Bounding and estimating MCMC convergence rates using common random number simulations

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Abstract

This paper explores how and when to use common random number (CRN) simulation to evaluate Markov chain Monte Carlo (MCMC) convergence rates. We discuss how CRN simulation is closely related to theoretical convergence rate techniques such as one-shot coupling and coupling from the past. We present conditions under which the CRN technique generates an unbiased estimate of the squared Wasserstein distance between two random variables. We also discuss how unbiasedness of the squared Wasserstein distance between two Markov chains over a single iteration does not extend to unbiasedness over multiple iterations. We provide an upper bound on the Wasserstein distance of a Markov chain to its stationary distribution after N steps in terms of averages over CRN simulations. Finally, we apply our result to a Gibbs sampler for Bayesian regression.

Keywords: Common random number; Convergence rate; Iterated random functions; Wasserstein distance; Gibbs sampler;

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1 Introduction

Markov chain Monte Carlo (MCMC) algorithms are often used to simulate from a stationary distribution of interest (see e.g. Brooks et al. [2011]). One of the primary questions when using these Markov chains is, after how many iterations is the distribution of the Markov chain sufficiently close to the stationary distribution of interest, i.e. when should actual sampling begin Hobert and Jones [2001]. The number of iterations it takes for the distribution of the Markov chain to be sufficiently close to stationarity is called the burn-in period. Various informal methods are available for estimating the burn-in period, such as effective sample size estimation, the Gelman-Rubin diagnostic, and visual checks using traceplots or autocorrelation graphs Dobson and Barnett [2008], Hoff [2009], Rachev et al. [2008], Roy [2020]. However, none of these methods provide a formal estimate of the distance between the distribution of the Markov chain and the stationary distribution.

From a theoretical perspective, distance to stationarity is traditionally measured in terms of total variation distance (e.g. Roberts and Rosenthal [2004], Tierney [1994]), though more recently the Wasserstein distance has been considered Gibbs [2004], Jin and Hobert [2022], Madras and Sezer [2010], Qin and Hobert [2022b]. However, finding upper bounds on either distance can be quite difficult to establish Geyer [2011], Hobert and Jones [2001], and if an upper bound is known, it is usually based on complicated problem-specific calculations Jin and Hobert [2022], Qin and Hobert [2022a], Sixta and Rosenthal [2022], Steinsaltz [1999]. This motivates the desire to instead estimate convergence bounds from actual simulations of the Markov chain, which we consider here.

One common method for generating upper bounds on the Wasserstein distance is through a contraction condition (see Definition 2.1). This can often be established using the common random number (CRN) simulation technique, i.e. using the same random variables to simulate two copies of a Markov chain with different initial values (see Section 2). Estimating Markov chain convergence rates using CRN simulation was first proposed in Johnson [1996] to find estimates of mixing times in total variation distance; see also Biswas et al. [2019],

Jacob [2020]. This approach falls under the general framework of "auxiliary simulation" Cowles and Rosenthal [1998], i.e. using extra preliminary Markov chain runs to estimate the convergence time needed in the final run. More recently, Biswas and Mackey [2021] showed how CRN simulation could be used for estimating an upper bound on the Wasserstein distance (their Proposition 3.1), and provided useful applications of the CRN method to high-dimensional and tall data (their Section 4). Simulation using the CRN technique is useful since for random variables under certain conditions it induces an unbiased estimate of the squared Wasserstein distance (see equation 3) and for Markov chains under certain conditions it produces a conditionally unbiased estimate of the squared Wasserstein distance (see equation 9). It was shown in Glasserman and Yao [1992] that simulated Euclidean distance between two random variables generated using the CRN technique is an unbiased estimate of the squared Wasserstein distance when the random transformation is an increasing function of the uniform random variable (see propositions 3.1 and 3.2 below).

In this paper, in Theorem 3.3 below, we generalize the result of Glasserman and Yao [1992] and conclude that the CRN technique generates an unbiased estimate of the squared Wasserstein distance whenever the intervals over which the transformation of a random variable in $\mathbb{R}$ are increasing and decreasing are the same. This theorem should help establish whether the CRN technique is optimal for simulating the Wasserstein distance, or if another simulation technique such as Biswas et al. [2022], Cowles and Rosenthal [1998], Lee et al. [2020], Papp and Sherlock [2022], Wang et al. [2021], Xu et al. [2021] is merited. Within the context of Markov chains, unbiasedness is only proven over a single iteration. We show how it is more difficult to extend over multiple iterations in Section 3.3.

Then, in Theorem 4.4 below, we provide an estimated upper bound in terms of CRN simulation on the Wasserstein distance between a Markov chain and the corresponding stationary distribution when only the unnormalized density of the stationary distribution is known. We apply this theorem (Section 5) to a Gibbs sampler for a Bayesian regression model with semi-conjugate priors.

This paper is organized as follows. In Section 2, we present definitions and notation. We also discuss the relationship between the closely related notions of coupling from the past, one-shot coupling, and the CRN technique. In Section 3, we present a set of random functions (of real-valued random variables) that will generate unbiased estimates of the squared Wasserstein distance when the CRN technique is used. In Section 4, we establish convergence bounds of a Markov chain to its corresponding stationary distribution using the CRN technique when the initial distribution is not in stationarity. Finally, in Section 5, we apply our Theorem 4.4 to a Gibbs sampler for a Bayesian regression model with semi-conjugate priors. The code used to generate all of the tables and calculations can be found at github.com/sixter/CommonRandomNumber.

2 Background

2.1 Distances between measures

Let $X : \mathcal{X} \to \mathbb{R}$ and $Y : \mathcal{X} \to \mathbb{R}$ be two random variables defined on a common complete seperable metric space $(\mathcal{X}, \mathcal{F}, \lambda)$ where $\mathcal{X}$ is a Borel measurable set, $\mathcal{F}$ is the Borel sigma field on $\mathcal{X}$, and λ is a Borel probability measure on $\mathcal{X}$.We denote the law of the random variable X as $\mathcal{L}(X)$ and similarly for $\mathcal{L}(Y)$. Let π, ν be two probability measures on $\mathbb{R}$, and let $d : \mathcal{X} \times \mathcal{X} \to \mathbb{R}_+$ be a metric function. When not specified, the distance, d, refers to the Euclidean distance. The probabilistic definition of the L^1-Wasserstein distance between the two probability measures π and ν is the infimum of the expected distance between X and Y over all joint pairs of random variables (X, Y) with marginals $\mathcal{L}(X) = \pi$ and $\mathcal{L}(Y) = \nu$, $W_d(\pi, \nu) = \inf_{X\sim\pi, Y\sim\nu} E[d(X, Y)]$. The Wasserstein distance is finite if for some $x_0 \in \mathcal{X}$, $E[d(X, x_0)] < \infty$ and $E[d(Y, x_0)] < \infty$. When the infimum is attained at an optimal coupling, the Wasserstein distance is the random variable pair (X_M, Y_M) that minimizes the expected distance, $W_d(\pi, \nu) = E[d(X_M, Y_M)]$ such that $\mathcal{L}(X_M) = \pi, \mathcal{L}(Y_M) = \nu$. Total variation is a special case defined as $||\pi - \nu||_{TV} = \inf_{X\sim\pi, Y\sim\nu} \mathbb{P}(X \neq Y)$.

2.2 Essential supremum and infimum

Let $f : \mathcal{X} \to \mathbb{R}$ be a function on the measure space $(\mathcal{X}, \mathcal{F}, \lambda)$. The essential supremum is the smallest value $a \in \mathbb{R}$ such that $\lambda(x \mid f(x) < a) = 1$. More formally, $ess\sup_x f(x) = \inf_{a\in\mathbb{R}}\{a \mid \lambda(x \mid f(x) > a) = 0\}$. The essential infimum is likewise the largest value $a \in \mathbb{R}$ such that $\lambda(x \mid f(x) > a) = 1$. Or, $ess\inf_x f(x) = \sup_{a\in\mathbb{R}}\{a \mid \lambda(x \mid f(x) < a) = 0\}$ Poznyak [2008].

2.3 Iterative function systems: Backward and forward process

Define a Markov chain $\{X_n\}_{n\geq 1}$ initialized at X_0 on a complete separable metric space $(\mathcal{X}, d)$ such that $X_n = f_{\theta_n}(X_{n-1})$, where $\{\theta_n\}_{n\geq 1}$ are i.i.d. random variables on some measurable space Θ and random measurable mappings $f_{\theta_n} : \mathcal{X} \mapsto \mathbb{R}$. The set of random functions $f_{\theta_1}, f_{\theta_2}, \ldots$ is called an iterated function system. Any time-homogeneous Markov chain can be represented as an iterated function system Stenflo [2012].

The iterated function system defines the forward and backward processes. The forward process, $\{X_n\}_{n\geq 1}$, which is a Markov chain, is defined as follows,

$$X_n = f_{\theta_n}(f_{\theta_{n-1}}(\ldots f_{\theta_1}(X_0)))$$

The backward process, $\{\tilde{X}_n\}_{n\geq 1}$, which is not necessarily a Markov chain Steinsaltz [1999] with respect to the filtration for $X_0, \ldots, X_n$ but tends to converge pointwise to a limit, is defined as follows,

$$\tilde{X}_n = f_{\theta_1}(f_{\theta_2}(\ldots f_{\theta_n}(X_0)))$$

Figure 1 graphs the forward and backward process of an autoregressive process using the same random mappings. The point towards which the backwards process converges is itself random.

Despite the difference in behaviour of the two processes, the marginal distributions of

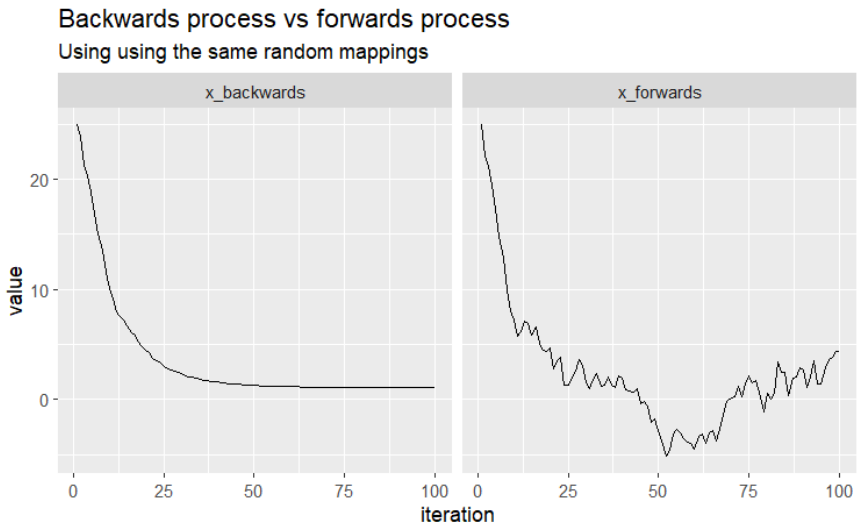

Figure 1: The backwards, $\{\tilde{X}_n\}_{n\geq 1}$, and forwards, $\{X_n\}_{n\geq 1}$, process of the autoregressive normal system where $X_n, \tilde{X}_n$ are simulated using the same random mappings, $X_n = 0.9X_{n-1} + Z_n, Z_n \sim N(0.1)$ and $X_0 = 25$.

the forward and backward processes are the same, $X_n \stackrel{d}{=} \tilde{X}_n$, so the backwards process is sometimes used when studying convergence properties of the forwards Markov chain Diaconis and Freedman [1999], Stenflo [2012], Steinsaltz [1999].

2.4 Convergence of forward and backward processes

When studying the convergence rates of iterated random functions, we are typically interested in establishing a contraction condition. The 'vanilla' contraction condition, sometimes referred to as global average Stenflo [2012] or strongly Steinsaltz [1999] contractive, is defined as the supremum over all x of the expected Lipschitz constant.

Definition 2.1 (Global average contraction condition)**.** There exists a $D \in (0, 1)$ such that for $n \geq 0$,

$$D \geq \sup_{x \neq x'} \frac{E[d(f_\theta(x), f_{\theta'}(x'))]}{d(x, x')}$$

Modifications to the above contraction condition have been widely studied and can be found in Diaconis and Freedman [1999], Ghosh and Marecek [2022], Jarner and Tweedie [2001], Leśniak et al. [2020], Steinsaltz [1999], Stenflo [2012]. Under strong conditions, the

mean value theorem can be used to show the global average contraction condition holds 2.1 and local contraction conditions exist Steinsaltz [1999].

Obtaining accurate calculations of the global contraction rate 2.1 is often difficult and alternatively estimating the convergence of the Markov chain through simulation may be appealing to practitioners. In particular, if two forward processes X_n, X'_n are simulated using the CRN technique (i.e., $X_n = f_{\theta_n}(X_{n-1})$ and $X'_n = f_{\theta_n}(X'_{n-1})$ for $n \in \mathbb{N}$) then the expected distance between the nth iteration of the two forward processes is equal to the expected distance between the nth and $n+1$th iteration of the backwards process, $\tilde{X}_n$.

$$
\begin{aligned}
&E[d(X_n, X'_{n+1}) \mid X_0 = x] \\
&= E[d[f_{\theta_n}(f_{\theta_{n-1}}(\dots f_{\theta_1}(x)\dots)), f_{\theta_n}(f_{\theta_{n-1}}(\dots f_{\theta_1}(f_{\theta_{n+1}}(x))\dots))] \mid X_0 = x] \\
&= E[d[f_{\theta_1}(f_{\theta_2}(\dots f_{\theta_n}(x)\dots)), f_{\theta_1}(f_{\theta_2}(\dots f_{\theta_n}(f_{\theta_{n+1}}(x))\dots))] \mid \tilde{X}_0 = x] \\
&= E[d(\tilde{X}_n, \tilde{X}_{n+1}) \mid \tilde{X}_0 = x]
\end{aligned}
$$

2.5 Common random numbers

Previously we defined the CRN technique to setting $\theta_n = \theta'_n$, i.e. using the same random variables $(\theta_n)_n$ to simulate both Markov chains. This is the intuitive definition of CRN for applications Biswas and Mackey [2021], Dai [2016], Heng and Jacob [2019]. However, we will first restrict our discussion to defining the CRN technique based on using uniform random variables as the common random number. Later on, we will discuss how expanding the definition of the CRN technique from a uniform random variable to θ_n affects the optimality of the CRN technique.

3 Conditionally unbiased estimates of the Wasserstein distance using the common random number technique

3.1 Common random number applied to a random variable

Suppose X is a random variables with cumulative distribution functions (CDF) F_X and Y is a random variable with CDF F_Y. Then we can represent $X_U \sim F_X$ and $Y_U \sim F_X$ with the inverse cumulative distribution function (CDF) of a uniform random variable U. That is $X_U = F_X^{-1}(U)$ where $F_X^{-1}(t) = \inf\{x \in \mathbb{R} : F_X(x) \geq t\}$ is a generalized inverse CDF of the marginal and $U \sim Unif(0,1)$. Similarly, $Y_U = F_Y^{-1}(U)$ with its generalized inverse CDF.

We first define CRN by jointly setting $(X_U, Y_U) = (F_X^{-1}(U), F_Y^{-1}(U))$ using a common uniform random variable $U \sim Unif(0,1)$ Glasserman and Yao [1992]. We will call this definition the InvCDF-CRN (inverse CDF - common random number). The InvCDF-CRN is the joint distribution that minimizes the expected square distance between two random variables. That is, the InvCDF-CRN solves the Monge-Kanterovich problem when $d(x,y) = (x-y)^2$ (see [Major, 1978, Theorem 8.1]). This definition stems from the following proposition which says that the maximum supermodular transform between the joint distribution of (X,Y) is attained with the random variables $(X_U, Y_U) = (F_X^{-1}(U), F_Y^{-1}(U))$. We say a function $h : \mathbb{R}^2 \to \mathbb{R}$ is right continuous if for every pair of decreasing sequences $x_n \to x$ and $y_n \to y$, $h(x_n, y_n) \to h(x,y)$.

Proposition 3.1 (Theorem 2 of Cambanis et al. [1976] and Proposition 2.1 of Glasserman and Yao [1992])**.** *Suppose that $\psi : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ is a measurable supermodular function ($\psi(x_1,y_1)+\psi(x_2,y_2) \geq \psi(x_1,y_2)+\psi(x_2,y_1)$ when $x_1 \leq x_2$ and $y_1 \leq y_2$) and right continuous. Let X and Y be real-valued random variables defined on $\mathcal{X}$ with distribution functions F_X*

and F_Y *respectively. If* $U \sim Unif(0,1)$ *and* $\sup_{X\sim F_X, Y\sim F_Y} E[\psi(X,Y)] < \infty$*, then*

$$\sup_{X\sim F_X, Y\sim F_Y} E[\psi(X,Y)] = E[\psi(F_X^{-1}(U), F_Y^{-1}(U))].$$

Proposition 3.1 is consistent with Theorem 2.9 of Santambrogio [2015]. Some examples of supermodular functions are $\psi(x,y) = xy$, $(x+y)^2$, $\min\{x,y\}$, and $f(x-y)$ where f is concave and continuous (see Section 4 of Cambanis et al. [1976]). In this paper, we focus on the functions $\psi(x,y) = xy$ and $\psi(x,y) = -|x-y|^2$. If the CRN generates the supremum expectation for the function $\psi(x,y) = xy$ (i.e., $\sup_{X\sim F_X, Y\sim F_Y} E[XY] = E[F_X^{-1}(U)F_Y^{-1}(U)]$), then the CRN generates the supremum covariance when the marginal distributions are fixed and X, Y have finite first moments as follows:

$$\sup_{X\sim F_X, Y\sim F_Y} Cov(X,Y) = \sup_{X\sim F_X, Y\sim F_Y} E[XY] - E[X]E[Y] \tag{1}$$

$$= Cov(F_X^{-1}(U), F_Y^{-1}(U)). \tag{2}$$

By the same reasoning, the function $\psi(x,y) = -|x-y|^2$ is supermodular since it is concave and continuous, then the CRN generates the L^2-Wasserstein distance (where $d(x,y) = |x-y|$) if X, Y have finite second moments:

$$W_2(\mathcal{L}(X), \mathcal{L}(Y))^2 = \inf_{X\sim F_X, Y\sim F_Y} E[(X-Y)^2] \tag{3}$$

$$= E[(F_X^{-1}(U) - F_Y^{-1}(U))^2]. \tag{4}$$

Note that the above result can be generalized from L^2-Wasserstein distance to L^p-Wasserstein distance Jacob [2020], Glasserman and Yao [1992].

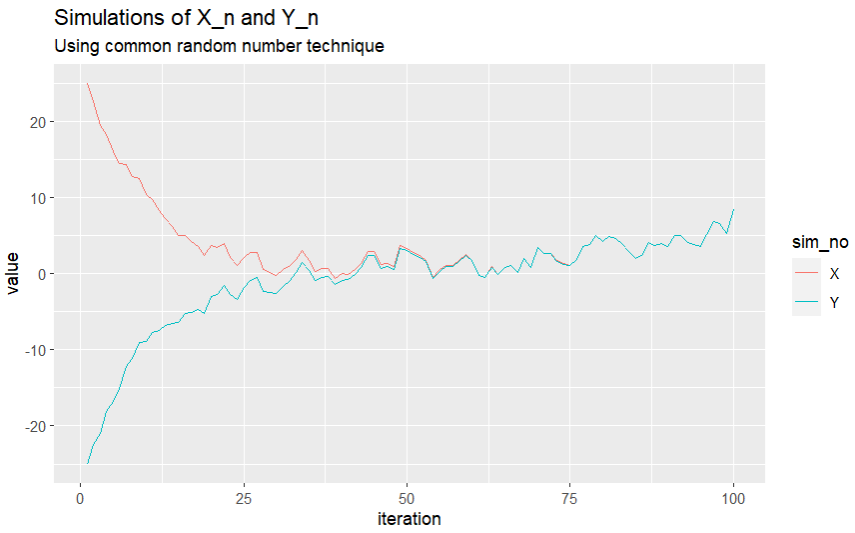

Figure 2: Two copies of the autoregressive process where X_n, Y_n are simulated using CRN, $X_n = 0.9X_{n-1} + Z_n, Z_n \sim N(0,1)$, and $X_0 = 25, Y_0 = -25$

3.2 Common random number in a Markov chain setting.

Within the context of a Markov chain, we define the CRN technique as follows. Let $\{X_n\}_{n\geq 0}$ be a Markov chain such that X_n is defined as an iterated function system and $X_n = f_{\theta_n}(X_{n-1}) = f(\theta_n, X_{n-1})$ where $\theta_1, \theta_2 \ldots$ are i.i.d. random variables. We assume that $\theta_U \sim F_\theta$ where F_θ is the distribution function of θ can be constructed from a uniform random variable, $\theta_U = F_\theta^{-1}(U)$, $U \sim Unif(0,1)$. Note that if $\vec{\theta} \in \mathbb{R}^p$ is a vector of independent random variables, then each coordinate can be constructed from a uniform random variable $\theta_{U,i} = F_{\theta_i}^{-1}(U_i), i \in \{1, \ldots p\}$ where $U_i \sim Unif(0,1)$ are i.i.d. (this is consistent with equation 3 of Glasserman and Yao [1992]). When used in simulation, the CRN technique visibly shows how two copies of a Markov chain converge. See figure 2 for an example of two autoregressive processes that converge.

Next, we extend Proposition 3.1 to non-decreasing functions of uniform random variables.

Proposition 3.2 (Proposition 2.2 of Glasserman and Yao [1992]). *Fix $x, y \in \mathcal{X}$ and let $X_1 = f(\theta_U, x)$ and $Y_1 = f(\theta_V, y)$ with measurable $f : \mathbb{R} \times \mathcal{X} \to \mathbb{R}$ where $\theta_U = F_\theta^{-1}(U)$, $\theta_V = F_\theta^{-1}(V)$ and $U, V \sim Unif(0,1)$. Suppose for $z = x, y$, $f(\cdot, z)$ is a non-decreasing*

continuous function with $E[X_1^2], E[Y_1^2] < \infty$. *Then*

$$\sup_{\substack{U\sim Unif(0,1)\\ V\sim Unif(0,1)}} E[f(\theta_U, x)f(\theta_V, y)] \tag{5}$$

is attained by setting $U = V$.

We relaxed the assumption that $f(\cdot, x)$ be increasing to assuming that $f(\cdot, x)$ is non-decreasing. The relaxed assumption generates the same conclusion since $\psi(f(\cdot, x), f(\cdot, x))$ remains supermodular if ψ is supermodular and $f(\cdot, x), f(\cdot, y)$ are non-decreasing (which is required in the proof of Proposition 2.2 of Glasserman and Yao [1992]). Note, for example that the distribution function F^{-1} in Proposition 2.1 of Glasserman and Yao [1992] is a non-decreasing function, not a strictly increasing function.

Similar to Proposition 3.1, the supremum covariance (equation 1) and infimum Euclidean distance (equation 3) are attained when $U = V$.

In practise, however, $f(\theta, x)$ and $f(\theta, y)$ are not always non-decreasing functions with respect to θ. Rather, the following theorem shows that the supremum is attained when $U = V$ if the functions $f(\theta, x)$ and $f(\theta, y)$ are both increasing and decreasing for the same values of $\theta \in \mathbb{R}$. A function $F : \mathbb{R} \to \mathbb{R}$ is of bounded variation if $T_F(x) = \sup\{\sum_{k=1}^{n} |F(x_k) - F(x_{k-1})| : -\infty < x_0 < x_1 < \cdots < x_n = x\}$ and $\lim_{x\to\infty} T_F(x)$ is finite. For a function $F : \mathbb{R} \to \mathbb{R}$, define the area over which F is a non-decreasing function, that is, for θ_0 there exists $\epsilon_0 > 0$ such that for $0 < \epsilon < \epsilon_0$, $F(\theta_0) \leq F(\theta_0 + \epsilon)$. Similarly, define the area over which F is a non-increasing function as the points θ_0 where there exists $\epsilon_0 > 0$ such that for $0 < \epsilon < \epsilon_0$, $F(\theta_0) \geq F(\theta_0 + \epsilon)$.

Theorem 3.3. *For fixed* $x, y \in \mathcal{X}$, *let* $X_1 = f(\theta_U, x)$ *and* $Y_1 = f(\theta_V, y)$ *be random functions with measurable* $f : \mathbb{R} \times \mathcal{X} \mapsto \mathbb{R}$ *and* $\theta_U = F_\theta^{-1}(U)$ *and* $\theta_V = F_\theta^{-1}(V)$ *with* $U, V \sim Unif(0, 1)$. *Define the set* $A_{x,y} = (I_x \cap I_y) \cup (D_x \cap D_y)$ *where for* $z = x, y$, I_z *is the area over which* $f(\cdot, z)$ *is a non-decreasing function and* D_z *is the area over which* $f(\cdot, z)$ *is a non-increasing function. If* $E[X_1^2], E[Y_1^2] < \infty$, *and both* $f(\cdot, x)$ *and* $f(\cdot, y)$ *are of bounded variation, then*

- *If* $P(A_{x,y}) = 1$ *(the intervals of positive measure over which* θ *is increasing and decreasing on* $f(\cdot, x)$ *and* $f(\cdot, y)$ *are the same),*

$$W_d(\mathcal{L}(X_1), \mathcal{L}(Y_1))^2 = E[(f(\theta_U, x) - f(\theta_U, y))^2] \tag{6}$$

i.e. $(f(\theta_U, x) - f(\theta_U, y))^2$ *is an unbiased estimator of* $W_d(\mathcal{L}(X_1), \mathcal{L}(Y_1))^2$.

- *If* $P(A_{x,y}) = 0$ *(that is the function* $f(\cdot, x)$ *is increasing and* $f(\cdot, y)$ *is decreasing over the same intervals of positive measure or vice versa),*

$$W_d(\mathcal{L}(X_1), \mathcal{L}(Y_1))^2 = E[(f(\theta_{1-U}, x) - f(\theta_U, y))^2] \tag{7}$$

i.e. $(f(\theta_{1-U}, x) - f(\theta_U, y))^2$ *is an unbiased estimator of* $W_d(\mathcal{L}(X_1), \mathcal{L}(Y_1))^2$.

- *If* $0 < P(A_{x,y}) < 1$ *(there are intervals of positive measure over which* θ *is increasing on* $f(\cdot, x)$ *and decreasing on* $f(\cdot, y)$ *or vice versa), then*

$$E[(f(\theta_U, x) - f(\theta_U, y))^2] - \epsilon \leq W_d(\mathcal{L}(X_1), \mathcal{L}(Y_1))^2 \leq E[(f(\theta_U, x) - f(\theta_U, y))^2] \tag{8}$$

where $\epsilon = 2E[(f(\theta_{1-U}, x) - f(\theta_U, x))f(\theta_U, y)1_{A^C}]$.

The proof is in Section 9.

The set $A_{x,y}$ is simpler to visualize. It is the values of θ for which either both $f(\theta, x)$ and $f(\theta, y)$ are increasing or decreasing for fixed x, y. See figure 3 for an example.

3.3 Conditionally unbiased estimates of the squared Wasserstein distance

Denote $X_n = f(\theta_n, X_{n-1})$ and $Y_n = f(\theta'_n, Y_{n-1})$ where $\theta_n, \theta'_n \in \mathbb{R}$ are random variables. Theorem 3.3 implies that if $P(A) = 1$ for all $X_{n-1} = x$ and $Y_{n-1} = y$, then applying the

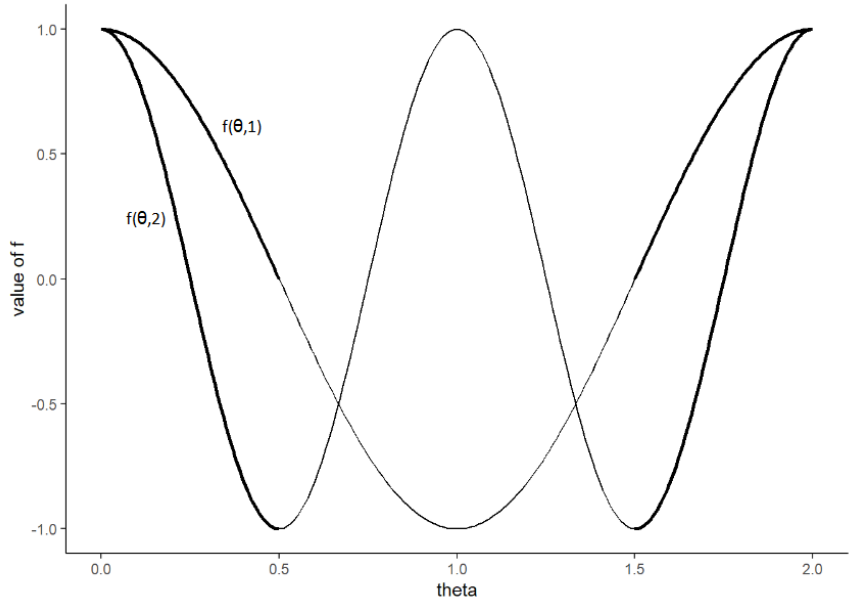

Figure 3: Denote $f(\theta, x) = \cos(\pi x \theta)$. The above graphs two functions: $f(\theta, 1) = \cos(\pi\theta)$ and $f(\theta, 2) = \cos(2\pi\theta)$. The set $A_{1,2}$ in this case is the value of θ where the function is bold. That is, $A = (0, 0.5) \cup (1.5, 2)$.

CRN technique to simulate $E[(X_n - Y_n)^2]$ will generate conditionally unbiased estimates of the squared Wasserstein distance. That is, for two copies of a Markov chain, X_n and Y_n, that were simulated by CRN ($X_n = f(\theta_n, X_{n-1})$ and $Y_n = f(\theta_n, Y_{n-1})$), the squared Wasserstein distance will be conditionally unbiased on X_{n-1} and Y_{n-1} as follows:

$$W_d(\mathcal{L}(X_n), \mathcal{L}(Y_n) \mid X_{n-1} = x, Y_{n-1} = y)^2 \tag{9}$$

$$:= \inf_{X_n \sim \mathcal{L}(X_n), Y_n \sim \mathcal{L}(Y_n)} E[(X_n - Y_n)^2 \mid X_{n-1} = x, Y_{n-1} = y] \tag{10}$$

$$= E[(f(\theta_n, X_{n-1}) - f(\theta_n, Y_{n-1}))^2 \mid X_{n-1} = x, Y_{n-1} = y] \tag{11}$$

This is the optimal coupling for the Wasserstein distance given the previous iteration.

Remark. Note that Markov chains that satisfy $P(A) = 1$ for all $X_{n-1} = x$ and $Y_{n-1} = y$ and are simulated by CRN may not be unconditionally unbiased. Unconditional unbiasedness is

defined as follows for $X_0 = x$ and $Y_0 = y$:

$$W_d(\mathcal{L}(X_n), \mathcal{L}(Y_n))^2 = E[(f(\theta_n, f(\theta_{n-1}, \dots f(\theta_1, x)\dots)) - f(\theta_n, f(\theta_{n-1}, \dots f(\theta_1, y)\dots)))^2].$$

To illustrate our point, fix $n = 2$ and initial values $X_0 = x, Y_0 = y$. Then

$$W_d(\mathcal{L}(X_2), \mathcal{L}(Y_2))^2 \coloneqq \inf_{\substack{\theta_1 \sim \mathcal{L}(\theta_1), \theta_1' \sim \mathcal{L}(\theta_1') \\ \theta_2 \sim \mathcal{L}(\theta_2), \theta_2' \sim \mathcal{L}(\theta_2')}} E[(f(\theta_2, f(\theta_1, x)) - f(\theta_2', f(\theta_1', y)))^2].$$

However, the function $f(\theta_2, \cdot)$ may be increasing for $f(\theta_1, x)$ and decreasing for $f(\theta_1, y)$ (or vice versa), which by Theorem 3.3 means that the function might not generate the infimum expectation.

Remark. Even if a Markov chain does not present itself as conditionally unbiased it might still be conditionally unbiased under different function construction. This is because the CRN technique depends on the function f. To quote Wang et al. [2021] "In most [...] scenarios the user must construct a coupling tailored to the problem at hand." For example, if X_1 and Y_1 have continuous distribution functions, then they can be written as transformations of the uniform distribution and thus a common random number that generates the maximum covariance exists. Generating such a function g such that $X_n = g(U), U \sim Unif(0, 1)$ may not be easy to calculate, however. For example, the Metropolis Hastings algorithm does not appear to converge in expectation when the heuristic algorithm for using the common random number on the proposal and accept/reject random variables is used Cowles and Carlin [1996]. Figure 4 shows that when we apply the heuristic algorithm on the CRN technique of a Metropolis algorithm, sample mean convergence is bounded away from 0. In Papp and Sherlock [2022], asymptotically optimal estimates using a variation of the CRN are provided for the Metropolis-Hastings algorithm when the target distribution is elliptical normal.

The following two examples use Theorem 3.3 to show that the CRN technique generates

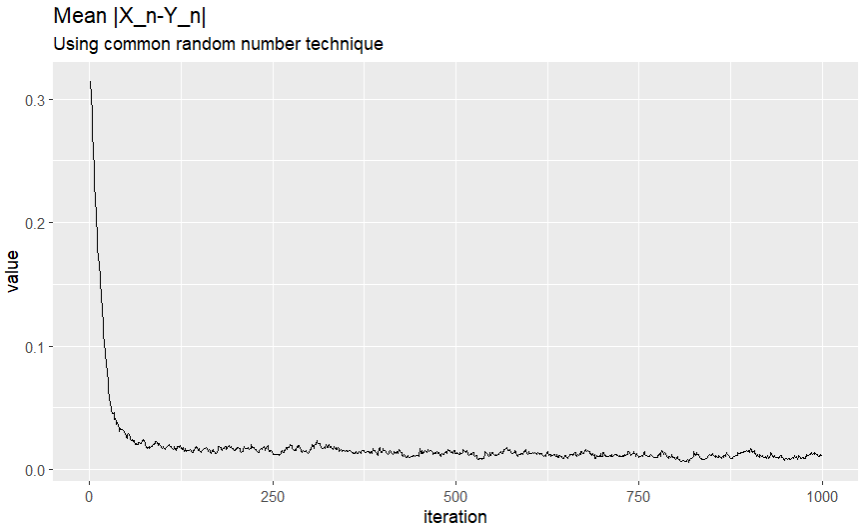

Figure 4: We apply a random-walk Metropolis algorithm on the unnormalized ($c > 0$) target density, $\pi(x) = cg(x)$ where $g(x) = x^3 \sin y^4 \cos y^5$ with proposal distribution $N(X_{n-1}, 0.01)$. The next iteration can be written as a function of $Z_n \sim N(0,1)$ and $U_n \sim Unif(0,1)$ as follows $X_n = (X_{n-1} + 0.1Z_n)I\{U_n < \pi(X_{n-1} + 0.1Z_n)/\pi(X_{n-1})\} + X_{n-1}I\{U_n \geq \pi(X_{n-1} + 0.1Z_n)/\pi(X_{n-1})\}$. When we use CRN on Z_n and U_n to simulate X_n and Y_n, $|X_n - Y_n|$ does not converge even though the Wasserstein distance does converge.

conditionally unbiased estimates of the squared Wasserstein distance.

Example 3.1 (Random logistic map)**.** Define $X_n \in [0,1]$ to be a random logistic map. That is, $X_n = f(\theta_n, X_{n-1}) = 4\theta_n X_{n-1}(1 - X_{n-1})$ and $\theta_n \sim Beta(a + 1/2, a - 1/2)$ for $a > 1/2$. Since $f(\theta_n, X_{n-1})$ is a non-decreasing function of θ_n for all values of $X_{n-1} \in [0,1]$, then by Theorem 3.3 the CRN technique provides simulated estimates of the Euclidean distance that are conditionally unbiased to the squared Wasserstein distance. That is, if $\hat{X}_n$ and $\hat{Y}_n$ are CRN simulations of the random logistics map then $W_d(\mathcal{L}(X_n), \mathcal{L}(Y_n))^2 = E[(\hat{X}_n - \hat{Y}_n)^2]$

See figure 5 for an example of two random logistic map processes that converge. See Section 7.4 of Steinsaltz [1999] for theoretical convergence diagnostics in total variation distance and example 2 of Madras and Sezer [2010] for upper bounds in Wasserstein distance as a function of total variation distance.

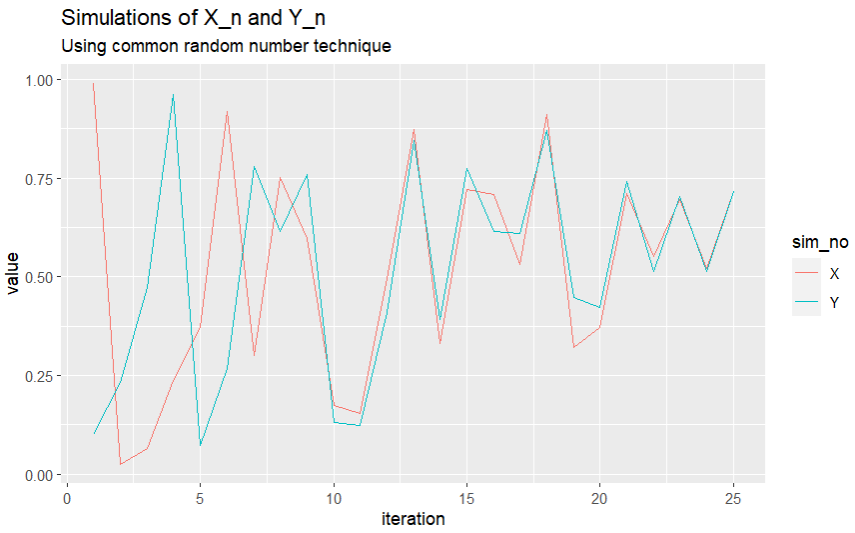

Figure 5: Two copies of the random logistic map where X_n, Y_n are simulated using CRN, $X_n = 4\theta_n X_{n-1}(1 - X_{n-1}), \theta \sim Beta(1.5, 0.5)$, and $X_0 = 0.99, Y_0 = 0.1$

Example 3.2. Define $X_n \in [-1, 1]$ to be a Markov chain such that

$$X_n = f(\theta_n, X_{n-1}) = \sin[(1 - |X_{n-1}|)\cos(\theta_n)]$$

where $\theta_n \sim Unif(-\pi/2, 3\pi/2)$. Since $f(\theta_n, X_{n-1})$ is increasing and decreasing over the same regions of θ for fixed $X_{n-1}, Y_{n-1} \in [-1, 1]$, then by Theorem 3.3 the CRN technique provides simulated estimates of the Euclidean distance that are conditionally unbiased to the squared Wasserstein distance.

Figure 6 provides an example of copies of this Markov chain converging when the CRN technique is used. Figure 7 shows that for initial values $X_0 = 0.75$ and $Y_0 = 0.05$ the functions $f(X_0, \theta)$ and $f(Y_0, \theta)$ are both increasing and decreasing over the same regions of θ.

Finally, note that Theorem 3.3 is only applicable for $\theta \in \mathbb{R}$. Further research needs to be done to extend the above results to $\theta \in \mathbb{R}^d$. However, we believe that a proof can be established using Proposition 3.2 and assuming that $f(\theta, x)$ is of bounded Arzelà-variation (see Definition 3.2.1 of Breneis [2020]). If a function defined in $\mathbb{R}^d$ is of bounded Arzelà-

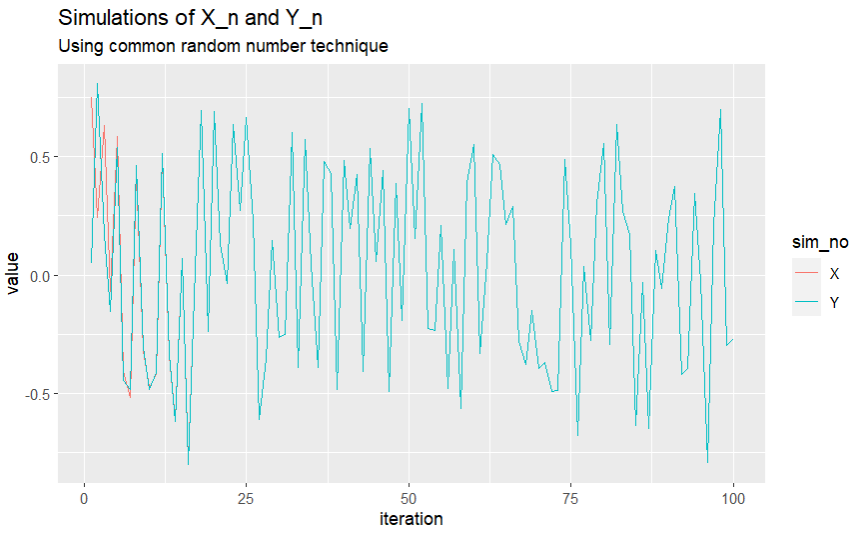

Figure 6: Two copies of a Markov chain $X_n = f(\theta_n, X_{n-1}) = \sin[(1 - |X_{n-1}|)\cos(\theta_n)]$ where $\theta_n \sim Unif(-\pi/2, 3\pi/2)$. X_n, Y_n are simulated using CRN, with initial values and $X_0 = 0.75, Y_0 = 0.05$

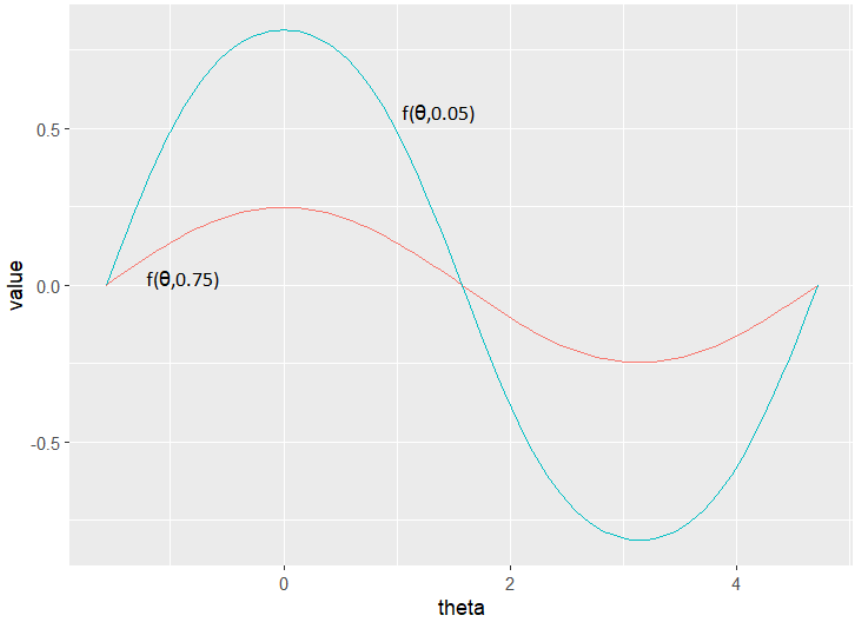

Figure 7: Denote $f(\theta, x) = \sin[(1-|x|)\cos(\theta)]$. The above graphs two functions: $f(\theta, 0.75) = \sin[0.25\cos(\theta)]$ and $f(\theta, 0.05) = \sin[0.95\cos(\theta)]$. Note that both functions are decreasing over the same region, $\theta = (0, \pi)$.

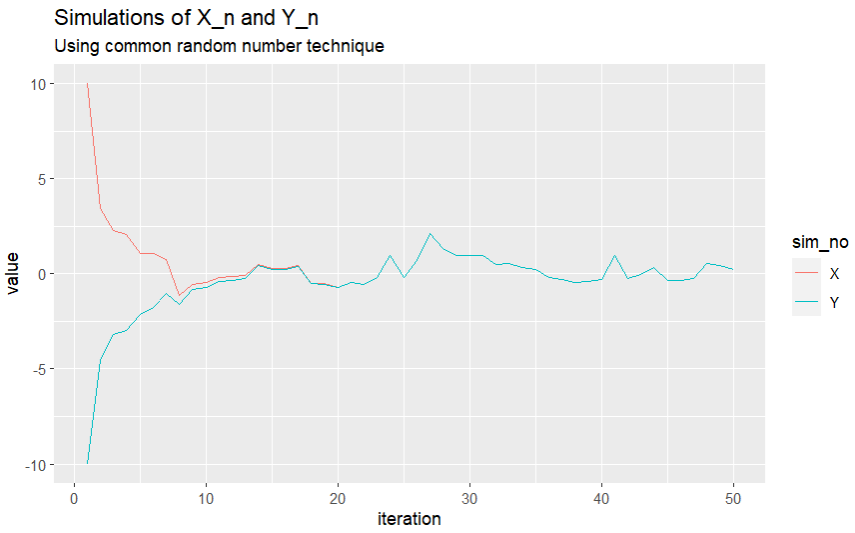

Figure 8: Two copies of a Markov chain with Dirichlet process means where X_n, Y_n are simulated using CRN, $X_n = (1-\theta_n)Z_n + \theta_n Z_{n-1}, \theta \sim Beta(1.5, 1), Z_n \sim N(0,1)$, and $X_0 = 10, Y_0 = -10$

variation, then it can be written as the difference of two coordinate-wise increasing functions (see Theorem 3.4.1 of Breneis [2020]) where Proposition 3.2 can then be applied. Example 3.3 is a Markov chain of Dirichlet process means where $\theta \in \mathbb{R}^2$ and $f(\theta, x)$ is not always an increasing function of θ, so none of the theorems in this text apply. The CRN technique still appears to generate converging Markov chains, however (see figure 8).

Example 3.3 (Dirichlet process means)**.** Define $X_n \in [0,1]$ to be a Markov chain of Dirichlet process means. That is $X_n = f(\theta_n, Z_n, X_{n-1}) = (1-\theta_n)Z_n + \theta_n X_{n-1}$ and $\theta_n \sim Beta(a, 1)$ for $a > 0$ and $Z_n \sim N(0,1)$. In this case $(\theta_n, Z_n) \in \mathbb{R}^2$, so Theorem 3.3 does not apply. Further, since $f(\theta_n, Z_n, X_{n-1})$ may not necessarily be an increasing function of (θ_n, Z_n), Proposition 3.2 also does not apply. The Markov chain of Dirichlet process means still seems to converge when the CRN technique is used. See figure figure 8 for an example of two Markov chains with Dirichlet processes means that converge. See section 7 of Roberts and Rosenthal [2002] for theoretical convergence diagnostics.

4 Common random number as a method of simulating Markov chain convergence rates

We propose estimating the L^1-Wasserstein distance between the nth iteration of a Markov chain X_n and the corresponding stationary distribution X_∞ through simulation using the CRN technique. Our method is outlined in Theorem 4.4. Using CRN simulation as a convergence diagnostic tool was first discussed in Johnson [1996] for bounding total variation distance.

Before providing a method for simulating an upper bound on $E[|X_n - X_\infty|]$, we must first provide a method of bounding the expected distance between two copies of a Markov chain ($E[|X_n - Y_n|]$) and their corresponding expected distance to stationarity, ($E[|X_n - X_\infty|]$). To do so, we will first define rejection sampling and separation distance and how they are related.

Definition 4.1 (Rejection sampling)**.** Suppose that we have a target distribution π, which we want to sample from, but is difficult to do, and we have a proposal distribution ν that is easier to sample from. Suppose also that $\pi << \nu$ (i.e., $\pi(A) = 0 \implies \nu(A) = 0$, where $A \in \mathcal{F}$) and $K \geq (d\pi/d\nu)(x), x \in \mathcal{X}$ for some known K. To generate a random variable $X_\pi, \mathcal{L}(X_\pi) = \pi$ we do the following,

1. Sample $X \sim \nu$ and $U \sim Unif(0,1)$ independently.
2. If $U \leq \frac{1}{K}\frac{d\pi}{d\nu}(X)$ then accept X as a draw from π. Otherwise reject X and restart from step 1.

Lemma 4.1 (Rejection sampler rejection rate)**.** *Denote the event*

$$A = \{X \text{ is accepted as a draw from } \pi\}$$

in the rejection sampler algorithm defined above. The rejection rate denoted as r is as follows

where $K = ess\sup_{x\in\mathcal{X}}(d\pi/d\nu)(x)$.

$$r(\pi,\nu) = 1 - P(A) = 1 - 1/K$$

Proof. See Section 11.2.2 of Ross [2010]. □

We further define the separation distance on the continuous state space $\mathcal{X}$ as follows. Separation distance was first defined in Aldous and Diaconis [1987] for discrete state spaces. As far as we know, separation distance was only recently defined on a continuous state space in Caputo et al. [2020]. We use the definition of separation distance defined in Caputo et al. [2020] where the density functions are known.

Definition 4.2 (Separation distance (Remark 5 of Caputo et al. [2020]))**.** Let ν and π be two distributions defined on the same measure space $(\mathcal{X},\mathcal{F},\lambda)$ such that $\nu << \pi$. The separation distance is,

$$s = s(\pi,\nu) = ess\sup_{x}\left(1 - \frac{d\nu}{d\pi}(x)\right)$$

It turns out that the separation distance and the rejection rate of the rejection sampler are the same.

Lemma 4.2. *Let* π *and* ν *be two probability measures defined on the same measure space* $(\mathcal{X},\mathcal{F},\lambda)$ *with positive density functions. If* ν *is the proposal distribution and* π *is the target distribution in a rejection sampler, then the rejection rate equals the separation distance,*

$$s(\pi,\nu) = r(\pi,\nu)$$

Proof. Let f be the probability density of π and g the probability density of ν. Then

$$s(\pi,\nu) = ess\sup_{x\in\mathcal{X}}\left(1 - \frac{g(x)}{f(x)}\right) = 1 - ess\inf_{x\in\mathcal{X}}\frac{g(x)}{f(x)} = 1 - \frac{1}{ess\sup_{x\in\mathcal{X}}\frac{f(x)}{g(x)}} \qquad = 1 - \frac{1}{K}$$
$$= r(\pi,\nu).$$

□

Now that we have defined separation distance and the rejection rate of the rejection sampler, we can apply upper bounds on the distance to stationarity as follows. The use of rejection sampling to generate an upper bound on the expected distance between a proposal distribution ν and a stationary distribution π was inspired by Johnson [1996], which used rejection sampling to generate similar upper bounds in total variation distance.

Theorem 4.3. *Let $\{X_n\}_{n\geq 1}$ and $\{Y_n\}_{n\geq 1}$ be two copies of a Markov chain in $\mathcal{X}$ with initial distribution $\mathcal{L}(X_0) = \mu, \mathcal{L}(Y_0) = \nu$. Assume π and ν are defined on the same support and let X_∞ be the corresponding stationary random variable with distribution π. Then*

$$W_{|\cdot|}(\mathcal{L}(Y_n), \mathcal{L}(X_\infty)) \leq E[|Y_n - X_\infty|] \leq KE[|X_n - Y_n|] \tag{12}$$

where the expectation is taken with respect to coupling using common random numbers $(\theta_n)_n$ such that X_0 and Y_0 are independent and $K = \frac{1}{1-s(\pi,\nu)} = \frac{1}{1-r(\pi,\nu)}$.

Proof. Let $A = \{\text{Accept } Y_0 \text{ as a draw from } \pi\}$. Note that $\mathcal{L}(Y_0|A) = \pi$ and so, $\mathcal{L}(Y_n|A) = \pi$. Then

$$\begin{aligned}
&\int_{\mathcal{X}\times\mathcal{X}} E[|X_n - Y_n| \;\big|\; X_0 = x, Y_0 = y]\mu(dx)\nu(dy) \\
&\geq \int_0^1 \int_{\mathcal{X}\times\mathcal{X}} E[|X_n - Y_n| \;\big|\; X_0 = x, Y_0 = y]\mu(dx)I_A(y,u)\nu(dy)du \\
&\geq \frac{1}{K}\int_{\mathcal{X}\times\mathcal{X}} E[|X_n - Y_n| \;\big|\; X_0 = x, Y_0 = y]\mu(dx)\pi(dy)
\end{aligned}$$

and so equation 12 follows. □

In many cases the normalizing constant for π is unknown. That is, we only know of a function $g(x)$ such that $cg(x)dx = \pi(dx)$ where c is unknown. In this case we must find a constant $L > 0$ such that $\int_{\mathcal{X}} g(x)dx \geq L$, which implies that $c \leq \frac{1}{L}$ and if h is the Lebesgue

density of ν,

$$K \leq \frac{1}{L} \sup_{x \in \mathcal{X}} \frac{g(x)}{h(x)}. \tag{13}$$

See Example 5.1 for a way of estimating K when the normalizing constant of π is unknown. In Section 5 we estimate L as the integral over a bounded subset of $\mathcal{X}$, $B \subset \mathcal{X}$. That is, $L = \int_B g(x)dx$. Caffo et al. [2002] presents an alternative approach to estimating the rejection rate, K, when the normalizing constant for π is unknown.

Next we define Algorithm 1 for generating an estimate of $\inf_{(X_N,Y_N)} E[|X_N - Y_N|]$, $N \geq 1$ where $\mathcal{L}(X_0) = \mu, \mathcal{L}(Y_0) = \nu$. The algorithm generates a conditionally unbiased estimate of the L^1-Wasserstein distance provided the conditions in Theorem 3.3 hold. This algorithm is similar to algorithm 1 in Biswas and Mackey [2021]. Combining algorithm 1 with Theorem

Algorithm 1 An estimate of $E[|X_N - Y_N|] \approx \frac{1}{I}\sum_{i=1}^{I} |x_{N,i} - y_{N,i}|$ using CRN

```
for i = 1, ..., I do
    x_{0,i} ~ μ, y_{0,i} ~ ν where x_{0,i} ⫫ y_{0,i}
    for n = 1, ..., N do
        θ_n ~ Θ
        x_{n,i} ← f_{θ_n}(x_{n-1,i})
        y_{n,i} ← f_{θ_n}(y_{n-1,i})
    end for
end for
return (1/I) Σ_{i=1}^{I} |x_{N,i} − y_{N,i}|
```

4.3, we can simulate an upper bound between a Markov chain at iteration N, X_N, and the corresponding stationary random variable, X_∞, as follows,

Theorem 4.4. *Suppose that the Markov chain $\{X_n\}_{n\geq 0}$ with stationary distribution $\mathcal{L}(X_\infty) = \pi$ can be written as an iterated function system $X_{n+1} = f_{\theta_{n+1}}(X_n)$ where $(\theta_n)_{n\geq 1}$ are i.i.d. random variables. Let (X_n, Y_n) be two copies of the Markov chain coupled using common random numbers $(\theta_n)_n$ with $\mathcal{L}(X_0) = \nu$ and $\mathcal{L}(Y_0) = \mu$. Suppose for each $n \geq 0$, $E[|X_n|], E[|Y_n|] < \infty$ and that the initial distribution of X_n, $\mathcal{L}(X_0) = \nu$ is defined on the*

same support as π. Then

$$W_{|\cdot|}(\mathcal{L}(X_N), \mathcal{L}(X_\infty)) \leq K \lim_{I\to\infty} \frac{1}{I} \sum_{i=1}^{I} |x_{N,i} - y_{N,i}| \tag{14}$$

holds almost surely where $\frac{1}{I}\sum_{i=1}^{I} |x_{N,i} - y_{N,i}|$ is defined as in algorithm 1 and $K = \frac{1}{1-s(\pi,\nu)} = \frac{1}{1-r(\pi,\nu)}$.

Proof. Fix $N \geq 1$. By the strong law of large numbers, $\lim_{I\to\infty} \frac{1}{I}\sum_{i=1}^{I} |x_{N,i} - y_{N,i}| \overset{a.s.}{=} E[|X_N - Y_N|]$. By Theorem 4.3, $E[|X_N - X_\infty|] \leq KE[|X_N - Y_N|]$ and so equation 14 follows. □

The consistency of $\lim_{I\to\infty} \frac{1}{I}\sum_{i=1}^{I} |x_{N,i} - y_{N,i}|$ is similarly proven in Proposition 3.1 of Biswas and Mackey [2021].

5 Gibbs sampler for a Bayesian regression model with semi-conjugate priors

Consider the Bayesian linear regression model with semi-conjugate priors (see Chapter 5 of Rachev et al. [2008]) for which we will apply Theorem 4.4 to simulate convergence bounds on the Wasserstein distance.

Example 5.1 (Gibbs sampler for Bayesian regression with semi-conjugate priors)**.** Suppose we have the following observed data $Y \in \mathbb{R}^k$ and $X \in \mathbb{R}^{k\times p}$ where

$$Y|\beta, \sigma \sim N_k(X\beta, \sigma^2 I_k)$$

for unknown parameters $\beta \in \mathbb{R}^p, \sigma^2 \in \mathbb{R}$. Suppose we apply the prior distributions on the unknown parameters,

$$\beta \sim N(m_\beta, \Sigma_\beta) \qquad\qquad \sigma^2 \sim \text{Inv-}\chi^2(\upsilon_0, c_0^2).$$

The joint posterior density function of $\beta, \sigma^2|Y, X$ is proportional to the following equation,

$$g(\beta, \sigma^2) \tag{15}$$

$$= \frac{1}{(\sigma^2)^{(n+\upsilon_0)/2+1}} \exp\left(-\frac{1}{2\sigma^2}(y - X\beta)^T(y - X\beta) - \frac{1}{2}(\beta - m_\beta)^T\Sigma_\beta^{-1}(\beta - m_\beta) - \frac{\upsilon_0 c_0^2}{2\sigma^2}\right). \tag{16}$$

The Bayesian regression two-variable deterministic scan Gibbs sampler is based on the conditional posterior distributions of β_n, σ_n^2 and is defined as follows initialized at β_0, σ_0^2:

1. $\beta_n|\sigma_{n-1}^2, Y, X \sim N(\tilde{\beta}_{\sigma_{n-1}^2}, V_{\sigma_{n-1}^2})$
2. $\sigma_n^2|\beta_n, Y, X \sim \Gamma^{-1}\left(\frac{k+\upsilon_0}{2}, \frac{1}{2}\left[\upsilon_0 c_0^2 + (Y - X\beta_n)^T(Y - X\beta_n)\right]\right)$

where

$$V_{\sigma_{n-1}^2} = \left(\frac{1}{\sigma_{n-1}^2}X^TX + \Sigma_\beta^{-1}\right)^{-1}, \qquad \tilde{\beta}_{\sigma_{n-1}^2} = V_{\sigma_{n-1}^2}\left(\frac{1}{\sigma_{n-1}^2}X^TY + \Sigma_\beta^{-1}m_\beta\right).$$

Here $\Gamma^{-1}(\alpha, \beta)$ represents the inverse gamma distribution with shape parameter α and rate parameter β. Replacing $\beta_n = \tilde{\beta}_{\sigma_{n-1}^2} + V_{\sigma_{n-1}^2}^{1/2} Z_n$, where $Z_n \sim N(0, I_p)$ into the equation for σ_n^2 and with $G_n \sim \Gamma(\frac{k+\upsilon_0}{2}, 1)$, we get that

$$\sigma_n^2|\sigma_{n-1}^2, Y, X = \left[\frac{\upsilon_0 c_0^2}{2} + \frac{(X\tilde{\beta}_{\sigma_{n-1}^2} - Y + XV_{\sigma_{n-1}^2}^{1/2} Z_n)^T(X\tilde{\beta}_{\sigma_{n-1}^2} - Y + XV_{\sigma_{n-1}^2}^{1/2} Z_n)}{2}\right]\frac{1}{G_n} \tag{17}$$

where $(Z_n, G_n)_n$ are independent for all n.

Although the joint Markov chain may be high-dimensional in both coordinates, special properties of the Gibbs sampler allow us to upper bound the total variation between two joint Markov chains in terms of only the a univariate marginals of the Markov chains using common random numbers.

Lemma 5.1. *Let $\beta_\infty, \sigma_\infty^2$ denote the stationary Gibbs Markov chain. The total variation*

distance can be bounded by the expected distance as follows,

$$\left\|\mathcal{L}(\beta_{n+1},\sigma^2_{n+1})-\mathcal{L}(\beta_\infty,\sigma^2_\infty)\right\|_{TV}\leq\frac{(k+\upsilon_0)^2}{2\upsilon_0 c_0^2}E[|\sigma^2_n-\sigma^2_\infty|]$$

where the expectation is with respect to coupling using common random numbers $(Z_n,G_n)_n$ *for* σ^2_n *and* $\sigma^2_\infty=\sigma^{'2}_n$ *such that* $\sigma^2_0\sim\mu$ *and* $\sigma^{'2}_0\sim\pi$ *are independent.*

Proof. It follows from the de-initializing property of the Markov chain [Roberts and Rosenthal, 2001, Example 3] that

$$\left\|\mathcal{L}(\beta_{n+1},\sigma^2_{n+1})-\mathcal{L}(\beta'_{n+1},\sigma^{'2}_{n+1})\right\|_{\mathrm{TV}}\leq\left\|\mathcal{L}(\sigma^2_n)-\mathcal{L}(\sigma^{'2}_n)\right\|_{\mathrm{TV}}.$$

Using common random numbers, let $G_n=G'_n$ where $G_n\sim\mathrm{Gamma}(\alpha,1)$ $Z_n\sim N(0,I_p)$ are independent and denote

$$\begin{aligned}W_n&=\frac{\upsilon_0c_0^2}{2}+\frac{\left\|X\tilde{\beta}_{\sigma^2_{n-1}}-Y+XV^{1/2}_{\sigma^2_{n-1}}Z_n\right\|^2}{2}\\W'_n&=\frac{\upsilon_0c_0^2}{2}+\frac{\left\|X\tilde{\beta}_{\sigma^{'2}_{n-1}}-Y+XV^{1/2}_{\sigma^{'2}_{n-1}}Z_n\right\|^2}{2},\end{aligned}$$

so that $\sigma^2_n|\sigma^2_{n-1}=W_n\frac{1}{G_n}$ and $\sigma^{'2}_n|\sigma^{'2}_{n-1}=W'_n\frac{1}{G'_n}$. Denote $\Delta=W'_n-W_n$ and without loss of generality, assume $W'_n>W_n$. Since $G_n\sim\mathrm{Gamma}(\alpha,1)$ where $\alpha=\frac{k+\upsilon_0}{2}$, let π_{1/G_n} denote the density of $1/G_n$ and similarly denote the density $\pi_{(1+\Delta/W_n)/G_n}$ for $(1+\Delta/W_n)/G_n$. So we have

$$\begin{aligned}\pi_{1/G_n}(x)&\propto x^{-\alpha-1}e^{-1/x}\\\pi_{(1+\Delta/W_n)/G_n}(x)&\propto\frac{1}{1+\Delta/W_n}\left(\frac{x}{1+\Delta/W_n}\right)^{-\alpha-1}e^{-(1+\Delta/W_n)/x}\\&\propto(1+\Delta/W_n)^\alpha x^{-\alpha-1}e^{-(1+\Delta/W_n)/x}.\end{aligned}$$

Using the coupling characterization of total variation

$$
\begin{aligned}
&||\mathcal{L}(\sigma_n^2) - \mathcal{L}(\sigma_n^{'2})||_{TV} \\
&\leq E\left[||\mathcal{L}(W_n\frac{1}{G_n}) - \mathcal{L}(W_n'\frac{1}{G_n})||_{TV} \mid Z_n, \sigma_{n-1}^2, \sigma_{n-1}^{'2}\right] \\
&= E\left[||\mathcal{L}(W_n\frac{1}{G_n}) - \mathcal{L}((W_n+\Delta)\frac{1}{G_n})||_{TV} \mid Z_n, \sigma_{n-1}^2, \sigma_{n-1}^{'2}\right] \\
&\qquad \text{By Proposition 2.2 of Sixta and Rosenthal [2022]} \\
&= E\left[||\mathcal{L}\left(\frac{1}{G_n}\right) - \mathcal{L}\left(\left(1+\frac{\Delta}{W_n}\right)\frac{1}{G_n}\right)||_{TV} \mid Z_n, \sigma_{n-1}^2, \sigma_{n-1}^{'2}\right] \\
&\qquad \text{By Proposition 2.1 of Sixta and Rosenthal [2022]} \\
&\leq E\left[\sup_{x>0}\left\{1 - \frac{\pi_{1/G_n}(x)}{\pi_{(1+\Delta/W_n)/G_n}(x)}\right\} \mid Z_n, \sigma_{n-1}^2, \sigma_{n-1}^{'2}\right] \\
&\qquad \text{By Lemma 6.16 of of Levin et al. [2017]}
\end{aligned}
$$

So,

$$
\begin{aligned}
||\mathcal{L}(\sigma_n^2) - \mathcal{L}(\sigma_n^{'2})||_{TV} &\leq E\left[\sup_{x>0}\left\{1 - \frac{x^{-\alpha-1}e^{-1/x}}{(1+\Delta/W_n)^\alpha x^{-\alpha-1}e^{-(1+\Delta/W_n)/x}}\right\}\right] \\
&= E\left[\sup_{x>0}\left\{1 - \frac{e^{\Delta/W_n/x}}{(1+\Delta/W_n)^\alpha}\right\}\right] \\
&= E\left[1 - \frac{1}{(1+\Delta/W_n)^\alpha}\right].
\end{aligned}
$$

Define $f(x) = \frac{1}{x^\alpha}, f'(x) = -\alpha\frac{1}{x^{\alpha+1}}$. By the mean value theorem, $f(1+\Delta/W_n) = f(1) -$

$\frac{\Delta}{W_n}\frac{\alpha}{\xi^{\alpha+1}}, \xi \in (1, 1+\Delta/W_n)$. So, $f(1+\Delta/W_n) \geq 1-\alpha\frac{\Delta}{W_n}$. Now,

$$
\begin{aligned}
&||\mathcal{L}(\sigma_n^2) - \mathcal{L}(\sigma_n^{'2})||_{TV} \\
&\leq E[1-(1-\alpha\frac{\Delta}{W_n})] = E[\alpha\frac{\Delta}{W_n}] \\
&\leq E[\frac{k+\upsilon_0}{2}\Delta\frac{2}{\upsilon_0 c_0^2}] && \text{since } \alpha = \frac{k+\upsilon_0}{2} \text{ and } W_n \geq \frac{\upsilon_0 c_0^2}{2} \\
&= \frac{k+\upsilon_0}{\upsilon_0 c_0^2} E[|W_n - W_n'|] \\
&= \frac{k+\upsilon_0}{\upsilon_0 c_0^2} E[|W_n - W_n'|] E[G_n^{-1}] E[G_n^{-1}]^{-1} \\
&= \frac{k+\upsilon_0}{\upsilon_0 c_0^2} E[|W_n/G_n - W_n'/G_n|] E[G_n^{-1}]^{-1} && \text{by independence} \\
&\leq \frac{(k+\upsilon_0)^2}{2\upsilon_0 c_0^2} E[|W_n/G_n - W_n'/G_n|].
\end{aligned}
$$

□

Using Lemma 5.1, we can apply Theorem 4.4 to only the one-dimensional initialization of the marginal Gibbs Markov chain (σ_n^2) to estimate the total variation of the possibly high-dimensional joint Markov chain.

Lemma 5.2. *Let $(\sigma_n^2)_n$ and $(\sigma_n^{'2})_n$ be two copies of the deterministic scan Gibbs Markov chain initialized with $\sigma^2 \sim \nu$ and $\sigma^{'2} \sim \mu$. Assume $\sigma_0^2 \sim \nu$ is a distributed $\Gamma^{-1}(\alpha', \beta')$ with parameters $\alpha' = (k+\upsilon_0)/2$ and $\beta' = \upsilon_0 c_0^2$. Let $\sigma_\infty^2 \sim \pi$ be from stationary Markov chain started from the the marginal posterior distribution. Then*

$$E[|\sigma_n^{'2} - \sigma_\infty^2|] \leq \frac{(2\pi)^{p/2}\det(\Sigma_\beta)^{1/2}}{\int_{\mathbb{R}^p \times \mathbb{R}_+} g(\beta, \sigma^2) d(\beta \times \sigma^2)} \frac{\Gamma(\alpha')}{\beta'^{\alpha'}} E[|\sigma_n^2 - \sigma_n^{'2}]$$

where the expectation is taken with respect to coupling using common random numbers and σ_0^2 and $\sigma_0^{'2}$ are independent.

Proof. Define f as the corresponding density function of ν, $f(\sigma^2) = \frac{\beta'^{\alpha'}}{\Gamma(\alpha')}\frac{1}{(\sigma^2)^{\alpha'+1}}e^{-\beta'/\sigma^2}$ where

$\alpha' = (k+\upsilon)/2$ and $\beta' = \upsilon_0 c_0^2/2$. Note that

$$\begin{aligned}\int g(\beta, \sigma^2) d\beta &\leq (2\pi)^{p/2} \det(\Sigma_\beta)^{1/2} \frac{1}{(\sigma^2)^{(k+\upsilon_0)/2+1}} \exp\left(-\frac{\upsilon_0 c_0^2}{2\sigma^2}\right) \\ &= (2\pi)^{p/2} \det(\Sigma_\beta)^{1/2} \frac{\Gamma(\alpha')}{\beta'^{\alpha'}} f(\sigma^2).\end{aligned}$$

By equation 13 the value for K follows. By equation 12 the inequality follows. □

Given Theorem 4.4 and Lemma 5.2 we show how an upper bound on the convergence rate in Wasserstein distance can be simulated for a numerical example of the Gibbs sampler for Bayesian regression with semi-conjugate priors, Example 5.1. We further provide an estimate of the upper bound in total variation using Lemma 5.1.

Numerical Example 5.1. Suppose that we are interested in evaluating the carbohydrate consumption (Y) by age, relative weight, and protein consumption (X) for twenty male insulin-dependent diabetics. For more information on this example, see Section 6.3.1 of Dobson and Barnett [2008].

We want to find the estimated upper bound on the total variation distance for a Gibbs sampler for Bayesian regression with semi-conjugate priors fitted to this model. In this case, there are 20 observed values and 4 parameters ($k = 20, p = 4$). We set the priors to $m_\beta = \vec{0}$, $\Sigma_\beta = I_4$, $\upsilon_0 = 1$, $c_0^2 = 10$. Using cubature approximation Narasimhan et al. [2023] with the R programming language R Core Team [2024], we can set $\int g(\beta, \sigma^2) d(\beta \times \sigma^2) = L \approx 0.9687$, where L is defined in equation 13. Using the bound in Lemma 5.2 $K \leq 2.1150$ and,

$$E[|\sigma_n^2 - \sigma_\infty^{'2}|] \leq 2.1150 \lim_{I\to\infty} \frac{1}{I} \sum_{i=1}^{I} |\sigma_{n,i}^2 - \sigma_{n,i}^{'2}|$$

holds almost surely.

Using the CRN technique, we simulated $E[|\sigma_{n,i}^2 - \sigma_{n,i}^{'2}|]$ one thousand times ($I = 1000$) over 100 iterations ($N = 100$). Figure 9 graphs the 1000 simulations and shows that the absolute differences spike at the second iteration, $|\sigma_{2,i}^2 - \sigma_{2,i}^{'2}|$, but converge quite quickly after

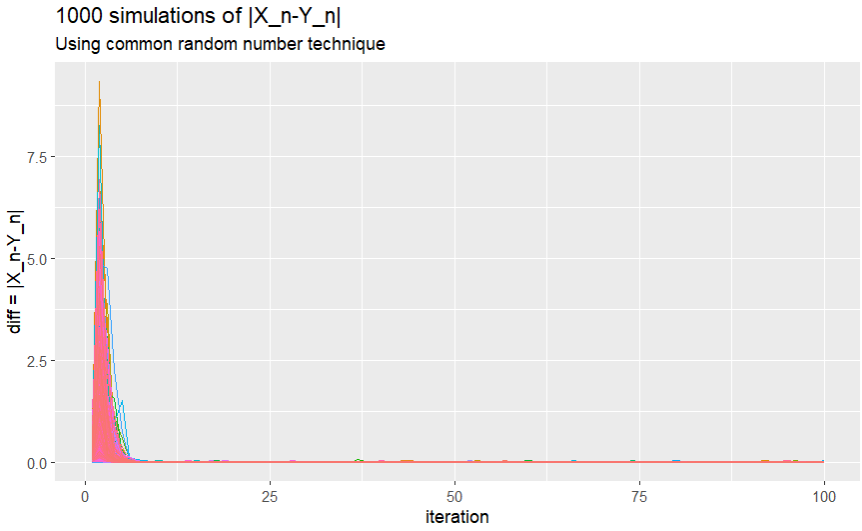

Figure 9: 1000 simulations of $|\sigma^2_{n,i} - \sigma'^2_{n,i}|$ where n =iteration.

this. At iteration 25, $E[|\sigma^2_{25} - \sigma^2_{\infty}|] \leq K\frac{1}{1000}\sum_{i=1}^{1000}|\sigma^2_{25,i} - \sigma'^2_{25,i}| = 2.1150 \times 0.0014 \approx 0.00291$. Figure 10 graphs the histogram of $|\sigma^2_{25,i} - \sigma'^2_{25,i}|$. Further, by Lemma 5.1 the total variation distance is bounded above by $\frac{(k+\upsilon_0)^2}{2\upsilon_0 c_0^2} = 22.05$ times the expected distance,

$$||\mathcal{L}(\sigma^2_n) - \mathcal{L}(\sigma'^2_{\infty})||_{TV} \leq 22.05E[|\sigma^2_n - \sigma^2_{\infty}|]$$

So at the 25th iteration, $||\mathcal{L}(\sigma^2_{25}) - \mathcal{L}(\sigma'^2_{\infty})||_{TV} \leq 0.0642$.

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7 Disclosure statement

The authors report there are no competing interests to declare.

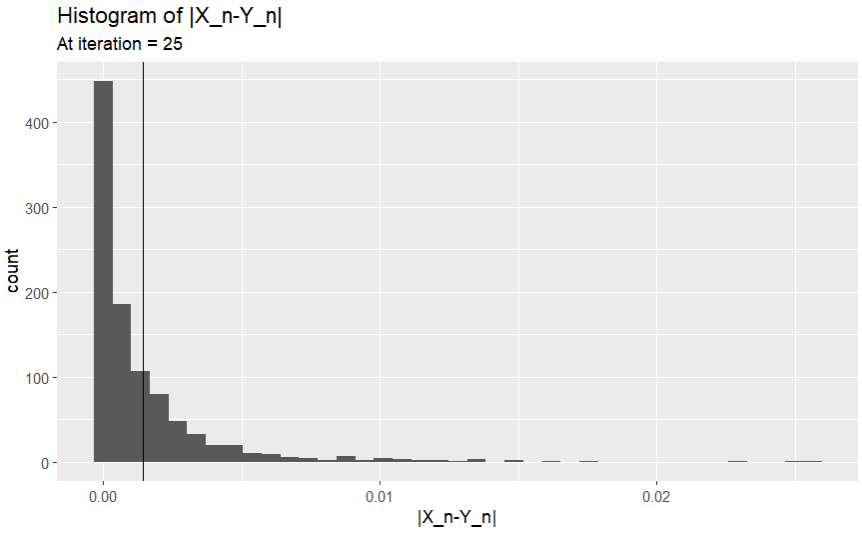

Figure 10: The following histogram graphs 1000 simulations of $|\sigma^2_{25,i} - \sigma'^2_{25,i}|$. The vertical line and sample mean difference is $\frac{1}{1000}\sum_{k=1}^{1000} |\sigma^2_{25,i} - \sigma'^2_{25,i}| = 0.0014$

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9 Proof of Theorem 3.3

Proof of Theorem 3.3. Fix x, y and denote $g(U) = f(F_\theta^{-1}(U), x)$ and $h(V) = f(F_\theta^{-1}(V), y)$. We write U, V as uniform random variables such that $\mathcal{L}(U) = Unif(0,1), \mathcal{L}(V) = Unif(0,1)$. Note that since $\theta_U = F^{-1}(U)$ where F is invertible, we interchangeably write the set A to signify A (defined on θ) and $F(A)$ (defined on U, V). Also note that since $g(U), h(V)$ are assumed to be of bounded variation, the sets I_x, I_y, D_x, D_y can be written as the union of countable intervals by Corollary 3.6 of Stein and Shakarchi [2005].

First we show that

$$\sup_{U\sim\mathcal{L}(U),V\sim\mathcal{L}(V)} E[g(U)h(V)1_A] = E[g(U)h(U)1_A] \tag{18}$$

Denote $I_x \cap I_y = \cup_{k\geq 1} J_k$ and $A \setminus (I_x \cap I_y) = \cup_{k\geq 1} L_k$ where J and L are intervals. We have

$$
\begin{aligned}
&\sup_{(U,V)} E[g(U)h(V)1_A] \\
&\leq \sup_{(U,V)} E[g(U)h(V)1_{I_x\cap I_y}] + \sup_{(U,V)} E[g(U)h(V)1_{A\setminus(I_x\cap I_y)}] \\
&= \sup_{(U,V)} E[g(U)h(V)1_{I_x\cap I_y}] + \sup_{(U,V)} E[(-g(U))(-h(V))1_{A\setminus(I_x\cap I_y)}] \\
&= \sup_{(U,V)} E[\sum_{k\geq 1} g(U)h(V)1_{J_k}] + \sup_{(U,V)} E[\sum_{k\geq 1}(-g(U))(-h(V))1_{L_k}] \\
&= \sup_{(U,V)} \sum_{k\geq 1} E[g(U)h(V)1_{J_k}] + \sup_{(U,V)} \sum_{k\geq 1} E[(-g(U))(-h(V))1_{L_k}] \\
&\leq \sum_{k\geq 1} \sup_{(U,V)} E[g(U)h(V)1_{J_k}] + \sum_{k\geq 1} \sup_{(U,V)} E[(-g(U))(-h(V))1_{L_k}] \\
&= \sum_{k\geq 1} E[g(U)h(U)1_{J_k}] + \sum_{k\geq 1} E[(-g(U))(-h(U))1_{L_k}] \\
&= E[g(U)h(U)1_{I_x\cap I_y}] + E[(-g(U))(-h(U))1_{A\setminus(I_x\cap I_y)}] \\
&= E[g(U)h(U)1_A]
\end{aligned}
$$

The third equality is by the Dominated Convergence Theorem, Theorem 1.5.8 of Durrett [2010], and the second last equality is by Proposition 3.2.

Since $E[g(U)h(U)] \leq \sup_{(U,V)} E[g(U)h(V)] \leq E[g(U)h(U)]$, equality follows. Note that Proposition 3.2 can still be applied even if $g(U)h(U)1_{J_k}$ and $g(U)h(U)1_{L_k}$ are no longer the product of right continuous functions, which is a result of the fact that 1_{J_k} may not necessarily be right continuous. This is because the theorem still applies by discussions in Section 4 of Cambanis et al. [1976] that note that rather than requiring that $f(\cdot, x)$ be right continuous it is simply necessary to assume that the discontinuous points are countable and have left and right limits. This is a necessary condition for bounded variation (assumed in the theorem). Since the function I_A has countably many discontinuities, Proposition 3.2 can be used.

Second we show that

$$\sup_{(U,V)} E[g(U)h(V)1_{A^c}] = E[g(U)h(1-U)1_{A^c}] \tag{19}$$

Suppose A^c can also be written as countable intervals. The set A^c represents areas where either g is increasing and h is decreasing or vice versa. By similar reasoning to equation 18,

$$\begin{aligned}
\sup_{(U,V)} E[g(U)h(V)1_{A^c}] &= -\inf_{(U,V)} E[g(U)(-h(V))1_{A^c}] \\
&= -\inf_{(U,V)} E[\sum_{I\in A^c} g(U)(-h(1-U))I] \\
&= -\inf_{(U,V)} \sum_{I\in A^c} E[g(U)(-h(1-U))I] \\
&\leq -\sum_{I\in A^c} \inf_{(U,V)} E[g(U)(-h(1-U))I] \\
&= -\sum_{I\in A^c} E[g(U)(-h(1-U))I] \\
&= -E[g(U)(-h(1-U))1_{A^c}] \\
&= E[g(U)h(1-U)1_{A^c}]
\end{aligned}$$

The third equality is by the Dominated Convergence Theorem, Theorem 1.5.8 of Durrett [2010], and the third last equality is by Theorem 2 of Cambanis et al. [1976].

Again, since $E[g(U)h(1-U)1_{A^c}] \leq \sup_{(U,V)} E[g(U)h(V)1_{A^c}] \leq E[g(U)h(1-U)1_{A^c}]$, equality follows.

Case 1: Suppose $P(A) = 1$. We write $P(A^c) = P(U,V) \in F(A^c))$

$$\begin{aligned}
&\sup_{(U,V)} E[g(U)h(V)] \\
&= \sup_{(U,V)} E[g(U)h(V)1_A] + E[g(U)h(V)1_{A^c}] \\
&= \sup_{(U,V)} E[g(U)h(V)1_A] + E[g(U)h(V) \mid (U,V) \in F(A^c)]P(A^c) \\
&= \sup_{(U,V)} E[g(U)h(V)1_A] && \text{Since } P(A^c) = 0 \\
&= E[g(U)h(U)1_A] && \text{by equation 18} \\
&= E[g(U)h(U)]
\end{aligned}$$

By equation 3, equation 6 follows.

Case 2: Suppose $P(A) = 0$.

$$\begin{aligned}
&\sup_{(U,V)} E[g(U)h(V)] \\
&= E[g(U)h(1-U)1_{A^c}] && \text{by equation 19} \\
&= E[g(U)h(1-U)]
\end{aligned}$$

By equation 3, equation 7 follows.

Case 3: Suppose $0 < P(A) < 1$.

$$\begin{aligned}
&\sup_{(U,V)} E[g(U)h(V)] \\
&\leq \sup_{(U,V)} E[g(U)h(V)1_A] + \sup_{(U,V)} E[g(U)h(V)1_{A^c}] \\
&= E[g(U)h(U)1_A] + E[g(U)h(1-U)1_{A^c}] && \text{by equations 18 and 19}
\end{aligned}$$

By equation 3, equation 8 follows. □

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