Convergence rates for Metropolis-Hastings algorithms in the Wasserstein distance

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Abstract

We develop necessary conditions for geometrically fast convergence in the Wasserstein distance for Metropolis-Hastings algorithms on $\mathbb{R}^d$ when the metric used is a norm. This is accomplished through a lower bound which is of independent interest. We show exact convergence expressions in more general Wasserstein distances (e.g. total variation) can be achieved for a large class of distributions by centering an independent Gaussian proposal, that is, matching the optimal points of the proposal and target densities. This approach has applications for sampling posteriors of many popular Bayesian generalized linear models. In the case of Bayesian binary response regression, we show when the sample size $n$ and the dimension $d$ grow in such a way that the ratio $d/n \to \gamma \in (0, +\infty)$, the exact convergence rate can be upper bounded asymptotically.

1 Introduction

Applications in modern Bayesian statistics often require generating Monte Carlo samples from a posterior distribution defined on $\Theta \subseteq \mathbb{R}^d$, which may mean using a version of the Metropolis-Hastings algorithm [2, 11, 21]. Popular versions of Metropolis-Hastings
include, among many others, the random walk Metropolis-Hastings, Metropolis-adjusted Langevin, and Metropolis-Hastings independence (MHI) algorithms, and Hamiltonian Monte Carlo.

Convergence analyses of Metropolis-Hastings Markov chains has traditionally focused on studying their convergence rates in total variation distances [14, 20, 29, 33, 37]. These convergence rates have received significant attention, at least in part, because they provide a key sufficient condition for the existence of central limit theorems [17] and validity of methods for assessing the reliability of the simulation effort [1, 13, 30, 35]. However, there has been significant recent interest in the convergence properties of Monte Carlo Markov chains in high-dimensional settings [5, 6, 10, 16, 24, 28, 38] and the standard approaches based on drift and minorization conditions [22, 31] have shown limitations in this regime [26]. This has led to interest in considering the convergence rates of Monte Carlo Markov chains using alternative Wasserstein distances [4, 10, 15, 25, 27] which can result in many similar benefits [10, 15, 18, 19].

We derive necessary conditions for geometrically fast convergence in the Wasserstein distance for general Metropolis-Hastings Markov chains when the metric used to define the Wasserstein distance is a norm. This requires uniform control over the rejection in the Metropolis-Hastings algorithm and essentially matches previous results with total variation distances [20, 29], suggesting a fundamental requirement for fast convergence of these algorithms. We accomplish this analysis through a lower bound in the Wasserstein distance for Metropolis-Hastings algorithms on $\mathbb{R}^d$ which is of independent interest. We then use this insight to motivate a new centered proposal for the MHI algorithm. That is, we match the maximal point of the proposal density with that of the target density. By centering the proposal, we directly imbue the Markov chain with a strong attraction to a set where the target distribution has high probability eliminating the need to develop a drift condition to study the convergence rate of the Markov chain. Using this centered proposal in the MHI algorithm, we derive exact convergence expressions which are universal across more general Wasserstein distances (e.g. total variation) and provide readily verifiable conditions when this is achievable.

We apply our theoretical work on the MHI algorithm with a centered Gaussian proposal to the problem of sampling posteriors of Bayesian generalized linear models and derive
exact convergence rates in general Wasserstein distances for many such models. We then consider high-dimensional Bayesian binary response regression with Gaussian priors and derive an asymptotic upper bound for general Wasserstein distances when the sample size and the dimension grow together. To the best of our knowledge, this work is the first to successfully address the setting where both the sample size and the dimension increase in unison. For example, previous results investigated the convergence rates of certain Gibbs samplers in the case where either the dimension or the sample size increase individually [6, 27].

2 Metropolis-Hastings and Wasserstein distance

As they will be considered here, Metropolis-Hastings algorithms simulate a Markov chain with invariant distribution $\Pi$ on a nonempty closed set $\Theta \subseteq \mathbb{R}^d$ using a proposal distribution $Q$ which, to avoid trivialities, is assumed throughout to be different than $\Pi$. We will assume $\Pi$ has Lebesgue density $\pi$ and for each $\theta \in \Theta$, $Q(\theta, \cdot)$ has Lebesgue density $q(\theta, \cdot)$. We will further assume for each $\theta' \in \Theta$, if $\pi(\theta') > 0$ then for each $\theta \in \Theta$, $q(\theta, \theta') > 0$. Define

$$a(\theta, \theta') = \begin{cases} 
\min \left\{ \frac{\pi(\theta')q(\theta', \theta)}{\pi(\theta)q(\theta, \theta')}, 1 \right\}, & \text{if } \pi(\theta)q(\theta, \theta') > 0 \\
1, & \text{if } \pi(\theta)q(\theta, \theta') = 0
\end{cases}.$$

We will consider Metropolis-Hastings algorithms initialized at a point $\theta_0 \in \Theta$. Metropolis-Hastings proceeds as follows: for $t \in \{1, 2, \ldots \}$, given $\theta_{t-1}$, draw $\theta'_t \sim Q(\theta_{t-1}, \cdot)$ and $U_t \sim \text{Unif}(0, 1)$ so that

$$\theta_t = \begin{cases} 
\theta'_t, & \text{if } U_t \leq a(\theta_{t-1}, \theta'_t) \\
\theta_{t-1}, & \text{otherwise}
\end{cases}.$$

If $\delta_\theta$ denotes the Dirac measure at the point $\theta$ and $A(\theta) = \int_{\Theta} a(\theta, \theta') q(\theta, \theta') d\theta'$, the Metropolis-Hastings Markov kernel $P$ is defined for $\theta \in \Theta$ and $B \subseteq \Theta$ by

$$P(\theta, B) = \int_B a(\theta, \theta') q(\theta, \theta') d\theta' + \delta_\theta(B) (1 - A(\theta)).$$
For $\theta \in \Theta$, define the Markov kernel at iteration time $t \geq 2$ recursively by

$$P_t(\theta, B) = \int_{\Theta} P(\theta, d\theta') P_{t-1}(\theta', B).$$

Let $C(P^t(\theta, \cdot), \Pi)$ be the set of all probability measures on $\Theta \times \Theta$ with marginals $P^t(\theta, \cdot)$ and $\Pi$ and $\rho$ be a lower semicontinuous metric. The $L_1$ Wasserstein distance, or $L_1$ transportation distance with metric $\rho$, which we call simply the Wasserstein distance, is

$$W_\rho(P^t(\theta, \cdot), \Pi) = \inf_{\xi \in C(P^t(\theta, \cdot), \Pi)} \int_{\Theta \times \Theta} \rho(\theta, \omega) d\xi(\theta, \omega).$$

Our focus will be on bounding or expressing exactly $W_\rho(P^t(\theta, \cdot), \Pi)$. In particular, we will sometimes be concerned with settings where the Markov kernel $P$ is Wasserstein geometrically ergodic meaning there is an $\epsilon \in (0, 1)$ and for every $\theta \in \Theta$, there is a $M_\theta \in (0, +\infty)$ such that

$$W_\rho(P^t(\theta, \cdot), \Pi) \leq M_\theta \epsilon^t.$$

### 3 Necessary conditions for Wasserstein geometric ergodicity

Necessary conditions for the geometric ergodicity in total variation of Metropolis-Hastings algorithms rely on controlling the rejection probability $1 - A(\theta)$ [20, 29]. If this rejection probability cannot be bounded below one, that is, if $\inf_{\theta \in \Theta} A(\theta) = 0$, then a Metropolis-Hastings algorithm fails to be geometrically ergodic [20, 29]. It is generally however an onerous task to uniformly control this rejection probability. Using a lower bound on the Wasserstein distance, we will establish necessary conditions for Metropolis-Hastings algorithm to be Wasserstein geometrically ergodic. As we shall see, this also requires uniform control of the rejection probability. We will denote norms by $\| \cdot \|$ and the standard $p$-norms by $\| \cdot \|_p$.

**Theorem 1.** Suppose there exists a constant $M \in (0, +\infty)$ such that $\pi \leq M$. If $C_0 \in$
(0, +∞) such that ||·|| ≥ C₀ ||·||₁ and
\[
C₀ = C₀'||\frac{(1 - \frac{1}{1+d})}{2M^\frac{1}{d} (1 + d)^\frac{1}{2}}.
\]
then
\[
\mathcal{W}_{||·||}(P^t(θ, ·), Π) ≥ C₀ (1 − A(θ))^{t(1+\frac{1}{2})}.
\]

**Proof.** We will first construct a suitable Lipschitz function. Fix θ ∈ Θ, and fix α ∈ (0, +∞). Define the function \( ϕ_{α,θ} : Θ → R \) by \( ϕ_{α,θ}(ω) = \exp (-α ||ω − θ||₁) \). We have for every \((ω, ω') ∈ Θ × Θ,\)
\[
|ϕ_{α,θ}(ω) − ϕ_{α,θ}(ω')| = |\exp (-α ||ω − θ||₁) − \exp (-α ||ω' − θ||₁)|
\]
\[
≤ α ||ω − θ||₁ − ||ω' − θ||₁
\]
\[
≤ α ||ω − ω'||₁.
\]
Therefore, \( α^{-1}φ_{α,θ} \) is a bounded Lipschitz function with respect to the distance ||·||₁ and the Lipschitz constant is 1. By assumption there exists \( M \) such that \( π ≤ M \) and \( Θ ⊆ R^d \). Then, using the fact that \( \int_{R^d} \exp (-α ||θ' − θ||₁) dθ' = 2^d α^{-d} \), we obtain
\[
\int_Θ ϕ_{α,θ} dΠ = \int_Θ ϕ_{α,θ}(θ') π(θ') dθ'
\]
\[
≤ M \int_Θ \exp (-α ||θ' − θ||₁) dθ'
\]
\[
≤ M \int_{R^d} \exp (-α ||θ' − θ||₁) dθ'
\]
\[
= M 2^d α^{-d}.
\] (1)

Fix a positive integer \( t \). Then, for each \( s ∈ \{0, \ldots, t - 1\} \) and each \( ω ∈ Θ \), we obtain the
lower bound

\[ \int_{\Theta} \varphi_{\alpha,\theta}(\theta') (1 - A(\theta'))^{s} P(\omega; d\theta') = \int_{\Theta} \varphi_{\alpha,\theta}(\theta') (1 - A(\theta'))^{s} \min \left\{ \frac{\pi(\theta') q(\theta', \omega)}{\pi(\omega) q(\omega, \theta')}, 1 \right\} q(\omega, \theta') d\theta' + \varphi_{\alpha,\theta}(\omega) (1 - A(\omega))^{s+1} \geq \varphi_{\alpha,\theta}(\omega) (1 - A(\omega))^{s+1}. \]

We now apply this lower bound multiple times for however large \( t \) is using the Fubini-Tonelli theorem [7, Theorem 2.37]:

\[ \int_{\Theta} \varphi_{\alpha,\theta}(\theta_t) P^t(\theta, d\theta_t) = \int_{\Theta} \left\{ \int_{\Theta} \varphi_{\alpha,\theta}(\theta_{t-1}) P(\theta_{t-1}, d\theta_t) \right\} P^{t-1}(\theta, d\theta_{t-1}) \geq \int_{\Theta} \varphi_{\alpha,\theta}(\theta_{t-1}) (1 - A(\theta_{t-1})) P^{t-1}(\theta, d\theta_{t-1}) = \int_{\Theta} \left\{ \int_{\Theta} \varphi_{\alpha,\theta}(\theta_{t-2}) (1 - A(\theta_{t-2})) P(\theta_{t-2}, d\theta_{t-1}) \right\} P^{t-2}(\theta, d\theta_{t-2}) \geq \int_{\Theta} \varphi_{\alpha,\theta}(\theta_{t-2}) (1 - A(\theta_{t-2}))^{2} P^{t-2}(\theta, d\theta_{t-2}) \geq \int_{\Theta} \varphi_{\alpha,\theta}(\theta_{t-2}) (1 - A(\theta_{t-2}))^{t} \]

\[ = (1 - A(\theta))^t. \quad (2) \]

The final step follows from the fact that \( \varphi_{\alpha,\theta}(\theta) = 1 \). Combining (1) and (2), we then have the lower bound,

\[ \int_{\Theta} \left( \frac{1}{\alpha} \varphi_{\alpha,\theta} \right) dP^t(\theta, \cdot) - \int_{\Theta} \left( \frac{1}{\alpha} \varphi_{\alpha,\theta} \right) d\Pi \geq \frac{(1 - A(\theta))^t - M^2\alpha^{-d}}{\alpha}. \quad (3) \]

The case where \( \mathcal{W}_{\|\cdot\|_1}(P^t(\theta, \cdot), \Pi) = +\infty \) is trivial so we assume that \( \mathcal{W}_{\|\cdot\|_1}(P^t(\theta, \cdot), \Pi) < \infty \). Let \( M_b(\Theta) \) be the set of bounded, measurable functions on \( \Theta \) and Lip(\( \rho \)) be the Lipschitz norm measuring the maximum Lipschitz constant for a function of interest. We then have by the Kantovorich-Rubinstein theorem [36, Theorem 1.14] and the lower
If $A(\theta) = 1$, then taking the limit of $\alpha \to +\infty$, completes the proof. Suppose then that $A(\theta) < 1$. Maximizing this lower bound with respect to $\alpha$ yields

$$
\alpha = 2M^2(1 - A(\theta))^{-d/2}.
$$

We then have

$$
W_{\|\cdot\|_1}(P^t(\theta, \cdot), \Pi) = \frac{(1 - A(\theta))^t}{\alpha} \left( 1 - \frac{1}{1+d} \right) \frac{(1 - \frac{1}{1+d})}{2M^2 (1 + d)^{\frac{d}{2}}} (1 - A(\theta))^{t(1 + \frac{1}{d})}.
$$

This completes the proof for the norm $\|\cdot\|_1$.

Since all norms on $\mathbb{R}^d$ are equivalent, there is a positive real number $C'_0$ such that $W_{\|\cdot\|}(P^t(\theta, \cdot), \Pi) \geq C'_0 W_{\|\cdot\|_1}(P^t(\theta, \cdot), \Pi)$ and the proof for any norm on $\mathbb{R}^d$ follows from the case we have proved for the norm $\|\cdot\|_1$. 

Using Theorem 1, we now establish necessary conditions for the Wasserstein geometric ergodicity of Metropolis-Hastings Markov chains.

**Proposition 1.** Under the same conditions as Theorem 1 with the additional assumption that $\inf_{\theta \in \Theta} A(\theta) = 0$, the Metropolis-Hastings kernel is not Wasserstein geometrically ergodic for any norm $\|\cdot\|$.

**Proof.** Assume by way of contradiction that the Metropolis-Hastings algorithm is Wasserstein geometrically ergodic for some norm $\|\cdot\|$. Then there is an $\epsilon \in (0, 1)$ where for every $\theta \in \Theta$, there is a constant $R_\theta$ such that

$$
W_{\|\cdot\|} \left( P^t(\theta, \cdot), \Pi \right) \leq R_\theta (1 - \epsilon)^t.
$$
From the lower bound in Theorem 1, we have
\[ C_0 (1 - A(\theta))^t \leq W_{\|\cdot\|}(P^t(\theta, \cdot), \Pi) \leq R_{\theta}(1 - \epsilon)^t \]

But this implies that
\[ 1 - A(\theta) \leq (1 - \epsilon)^{1/(1+1/d)}. \]

Write \((1 - \epsilon)^{1/(1+1/d)} = 1 - \epsilon'\) where \(\epsilon' \in (0, 1)\). We then must have that \(A(\theta) \geq \epsilon'\) for every \(\theta \in \Theta\). But this is a contradiction to the assumption that \(\inf_{\theta \in \Theta} A(\theta) = 0\). \(\square\)

There is in fact an elementary example which fails to be geometrically ergodic and also fails to be Wasserstein geometrically ergodic.

**Example 1.** Consider the RWM algorithm with target distribution \(\Pi\) on \(\mathbb{R}^d\) with density \(\pi(x,z) \propto \exp[-(x^2 + x^2 z^2 + z^2)]\). This algorithm has been shown to not be geometrically ergodic [29, Proposition 5.2]. The conditions are also met for Proposition 1 in this example and this algorithm also fails to be Wasserstein geometrically ergodic for any norm.

For the MHI algorithm, we have the following necessary condition for Wasserstein geometric ergodicity.

**Proposition 2.** Assume the proposal distribution \(Q\) has density \(q\) and is independent of the previous iteration. Under the same conditions as Theorem 1 with the additional assumption that \(\inf_{\theta \in \Theta} \{q(\theta)/\pi(\theta)\} = 0\), the MHI kernel is not Wasserstein geometrically ergodic for any norm \(\|\cdot\|\).

*Proof.* Since \(\inf_{\theta \in \Theta} \{q(\theta)/\pi(\theta)\}\), choose a monotonically decreasing sequence \((\theta_n)_n \subset \Theta\) such that
\[ \lim_{n \to +\infty} \frac{q(\theta_n)}{\pi(\theta_n)} = 0. \]

Since \(A(\theta)\) is bounded by 1, the monotone convergence theorem [7, Theorem 2.14] ensures
\[ \lim_{n \to +\infty} A(\theta_n) = 0. \]

We then have that
\[ 0 \leq \inf_{\theta \in \Theta} A(\theta) \leq \inf_n A(\theta_n) \leq \lim_{n \to +\infty} \inf A(\theta_n) = 0. \]
An application of Proposition 1 completes the proof.

The following example for the MHI algorithm fails to be geometrically ergodic \([20]\) and also fails to be Wasserstein geometrically ergodic.

**Example 2.** Consider the target distribution \(N(0, 1)\) in one dimension with independent proposal \(N(1, 1)\). It has been shown previously that the ratio of the proposal and target density cannot be uniformly bounded above 0 \([20]\). This algorithm then satisfies the conditions in Proposition 2 and cannot be Wasserstein geometrically ergodic for any norm.

### 4 Exact convergence rates in Wasserstein distances with centered proposals

Recently there have been attempts at using centered drift functions to improve convergence analyses of some Monte Carlo Markov chains in high-dimensional settings \([6, 24, 27]\). Our approach is to center the proposal distribution, that is, matching the optimal points of the proposal and target densities. We first consider the following assumption which has been considered previously \([37]\).

**Assumption 1.** The proposal \(Q\) is independent of the previous iteration, and there exists a solution \(\theta^* = \arg\min \{q(\theta)/\pi(\theta) : \theta \in \Theta, \pi(\theta) > 0\}\).

If \(\epsilon_{\theta^*} = q(\theta^*)/\pi(\theta^*)\), then Assumption 1 implies uniform ergodicity of the MHI algorithm by \([33, Corollary 4]\). Assumption 1 also implies that \(P^t(\theta^*, \cdot)\) can be represented as a convex combination of the target distribution and the Dirac measure at the point \(\theta^*\) \([37, Remark 1, Theorem 2]\), that is,

\[
P^t(\theta^*, \cdot) = (1 - (1 - \epsilon_{\theta^*})t) \Pi + (1 - \epsilon_{\theta^*})^t \delta_{\theta^*}.
\]

This representation gives way to an exact convergence rate in total variation if the algorithm is started at the point \(\theta^*\) \([37, Remark 1, Theorem 2]\). We now show that it is also possible to derive exact convergence rates for more general Wasserstein distances.
Proposition 3. Under Assumption 1,
\[ W_\rho \left( P^t(\theta^*, \cdot), \Pi \right) = (1 - \epsilon_{\theta^*})^t \int_\Theta \rho(\theta, \theta^*) d\Pi(\theta). \]

Proof. Let \( \psi : \Theta \rightarrow \mathbb{R} \) be a function such that \( \int_\Theta |\psi| d\Pi < \infty \). We have the identity,
\[ \int_\Theta \psi dP^t(\theta^*, \cdot) = (1 - (1 - \epsilon_{\theta^*})^t) \int_\Theta \psi d\Pi(B) + (1 - \epsilon_{\theta^*})^t \psi(\theta^*). \] (5)

It can be shown that \( W_\rho(\delta_{\theta^*}, \Pi) = \int_\Theta \rho(\theta, \theta^*) d\Pi(\theta) \). Since \( q \) is not exactly \( \pi \), then \( \epsilon_{\theta^*} \in (0, 1) \). Denoting \( M_b(\Theta) \) by the set of bounded measurable functions on \( \Theta \) and \( \|\cdot\|_{\text{Lip}(\rho)} \) denoting the Lipschitz norm with the distance \( \rho \), applying the Kantovorich-Rubinstein theorem [36, Theorem 1.14],
\[ W_\rho \left( P^t(\theta^*, \cdot), \Pi \right) = \sup_{\varphi \in M_b(\Theta)} \frac{1}{\|\varphi\|_{\text{Lip}(\rho)}} \int_\Theta \varphi \left( P^t(\theta^*, \cdot) - \Pi \right) \]
\[ = \sup_{\varphi \in M_b(\Theta)} \left\{ (1 - \epsilon_{\theta^*})^t \int_\Theta \varphi \left( \delta_{\theta^*} - \Pi \right) \right\} \]
\[ = (1 - \epsilon_{\theta^*})^t \sup_{\varphi \in M_b(\Theta)} \frac{1}{\|\varphi\|_{\text{Lip}(\rho)}} \int_\Theta \varphi \left( \delta_{\theta^*} - \Pi \right) \]
\[ = (1 - \epsilon_{\theta^*})^t \frac{1}{\|\cdot\|_{\text{Lip}(\rho)}} \sup_{\varphi \in M_b(\Theta)} \int_\Theta \varphi \left( \delta_{\theta^*} - \Pi \right) \]
\[ = (1 - \epsilon_{\theta^*})^t W_\rho \left( \delta_{\theta^*}, \Pi \right) \]
\[ = (1 - \epsilon_{\theta^*})^t \int_\Theta \rho(\theta, \theta^*) d\Pi(\theta). \]

Under Assumption 1, Proposition 3 shows the convergence rate in total variation matches the convergence rate in other Wasserstein distances. This means it cannot be improved using “weaker” Wasserstein distances alternative to the total variation distance. On the other hand, it also says the rate does not worsen when looking at “stronger” Wasserstein distances such as those controlled using drift and minorization conditions [9].

We shall see in the next section that by centering a Gaussian proposal, we may satisfy Assumption 1 for a general class of target distributions with \( \theta^* \) being the optimum of
the target’s density. While we focus on Gaussian proposals, the technique of centering proposals is in fact more general.

4.1 Centered MHI with Gaussian proposals

We now provide general conditions where Proposition 3 may be applied with centered Gaussian proposals. We will assume the target distribution $\Pi$ is a probability distribution supported on $\mathbb{R}^d$. With $f : \mathbb{R}^d \rightarrow \mathbb{R}$ and normalizing constant $Z_\Pi$, we may then define the density $\pi$ by $\pi(\theta) = Z^{-1}_\Pi \exp(-f(\theta))$. Let $\theta^*$ be the unique maximum of $\pi$, $\alpha \in (0, +\infty)$, and $C \in \mathbb{R}^{d \times d}$ be a symmetric, positive-definite matrix. Under suitable conditions, the point $\theta^*$ may be found, at least approximately, by means of optimization. Let the proposal distribution $Q$ with density $q$ correspond to a $d$-dimensional Gaussian distribution, $N_d(\theta^*, \alpha^{-1}C)$ and finally, define $\epsilon_{\theta^*} = (2\pi)^{-d/2}\alpha^{d/2} \det(C)^{-1/2} Z_\Pi \exp(f(\theta^*))$.

Proposition 4. If $\theta^*$ exists and satisfies $f(\theta) \geq f(\theta^*) + \alpha (\theta - \theta^*)^T C^{-1} (\theta - \theta^*)/2$ for any $\theta \in \mathbb{R}^d$, then

$$W_\rho \left( P^d(\theta^*, \cdot), \Pi \right) = (1 - \epsilon_{\theta^*}) \int_{\mathbb{R}^d} \rho(\theta, \theta^*) d\Pi(\theta).$$

Proof. Since the proposal density has been centered at the point $\theta^*$, it then satisfies $q(\theta^*) = (2\pi)^{-d/2}\alpha^{d/2} \det(C)^{-1/2}$. For every $\theta \in \mathbb{R}^d$, we have the lower bound

$$\frac{q(\theta)}{\pi(\theta)} = (2\pi)^{-d/2}\alpha^{d/2} \det(C)^{-1/2} Z_\Pi \exp \left( f(\theta) - \frac{\alpha}{2} (\theta - \theta^*)^T C^{-1} (\theta - \theta^*) \right) \\
\geq (2\pi)^{-d/2}\alpha^{d/2} \det(C)^{-1/2} Z_\Pi \exp(f(\theta^*)) \\
= \frac{q(\theta^*)}{\pi(\theta^*)}.$$ 

Since both densities are positive and the proposal is independent of the previous iteration, we have shown that Assumption 1 is satisfied. An application of Proposition 3 with the the proposal and target distribution $Q$ and $\Pi$ as we have defined them in this section completes the proof.

The point $\theta^*$ is guaranteed to exist if the function $f$ satisfies a convexity property. A function $h : \mathbb{R}^d \rightarrow \mathbb{R}$ is strongly convex with parameter $\alpha$ if there is an $\alpha \in (0, +\infty)$ so
that $h(\cdot) - \alpha \|\cdot\|^2 / 2$ is convex [12, 23]. The norm in this definition is often taken to be the standard Euclidean norm, but we will use the norm induced by the matrix $C^{-1}$. We obtain the following general conditions for Proposition 4 to hold.

**Proposition 5.** If the function $\theta \mapsto f(\theta) - \alpha \theta^T C^{-1}\theta / 2$ is convex for all points on $\mathbb{R}^d$, then

$$W_{\rho} \left(P^I(\theta^*, \cdot), \Pi \right) = (1 - \epsilon_{\theta^*}) \int_{\mathbb{R}^d} \rho(\theta, \theta^*) d\Pi(\theta).$$

**Proof.** Since the function $f(\theta) - \alpha \theta^T C^{-1}\theta / 2$ is convex for all points on $\mathbb{R}^d$, it follows that for any $\lambda \in [0, 1]$ and any $(\theta, \theta') \in \mathbb{R}^d \times \mathbb{R}^d$,

$$f(\lambda \theta + (1 - \lambda)\theta') \leq \lambda f(\theta) + (1 - \lambda)f(\theta') - \frac{\alpha}{2} \lambda(1 - \lambda)(\theta' - \theta)^T C^{-1}(\theta' - \theta).$$

Since $C^{-1}$ is positive-definite, then $\alpha \lambda(1 - \lambda)(\theta' - \theta)^T C^{-1}(\theta' - \theta) / 2$ is nonnegative and this implies that $f$ is a convex function. It can also be shown that $\lim_{\|\theta\| \to \infty} f(\theta) = +\infty$ and since $f$ is lower semicontinuous, then $f$ attains its minimum $\theta^* \in \mathbb{R}^d$. The right directional derivative $f'(\theta^*; \theta) = \lim_{t \downarrow 0} t^{-1} [f(\theta^* + t\theta) - f(\theta^*)]$ exists for all points $\theta \in \mathbb{R}^d$ [23, Theorem 3.1.12]. For $\lambda \in (0, 1)$, we have

$$\frac{1}{1 - \lambda} \frac{1}{\lambda} [f(\theta^* + \lambda(\theta - \theta^*)) - f(\theta^*)] - \frac{1}{1 - \lambda} (f(\theta) - f(\theta^*)) \leq -\frac{\alpha}{2} (\theta - \theta^*)^T C^{-1}(\theta - \theta^*).$$

Taking the limit with $\lambda \downarrow 0$, we have that

$$f'(\theta^*; \theta - \theta^*) - f(\theta) + f(\theta^*) \leq -\frac{\alpha}{2} (\theta - \theta^*)^T C^{-1}(\theta - \theta^*).$$

Since $\theta^*$ is the minimum of $f$, then the right directional derivative satisfies $f'(\theta^*; \theta - \theta^*) \geq 0$ for all $\theta \in \mathbb{R}^d$. Therefore for all $\theta \in \mathbb{R}^d$,

$$f(\theta) \geq f(\theta^*) + \frac{\alpha}{2} (\theta - \theta^*)^T C^{-1}(\theta - \theta^*).$$

This inequality implies the minimum is unique. An application of Proposition 4 completes the proof.
5 Applications to Bayesian generalized linear models

We consider Bayesian Poisson and negative-binomial regression for count response regression and Bayesian logistic and probit regression for binary response regression. Suppose there are \( n \) discrete-valued responses \( Y_i \) with features \( X_i \in \mathbb{R}^d \), and a parameter \( \beta \in \mathbb{R}^d \). For Poisson regression, assume the \( Y_i \)'s are conditionally independent with \( Y_i | X_i, \beta \sim \text{Poisson} \left( \exp \left( \beta^T X_i \right) \right) \).

Similarly, for negative-binomial regression, if \( \xi \in (0, +\infty) \), assume \( Y_i | X_i, \beta \sim \text{Negative-Binomial} \left( \xi, \left( 1 + \exp \left( -\beta^T X_i \right) \right)^{-1} \right) \).

For binary response regression, if \( S : \mathbb{R} \rightarrow (0, 1) \), assume \( Y_i | X_i, \beta \sim \text{Bernoulli} \left( S \left( \beta^T X_i \right) \right) \). For logistic regression, we will consider \( S(x) = \left( 1 + \exp \left( x \right) \right)^{-1} \) and for probit regression, we will consider \( S(x) \) to be the cumulative distribution function of a standard Gaussian random variable. Suppose \( \beta \sim N_d(0, \alpha^{-1}C) \) where \( \alpha \in (0, +\infty) \) and \( C \in \mathbb{R}^{d \times d} \) is a symmetric, positive-definite matrix. Both \( \alpha \) and \( C \) are assumed to be known. Define the vector \( Y = (Y_1, \ldots, Y_n)^T \) and the matrix \( X = (X_1, \ldots, X_n)^T \). Let \( \Pi(\cdot | X, Y) \) denote the posterior with density \( \pi(\cdot | X, Y) \). If \( \ell_n \) denotes the negative log-likelihood for each model, the posterior density is characterized by

\[
\pi(\beta | X, Y) = Z_{\Pi(\cdot | X, Y)}^{-1} \exp \left( -\ell_n(\beta) - \frac{\alpha}{2} \beta^T C^{-1} \beta \right).
\]

Observe that the function \( \ell_n \) is convex in all four models we consider. Let \( \beta^* \) denote the unique maximum of \( \pi(\cdot | X, Y) \). For the MHI algorithm, we use a \( N_d(\beta^*, \alpha^{-1}C) \) proposal distribution, and Proposition 5 immediately yields the following for each posterior.

**Corollary 1.** Let \( \epsilon_{\beta^*} = \exp(\ell_n(\beta^*) + \frac{\alpha}{2} \beta^{*T} C^{-1} \beta^*) Z_{\Pi(\cdot | X, Y)} \left( (2\pi)^{d/2} \det (\alpha^{-1}C)^{1/2} \right)^{-1} \). Then

\[
W_\rho \left( P^t(\beta^*, \cdot), \Pi(\cdot | X, Y) \right) = (1 - \epsilon_{\beta^*})^t \int_{\mathbb{R}^d} \rho(\beta, \beta^*) d\Pi(\beta | X, Y).
\]
5.1 High-dimensional binary response regression

Our goal now is to obtain an upper bound on the rate of convergence established in Corollary 1 in high dimensions for binary response regression. In this context, it is more natural to treat the \((Y_i, X_i)_{i=1}^n\) as stochastic; each time the sample size increases, the additional observation is randomly generated. Specifically, we will assume that \((Y_i, X_i)_{i=1}^n\) are independent with \(Y_i | X_i, \beta \sim \text{Bernoulli}(S(\beta^T X_i))\) and \(X_i \sim N_d(0, \sigma^2 n^{-1} I_d)\) with \(\sigma^2 \in (0, +\infty)\). Similar scaling assumptions on the data are used for high-dimensional maximum-likelihood theory in logistic regression [32]. We will also assume the limit of the trace of the covariance matrix used in our prior is finite, that is, \(\text{tr}(C) \rightarrow s_0 \in (0, +\infty)\) as \(d \rightarrow +\infty\). This assumption is natural as for the Gaussian prior to exist in any infinite-dimensional Hilbert space, it is a necessary condition that the trace of the covariance is finite. Under this model, if the dimension and sample size grow proportionally, we now provide an explicit high-dimensional asymptotic upper bound on the Wasserstein distance.

**Theorem 2.** Suppose that:

1. The negative log-likelihood \(\ell_n\) is a twice continuously differentiable convex function with Hessian \(H_{\ell_n}\).

2. There is a universal constant \(r_0 \in (0, +\infty)\) such that \(\lambda_{\text{max}}(H_{\ell_n}(\beta)) \leq r_0 \lambda_{\text{max}}(X^T X)\) for every \(\beta \in \mathbb{R}^d\).

Let \(a_0 = r_0(1 + \gamma^{1/2})^2 \sigma^2 s_0/(2\alpha)\). If \(d, n \rightarrow +\infty\) in such a way that \(d/n \rightarrow \gamma \in (0, +\infty)\), then, almost surely

\[
\limsup_{d,n \to \infty} d \frac{W_\rho(P^*(\beta^*, \cdot), \Pi(\cdot | X, Y))}{\gamma} \leq (1 - \exp(-a_0))^t \limsup_{d,n \to \infty} \int_{\mathbb{R}^d} \rho(\beta, \beta^*) d\Pi(\beta | X, Y).
\]

**Proof.** Under our assumption, we may write the matrix \(X = n^{-1/2}G\) where \(G\) is a matrix with i.i.d Gaussian entries with mean 0 and variance \(\sigma^2\). Denote the largest eigenvalue of the matrix \(X^T X\) by \(\lambda_{\text{max}}(X^T X)\). Therefore, as \(d, n \rightarrow \infty\) in such a way that \(d/n \rightarrow \)
\[ \gamma \in (0, +\infty), \]
\[ \lambda_{\max} (X^T X) = \lambda_{\max} \left( \frac{1}{n} G^T G \right) = \frac{1}{n} \sup_{v \in \mathbb{R}^d, \|v\|_2 = 1} \| G^T G v \|_2 \to (1 + \gamma^{1/2})^2 \sigma^2 \]
almost surely [8, Theorem 1].

Define the function \( f : \mathbb{R}^d \to \mathbb{R} \) by
\[ f(\beta) = \ell_n(\beta) + \frac{\alpha}{2} \beta^T C^{-1} \beta \]
where \( \ell_n \) is the negative log-likelihood loss function and define \( Z_Q = (2\pi)^{-d/2} \det (\alpha^{-1} C)^{-1/2} \). We will first lower bound the quantity \( \exp(f(\beta^*)) Z_{\Pi(\cdot|X,Y)}/Z_Q \).

We have that for any \( \beta \in \mathbb{R}^d \) and any \( v \in \mathbb{R}^d \),
\[ v^T H_{\ell_n}(\beta) v \leq r_0 \lambda_{\max} (X^T X) \| v \|_2^2. \]

This implies that for any \( \beta \in \mathbb{R}^d \) and any \( v \in \mathbb{R}^d \), the Hessian of \( f \), denoted by \( H_f \), satisfies
\[ v^T H_f(\beta) v \leq v^T \left( r_0 \lambda_{\max} (X^T X) I_d + \alpha C^{-1} \right) v. \]

Since the function \( \ell_n \) is twice continuously differentiable, then \( f \) is also twice continuously differentiable. Since both the gradient \( \nabla f \) and Hessian \( H_f \) are continuous and \( \nabla f(\beta^*) = 0 \), we use a Taylor expansion to obtain the upper bound
\[ f(\beta) = f(\beta^*) + \int_0^1 \int_0^t (\beta - \beta^*)^T H_f(\beta^* + s(\beta - \beta^*)) (\beta - \beta^*) ds dt \leq f(\beta^*) + \frac{1}{2} (\beta - \beta^*)^T (r_0 \lambda_{\max} (X^T X) I_d + \alpha C^{-1}) (\beta - \beta^*). \]

We then have a lower bound on the normalizing constant of the target posterior
\[ Z_{\Pi(\cdot|X,Y)} = \int_{\mathbb{R}^d} \exp(-f(\beta)) d\beta \geq \frac{\exp(-f(\beta^*)) (2\pi)^{d/2}}{\det (r_0 \lambda_{\max} (X^T X) I_d + \alpha C^{-1})^{1/2}}. \]

This in turn yields a lower bound on the ratio
\[ \frac{Z_{\Pi(\cdot|X,Y)}}{Z_Q} \exp(f(\beta^*)) \geq \frac{\det (\alpha C^{-1})^{1/2}}{\det (r_0 \lambda_{\max} (X^T X) I_d + \alpha C^{-1})^{1/2}}. \tag{6} \]

The matrix \( C \) is symmetric and positive-definite and so its eigenvalues exist and are positive. Let \( (\lambda_i(C))_{i=1}^d \) be the eigenvalues of \( C \). It is readily verified that the eigenvalues
of the matrix \( r_0 \lambda_{\max}(X^T X) I_d + \alpha C^{-1} \) exist and are \( \left( r_0 \lambda_{\max}(X^T X) + \frac{\alpha}{\lambda_i(C)} \right)_{i=1}^d \). Then

\[
\frac{\det(\alpha C^{-1})}{\det(r_0 \lambda_{\max}(X^T X) I_d + \alpha C^{-1})} = \prod_{i=1}^d \frac{\alpha}{\lambda_i(C)} \left( r_0 \lambda_{\max}(X^T X) + \frac{\alpha}{\lambda_i(C)} \right) \\
= \prod_{i=1}^d \frac{r_0 \lambda_{\max}(X^T X) + \alpha}{\lambda_i(C)} \\
= \prod_{i=1}^d \frac{1}{r_0 \lambda_{\max}(X^T X) \lambda_i(C) + 1} \\
= \exp\left( -\sum_{i=1}^d \log \left( r_0 \lambda_{\max}(X^T X) \lambda_i(C) + 1 \right) \right). \tag{7}
\]

We have the basic inequality \( \log(x + 1) \leq x \) for any \( x \in [0, +\infty) \). Since the eigenvalues of \( C \) are positive and \( \lambda_{\max}(X^T X) \) is nonnegative, we have the upper bound

\[
\sum_{i=1}^d \log \left( \frac{r_0}{\alpha} \lambda_{\max}(X^T X) \lambda_i(C) + 1 \right) \leq \frac{r_0}{\alpha} \lambda_{\max}(X^T X) \sum_{i=1}^d \lambda_i(C). \tag{8}
\]

This yields a lower bound on (7). Define the doubly-indexed sequence \( (a_{d,n}) \) by

\[
a_{d,n} = \frac{r_0}{2\alpha} \lambda_{\max}(X^T X) \sum_{i=1}^d \lambda_i(C).
\]

We have then shown that

\[
\frac{Z_{\Pi|X,Y}}{Z_Q} \exp(f(\beta^*)) \geq \exp(-a_{d,n}) \cdot \tag{9}
\]

By our assumption, \( tr(C) \to s_0 \) as \( d \to \infty \). That is to say that \( \lim_{d \to +\infty} \sum_{i=1}^d \lambda_i(C) = s_0 \). Then as \( d, n \to \infty \) in such a way that \( d/n \to \gamma \in (0, +\infty) \), by continuity

\[
a_{d,n} \to \frac{r_0}{2\alpha} (1 + \gamma^{1/2})^2 \sigma^2 s_0
\]
almost surely. This implies using continuity that almost surely,
\[
\lim_{d,n \to \infty} (1 - \exp(-a_{n,d}))^t = (1 - \exp(-a_0))^t.
\]

By Corollary 1, we have the upper bound on the Wasserstein distance for each \(d\) and each \(n\):
\[
\mathcal{W}_\rho(P^t(\beta^*, \cdot), \Pi(\cdot | X, Y)) = \left(1 - \exp(f(\beta^*)) \frac{Z_{\Pi(\cdot | X, Y)}}{Z_Q}\right)^t \int_{\mathbb{R}^d} \rho(\beta, \beta^*) d\Pi(\beta | X, Y)
\]
\[
\leq (1 - \exp(-a_{n,d}))^t \int_{\mathbb{R}^d} \rho(\beta, \beta^*) d\Pi(\beta | X, Y).
\]

Suppose that \(\limsup_{d,n \to \infty} \int_{\mathbb{R}^d} \rho(\beta, \beta^*) d\Pi(\beta | X, Y) < \infty\). Using properties of the limit superior,
\[
\limsup_{d,n \to \infty} \mathcal{W}_\rho(P^t(\beta^*, \cdot), \Pi(\cdot | X, Y)) = \lim_{d,n \to \infty} (1 - \exp(-a_{n,d}))^t \int_{\mathbb{R}^d} \rho(\beta, \beta^*) d\Pi(\beta | X, Y).
\]

The other case when \(\limsup_{d,n \to \infty} \int_{\mathbb{R}^d} \rho(\beta, \beta^*) d\Pi(\beta | X, Y) = +\infty\) is trivial. \(\square\)

If \(tr(C) \to s_0\) as \(d \to +\infty\), the previous Theorem applies to both Bayesian logistic and probit regression. For logistic regression, \(\ell_n\) is a twice continuously differentiable convex function and we may choose \(r_0 = 4^{-1}\). Similarly for probit regression, \(\ell_n\) is also a twice continuously differentiable convex function and we may choose \(r_0 = 1\) [3].

In Figure 1, we plot \((1 - \exp(-a_0))^t\), the limiting decrease in the Wasserstein distance
according to our upper bound, with varying values of the limiting ratio $\gamma$. We observe that as this ratio increases, the number of iterations needed to converge may still increase rapidly.

![Figure 1: The limiting decrease in the Wasserstein distance using different values of $\gamma$, the limiting ratio of the dimension and sample size, versus the number of iterations.](image)

6 Final remarks

By centering the proposal, we directly imbue the Markov chain with a strong attraction to a set where the target distribution has high probability. In certain situations, our technique provided uniform control over the ratio between the proposal and target densities yielding exact convergence rates which are universal across general Wasserstein distances. We have also demonstrated that control of this ratio is necessary for Wasserstein geometric ergodicity in possibly “weaker” Wasserstein distances. This ratio appears at the core of the MHI algorithm.

The centered MHI algorithm turns out to have many applications for posteriors that arise in Bayesian generalized linear models. We have shown this algorithm is quite capable of sampling high-dimensional posteriors in Bayesian binary response regression. Our technique of centering a Gaussian proposal at the posterior maximum was key to our
analysis, but the approach seems more general and worthy of future research.

7 Supplementary material and code availability

The Python [34] package “cmhi” is available for download and all simulation code is available at github.com/austindavidbrown/Centered-Metropolis-Hastings.

References

[1] Niloy Biswas, Pierre E. Jacob, and Paul Vanetti. Estimating convergence of Markov chains with L-lag couplings. Advances in Neural Information Processing Systems 32, pages 7389–7399, 2019.

[2] Steve Brooks, Andrew Gelman, Galin L. Jones, and Xiao-Li Meng. Handbook of Markov chain Monte Carlo. Chapman and Hall/CRC, 1 edition, 2011.

[3] Eugene Demidenko. Computational aspects of probit model. Mathematical Communications, 6:233–247, 2001.

[4] Alain Durmus and Éric Moulines. Quantitative bounds of convergence for geometrically ergodic Markov chain in the Wasserstein distance with application to the Metropolis adjusted Langevin algorithm. Statistics and Computing, 25:5–19, 2015.

[5] Alain Durmus and Éric Moulines. High-dimensional Bayesian inference via the un-adjusted Langevin algorithm. Bernoulli, 25:2854–2882, 2019.

[6] Karl Oskar Ekvall and Galin L. Jones. Convergence analysis of a collapsed Gibbs sampler for Bayesian vector autoregressions. Electronic Journal of Statistics, 15:691–721, 2021.

[7] Gerald B. Folland. Real Analysis: Modern Techniques and Their Applications. Wiley, 2 edition, 1999.

[8] Stuart Geman. A limit theorem for the norm of random matrices. The Annals of Probability, 8:252–261, 1980.
[9] Martin Hairer and Jonathan C. Mattingly. Yet Another Look at Harris’ Ergodic Theorem for Markov Chains, volume 63. Springer Basel, 2011.

[10] Martin Hairer, Andrew M. Stuart, and Sebastian J. Vollmer. Spectral gaps for a Metropolis–Hastings algorithm in infinite dimensions. The Annals of Applied Probability, 24:2455–2490, 2014.

[11] Wilfred K. Hastings. Monte Carlo sampling methods using Markov chains and their applications. Biometrika, 57:97–109, 1970.

[12] Jean-Baptiste Hiriart-Urruty and Claude Leméchal. Fundamentals of Convex Analysis. Springer-Verlag Berlin Heidelberg, 1 edition, 2001.

[13] Pierre E. Jacob, John O’Leary, and Yves F. Atchadé. Unbiased Markov chain Monte Carlo methods with couplings. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 82:543–600, 2020.

[14] Søren Fiig Jarner and Ernst Hansen. Geometric ergodicity of Metropolis algorithms. Stochastic Processes and their Applications, 85:341–361, 2000.

[15] Rui Jin and Aixin Tan. Central limit theorems for Markov chains based on their convergence rates in Wasserstein distance. arXiv:2002.09427, 2020.

[16] James E. Johndrow, Aaron Smith, Natesh Pillai, and David B. Dunson. MCMC for imbalanced categorical data. Journal of the American Statistical Association, 114:1394–1403, 2019.

[17] Galin L. Jones. On the Markov chain central limit theorem. Probability Surveys, 1:299–320, 2004.

[18] Aldéric Joulin and Yann Ollivier. Curvature, concentration and error estimates for Markov chain Monte Carlo. The Annals of Probability, 38:2418–2442, 2010.

[19] Tomasz Komorowski and Anna Walczuk. Central limit theorem for Markov processes with spectral gap in the Wasserstein metric. Stochastic Processes and their Applications, 122:2155–2184, 2011.
[20] Kerrie L. Mengersen and Richard L. Tweedie. Rates of convergence of the Hastings and Metropolis algorithms. *The Annals of Statistics*, 24:101–121, 1996.

[21] Nicholas Metropolis, Arianna W. Rosenbluth, Marshall N. Rosenbluth, Augusta H. Teller, and Edward Teller. Equation of state calculations by fast computing machines. *The Journal of Chemical Physics*, 21:1087–1092, 1953.

[22] Sean P. Meyn and Richard L. Tweedie. *Markov Chains and Stochastic Stability*. Cambridge University Press, USA, 2 edition, 2009.

[23] Yurii Nesterov. *Lectures on Convex Optimization*. Springer International Publishing, 2 edition, 2018.

[24] Qian Qin and James P Hobert. Convergence complexity analysis of Albert and Chib’s algorithm for Bayesian probit regression. *Annals of Statistics*, 47:2320–2347, 2019.

[25] Qian Qin and James P Hobert. Geometric convergence bounds for Markov chains in Wasserstein distance based on generalized drift and contraction conditions. To appear in *Annales de l’Instute Henri Poincaré*, 2021.

[26] Qian Qin and James P Hobert. On the limitations of single-step drift and minorization in Markov chain convergence analysis. To appear in *Annals of Applied Probability*, 2021.

[27] Qian Qin and James P Hobert. Wasserstein-based methods for convergence complexity analysis of MCMC with applications. To appear in *Annals of Applied Probability*, 2021.

[28] Bala Rajaratnam and Doug Sparks. MCMC-based inference in the era of big data: A fundamental analysis of the convergence complexity of high-dimensional chains. *arXiv:1508.00947*, 2015.

[29] Gareth O. Roberts and Richard L. Tweedie. Geometric convergence and central limit theorems for multidimensional Hastings and Metropolis algorithms. *Biometrika*, 83:95–110, 1996.
[30] Nathan Robertson, James M. Flegal, Dootika Vats, and Galin L. Jones. Assessing and visualizing simultaneous simulation error. *Journal of Computational and Graphical Statistics*, 30:324–334, 2021.

[31] Jeffrey S. Rosenthal. Minorization conditions and convergence rates for Markov chain Monte Carlo. *Journal of the American Statistical Association*, 90:558–566, 1995.

[32] Pragya Sur and Emmanuel J. Candès. A modern maximum-likelihood theory for high-dimensional logistic regression. *Proceedings of the National Academy of Sciences*, 116:14516–14525, 2019.

[33] Luke Tierney. Markov chains for exploring posterior distributions. *The Annals of Statistics*, 22:1701–1728, 1994.

[34] Guido Van Rossum and Fred L. Drake. *Python 3 Reference Manual*. CreateSpace, 2009.

[35] Dootika Vats, James M. Flegal, and Galin L. Jones. Multivariate output analysis for Markov chain Monte Carlo. *Biometrika*, 106:321–337, 2019.

[36] Cédric Villani. *Topics in Optimal Transportation*. Graduate studies in mathematics. American Mathematical Society, 2003.

[37] Guanyang Wang. Exact convergence rate analysis of the independent Metropolis-Hastings algorithms. *arXiv:2008.02455*, 2020.

[38] Yun Yang, Martin J. Wainwright, and Michael I. Jordan. On the computational complexity of high-dimensional Bayesian variable selection. *Annals of Statistics*, 44:2497–2532, 2016.