ODE methods for Markov chain stability with applications to MCMC

G. Fort, E. Moulines
ENST, LTCI UMR 5141
46 rue Barrault
75634 Paris Cedex 13, France
gfort,moulines@tsi.enst.fr

S. Meyn
CSL, University of Illinois
1308 West Main Street
Urbana, IL 61801
meyn@uiuc.edu

P. Priouret
LPMA, UMR 7599
Université Paris VI
4, Place Jussieu, 75252 PARIS Cedex 05
priouret@ccr.jussieu.fr

ABSTRACT

Fluid limit techniques have become a central tool to analyze queueing networks over the last decade, with applications to performance analysis, simulation, and optimization.

In this paper some of these techniques are extended to a general class of skip-free Markov chains. As in the case of queueing models, a fluid approximation is obtained by scaling time, space, and the initial condition by a large constant. The resulting fluid limit is the solution of an ODE in “most” of the state space. Stability and finer ergodic properties for the stochastic model then follow from stability of the set of fluid limits. Moreover, similar to the queueing context where fluid models are routinely used to design control policies, the structure of the limiting ODE in this general setting provides an understanding of the dynamics of the Markov chain. These results are illustrated through application to Markov Chain Monte Carlo.

KEYWORDS

Markov Chain Monte-Carlo, Metropolis-Hastings algorithm, fluid limits for general state-space Markov chains, fluid limit stability.

1 INTRODUCTION

Although fluid approximations for queueing networks were advocated almost 25 years ago in the book of Newell [1], this viewpoint has been slow to take hold in the queueing research community. Beginning in the 1990s fluid models have been used to address delay in complex networks [2] and bottleneck analysis in [3]. The latter work followed an already extensive research program on diffusion approximations for networks (see [4] and the references therein).

In this paper we extend the application of fluid approximations for analysis of a general class of discrete-time Markov chains \{Φ_k\} on \(d\)-dimensional Euclidean state-space. Recall that a Markov chain is called skip-free if the increments \((Φ_{k+1}−Φ_k)\) are uniformly bounded in norm by a deterministic constant for each \(k\) and each initial condition. For example, Markov chain models of queueing systems are typically skip-free. Here we consider a relaxation of this assumption in which the increments are assumed bounded in an \(L^p\)-sense. Consequently, we find that the chain can be represented by the additive noise model,

\[
Φ_{k+1} = Φ_k + Δ(Φ_k) + ϵ_{k+1}, \quad k \geq 0,
\]

where \(\{ϵ_k\}\) is a martingale increment sequence w.r.t. the natural filtration of the process \{Φ_k\}, and \(Δ: X \to X\) is bounded. Associated to this chain, we consider the following sequence of continuous time process

\[
η^n_r(t; x) \overset{\text{def}}{=} r^{-1} Φ_{[rt]+α}, \quad η^n_r(0; x) \overset{\text{def}}{=} r^{-1} Φ_0 = x,
\]

for \(r \geq 0, α \geq 0\) and \(x \in X\), obtained by interpolating and scaling the Markov chain in space and time. \([\cdot]\) stands for the lower integer part. A fluid limit is obtained as a subsequential weak-limit, and the set of all such limits is called the fluid limit model. In queueing network applications, a fluid limit is easy to interpret in terms of mean flows; in most situations it is a solution of a deterministic set of equations depending on network characteristics as well as the control policy (see e.g. [3, 5, 6, 7, 8]). The existence of limits and the continuity of the fluid limit model may be established under general conditions on the increments (see Theorem 2.2).

The fact that stability of the fluid limit model implies stability of the stochastic network was established in a limited setting in [9], and then extended to a particular two-station, two-class network in [10]. This technique was generalized to a very broad class of multi-class networks in [5]. A key step in the proof of these results is a multi-step state-dependent version of Foster’s criterion introduced in [9] for countable state space models, and later extended to general state-space in [11, 12] (see also [13] for an in-depth discussion). The main result of [5] only established positive recurrence. Moments and rates of convergence to stationarity of the Markovian network model were obtained in [6] based on an extension.
Figure 1: Blue lines: trajectories of the interpolated process \( (2) \) for the Symmetric Random Walk Metropolis Hastings (SRWM) algorithm for a set of initial conditions on the unit sphere between \((0,0,\pi/2)\) for the target density (23). Red lines: flow of the associated ODE.

Figure 2: Blue lines: trajectories of the interpolated process \( (2) \) for the SRWM with target density (24) and initial condition \( x = (1/\sqrt{2},1/\sqrt{2}) \). Red lines: support of the fluid limits associated to this initial condition.

An advantage of the ODE approach over the usual Foster-Lyapunov approach to stability is that the ODE model provides insight into Markov chain dynamics, especially transient behavior starting from a ‘large initial condition’. In the queueing context, the ODE model has many other applications, such as simulation variance reduction [21] and optimization [22].

The remainder of the paper is organized as follows. Section 2.1 contains notations and assumptions, along with a construction of the fluid limit model. The main result is contained in Section 2.2, where it is shown that stability of the fluid limit model implies the existence of polynomial moments as well as polynomial rates of convergence to stationarity (known as \((f,r)\)-ergodicity.) Fluid limits are characterized in Section 2.3. Proposition 2.5 provides conditions that guarantee that a fluid limit coincides with the weak solutions of the ODE (3). The proofs are omitted due to lack of space and can be found in [23].

These results are applied to establish \((f,r)\)-ergodicity of the random-walk Metropolis-Hastings algorithm for super-exponential densities in Section 3.1 and for sub-exponential densities in Section 3.2. In example 3.2 the fluid limit model is stable, and any fluid limit is a weak solution of the ODE (3), yet some fluid limits are non-deterministic.

2 ASSUMPTIONS AND STATEMENT OF THE RESULTS

2.1 Fluid Limit: definitions

We consider a Markov chain \( \Phi \) on a \( d \)-dimensional Euclidean space \( X \) equipped with its Borel sigma-field \( \mathcal{X} \). The distribution of \( \Phi \) is specified by its initial state \( \Phi_0 = x \in X \) and its transition kernel \( P \). We write \( P_x \) for the distribution of the chain conditional on the initial state \( \Phi_0 = x \) and \( E_x \) for the corresponding expectation.

Denote by \( C(R^+,X) \) the space of continuous \( X \)-valued functions on the infinite time interval \([0,\infty)\). We equip \( C(R^+,X) \) with the local uniform topology. Denote by \( D(R^+,X) \) space of \( X \)-valued right-continuous functions with left limits on the infinite time interval \([0,\infty), \) hereafter cadlag functions. This space is endowed with the Skorokhod topology. For \( 0 < T < +\infty \), denote by \( C([0,T],X) \) (resp. \( D([0,T],X) \)) the space of \( X \)-valued continuous functions (resp. cadlag functions) defined on \([0,T]\) equipped with the uniform (resp. Skorokhod) topology.

For \( x \in X \) and \( \alpha > 0 \), consider the following interpolated process,

\[
\eta^\alpha_x(t;x) \triangleq r^{-1}\eta(t;x) = r^{-1}\Phi \left( t + r\alpha \right) = \Phi(t) \left. \right| \Phi_{t+r\alpha} = x.
\]  

Denote by \( \mathcal{Q}^\alpha_{x,z} \) the image probability on \( D(R^+,X) \) of \( P_x \) by \( \eta^\alpha_x(\cdot;x) \). In words, the renormalized process is obtained by scaling the Markov chain in space, time and initial condition. This is made precise in the following.

Definition 2.1 (\( \alpha \)-Fluid Limit). Let \( \alpha \geq 0 \) and \( x \in X \). A probability measure \( \mathcal{Q}^\alpha_x \) on \( D(R^+,X) \) is said to be an \( \alpha \)-fluid limit if there exist sequences of scaling factors \( \{r_n\} \subset \mathbb{R}_+ \) and initial states \( \{x_n\} \subset X \) satisfying \( \lim_{n \to \infty} r_n = +\infty \) and
lim_{n \to \infty} x_n = x such that Q_x^{x_n} converges weakly to Q_x^x on D(\mathbb{R}^+, X), which we denote Q_x^{x_n} \Rightarrow Q_x^x.

The set \( \mathcal{L}^a \) is an open set \( \{Q_x^x, x \in X\} \) of all such limits is referred to as the \( \alpha \)-fluid limit model. An \( \alpha \)-fluid limit \( Q_x^x \) is said to be continuous if \( Q_x^x(\mathcal{C}(\mathbb{R}^+, X)) = 1 \). An \( \alpha \)-fluid limit \( Q_x^x \) is said to be deterministic if there exists a function \( g \in D(\mathbb{R}^+, X) \) such that \( Q_x^x = \delta_g \), the Dirac mass at \( g \).

Assume that \( E_x[|\Phi_1|] < \infty \) for all \( x \in X \), and consider the decomposition (1) where

\[
\Delta(x) \overset{\text{def}}{=} E_x[|\Phi_1 - \Phi_0|] = E_x[|\Phi_1|] - x \quad \text{for all } x \in X, \quad (5)
\]

\[
\epsilon_k \overset{\text{def}}{=} \Phi_k - E[\Phi_k|\mathcal{F}_{k-1}] \quad \text{for all } k \geq 1. \quad (6)
\]

In the sequel, we assume that

B1 There exists \( p > 1 \) such that

\[
\lim_{K \to \infty} \sup_{x \in X} E_x[|\epsilon_1|^p \{ |\epsilon_1| \geq K \}] = 0.
\]

B2 There exists \( \beta \in [0, 1 \wedge (p - 1]) \) such that

\[
N(\beta, \Delta) \overset{\text{def}}{=} \sup_{x \in X} \{ (1 + |x|^\beta) |\Delta(x)| \} < \infty. \quad (7)
\]

The condition B2 implies that the function \( \Delta \) is bounded on \( X \).

A sequence of probability measure \( \{S_n\}_{n \in \mathbb{N}} \) on \( D(\mathbb{R}^+, X) \) is said to be \( \mathcal{C} \)-tight if it is tight in \( D(\mathbb{R}^+, X) \) and if every weak limit \( S \) of a subsequence of \( \{S_n\}_{n \in \mathbb{N}} \) is continuous.

**Theorem 2.2.** Assume B1 and B2. Then, for any sequences \( \{r_n\} \subset \mathbb{R}^+ \) and \( \{x_n\} \subset X \) such that \( \lim_{n \to \infty} r_n = +\infty \) and \( \lim_{n \to \infty} x_n = x \), \( \{Q_{x_n, x_n}^x\}_{n \in \mathbb{N}} \) is \( \mathcal{C} \)-tight for all \( 0 \leq \alpha \leq \beta \). Furthermore, for all \( 0 \leq \alpha < \beta \), the \( \alpha \)-fluid limits are trivial in the sense that \( Q_x^x = \delta_0 \) with \( g(t) \equiv x \).

### 2.2 Stability of Fluid Limits and Markov Chain Stability

There are several notions of stability that appeared in the literature (see [24, Theorem 3] and the surrounding discussion). We adopt the notion of stability introduced in [25].

**Definition 2.3** (Stability). The \( \alpha \)-fluid limit model \( \mathcal{L}^a \) is said to be stable if there exist \( T > 0 \) and \( \rho < 1 \) such that for any \( x \in X \) with \( |x| = 1 \),

\[
Q_x^x \left( \eta \in D(\mathbb{R}^+, X), \inf_{0 \leq t \leq T} |\eta(t)| \leq \rho \right) = 1. \quad (8)
\]

Let \( f : X \to [1, \infty) \) be a function and \( \{r(n)\}_{n \in \mathbb{N}} \) be a sequence of positive real numbers. Denote by \( ||.||_f \) the \( f \)-total variation norm, defined for any finite signed measure \( \nu \) as \( ||\nu||_f = \sup_{|g| \leq f} ||\nu(g)|| \). When \( f \equiv 1 \), \( ||.||_1 = ||.||_{TV} \) is the total variation norm. An aperiodic phi-irreducible positive Harris chain with stationary distribution \( \pi \) is called \((f, r)\)-ergodic if \( \lim_{n \to \infty} r(n) ||P^n(x, \cdot) - \pi||_f = 0 \) for all \( x \in X \). If \( P \) is positive Harris recurrent with invariant probability \( \pi \), the fundamental kernel \( Z \) is defined as \( Z \overset{\text{def}}{=} (\text{Id} - P + \Pi)^{-1} \), where the kernel \( \Pi \) is \( \Pi(x, \cdot) \equiv \pi(\cdot) \), for all \( x \in X \) and \( \Pi \) is the identity kernel. For any measurable function \( g \) on \( X \), the function \( \hat{g} = Zg \) is a solution to the Poisson equation, whenever the inverse is well defined. The unfamiliar reader can refer to [11]) for the definitions of aperiodicity, phi-irreducibility, positive Harris chain, \( \cdots \).

Let \( f \geq 1 \) be a finite valued function on \( X \) and let \( L_{2\infty}^f \) denote the vector space of all measurable functions \( g \) on \( X \) such that \( \sup_{x \in X} |g(x)| / f(x) \) is finite. This vector space is a Banach space with the associated norm \( ||g||_f \overset{\text{def}}{=} \sup_{x \in X} |g(x)| / f(x) \). The following theorem may be seen as an extension of [6, Theorem 5.5], which relates the stability of the fluid limit to the \( (f, r) \)-ergodicity of the original chain.

**Theorem 2.4.** Let \( \{\Phi_k\}_{k \in \mathbb{N}} \) be a phi-irreducible and aperiodic Markov chain such that compact sets are petite. Assume B1 and B2 and the \( \beta \)-fluid limit model \( \mathcal{L}^\beta \) is stable. Then, for any \( 1 \leq q \leq (1 + \beta)^{-1} \),

(i) the \( \beta \)-fluid chain \( \{\Phi_k\}_{k \in \mathbb{N}} \) is \((f_q, r_q)\)-ergodic with \( f_q(x) \overset{\text{def}}{=} 1 + x^{p-q(1+\beta)} \) and \( r_q(n) = n^{q-1} \).

(ii) the fundamental kernel \( Z \) is a bounded linear transformation from \( L_{2\infty}^f \) to \( L_{2\infty}^{f_q} \).

### 2.3 Characterization of the fluid limits

Theorem 2.4 relates the ergodicity of the Markov chain to the stability of the fluid limit and begs the question: how can we determine if the \( \beta \)-fluid limit model is stable? To answer this question we first characterize the set of fluid limits.

In addition to Assumptions B1-B2 we require conditions on the limiting behavior of the function \( \Delta \).

**B3** There exist an open set \( O \subset X \setminus \{0\} \) and a continuous function \( \Delta_\infty : O \to X \) such that, for any compact subset \( H \subset O \),

\[
\lim_{r \to +\infty} \sup_{x \in H} |x|^{\beta} \Delta(r(x) - \Delta_\infty(x)) = 0,
\]

where \( \beta \) is given by B2.

The characterization of fluid limits is elementary when \( O = X \setminus \{0\} \), in which case the radial limit \( \lim_{r \to +\infty} r^{\beta} |x|^{\beta} \Delta(r(x)) \) exists for \( x \neq 0 \). Though this condition is met in many examples, there are cases where radial limits do not exist for directions belonging to some low-dimensional manifolds of the unit sphere.

We consider the ODE (3), where the function \( h \) is given by

\[
h(x) \overset{\text{def}}{=} |x|^{-\beta} \Delta_\infty(x). \quad (9)
\]

A function \( \mu : I \to X \) (where \( I \subset \mathbb{R}^+ \) is an interval which can be open or closed, bounded or unbounded) is said to be a solution of the ODE (3) on \( I \) with initial condition \( x \) if \( \mu \) is continuously differentiable on \( I \), for all \( t \in I \) \( \mu(t) \in O \), \( \mu(0) = x \) and \( \dot{\mu}(t) = h \circ \mu(t) \). The following proposition shows that the fluid limit in \( O \) coincides with the solutions of the ODE.

**Proposition 2.5.** Assume B1, B2 and B3. Let \( Q^0 \) be a \( \beta \)-fluid limit and for any \( 0 \leq s \leq t \), define

\[
A(s,t) \overset{\text{def}}{=} \{ \eta \in C(\mathbb{R}^+, X) : \eta(u) \in O \text{ for all } u \in [s,t] \}. \quad (10)
\]
Then, on $A(s,t)$,
\[
\sup_{s \leq t \leq T} \left| \eta(u) - \eta(s) - \int_s^u h \circ \eta(v)dv \right| = 0, \quad \mathbb{Q}^\beta \text{-} a.s.
\]

Under very weak additional conditions one may deduce a first elementary stability condition which says such solutions are well-defined. From the discussion above, \cite[(8)]{26} to the behavior of the solutions of the ODE when \( \rho < \beta \) to a sphere of radius \( r \) before a given time \( \rho(0) \). Assume that \( B1 \) to \( B4 \) hold with \( O \) and \( \{ \mu_n \} \) \( \beta \) fluid limits are stable and the conclusions of Theorem 2.4 hold.

B4 Assume that for all \( x \in O \), there exists \( T_x \) such that the ODE (3) with initial condition \( x \in O \) exist and are unique on a non-vanishing interval \([0, T_x]\). In such case, Proposition 2.5 provides a handy description of the fluid limit.

Assumption B4 is satisfied if \( \Delta_x \) is locally Lipschitz on \( O \); in such case, \( h \) is locally Lipschitz on \( O \) and it then follows from classical results on the existence of solutions of the ODE \( (\text{see e.g. } [26]) \) that, for any \( x \in O \), there exists \( T_x \) such that, on the interval \([0, T_x]\), the ODE (3) has a unique solution \( \mu \) with initial condition \( \mu(0) = x \). In addition, if the ODE (3) has two solutions \( \mu_1 \) and \( \mu_2 \) on an interval \( I \) which satisfy \( \mu_1(t_0) = \mu_2(t_0) = x_0 \) for some \( t_0 \in I \), then \( \mu_1(t) = \mu_2(t) \) for any \( t \in I \).

An elementary application of Proposition 2.5 shows that, under this additional assumption, a fluid limit starting at \( x_0 \in O \) coincides with the solution of the ODE (3) with initial condition \( x_0 \) on a non-vanishing interval.

**Theorem 2.6.** Assume \( B1 \) to \( B4 \). Then, for each \( x_0 \in O \) there exists \( T_{x_0} \) such that \( \mathbb{Q}^\beta_{x_0} = \delta_{\mu(\cdot; x_0)} \) on \( D([0, T_{x_0}], X) \).

If we can take \( O = X \setminus \{0\} \) in B3 then all \( \beta \)-fluid limits are deterministic and solve the ODE (3). Furthermore, for any \( \epsilon > 0 \) and \( x \in X \), and any convergent sequences \( \{r_n\} \subset \mathbb{R}_+ \) and \( \{x_n\} \subset X \),
\[
\lim_{n \to \infty} \mathbb{P}_{r_n \to \infty} \left( \sup_{0 \leq t \leq T_{r_n}} |\eta(t; r_n) - \eta(t; x_n)| \geq \epsilon \right) = 0.
\]

Hence, the fluid limit only depends on the initial value \( x \) and does not depend upon the choice of the sequences \( \{r_n\} \) and \( \{x_n\} \).

The last step is to relate the stability of the fluid limit \( (\text{see } (8)) \) to the behavior of the solutions of the ODE when such solutions are well-defined. From the discussion above, we may deduce a first elementary stability condition which holds under B3 with \( O = X \setminus \{0\} \). In this case, the stability of the fluid limit is implied upon assuming that the solution of the ODE with initial condition \( x \in X \setminus \{0\} \) enters a sphere of radius \( r \) before 1 before a given time \( T \).

**Theorem 2.7.** Let \( \{\Phi_k\}_{k \in \mathbb{N}} \) be a phi-irreducible and aperiodic Markov chain such that compact sets are petite. Let \( \rho \in (0,1) \) and \( T > 0 \). Assume that \( B1 \) to \( B4 \) hold with \( O = X \setminus \{0\} \). Assume in addition that, for any \( x_0 \) satisfying \( |x_0| = 1 \) the solution \( \mu(\cdot; x) \) is such that
\[
\inf_{0 \leq t \leq T} \|\mu(t; x)\| \leq \rho.
\]

Then, the \( \beta \)-fluid limit model is stable and the conclusions of Theorem 2.4 hold.

When B3 holds for a strict subset of the state space \( O \subsetneq X \setminus \{0\} \), the situation is more difficult, because some fluid limits are not solutions of the ODE. Regardless, under general assumptions stability of the ODE implies stability of the fluid limit model.

**Theorem 2.8.** Let \( \{\Phi_k\}_{k \in \mathbb{N}} \) be a phi-irreducible and aperiodic Markov chain such that compact sets are petite. Assume that \( B1 \) to \( B4 \) hold with \( O \subseteq X \setminus \{0\} \). Assume in addition that

(i) there exists \( T_0 > 0 \) such that, for any \( x \), \( |x| = 1 \),
\[
\mathbb{Q}_x^\beta (\eta(\cdot; [0, T_0]) \cap O \neq \emptyset) = 1.
\]

(ii) for any \( K > 0 \), there exist \( T_K \) and \( \rho_K < 1 \) such that
\[
\inf_{[0,T_K]} \|\mu(\cdot; x)\| \leq \rho_K.
\]

(iii) for any compact set \( H \subset O \) and any \( K \),
\[
\Omega_H \overset{\text{def}}{=} \{\mu(\cdot; x), x \in H\}
\]

is a compact subset of \( O \).

Then, the set of all \( \beta \)-fluid limits is stable and the conclusions of Theorem 2.4 hold.

The first condition (i) implies that each \( \beta \)-fluid limit reaches the set \( O \) in finite time. When the initial point \( x \) of the fluid limit lies in the set \( O \), this condition is automatically fulfilled. When \( x \neq 0 \) does not belong to \( O \), this condition typically requires that there is a force driving the chain away from the singular set. The verification of this property generally requires some problem-dependent and sometimes intricate constructions \( (\text{see e.g. Example 3.2}) \). The second condition (ii) implies that the solution \( \mu(\cdot; x) \) of the ODE with initial point in \( x \in O \) reaches a ball inside the unit sphere before approaching the singularity. This also means that the singular set is repulsive for solutions of the ODE.

**3 THE ODE METHOD FOR THE METROPOLIS-HASTINGS ALGORITHM**

The Metropolis-Hastings (MH) algorithm is a popular computational method for generating samples from virtually any distribution \( \pi \) \( (\text{see } [27] \text{ and the references therein}) \). In particular there is no need for the normalising constant to be known and the space \( X = \mathbb{R}^d \) on which it is defined can be high dimensional \( (\text{i.e. the integer } d \text{ can be large}) \). The method consists of simulating an ergodic Markov chain \( \{\Phi_k\}_{k \geq 0} \) on \( X \) with transition probability \( P \) such that \( \pi \) is the stationary distribution for this chain, \( i.e. \pi P = \pi \).

The MH algorithm requires the choice of a proposal kernel \( q \). In order to simplify the discussion, we will here assume that \( \pi \) and \( q \) admit densities with respect to Lebesgue measure \( \lambda^{\text{Leb}} \), denoted with an abuse of notation \( \pi \) and \( q \) hereafter. The rôle of the distribution \( q \) consists of proposing potential transitions for the Markov chain \( \{\Phi_k\} \). Given that the chain is currently at \( x \), a candidate \( y \) is accepted
with probability $\alpha(x, y)$ defined as $\alpha(x, y) = 1 \wedge \frac{q(y)q(x, y)}{q(x)q(y, x)}$. Otherwise it is rejected and the Markov chain stays at its current location $x$. The transition kernel $P$ of this Markov chain takes the form for $x \in X$ and $A \in \mathcal{B}(X)$

$$P(x, A) = \int_{A - x} \alpha(x, x + y)q(x, x + y)\lambda^{\text{Leb}}(dy) + \mathbb{1}_A(x) \int_{X - x} \{1 - \alpha(x, x + y)\}q(x, x + y)\lambda^{\text{Leb}}(dy),$$

where $A - x \overset{\text{def}}{=} \{y \in X, x + y \in A\}$. The Markov chain $P$ is reversible with respect to $\pi$, and therefore admits $\pi$ as invariant distribution. For the purpose of illustration, we focus on the symmetric increments random-walk MH algorithm (hereafter SRWM), in which $q(x, y) = q(y - x)$ for some symmetric distribution $q$ on $\mathbb{R}^d$. Under these assumptions the acceptance probability simplifies to $\alpha(x, y) = 1 \wedge [\pi(y)/\pi(x)]$.

For any measurable function $V : X \to \mathbb{R}$,

$$\mathbb{E}_x [V(\Phi_1)] - V(x) = \int_{A_x} \{V(x + y) - V(x)\}q(x)\lambda^{\text{Leb}}(dy) + \int_{R_x} \{V(x + y) - V(x)\} \frac{\pi(x + y)}{\pi(x)}q(x)\lambda^{\text{Leb}}(dy),$$

where $A_x \overset{\text{def}}{=} \{y \in X, \pi(x + y) \geq \pi(x)\}$ is the acceptance region (moves toward $x + A_x$ are accepted with probability one) and $R_x \overset{\text{def}}{=} X \setminus A_x$ is the potential rejection region. From [28, Theorem 2.2], we obtain the following basic result.

**Theorem 3.1.** Suppose the target density $\pi$ is positive and continuous and that $q$ is bounded away from zero, i.e. there exist $\delta_q > 0$ and $\epsilon_q > 0$ such that $q(x) \geq \epsilon_q$ for $|x| \leq \delta_q$. Then, the random-walk-based Metropolis algorithm on $(X, \mathcal{X})$ is $\lambda^{\text{Leb}}$-irreducible, aperiodic and every non-empty bounded set is small.

In the sequel, we assume that $q$ has a moment of order $p > 1$. To apply the results presented in section 2, we must first compute $\Delta(x) = \mathbb{E}_x[\Phi_1] - x$, i.e. to set $V(x) = x$ in the previous formula. Since $q$ is symmetric and therefore zero-mean, the previous relation boils down to

$$\Delta(x) = \int_{R_x} y \left(\frac{\pi(x + y)}{\pi(x)} - 1\right)q(y)\lambda^{\text{Leb}}(dy).$$

Note that, for any $x \in X$, $|\epsilon_1| \leq |\Phi_1 - \Phi_0| + m \mathbb{P}_\delta$-a.s. where $m = \int |y|q(y)\lambda^{\text{Leb}}(dy)$. Therefore, for any $K > 0$,

$$\mathbb{E}_x [|\epsilon_1|^p 1\{|\epsilon_1| \geq K\}] \leq 2^p \mathbb{E}_x[\{|\Phi_1 - \Phi_0|^p + m^p|\{\Phi_1 - \Phi_0| \geq K - m\}\}] \leq 2^p \int |y|^p 1\{|y| \geq K - m\}q(y)\lambda^{\text{Leb}}(dy).$$

showing that assumption B1 is satisfied as soon as the increment distribution has a bounded $p$-th moment. Because on the set $R_x$, $\pi(x + y) \leq \pi(x)$, we similarly have $|\Delta(x)| \leq \int |y|q(y)\lambda^{\text{Leb}}(dy)$ showing that B2 is satisfied with $\beta = 0$; nevertheless, in some examples, for $\beta = 0$, $\Delta_\infty$ can be zero and the fluid limit model is unstable. In these cases, it is required to use larger $\beta$ (see section 3.2).

### 3.1 Super-exponential target densities

In this section, we focus on target density $\pi$ on $\mathbb{R}^d$ which are super-exponential.

**Definition 3.2 (Super-exponential pdf).** A probability density function $\pi$ is said to be super-exponential if $\pi$ is positive with continuous first derivatives and is such that

$$\lim_{|x| \to \infty} \langle n(x), \ell(x) \rangle = -\infty,$$

where $n(x) = x/|x|$ and

$$\ell(x) \overset{\text{def}}{=} \nabla \log \pi(x).$$

The condition implies that for any $H > 0$ there exists $R > 0$ such that

$$\frac{\pi(x + an(x))}{\pi(x)} \leq \exp(-aH) \quad \text{for } |x| \geq R, a \geq 0,$$

that is, $\pi(x)$ is at least exponentially decaying along any ray with the rate $H$ tending to infinity as $|x|$ goes to infinity.

It also implies that for $x$ large enough the contour manifold $C_x \overset{\text{def}}{=} \{y \in X, \pi(x + y) = \pi(x)\}$ can be parameterized by the unit sphere $\mathbb{S}$, since each ray meets $C_x$ at exactly one point. (see Fig. 3). Denote by $A \subset B$ the symmetric difference of the sets $A$ and $B$ and for any measurable set $A$, denote $Q(A) = \int_A q(y)\lambda^{\text{Leb}}(dy)$.

**Definition 3.3 (Radial limit).** We say that the family of rejection regions $\{R_x, x \geq 0, x \in \mathbb{R}\}$ has radial limits over the open cone $\mathcal{O} \subseteq X \setminus \{0\}$ if there exists a collection of sets $\{R_x, x \in \mathcal{O}\}$ such that, for any compact subset $H \subseteq \mathbb{O}$, $\lim_{r \to \infty} \text{sup}_{x \in \mathcal{O}} Q(R_{rx} \cup R_{rx}, x = 0) = 0$.

**Proposition 3.4.** Assume that the target density $\pi$ is super-exponential. Assume in addition that the family $\{R_x, x \geq 0, x \in \mathcal{O}\}$ has a radial limit over an open cone $\mathcal{O} \subseteq X \setminus \{0\}$. Then, for any compact set $H \subset \mathcal{O}$, $\lim_{r \to \infty} \text{sup}_{x \in \mathcal{O}} |\Delta(rx) - \Delta_\infty(x)| = 0$, where $\Delta_\infty(x) \overset{\text{def}}{=} -\int_{R_{\infty,x}} yq(y)\lambda^{\text{Leb}}(dy)$.

The definition of the limiting field $\Delta_\infty$ becomes simple when the rejection region radially converges to an half-space.
Definition 3.5 (regularity in the tails). We say that the target density $\pi$ is regular in the tails over $O$ if the family $\{R_x, r \geq 0, x \in O\}$ has radial limits over an open cone $O \subseteq X \setminus \{0\}$ and there exists a continuous function $\ell_\infty : X \setminus \{0\} \to X$ such that, for all $x \in O$,

$$Q(R_{x,0} \cap \{y \in X, (y, \ell_\infty(x)) < 0\}) = 0.$$  

(18)

Regularity in the tails holds when the curvature of the contour manifold $C_x$ goes to zero as $r \to \infty$; nevertheless, this condition may still hold in situations where the curvature of the contour manifolds can grow to infinity in some directions (see Fig. 5).

Assume that:

$$q(x) = \det^{-1/2}(\Sigma) q_0(\Sigma^{-1/2} x),$$  

(19)

where $\Sigma$ is a positive definite matrix and $q_0$ is a rotationally invariant distribution, i.e. $q_0(Ux) = q_0(x)$ for any unitary matrix $U$.

Proposition 3.6. Assume that the target density $\pi$ is super-exponential and regular in the tails over the open cone $O \subseteq X \setminus \{0\}$. Then, the SRWM algorithm with proposal $q$ given in (19) satisfies assumption B3 on $O$ with

$$\Delta_\infty(x) = m_1(q_0) \frac{\sum_\ell_\infty(x)}{\sqrt{\sum_\ell_\infty(x)}},$$  

(20)

where $\ell_\infty$ is defined in (18) and $m_1(q_0) \equiv \int_X y_1 \sum_{y \geq 0} q_0(y)^{1/2} dy > 0$, where $y = (y_1, \ldots, y_d)$.

If $\Sigma = I_d$ and $\ell_\infty(x) = \lim_{r \to \infty} n(\ell(rx))$ then the ODE is a version of steepest ascent algorithm to maximize log fluid limit $Q$. Following [28], define the class $P$ of such a positive conclusion for the algorithm itself (because we do not control the fluctuation of the algorithm around its limit). The tail regularity condition and the definition of the ODE limit are more transparent in a class of models which are very natural in many statistical contexts, namely, the exponential family. Following [28], define the class $P$ to consist of those everywhere positive densities with continuous second derivatives $\pi$ satisfying

$$\pi(x) \propto g(x) \exp \{-p(x)\},$$  

(21)

where

- $g$ is a positive function slowly varying at infinity, i.e. for any $K > 0$,

$$\limsup_{|x| \to \infty} \frac{g(x+y)}{g(x)} = \limsup_{|x| \to \infty} \frac{g(x+y)}{g(x)} = 1,$$

(22)

- $p$ is a positive polynomial in $X$ of even order $m$ and $\lim_{|x| \to \infty} p_m(x) = \infty$, where $p_m$ denotes the polynomial consisting only of the $p$'s $m$-th order terms.

Proposition 3.7. Assume that $\pi \in P$ and let $q$ be given by (19). Then, $\pi$ is super-exponential, regular in the tails over $X \setminus \{0\}$ with $\ell_\infty(x) = -n[\nabla p_m(n(x))]$. For any $x \in X \setminus \{0\}$, there exists $T_x > 0$ such that the ODE $\dot{\pi} = \Delta_\infty(\mu)$ with initial condition $x$ and $\Delta_\infty$ given by (20) has a unique solution on $[0, T_x)$ and $\lim_{t \to T_x^-} \mu(t; x) = 0$. In addition, the fluid limit $Q^\infty_\mu$ is deterministic on $D([0, T_x], X)$, with support function $\mu(\cdot; x)$.

Because all the solutions of the initial value problem $\dot{\mu} = -m_1(q_0)\nabla p_m(n(\mu))$, $\mu(0) = 0$ are zero after a fixed amount of time $T$ for any initial condition on the unit sphere, we may apply Theorem 2.7. We have, from Theorems 3.1 and 3.7

Theorem 3.8. Consider the SRWM Markov chain with target distribution $\pi \in P$ and increment distribution $q$ having a moment of order $p > 1$ and satisfying (19). Then for any $1 \leq u \leq p$, the SRWM Markov chain is $(f_u, r_u)$-ergodic with

$$f_u(x) = 1 + |x|^{p-u}, \quad r_u(t) \sim t^{u-1}.$$  

Example 3.1. To illustrate our findings, consider the target density, borrowed from [29, example 5.3]

$$\pi(x_1, x_2) \propto (1 + x_1^2 + x_2^2 + x_1^2 x_2^2) \exp(-x_1^2 + x_2^2).$$  

(23)

The contour curves are illustrated in Figure 4. They are almost circular except from some small wedges by the $x$-axis. Due to the wedges, the curvature of the contour manifold at $(x, 0)$ is $(x^2 - 1)/x$ and therefore tends to infinity along the $x$-axis. Since $\pi \in P$, Proposition 3.7 shows that $\pi$ is super-exponential, regular in the tails and $\ell_\infty(x) = \ell_\infty(x)$, taking $q \sim N(0, \sigma^2 I)$, $\Delta_\infty(x) = -\sigma^2(x)/\sqrt{2\pi}$ and (the Caratheodory) solution of the initial value problem $\dot{\mu} = \Delta_\infty(\mu)$, $\mu(0) = x$ are given by $\mu(x; t) = \left(\frac{|x| - \sigma t}{\sqrt{2\pi}}\right)^2 \{\sigma t < \sqrt{2\pi}|x| n(x)\}$. Along the sequence $\{x_k = (k \pm k^{-1})\}_{k \geq 0}$, the normed gradient $n(\ell(x_k))$ converges to $(0, \pm 1)$, showing that whereas $\ell_\infty$ is the radial limit of the normed gradient $n(\ell)$ (i.e. for any $u \in S$, $\lim_{\ell \to \infty} n(\ell(lu)) = \ell_\infty(u)$), $\lim_{|x| \to \infty} n(\ell(x)) - \ell_\infty(x)$ = 2. Therefore, the normed gradient $n(\ell(x))$ does not have a limit as $|x| \to \infty$ along the $x$-axis. Nevertheless the fluid limit exists, and is extremely simple to determine. Hence, the ergodicity of the SRWM sampler with target distribution (23) may be established (note that for this example the theory developed in [28] and [29] does not apply). The functions $\Delta$ and $\Delta_\infty$ are displayed in Figure 5. The flow of the initial value problem $\dot{\mu} = \Delta_\infty(\mu)$ for a set of initial conditions on the unit sphere between $(0, \pi/2)$ are displayed in Figure 1.

Example 3.2 (Mixture of Gaussian densities). In this example (also borrowed from [29]), we consider the mixture of two Gaussian distributions on $\mathbb{R}^2$. For some $a^2 > 1$ and $0 < \gamma < 1$, set

$$\pi(x) \propto \gamma \exp(-0.5x^T \Gamma_1^{-1} x) + (1 - \gamma) \exp(-0.5x^T \Gamma_2^{-1} x),$$  

(24)

where $\Gamma_1^{-1} \equiv \text{diag}(a^2, 1)$ and $\Gamma_2^{-1} \equiv \text{diag}(1, a^2)$. The contour curves for $\pi$ with $a = 4$ are illustrated on Figure 6. The contour curves have some sharp bends that do not disappear in the limit even though the contour curves of the two components of the mixtures are smooth ellipses. [29, Eq. (51)] have shown indeed that the curvature of the contour curves on the diagonals tend to infinity. As shown in the following Lemma, this target density is however regular in the tails over $O = X \setminus \{x = (x_1, x_2) \in \mathbb{R}^2, |x_1| = |x_2|\}$ (and not over $X \setminus \{0\}$). More precisely:
Lemma 3.9. For any $\varepsilon > 0$, there exist $M$ and $K$ such that
\[
\sup_{|x| > K, |x| - 2|x| \geq M} |\Delta(x) - \Delta_\infty(x)| \leq \varepsilon, 
\]
where $\Delta_\infty(x) \equiv -\int_{R_{\infty,x}} (y) yq(y)\lambda_{\text{Lab}}(dy)$ with $R_{\infty,x} \equiv \{y, (y, \Gamma_1^{-1}x) \geq 0\}$ if $|x_1| > |x_2|$ and $R_{\infty,x} \equiv \{y, (y, \Gamma_1^{-1}x) \geq 0\}$ otherwise.

Since $q$ satisfies (19), when $\Sigma = \text{Id}$, for any $x \in O$, $\Delta_\infty$ may be expressed as: $\Delta_\infty(x) = -c_n(\Gamma_2^{-1}x)$ if $|x_1| > |x_2|$ and $\Delta_\infty(x) = -c_n(\Gamma_1^{-1}x)$ if $|x_1| < |x_2|$, where $c_n$ is a constant depending on the proposal distribution $q$. This is illustrated in Figure 7 which displays the functions $\Delta$ and $\Delta_\infty$ and shows that these two functions are asymptotically close outside a band along the main diagonal. The flow of the initial value problem $\mu = \Delta_\infty(\mu)$ for a set of initial conditions on the unit sphere are displayed in Figure 8 together with trajectories of the interpolated process.

If we assume that $q$ is rotationally invariant and with compact support, it may be shown that $B_4$, and conditions (i), (ii), and (iii) of Proposition 2.8 hold. The proof of condition (i) is certainly the most difficult to check, and requires the construction of a local Lyapunov function to show that the fluid limit does not stay in a neighborhood of the diagonal. Note that the fluid limit model is not deterministic (see Fig. 3).

Proposition 3.12. Assume that the target density $\pi$ is subexponential and regular in the tails over an open cone $O \subseteq X \setminus \{0\}$ and that $q$ satisfies (19). Then, for any compact set $H \subset O$, $\lim_{n \to \infty} \sup_{x \in H} |r^\beta |x|^{\beta} \Delta_\infty(x) - \Delta_\infty(x)| = 0$, with
\[
\Delta_\infty(x)q \equiv \int_{O} y(\ell(x,y))dy = m_2(q_0)\Sigma_\ell(x), 
\]
where $m_2(q_0) \equiv \int_{x} y_2^2(y \geq 0)q_0(y)dy > 0$.

Once again, if the curvature of the contour curve goes to zero at infinity, $\ell_\infty(x)$ is for large $x$ asymptotically colinear to $n(\nabla \log \pi(x))$. However, whereas $|\nabla \log \pi(x)| \to 0$ as $|x| \to \infty$, the renormalization prevents $\ell_\infty(x)$ to vanish at $\infty$; on the contrary, it converges radially to a constant along each ray. As above, the tail regularity condition may still hold even when the curvature goes to infinity; see example 3.3. As above, the subexponential tail regularity condition and the definition of the ODE limit are more transparent in the weibullian family. Mimicking the construction above, define for $\delta > 0$ the class $P_3$ to consist of those everywhere positive densities with continuous second derivatives $\pi$ satisfying
\[
\pi(x) \propto g(x)\exp \left\{-p^\delta(x)\right\}, 
\]
where $g$ is a positive function slowly varying at infinity (see (22)), $p$ is a positive polynomial in $X$ of even order $m$ with $\lim_{|x| \to \infty} p_m(x) = +\infty$.

Proposition 3.13. Assume that $\pi \in P_3$ for some $0 < \delta < 1/m$ and let $q$ be given by (19). Then, $\pi$ is subexponential, regular in the tails with $\beta = 1 - m\delta$ and $\ell_\infty(x) = -\delta \Gamma_1^{-1}(n(x))\nabla p_m(n(x))$. For any $x \in X \setminus \{0\}$, there exists $T_x > 0$ such that the ODE $\dot{\mu} = h(\mu)$ with initial condition $x$ and $h$ given by
\[
h(x) = -\delta |x|^{-(1-m\delta)} m_2(q_0) p_m^{-1}(n(x)) \nabla p_m(n(x)), 
\]
has a unique solution on $[0,T_x)$ and $\lim_{t \to T^-} h(t; x) = 0$. In addition, the fluid limit $Q^\beta_x$ is deterministic on $D([0,T_x), X)$, with support function $\mu(\cdot; x)$.

Example 3.3. Consider the subexponential weibullian family derived from example 3.1
\[
\pi(x, x_2) \propto (1 + x_1^2 + x_2^2 + x_1^8 x_2^4) \exp \left\{-\left(x_1^2 + x_2^4\right)^\delta\right\}. 
\]

The contour curves are displayed in Figure 9. Since $\pi \in P_3$, Proposition 3.13 shows that $\pi$ is subexponential, regular in the tails with $\beta = 1 - 2\delta$ and $\ell_\infty(x) = -2\delta \Gamma_1^{-1}(n(x))$. Taking $q \sim N(0, \sigma^2 I)$, $\Delta_\infty(x) = -\sigma^2 \delta |x|$ and the (Caratheodory) solution of the initial value problem $\mu = |x|^{-(2-\delta)}\Delta_\infty(\mu)$, $\mu(0) = x$ are given by $\mu(t;x) = |x|^{2(1-\delta)} - 2\sigma^2\delta(1 - t)^{[\delta(1-\delta)^{-1}]} n(x) 1\{|x|^{2(1-\delta)} - 2\sigma^2\delta(1 - t)^{\delta(1-\delta)} \geq 0\}$. Here again, the
gradient \( f(x) \) (even properly normalized) does not have a limit as \( |x| \to \infty \) along the x-axis, but the fluid limit model is simple to determine. Hence, the ergodicity of the SRWM sampler with target distribution (28) may be established (note that for this example the theory developed in [30] and [15] do not apply). The functions \( \Delta \) and \( \Delta_{\infty} \) are displayed Figure 10. The flow of the initial value problem \( \mu = h\mu \) for a set of initial conditions on the unit sphere between \( (0, \pi/2) \) are displayed in Fig. 1.

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REFERENCES


Figure 4: Contour curves of the target density (23).

Figure 5: Blue lines: $\Delta_\infty$; Green lines: $\Delta$ for the target density (23).

Figure 6: Contour plot of the target density (24).

Figure 7: Blue lines: $\Delta_\infty$; Green lines: $\Delta$ for the target density (24).

Figure 8: Blue lines: interpolated process for a set of initial conditions on the unit sphere for the target density (24). Red lines: flow of the initial value problem $\dot{\mu} = h(\mu)$ with $h$ given in Lemma 3.9.


Figure 9: contour curves of the target density (28)

Figure 10: Blue lines: $\Delta_\infty$; Green lines: $\Delta$ for the target density (28)

Figure 11: Blue lines: interpolated process $\eta_1^{\beta}$ for a set of initial conditions on the unit sphere for the target density (28) with $\delta = 0.4$. Red lines: support of the fluid limits associated to these initial conditions.