let $M_{y}(t) = E_{y}(e^{tX_{1}})$ for $y \in D_{\eta}$. Then

by (1.11)(iii). Since $\nabla_t \log M_y(t(N, y, z)) \equiv z$ for $y, z \in D_\eta$ by (1.12), t(N, y, z) is analytic for $z \in \operatorname{int}(D_\eta)$ and

(2.8)
$$\nabla_z t(N, y, z) = \sum_{N, t(N, y, z)}^{-2} (y)$$
$$= \sum_{N}^{-2} (y) + O(|t(N, y, z)|) + O(N\beta_N)$$

by (1.11)(ii) and (2.7) whenever $|t(N, y, z)| < \omega N$ and ω is sufficiently small. Since $z \in D_\delta$, $B_z = \{u: |u-z| < \eta - \delta\} \subseteq D_\eta$. Similarly, $f_N(y) \in B_z$ for sufficiently small ω_1 since $|f_N(y) - z| \le |y - z| + O(\beta_N) \le C\omega_1$. Hence t(N, y, u) is defined and analytic for u in an open set containing the line between $f_N(y)$ and z, and $t(N, y, f_N(y)) = 0$. If $|t(N, y, u)| < \omega N$ for $|u - f_N(y)| < \omega_1$ as well, and

if $|z - f_N(y)| < \omega_1$, then

$$(2.9) |t(N, y, z)| = |t(N, y, z) - t(N, y, f_N(y))| \le C_6 N|z - f_N(y)|$$

by (2.8) and (1.11)(i, ii). Thus $|t(N, Y, z)| < \omega N$ is guaranteed by continuity if $|z - y| < \omega_1$ and $\beta_N < \omega_1$ for a perhaps smaller value of $\omega_1 > 0$, and Lemma 2.3(i) follows from (2.9) and (1.11)(i).

Finally, let $\Delta = \max\{|t(N, x, z)|, |t(N, y, z)|\}$. Then by (2.6)

$$\begin{split} |\lambda(N,x,z) - \lambda(N,y,z)| &\leq \sup \bigl\{|\log M_x(t) - \log M_y(t)| \colon |t| \leq \Delta\bigr\} \\ &\leq C_8 \Delta |x-y| \end{split}$$

by (1.17), and Lemma 2.3(ii) follows from Lemma 2.3(i). \Box

LEMMA 2.4. If $\beta_N \to 0$, there exists $\omega_2 > 0$ such that

$$\lambda(N, x, z) = \frac{1}{2} (z - f_N(x), \Sigma_N^{-2}(x)(z - f_N(x)))(1 + O(\gamma_N)),$$

uniformly for $x, z \in D_{\delta}$ with $|x - z| \le \gamma_N$, where $\beta_N \le \gamma_N < \omega_2$.

PROOF. As in the proof of Lemma 2.3, if $\gamma_N < \omega_1$, t(N, x, u) is defined and analytic for u in an open set containing the line between $f_N(x)$ and z. By assumption, $|z - f_N(x)| = O(|z - x| + \beta_N) = O(\gamma_N)$. Since $\nabla_z \lambda(N, x, z) = t(N, x, z)$ by (1.12),

$$(2.10) \qquad \nabla_z \nabla_z \lambda(N, x, z) = \nabla_z t(N, x, z) = \sum_{N=0}^{\infty} (x) + O(N \gamma_N)$$

by (2.8) and (2.9) whenever $|z-f_N(x)|<\omega_3$. Since $\lambda(N,x,f_N(x))=\nabla_z\lambda(N,x,f_N(x))=0$, by Taylor's theorem

(2.11)
$$\lambda(N, x, z) = \frac{1}{2} (z - f_N(x), \nabla_z \nabla_z \lambda(N, x, z_\theta) (z - f_N(x)))$$
$$= \frac{1}{2} (z - f_N(x), \Sigma_N^{-2}(x) (z - f_N(x)))$$
$$+ O(N\gamma_N |z - f_N(x)|^2)$$

by (2.10), where $z_{\theta} = \theta f_N(x) + (1 - \theta)z$ for $0 < \theta < 1$. Lemma 2.4 follows from (2.11) and (1.11)(ii). \Box

3. Tightness properties. In this section we prove two basic tightness results. The first is a uniform bound on the amount of time that an arbitrary trajectory can spend away from the stable equilibrium point before building up a large value of the action S(N, T, [u]). The second result finds the asymptotics of the minimal action A_N if $\beta_N \to 0$. In the following, "for sufficiently large N" will usually be understood.

PROPOSITION 3.1. There exists a function $c(\varepsilon, T)$ with $\lim_{T\to\infty} c(\varepsilon, T) = \infty$ for each $\varepsilon > 0$ such that

(3.1)
$$S(N, T, [u]) \ge N\beta_N c(\varepsilon, \beta_N T)$$

for all $T \ge 2$ for all trajectories $[u] = (u_n: 0 \le n \le T) \subseteq D_\delta$ with $|u_n - x_0| \ge \varepsilon > 0$ for $1 \le n \le T$.

PROOF. For $0 \le n \le T - 1$,

$$|u_{n+1} - x_0| \le |u_{n+1} - f_N(u_n)| + |f_N(u_n) - x_0| \le |u_{n+1} - f_N(u_n)| + (1 - \kappa \beta_N)|u_n - x_0|$$

by (1.15). The inequality

$$(x+y)^2 \le (1+a)x^2 + \left(1+\frac{1}{a}\right)y^2$$
, all $a > 0$,

summed in (3.2) yields

$$\begin{split} \sum_{n=0}^{T} |u_n - x_0|^2 &\leq |u_0 - x_0|^2 + (1+\alpha)(1-\kappa\beta_N)^2 \sum_{n=0}^{T-1} |u_n - x_0|^2 \\ &+ \left(1 + \frac{1}{a}\right) \sum_{n=0}^{T-1} |u_{n+1} - f_N(u_n)|^2 \\ &= |u_0 - x_0|^2 + (1-\kappa\beta_N) \sum_{n=0}^{T-1} |u_n - x_0|^2 \\ &+ \frac{1}{\kappa\beta_N} \sum_{n=0}^{T-1} |u_{n+1} - f_N(u_n)|^2 \end{split}$$

if $\alpha = \kappa \beta_N / (1 - \kappa \beta_N)$. Hence

(3.3)
$$\sum_{n=0}^{T-1} |u_{n+1} - f_N(u_N)|^2 \ge \kappa \beta_N \left(\kappa \beta_N \sum_{n=0}^T |u_n - x_0|^2 - |u_0 - x_0|^2 \right)$$

$$\ge \kappa \beta_N \left(\kappa \beta_N T \varepsilon^2 - C_Q \right)$$

since $|u_n-x_0|\geq \varepsilon$ for $1\leq n\leq T$ and $u_0,x_0\in Q$. Proposition 3.1 follows from (3.3) and Lemma 2.2(i) with $c(\varepsilon,T)=\alpha\kappa(\kappa T\varepsilon^2-C_Q)$. \square

REMARK. The contraction condition (1.15) in Proposition 3.1 can be generalized by assuming that there exist a sequence of functions $\{G_N(u)\}$ on sets $D_2(N) \supseteq D_\delta \cup f_N(D_\delta)$ such that:

- (i) $G_N(u) \ge 0$, $G_N(x_0) = 0$.
- (ii) $G_N(u) \ge \eta_{\varepsilon} > 0$ uniformly for $|u x_0| \ge \varepsilon > 0$.
- (3.4) (iii) $|\nabla G_N(u)| \le C$ uniformly for $N \ge 1$ and $u \in D_{\delta}$.
 - (iv) There exists $\gamma > 0$ such that

$$G_N(f_N(u)) \leq (1 - \gamma \beta_N) G_N(u)$$

for $N \ge 1$ and $u \in D_n$.

We now compute the asymptotic minimal action. Define

(3.5)
$$Q(L, x, y) = \inf \left\{ \int_0^L (u' - h(u), \sigma^{-2}(u)(u' - h(u))) dt : u(0) = x, u(L) = y, \{u(t)\} \subseteq D_\delta \right\}$$

so that $V(x, y) = \inf_{L>0} Q(L, x, y)$ for V(x, y) in (1.21).

PROPOSITION 3.2. If $\beta_N \to 0$, there exists $y_0 \in \partial D$ such that

(3.6)
$$\inf_{y \in D^c} V(x_0, y) = V(x_0, y_0) = V > 0$$

for V(x, y) in (1.21), where if $x_N \to x_0$,

$$\lim_{N\to\infty} \frac{A_N(x_N)}{N\beta_N} = \lim_{N\to\infty} \frac{A_N}{N\beta_N} = \inf_{L>0} Q(L, x_0, y_0) = V > 0$$

for A_N and V(N, x, y) in (1.20).

The proof depends on Lemmas 3.1–3.3 below. Since D_{δ} is open in \mathbb{R}^d , the first lemma can be proven by adjoining linear path segments with |u'(t)| = 1 between pairs of points that are close, and by using global bounds for pairs that are not close. Assume $\beta_N \to 0$ for the rest of Section 3.

Lemma 3.1. For each x_1 , $y_1 \in \text{int}(D_{\delta})$, there exists c > 0 such that for all $x_2, y_2 \in D_{\delta}$,

(i)
$$|V(x_2, y_2) - V(x_1, y_1)| \le c|x_1 - x_2| + c|y_1 - y_2|$$

and if L > 0 and $L' = L - |x_1 - x_2| - |y_1 - y_2| > 0$,

(ii)
$$Q(L, x_2, y_2) \le Q(L', x_1, y_1) + c|x_1 - x_2| + c|y_1 - y_2|.$$

Since every continuous path from x_0 to $y \in D^c$ must exit through a point of ∂D , Lemma 3.1(i) implies that $\inf_{y \in D^c} V(x_0, y)$ is attained at some point $y_0 \in \partial D$.

LEMMA 3.2. Assume $\{T_N\}$ satisfies

(3.7)
$$\beta_N T_N \to \infty, \qquad \beta_N^2 T_N \to 0 \quad and$$

$$\beta_N T_N \sup_{x \in D_n} \left(|h_N(x) - h(x)| + |N\Sigma_N^2(x) - \sigma^2(x)| \right) \to 0.$$

Then, for any sequence $x_N \to x_0$, there exist paths $[u^N] = (u_n: 0 \le n \le T_N')$ with $T_N' \le T_N$, $u_0 = x_N$, $u_n \in D$ for $0 \le n < T_N'$ and $u_{T_N'} = y_N \in \partial D$ such that $|u_{n+1} - u_n| \le C\beta_N$ for some absolute constant C and

$$\limsup_{N\to\infty}\frac{S(N,T_N',[u^N])}{N\beta_N}\leq V=V(x_0,y_0).$$

PROOF. If $L_N=\beta_N T_N$, then $L_N\to\infty$ by (3.7). Choose $y_0\in\partial D$ such that $V(x_0,y_0)=\inf_{y\in\partial D}V(x_0,y)$. Since $h(x_0)=0$, $V(x_0,y_0)=\inf_{L>0}Q(L,x_0,y_0)=\lim_{L\to\infty}Q(L,x_0,y_0)$. Hence by Lemma 3.1(ii)

$$V(x_0, y_0) = \lim_{N\to\infty} Q(L_N, x_N, y_0)$$

$$(3.8) \geq \limsup_{N \to \infty} \inf \left\{ \frac{1}{2} \int_{0}^{L} (u' - h(u), \sigma^{-2}(u)(u' - h(u))) dt : L \leq L_{N}, \\ u(0) = x_{N}, u(t) \in D(0 \leq t < L), u(L) \in \partial D \right\}$$

by stopping functions $(u(t): 0 \le t \le L_N)$ in the definition of $Q(L_N, x_N, y_0)$ at their first exit from D. Since each $L_N < \infty$ and the first exit time is lower semicontinuous with respect to uniform convergence, the infimum in (3.8) is attained for each N at functions $(u_N(t): 0 \le t \le L_N')$ where $L_N' \le L_N$. Since $h(x_0) = 0$ and $x_N \to x_0$, it is sufficient to assume $L_N' \to \infty$ and that $L_N'/\beta_N = T_N'$ are integers. The Euler equations in canonical form for the variational problem in (3.8) [see, e.g., Courant and Hilbelrt (1962), page 114] are

(3.9)
$$u' = L_{v}(v, u) = h(u) + \sigma^{2}(u)v,$$
$$v' = -L_{u}(v, u) = -(\nabla_{u}h(u), v) - \frac{1}{2}\nabla_{u}(\sigma^{2}(u)v, v)$$

for the Lagrangian

$$L(v, u) = (h(u), v) + \frac{1}{2}(\sigma^{2}(u)v, v).$$

Since $(d/dt)L[v(t), u(t)] \equiv 0$ by (3.9), there exists C_i depending only on the implicit constants in (1.11) such that for any solution of (3.9) in \overline{D} for $0 \le t \le A$,

$$(3.10) C_1|v(0)| - C_3 \le |v(t)| \le C_2|v(0)| + C_3, 0 \le t \le A.$$

Since by (3.8)

$$\limsup_{N\to\infty} \frac{1}{2} \int_0^{L_N'} \left(\sigma^2(u_N)v_N, v_N\right) dt \leq V < \infty,$$

where $L'_N \to \infty$, it follows from (3.10) and (1.11)(ii, iv) that v(0) is bounded in N. Thus, again by (3.10), v(t) is uniformly bounded in N, and by (3.9)

$$(3.11) |u_N''(t)| + |u_N'(t)| \le C_5 < \infty, 0 \le t \le L_N', \text{ all } N \ge 1.$$

Define sequences $[u^N] = (u_n: 0 \le n \le T'_N)$ by

$$u_n = u_N(n\beta_N), \qquad 0 \le n \le L'_N/\beta_N = T'_N \le T_N.$$

Thus $|u_{n+1} - u_n| \le C_5 \beta_N$ by (3.11), $u_0 = u_N(0) = x_N$, $u_n \in D$ for $0 \le n < T_N'$ by (3.8) and $u_{T_N'} = u_N(L_N') = y_N \in \partial D$. Thus by Lemma 2.4, (3.11), and (3.7)

$$\frac{1}{N\beta_{N}}S(N, T'_{N}, [u^{N}])$$

$$= \frac{1}{2N\beta_{N}} \sum_{n=0}^{T'_{N}-1} (u_{n+1} - f_{N}(u_{n}), \Sigma_{N}^{-2}(u_{n})(u_{n+1} - f_{N}(u_{n})))(1 + O(\beta_{N}))$$

$$= \frac{\beta_{N}}{2N} \sum_{n=0}^{T'_{N}-1} (u'_{N}(n\beta_{N}) - h_{N}(u_{n}), \Sigma_{N}^{-2}(u_{n})(u'_{N}(n\beta_{N}) - h_{N}(u_{n})))$$

$$+ O(\beta_{N}^{2}T_{N})$$

$$= \frac{1}{2} \int_{0}^{L'_{N}} (u'_{N} - h(u_{N}), \sigma^{-2}(u_{N})(u'_{N} - h(u_{N}))) dt + o(1)$$

$$\leq V(x_{0}, y_{0}) + o(1)$$

by (3.8), which completes the proof of Lemma 3.2. \square

LEMMA 3.3. Let $x_N \to x_0$ and $\{y_N\} \subseteq D_{\delta} - D$. Then, for any $\varepsilon > 0$, there exist $L < \infty$, $x_1 \in D$ and $y \in D_{\delta} - D$ such that $|x_1 - x_0| \le \varepsilon$ and

(3.12)
$$\liminf_{N\to\infty} \frac{V(N, x_N, y_N)}{N\beta_N} \ge Q(L, x_1, y) > 0.$$

PROOF. Choose $[u^N] = (u_n: 0 \le n \le T_N) \subseteq D_\delta$ such that $u_0 = x_N, u_{T_N} = y_N$ and

(3.13)
$$S(N, T_N, [u^N]) = V(N, x_N, y_N) + O(\beta_N 2^{-N}).$$

Define $k_N = \max\{n: |u_n - x_0| \le \varepsilon\}$ for some $\varepsilon > 0$, and set $v_n = u_{n+k_N}$ for $0 \le n \le M_N = T_N - k_N$. Thus $|v_0 - x_0| \le \varepsilon$, $|v_n - x_0| > \varepsilon$ for $1 \le n \le M_N$ and $v_{M_N} = u_{T_N} = y_N$. Since there is nothing to prove if the left-hand side of (3.12) is infinite, and $\lambda(N, u_i, u_{i+1}) \ge 0$, it is sufficient to assume

$$(3.14) \quad \frac{S(N, M_N, [v^N])}{N\beta_N} \leq \frac{S(N, T_N, [u^N])}{N\beta_N} \leq S < \infty, \quad \text{all } N \geq 1.$$

Since $|v_n - x_0| > \varepsilon$ for $1 \le n \le M_N$, $S(N, M_N, [v^N]) \ge N\beta_N c(\varepsilon, \beta_N M_N)$ by Proposition 3.1, and $c(\varepsilon, \beta_N M_N) \le S$ by (3.14). Since $\lim_{T \to \infty} c(\varepsilon, T) = \infty$,

$$(3.15) L_N = \beta_N M_N \le L(\varepsilon, S) < \infty.$$

Define piecewise linear functions $\{v_N(t): 0 \le t \le L_N\}$ with nodes

$$v_N(n\beta_N) = v_n \text{ for } 0 \le n \le M_N.$$

Since $\lambda(N,v_n,v_{n+1}) \leq S(N,M_N,[v^N]) \leq N\beta_N S$ by (3.14), $|v_{n+1}-v_n| \leq C\sqrt{\beta_N}$ by Lemma 2.2(i). By Lemma 2.4

and by (3.14) and (1.11)(ii)

(3.16)
$$\int_{0}^{L_{N}} v_{N}'(t)^{2} dt = O(1).$$

Hence by (3.15) and (3.16)

(3.17)
$$\frac{1}{N\beta_{N}}S(N, M_{N}, [v^{N}])$$

$$= \frac{1}{2}\int_{0}^{L_{N}}(v'_{N} - h(v_{N}), \sigma^{-2}(v_{N})(v'_{N} - h(v_{N}))) dt + o(1).$$

Choosing a subsequence if necessary, we can assume $L_N \to L < \infty$ by (3.15),

 $v_N(0) \to x_1$ where $|x_1 - x_0| \le \varepsilon$, $y_N \to y \in D_\delta - D$ and $v_N'(t) \to v'(t)$ weakly in $L^2[0, L]$, where $v(0) = x_1$ and v(L) = y. Then by (3.13) and (3.17)

(3.18)
$$\liminf_{N \to \infty} \frac{V(N, x_N, y_N)}{N\beta_N} \ge \frac{1}{2} \int_0^L (v' - h(v), \sigma^{-2}(v)(v' - h(v))) dt$$
$$\ge Q(L, x_1, y).$$

Since $L<\infty$, there exists $(w(t)\colon 0\leq t\leq L)\subseteq D_\delta$ with $w(0)=x_1,\ w(L)=y$ such that the integral on the right-hand side of (3.18) (with w in place of v) equals $Q(L,x_1,y)$. If $Q(L,x_1,y)=0$, then w'(t)=h(w(t)) for $0\leq t\leq L$ with $w(0)\in D$ but $w(L)\notin D$, which violates (1.16). Hence $Q(L,x_1,y)>0$ and Lemma 3.3 follows. \square

Proof of Proposition 3.2. By (3.18), $Q(L, x_1, y) \ge V(x_1, y) = V(x_0, y) + O(\varepsilon)$ by Lemma 3.1(i), while $V(x_0, y) \ge V$ by definition. Hence Proposition 3.2 follows from Lemmas 3.2 and 3.3, with V > 0 by (3.18) and Lemma 3.2. \square

The argument of (3.18) applied to Lemma 3.2 yields the following corollary.

COROLLARY 3.1. Let $\{[u^N]\}$ be the sequence of paths constructed in the proof of Lemma 3.2. Then

(3.19)
$$\lim_{N \to \infty} \frac{S(N, T'_N, [u^N])}{N\beta_N} = V$$

and $V(x_0, y_1) = V$ for any limit point y_1 of $y_N = u_{T_N}$.

4. Upper and lower large deviation bounds. This section derives uniform upper and lower bounds for the Markov chains $\{X_n\}$ for $\beta_N \to 0$. We begin with results for the upper bound. Recall $T_e = \inf\{n \geq 1 \colon X_n \notin D\}$, and let [X] be the (random) trajectory $(X_n \colon 0 \leq n \leq T)$.

Proposition 4.1. For q_N in (1.19) and all s > 0 and $T < \infty$,

(i)
$$\sup_{x \in D} P_x(S(N, T, [X]) \ge s, X_k \in D \ (0 \le k < T), X_T \in D_{\delta})$$
$$\le e^{-s}q_N^T$$

and

$$\sup_{x \in D} P_x \Big(S \big(N, \, T_e, \big[\, X \, \big] \big) \geq s \, , \, X_{T_e} \in D_\delta, \, T_e \leq T \, \Big)$$

$$\leq T e^{-s} \big(1 + q_N \big)^T .$$

PROOF. The probability in Proposition 4.1(i) is bounded by

$$\begin{split} e^{-s} \sup_{x \in D} E_x & \left(\exp \left(\sum_{k=0}^{T-1} \lambda(N, X_k, X_{k+1}) \right) \prod_{k=0}^{T-1} I(X_k \in D) I(X_T \in D_{\delta}) \right) \\ & \leq e^{-s} \sup_{x \in D} E_x \left(e^{\lambda(N, x, X_1)} I(X_1 \in D_{\delta}) \right)^T = e^{-s} q_N^T \end{split}$$

by the Markov property. For Proposition 4.1(ii), write $\{T_e \leq T\}$ as the union of the events $\{T_e = n\}$ for $1 \leq n \leq T$ and apply Proposition 4.1(i). \square

Remarks. If d=1, $q_N=O(N)$. If $\{X_n\}$ is multinomial, $q_N=O(N^{d/2})$ for $d\geq 1$. If $D_\delta=Q$, then $q_N\sim C_dN^{d/2}$, and in particular $\log q_N=O(\log N)$ cannot be improved. The first statement follows by adapting a standard argument [Freidlin and Wentzell (1984), Chapter 5, Theorem 1.1]. Fix $N\geq 1$ and $x\in D$, assume d=1, and set $m(t)=\log M(t)$ for $M(t)=E_x(e^{tX_1})$. If $x\in D$, $f_N(x)$ is in the interior of D_δ for sufficiently small β_N if $\beta_N\to 0$; since $f\colon D\to D$, where $f_N\to f$ uniformly in Q if $\beta_N\equiv 1$, $f_N(x)\in \mathrm{int}(D_\delta)$ in all cases. Since $\lambda(N,x,u)$ is convex in u,

$$\{u \in D_{\delta}: \lambda(N, x, u) \le s\} = [u_1(s), u_2(s)], \text{ any } s > 0,$$

where $u_1(s) < f_N(x) < u_2(s)$. Since $t_1(s) < 0 < t_2(s)$ for $t_i(s) = t(N, x, u_i(s))$, $u_1(s) \le u \le u_2(s)$ if and only if $t_i(s)u - m(t_i(s)) \le s$ for i = 1, 2 and $u \in D_{\delta}$. Hence by Chebyshev's inequality

$$\begin{aligned} P_x(\lambda(N, x, X_1) > s, \ X_1 &\in D_{\delta}) \\ &\leq \sum_{i=1}^2 P_x(t_i X_1 - m(t_i) > s) \leq 2 \sup_t P_x(t X_1 - m(t) > s) \\ &\leq 2 \sup_t e^{-s} E(e^{t X_1}) e^{-m(t)} = 2e^{-s}. \end{aligned}$$

By (1.14), $|\lambda(N, x, u)| \leq C_4 N$ for $x, u \in D_{\eta}$, so by (4.1) and integrating by parts $E_x(e^{\lambda(N, x, X_1)}I(X_1 \in D_{\delta}))$

$$egin{aligned} &= \int_{0-}^{CN} & e^s P_x ig(\lambda(N,x,X_1) \in ds, \ X_1 \in D_\delta ig) \ &\leq 1 + \int_{0}^{CN} & e^s P_x ig(\lambda(N,x,X_1) > s, \ X_1 \in D_\delta ig) \ ds \leq 1 + 2NC. \end{aligned}$$

Hence $q_N \leq 1 + 2CN$ if d = 1.

If $\{X_n\}$ is multinomial for d=1, and if

$$P(Y = 1) = f$$
, $P(Y = 0) = 1 - f$, where $0 < f < 1$,

the Legendre function of Y is

$$\lambda^{Y}(u) = u \log \left(\frac{u}{f}\right) + (1-u) \log \left(\frac{1-u}{1-f}\right).$$

The Legendre function of X_1 in (1.6) is $\lambda(u) = N\lambda^{Y}(u)$ by (1.31), and

$$\begin{split} E\left(e^{\lambda(X_1)}\right) &= E\left(\left(\frac{X_1}{f}\right)^{NX_1} \left(\frac{1-X_1}{1-f}\right)^{N-NX_1}\right) \,. \\ &= N^{-N} \sum_{k=0}^{N} \cdot \left(\frac{k}{f}\right)^k \left(\frac{N-k}{1-f}\right)^{N-k} \left(\frac{N}{k}\right) f^k (1-f)^{N-k} \\ &\sim \sqrt{\frac{N}{2\pi}} \sum_{k=0}^{N} \frac{1}{\sqrt{k(N-k)}} \sim \sqrt{N\pi/2} \end{split}$$

by Stirling's formula, where $\binom{N}{k}$ are binomial coefficients. In particular, $E(e^{\lambda(X_1)})$ is independent of f for 0 < f < 1. Note that (1.11)(ii) excludes singular values of f. If Y is multinomial for $d \ge 2$, that is,

$$P(Y = \mathbf{e}_i) = f_i, \qquad 1 \le i \le d,$$

$$P(Y = \mathbf{0}) = f_{d+1} = 1 - \sum_{k=1}^{d} f_k,$$

the Legendre function is $\sum_{j=1}^{d+1} u_j \log(u_j/f_j)$, where $u_{d+1} = 1 - \sum_{j=1}^{d} u_j$. By a similar argument $E(e^{\lambda(X_1)})$ is independent of $\{f_i\}$ if $f_i > 0$, $1 \le i \le d+1$, and

$$E(e^{\lambda(X_1)}) \sim C_d N^{d/2}$$
 as $N \to \infty$.

In particular $q_N = O(N^{d/2})$ for multinomial $\{X_n\}$ for any $D_{\delta} \subseteq Q$, and $q'_N \sim C_d N^{d/2}$ for q'_N in (1.27).

The next proposition is the large deviation lower bound.

Proposition 4.2. Assume $\beta_N \to 0$, and let $[u] = (u_n: 0 \le n \le T) \subseteq D_\delta$ be a trajectory with $|u_{n+1} - u_n| \le C\beta_N$ for $0 \le n \le T - 1$. Then

$$(4.2) P_x \Big(\max_{1 \le n \le T} |X_n - u_n| \le r \Big) \ge \Big(1 - 2de^{-cNr^2} \Big)^T e^{-S(N, T, [u]) + O(TNr\beta_N)}$$

for $|x - u_0| \le r \le C\beta_N$ and c > 0 in Lemma 2.1.

Proof. By the Markov property

$$\begin{split} P_x \Big(\max_{1 \leq n \leq T} |X_n - u_n| \leq r \Big) \\ &\geq P_x \Big(\max_{1 \leq n \leq T-1} |X_n - u_n| \leq r \Big) \inf_{|\gamma - u_{T-1}| \leq r} P_y \big(|X_1 - u_T| \leq r \big). \end{split}$$

Since $S(N, T, [u]) = \sum_{n=0}^{T-1} \lambda(N, u_n, u_{n+1})$, it is sufficient by induction to prove

$$(4.3) P_{y}(|X_{1}-z| \leq r) \geq (1-2de^{-cNr^{2}})e^{-\lambda(N,x,z)+O(Nr\beta_{N})}$$
 uniformly for $x, z \in D_{\delta}$, $|y-x| \leq r$ and $|x-z| \leq C\beta_{N}$.

The proof of (4.3) will be via the standard Cramér transformation. Let $B = \{u: |u-z| \le r\}$ and $M_y(t) = E_y(e^{tX_1})$. Since $x \in D_\delta$ and $|y-x| \le r$, $y \in D_\eta$ for sufficiently large N. Using the associated distribution (1.10) with t = t(N, y, z),

$$\begin{aligned} P_{y}(|X_{1}-z| \leq r) &= P_{y}(B) = E_{y,t}(1_{B}e^{-tX_{1}})M_{y}(t) \\ &\geq P_{y,t}(B)\inf_{|\omega|=1}e^{-t(z+r\omega)}M_{y}(t) \\ &= P_{y,t}(B)e^{-\lambda(N,y,z)}e^{-|t|r}, \qquad t = t(N,y,z), \end{aligned}$$

since $\lambda(N, y, z) = tz - \log M_{\nu}(t)$ by (1.12). Since

$$E_{y,t}(X_1) = \nabla_t \log M_y(t(N, yz)) = z$$

by the choice of t,

$$(4.5) P_{y,t}(B) = 1 - P_{y,t}(|X_1 - E_{y,t}(X_1)| > r) \ge 1 - 2de^{-cNr^2}$$

by Lemma 2.1 if $r < \omega_0$. By (4.3), $x, z \in D_\delta$ and $|x - z| + |y - z| = O(\beta_N)$, and Lemma 2.3 implies $|t| = O(N\beta_N)$ and $|\lambda(N, y, z) - \lambda(N, x, z)| = O(N\beta_N r)$ for sufficiently small β_N . Thus (4.3) follows from (4.4) and (4.5), and Proposition 4.2 follows. \square

5. Conclusion of proofs. In this section we put together the arguments of Sections 3 and 4 to prove our main results. It is useful to think of the escape time T_e from D as analogous to an exponential variable with mean $e^{A_N(1+o(1))}$ for A_N in (1.20). Recall that Theorem 1.1 assumes $\beta_N \to 0$.

LEMMA 5.1. Under the hypotheses of Theorem 1.1,

(i)
$$E_r(T_o) \le e^{A_N(1+o(1))}$$

and

(ii)
$$P_x(T_e \ge e^{A_N(1+r)}) = O(e^{-rA_N/2}), \quad all \ r > 0,$$

uniformly for $x \in D$.

PROOF. Note that (ii) follows from (i) by Chebyshev's inequality. For (i), choose $T_N \to \infty$ and then $\varepsilon_N \to 0$ such that $\beta_N T_N \to \infty$ and

(5.1)
$$(3.7) \text{ holds, } \beta_N T_N = o\left(\left(\frac{N\beta_N^2}{\log(N+q_N)}\right)^{1/3}\right),$$

$$\varepsilon_N \to 0, \qquad c(\varepsilon_N, \beta_N T_N) \to \infty,$$

for $c(\varepsilon, T)$ in Proposition 3.1. Set $B = \{x: |x - x_0| \le \varepsilon_N\}$ and $\tau_1 = \min\{n \ge 1: X_n \in B \cup D^c\}$. The key step in the proof of Lemma 5.1 is to show

(5.2)
$$\sup_{x \in D} P_x(T_e > 2T_N) \le 1 - e^{-A_N(1 + o(1))}.$$

By the Markov property

(5.3)
$$P_{x}(T_{e} \leq 2T_{N}) \geq P_{x}(\tau_{1} \leq T_{N}) \inf_{z \in R} P_{z}(T_{e} \leq T_{N}).$$

The first step is to show

(5.4)
$$\lim_{N\to\infty} \sup_{x\in D} P_x(\tau_1 > T_N) = 0.$$

By Proposition 3.1

$$\begin{split} P_x(\tau_1 > T_N) &= P_x(X_n \in D, |X_n - x_0| > \varepsilon_N \text{ for } 1 \le n \le T_N) \\ &\le P_x(S(N, T_N, [X]) \ge N\beta_N c(\varepsilon_N, \beta_N T_N), \ X_n \in D \text{ for } 1 \le n \le T_N) \\ &\le e^{-N\beta_N c(\varepsilon_N, \beta_N T_N)} q_N^{T_N} \end{split}$$

by Proposition 4.1(i). Since $c(\varepsilon_N, \beta_N T_N) \to \infty$ and $T_N \log q_N = o(N\beta_N)$ by (5.1)

(5.5)
$$\sup_{x \in D} P_x(\tau_1 > T_N) = O(e^{-CN\beta_N}), \text{ all } C < \infty,$$

and (5.4) follows. For the second factor in (5.3), set $\lambda_N = (N\beta_N^2/\log N)^{-1/3}$. Then by (5.1)

(5.6)
$$\lambda_N \to 0, \qquad \beta_N T_N \lambda_N \to 0, \qquad \frac{N \beta_N^2 \lambda_N^2}{\log N} \to \infty.$$

Let $[u^N]$ be the trajectories guaranteed by Lemma 3.2, where $\{x_N\}$ is an asymptotically minimizing sequence for the second factor in (5.3). Choosing a subsequence if necessary, we can assume $y_N=u_{T_N'}\to y_1\in\partial D$, where $V(x_0,\,y_1)=V$ by Corollary 3.1. By the "well-sharpened pencil condition" at y_1 [see the remarks after (1.22) in Section 1], there exist $z_N\in D_\delta$ such that $|z_N-D|\geq 2\beta_N\lambda_N$ and $|z_N-y_1|\leq C\beta_N\lambda_N$. Define $[v^N]$ by $v_n\equiv u_n,\,0\leq n< T$), $v_T=z_N$ for $T=T_N'$. Since $|\lambda(N,u_{T-1},\,y_1)-\lambda(N,u_{T-1},\,z_N)|\leq C_1N\beta_N\lambda_N$ by Lemma 2.2(ii), $\{[v^N]\}$ also satisfies

$$\lim_{N\to\infty}\frac{S(N,T_N',\lceil v^N\rceil)}{N\beta_N}=V>0.$$

Hence by Proposition 4.2 and (5.1)

$$\inf_{z \in B} P_z(T_e \le T_N) \ge P_{x_N} \Big(\max_{1 \le n \le T_N'} |X_n - v_n| \le \beta_N \lambda_N \Big) (1 + o(1)) \\
\ge (1 - 2de^{-cN\beta_N^2 \lambda_N^2})^{T_N'} e^{-S(N, T_N', [v^N]) + O(T_N N\beta_N^2 \lambda_N)} \\
= e^{-N\beta_N (V + o(1))} = e^{-A_N (1 + o(1))}$$

by (5.6). Note $T_N = O(\sqrt{N})$ since $\beta_N T_N = O(\sqrt{N}\beta_N^2)$ by (5.1), and similarly $N\beta_N \ge \sqrt{N}$. The relation (5.2) follows from (5.7) and (5.5).

We complete the proof of Lemma 5.1 as in Freidlin and Wentzell (1984). By (5.2) and the Markov property, $P_x(T_e \ge 3nT_N) \le (1 - e^{-A_N(1+o(1))})^n$ uniformly for $x \in D$ and $n \ge 1$, so

$$\begin{split} E_x(T_e) &\leq 3T_N \sum_{n=0}^{\infty} P_x(T_e \geq 3nT_N) \leq 3T_N \sum_{n=0}^{\infty} \left(1 - e^{-A_N(1+o(1))}\right)^n \\ &= 3T_N e^{A_N(1+o(1))} = e^{A_N(1+o(1))}. \end{split}$$

This implies Lemma 5.1(i), and since Lemma 5.1(ii) follows from Chebyshev's inequality, the proof of Lemma 5.1 is complete. \Box

LEMMA 5.2. Under the hypotheses of Theorem 1.1, uniformly for $x \in K$ for any compact set $K \subset D$,

(i)
$$E_r(T_e) \ge e^{A_N(1+o(1))}$$

and

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(ii)
$$P_x(T_e \le e^{A_N(1-r)}) = O(e^{-rA_N/2}), \quad 0 < r < \alpha(K).$$

PROOF. Let T_N , ε_N and B be as in the proof of Lemma 5.1. As in Freidlin and Wentzell (1984), define stopping times $\{\tau_k\}$ by $\tau_0=0$ and by induction

$$au_{k+1} = egin{cases} \min\{n \geq au_k + 1 \colon X_n \in B \cup D^c\} & ext{if } au_k < T_e, \ T_e & ext{if } au_k = T_e. \end{cases}$$

Then $\tau_k < \tau_{k+1}$ if and only if $\tau_k < T_e$, and

$$T_e = au_1 + \sum_{k=1}^{\infty} (au_{k+1} - au_k) \ge 1 + \sum_{k=1}^{\infty} I(au_k < T_e),$$

where I(A) is the indicator function, since $\tau_{k+1} - \tau_k \ge 1$ if $\tau_k < T_e$. Hence by the Markov property

(5.8)
$$\inf_{x \in K} E_x(T_e) \ge \inf_{x \in K} P_x(\tau_1 < T_e) \sum_{k=1}^{\infty} \inf_{z \in B} P_z(\tau_1 < T_e)^k.$$

The first step is to show

(5.9)
$$\sup_{x \in K} P_x(\tau_1 = T_e) = O(e^{-\alpha A_n}), \qquad \alpha = \alpha(K) > 0.$$

For $x \in D$ and $\{T_N\}$ in (5.1)

$$\begin{split} P_x(\tau_1 = T_e) &\leq P_x(\tau_1 = T_e \leq T_N) + P_x(\tau_1 > T_N) \\ &\leq P_x(T_e \leq T_N, \ X_{T_e} \in D_\delta) + P_x(T_e \leq T_N, \ X_{T_e} \notin D_\delta) \\ &+ P_x(\tau_1 > T_N). \end{split}$$

The last term in (5.10) is $O(e^{-CN\beta_N})$ for all $C < \infty$ by (5.5). Also

$$\begin{split} P_x\big(T_e \leq T_N, \ X_{T_e} \notin D_\delta\big) &\leq T_N \sup_{x \in D} P_x\big(X_1 \notin D_\delta\big) \\ &\leq T_N \sup_{x \in D} P_x\big(|X_1 - f_N(x)| > \delta - O(\beta_N)\big) \\ &= O(e^{-cN\delta_1^2}) \end{split}$$

by Lemma 2.1 and (1.11)(i) for sufficiently small $\delta_1 > 0$.

For paths $[u] \subseteq D_{\delta}$ with $u_0 = x \in D$ and $u_T \in D_{\delta} - D$, $S(N, T, [u]) \ge A_N(x)$ by definition. Hence the first term on the right-hand side of (5.10) equals

$$\begin{split} P_x \Big(S(N, T_e, [X]) &\geq A_N(x), \, T_e \leq T_N, \, X_{T_e} \in D_\delta \Big) \\ &\leq T_N e^{-A_N(x)} (1 + q_N)^{T_N} \\ &= \exp \left[-N\beta_N \left(\frac{A_N(x)}{N\beta_N} + o(1) \right) \right] \end{split}$$

by Propositions 4.1(ii) and 3.2, since $T_N \log(1 + q_N) = o(N\beta_N)$ by (5.1). As in the proof of Lemma 3.3,

$$\liminf_{N\to\infty}\inf_{x\in K}\frac{A_N(x)}{N\beta_N}>\alpha(K)=\frac{1}{2}Q(L,x_K,y_1)>0$$

for some $x_K \in K \cup \{x_0\}$ and $y_1 \in \partial D$, and (5.9) follows. By the same argument

(5.12)
$$\sup_{z \in B} P_z(\tau_1 = T_e) = O(e^{-A_N(1+o(1))})$$

since

$$\lim_{N \to \infty} \inf_{z \in B} \frac{A_N(z)}{N\beta_N} = V > 0$$

by Proposition 3.2. Hence by (5.9) and (5.12)

$$\inf_{x \in K} E_x(T_e) \geq \inf_{x \in K} P_x(\tau_1 < T_e) \sum_{k=1}^{\infty} \left(1 - e^{-A_N(1+o(1))}\right)^n = e^{A_N(1+o(1))},$$

which implies Lemma 5.2(i). Finally, if $M_N=e^{A_N(1-r)}$, then $P_x(T_e\leq M_N)\leq P_x(\tau_1< T_e\leq M_N)+P_x(\tau_1=T_e)$. The second term is $O(e^{-\alpha A_N})$ by (5.9), while the first is bounded by

$$P_x(\tau_{M_N} = T_e) \le M_N \sup_{z \in B} P_z(\tau_1 = T_e) = O(e^{-rA_N(1+o(1))})$$

and Lemma 5.2(ii) follows. □

PROOF OF THEOREM 1.1. This follows from Lemmas 5.1 and 5.2. \Box

PROOF OF THEOREM 1.2. The first step is to show $\lim_{N \to \infty} A_N/N = V > 0$ if $\beta_N \equiv 1$. Since $\lambda(N,x,u)/N \to \lambda(x,u)$ pointwise for $x \in D$ and $u \in Q$, $\limsup_{N \to \infty} A_N/N \le V$ by (1.28). Choose paths $(v_i \colon 0 \le i \le M_N)$ (depending on N) such that $v_0 = x_0, \ v_i \in D, \ 0 \le i < M_N, \ v_{M_N} \notin D$ and

(5.13)
$$\frac{A_N}{N} = \frac{S(N, M_N, [v])}{N} + o(1) = \sum_{i=0}^{M_N-1} \frac{\lambda(N, v_i, v_{i+1})}{N} + o(1).$$

Set $u_i = v_{i+k_N}$ for $0 \le i \le T_N = M_N - k_N$ for $k_N = \max\{i: |v_i - x_0| \le \varepsilon\}$ for fixed $\varepsilon > 0$. In particular, $|u_0 - x_0| \le \varepsilon$ and $|u_i - x_0| > \varepsilon$ for $1 \le i < T_N$. Hence by Lemma 2.2(i, ii) and the proof of Proposition 3.1, $c(\varepsilon, T_N) \le S(N, T_N, [u])/N \le A_N/N + o(1) \le C_4 + o(1)$ by (5.13), (1.14) and the nonnegativity of $\lambda(N, v, w)$. In particular $T_N \le C(\varepsilon) < \infty$ by Proposition 3.1. Since $\lambda(N, x, u)/N$ are equicontinuous on $D \times Q$ by Lemma 2.2(ii), $\lim_{N\to\infty} A_N/N \ge V$ follows within terms of order ε by (5.13), Lemma 2.2(ii) and compactness [recall u_i depends on N for $0 \le i \le T_N \le C(\varepsilon) < \infty$, and $|u_0 - x_0| \le \varepsilon$]. Similarly, V > 0 by arguing as in the proof of Proposition 3.2 and (5.13), with $f: D \to D$ or (1.15) replacing (1.16).

For the analog of Lemma 5.1, let $(u_i: 0 \le i \le T)$ be a path such that $u_0 = x_0$, $u_i \in D$ for $0 \le i < T$, $u_T = y_0$ where y_0 satisfies (1.22) and

$$(5.14) V \leq \sum_{i=0}^{T-1} \lambda(u_i, u_{i+1}) \leq V + \varepsilon/2.$$

Since (5.14) will be used instead of Lemma 3.2, conditions (3.7) are not needed in (5.1). Since $\{\lambda(N,x,y)/N\}$ are uniformly Lipschitz, it is sufficient in (5.14) to assume $|u_T-D|\geq 2\lambda_N$ for $\{\lambda_N\}$ in (5.6). Since $P=(u_i\colon 0\leq i< T)\subseteq D$ is finite and independent of N, also $|P-D^c|\geq 2\lambda_N$ for sufficiently large N. The proof of Proposition 4.2 now carries over for u_i if $\beta_N\equiv 1$ and $r\leq \lambda_N\to 0$, since then |t(N,y,z)|=O(N) by (1.13) and $|\lambda(N,y,z)-\lambda(N,x,z)|=O(Nr)$ by Lemma 2.2(ii). Since q_N' is used in place of q_N in the analog of Lemma 5.2, only two terms are needed on the right-hand side of (5.10), and (5.11) is not required. The rest of the proof of Theorem 1.1 extends to the case $\beta_N\equiv 1$ without modification. \square

PROOF OF THEOREM 1.3. For ε_N , T_N and B as in the proof of Lemma 5.1, let $\sigma_{k+1} = \min\{n \geq \sigma_k + 1: X_n \in B\}$. The conditions stated just before Theorem 1.3 imply (5.5) for σ_1 and hence

(5.15)
$$\sup_{x \in Q} E_x(\sigma_1) = O(T_N) = O(\sqrt{N})$$

by (5.1). The constant v(E) > 0 in (1.30) providing that some open set containing x_0 but disjoint from E is stable in the sense of (1.16). Hence v(E) > 0 by Lemma 5.3 below. The proof of (1.30) then follows from (5.15) by proceeding along the lines of Freidlin and Wentzell (1984), Chapter 4, Theorem 4.3. \square

Lemma 5.3. Given (1.15), the stability condition (1.16) holds if $\beta_N \to 0$, and (1.25)(iv) holds if $\beta_N \equiv 1$, for any set $D = \{x: |x - x_0| < r\} \subseteq D_n$ for r > 0.

PROOF. If $\beta_N \equiv 1$, $|f(u) - x_0| \le (1 - \kappa)|u - x_0|$ implies $f \colon D \to D$ directly. If $\beta_N \to 0$, $(v - x_0, f_N(u) - x_0) \le (1 - \kappa \beta_N)(u - x_0, u - x_0)$ by Cauchy's inequality and (1.15) is $(u - x_0, h_N(u)) \le -\kappa(u - x_0, u - x_0)$ by (1.11)(i). This holds for the direction h(u) as well, so if $u'(t) \equiv h(u(t))$,

$$\frac{d}{dt}|u(t)-x_0|^2=2(u(t)-x_0, \dot{n}(u(t)))\leq -2\kappa|u(t)-x_0|^2\leq 0.$$

This implies $|u(t)-x_0| \le e^{-\kappa t}|u(0)-x_0|$ for $t \ge 0$, so $u(t) \in D$ for all $t \ge 0$ if $u(0) \in D$. \square

Added in proof. The martingale arguments of Ventsel' (1976a, b) and Darden (1983) may allow (1.18) to be replaced by $N\beta_N \to \infty$ and a uniform Lipschitz condition on $N\Sigma_N^2(x)$ in (1.11).

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