

OPTIMAL SCALING OF METROPOLIS ALGORITHMS ON GENERAL TARGET DISTRIBUTIONS

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ABSTRACT. The main limitation of the existing optimal scaling results for Metropolis–Hastings algorithms is that the assumptions on the target distribution are unrealistic. In this paper, we consider optimal scaling of random-walk Metropolis algorithms on general target distributions in high dimensions arising from realistic MCMC models. For optimal scaling by maximizing expected squared jumping distance (ESJD), we show the asymptotically optimal acceptance rate 0.234 can be obtained under general realistic sufficient conditions on the target distribution. The new sufficient conditions are easy to be verified and may hold for some general classes of realistic MCMC models, which substantially generalize the product i.i.d. condition required in most existing literature of optimal scaling. Furthermore, we show one-dimensional diffusion limits can be obtained under slightly stronger conditions, which still allow dependent coordinates of the target distribution. We also connect the new diffusion limit results to complexity bounds of Metropolis algorithms in high dimensions.

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1. INTRODUCTION

Markov chain Monte Carlo (MCMC) algorithms [BGJM11; GRS95; Liu08; MT12; RC04] are now routinely used in many fields to obtain approximations of integrals that could not be tackled by common numerical methods, because of the simplicity and the scalability to high-dimensional settings. The running times of MCMC algorithms are an extremely important issue of practice. They have been studied from a variety of perspectives, including convergence “diagnostics” via the Markov chain output [GR92], proving weak convergence limits of sped-up versions of the algorithms to diffusion limits [RGG97; RR98], and directly bounding the convergence in total variation distance [MT94; Ros95; Ros96; RT99; JH01; Ros02; JH04; Bax05; FHJ08].

The optimal scaling framework [RGG97; RR98; RR01] is one of the most successful and practically useful ways of performing asymptotic analysis of MCMC methods in high-dimensions. Optimal scaling results (e.g. [CRR05; NR+06; Béd08; BR08; NR08; NR11; NRY12; JLM15; JLM14; RR14; ZBK17]) facilitate optimization of MCMC performance by providing clear and mathematically-based guidance on how to tune the parameters defining the proposal distribution for Metropolis–Hastings algorithms [MRRT+53; Has70]. For instance, classical results include tuning the acceptance probabilities to 0.234 for random-walk Metropolis algorithm (RWM) [RGG97] and 0.574 for Metropolis-adjusted Langevin algorithm (MALA) [RR98]. Moreover, optimal scaling results have been used to analyze and compare a wide variety of MCMC algorithms, such as Hamiltonian Monte Carlo (HMC) [BPRSS+13], Pseudo-Marginal MCMC [STRR15], multiple-try MCMC [BDM12]. This yields guidance which is widely used by practitioners, especially via self-tuning or Adaptive MCMC methodologies [AT08; Ros11].

In the original paper, Roberts, Gelman, and Gilks [RGG97] dealt with the RWM algorithm for target distributions which have i.i.d. product forms. The i.i.d. assumption is very restrictive and the main limitation of the optimal scaling framework. From a practitioner’s perspective, target distributions of the i.i.d. forms are too limited a class of probability distributions to be useful, since they can be tackled by sampling a single one-dimensional target due to the product structure. To this day, optimal scaling results have mainly been proved for target distributions with a product structure, which severely limits their applicability. On the other hand, practitioners use these tuning criteria far outside the class of target distributions of product i.i.d. forms. For example, extensive simulations [RR01; SFR10] show that these optimality results also hold for more complex target distributions.

There exists only a few extensions for correlated targets and most of them are derived for very specific models. For example, Breyer and Roberts [BR00] studied target densities which are Gibbs measures and Roberts and Rosenthal [RR01] studied inhomogeneous target densities. Breyer, Piccioni, and Scarlatti [BPS+04] studied

target distributions arising in nonlinear regression and have a mean field structure. Neal and Roberts [NR+06] considered the case where updates of high-dimensional Metropolis algorithms are lower dimensional than the target density itself. Later, Bédard and Rosenthal [BR08] studied independent targets with different scales [Béd07; Béd08] and hierarchical target distributions [Béd09]. Neal and Roberts [NR08] studied spherically constrained target distributions and non-Gaussian proposals [NR11]. Sherlock and Roberts [SR09] considered elliptically symmetric unimodal targets. Neal, Roberts, and Yuen [NRY12] studied densities with bounded support. Durmus, Le Corff, Moulines, and Roberts [DLCMR17] considered target distributions which are differentiable in L^p mean. Recently, Mattingly, Pillai, and Stuart [MPS12] studied diffusion limits for a class of high-dimensional measures found from the approximation of measures on a Hilbert space which are absolutely continuous with respect to a Gaussian reference measure (See also [PST12; BRS09; BRSV08]). The conditions on the target distribution might seem to be general at the first glance. However, it is not clear how to check if a target distribution belong to this class. So far, only a few limited applications, such as [HSV11; Stu10] are known to lead to target distributions have the form required by [MPS12].

In this paper, we consider optimal scaling of RWM algorithms on general target distributions in high dimensions arising from realistic MCMC models. First, for optimal scaling by maximizing expected squared jumping distance (ESJD), we show the asymptotically optimal acceptance rate 0.234 can be obtained under general sufficient conditions on the target distribution. The new sufficient conditions are easy to check in practice and may hold for some general classes of realistic MCMC models. Our results substantially generalize the commonly used product i.i.d. condition. Furthermore, we show one-dimensional diffusion limits can also be obtained under relaxed conditions which still allow dependent coordinates of the target distribution. Finally, we also connect the new results of diffusion limits to complexity bounds of RMW algorithms in high dimensions.

The paper is organized as follows. In Section 2, we give a brief background review of optimal scaling for Metropolis–Hastings algorithms and complexity bounds via diffusion limits. In Section 3, we present our main results, which include three parts: optimal scaling by maximizing ESJD, optimal scaling via diffusion limits, and complexity bounds via diffusion limits. In Section 4, we demonstrate the new optimal scaling result holds for some realistic MCMC models. In Section 5, we prove Theorem 3.9, which is one of our main results. The proofs of lemmas used for proving Theorem 3.9 and other main results, such as Theorems 3.18 and 3.20, are delayed to Appendices A to C.

2. BACKGROUND ON OPTIMAL SCALING

Practical implementations of Metropolis–Hastings algorithms suffer from slow mixing for at least two reasons: the Markov chain moves very slowly to the target distribution when the proposed jumps are too short; the Markov chain stays at a state for most of the time when the proposed jumps are long but the chain ends up in low probability areas of the target distribution. The optimal scaling problem [RGG97] considers the choice of proposed distribution to optimize mixing of the Metropolis–Hastings algorithm. Note that we don’t consider transient phase of the Metropolis–Hasting algorithms in this paper. The transient phase of high-dimensional Metropolis–Hasting algorithms are studied for example in [CRR05; JLM14; JLM15].

We focus on one of the most popular MCMC algorithms, the RWM algorithm. This algorithm proceeds by running a Markov chain $\{X^d(t), t = 0, \dots, \infty\}$ as follows. Given a target distribution π^d on the state space \mathbb{R}^d and the current state $X^d(t) = x^d$, a new state is proposed by $Y^d \sim \mathcal{N}(x^d, \sigma_d^2 I)$, which is sampled from a multivariate Gaussian distribution centered at x^d , then the proposal is accepted with probability $\min\{1, \pi^d(Y^d)/\pi^d(x^d)\}$ so that $X^d(t+1) = Y^d$. Otherwise the proposal is rejected and $X^d(t+1) = x^d$. This algorithm is easily seen to be irreducible and aperiodic and to leave π^d stationary. Therefore, it will converge asymptotically to π^d . Note that the only computational cost involved in calculating the acceptance probabilities is the relative ratio of densities. Within the class of all Metropolis–Hastings algorithms, the RWM algorithm is still widely used in many applications because of its simplicity and robustness.

2.1. Optimal Scaling via Diffusion Limits. The most common technique to prove optimal scaling results is to show a weak convergence to diffusion limits as the dimension of a sequence of target densities converges to infinity [RGG97; RR98]. More specifically, when the proposal is appropriately scaled according to the dimension, the sequence of sped-up stochastic processes formed by the first coordinate of each Markov chain converges to the appropriate limiting Langevin diffusion process. The limiting diffusion limit admits a straightforward efficiency maximization problem which leads to asymptotically optimal acceptance rate of the proposed moves for the Metropolis–Hastings algorithm. In [RGG97], the target distribution π^d is assumed to be an d -dimensional product density with respect to Lebesgue measure. That is

$$\pi^d(x^d) = \prod_{i=1}^d f(x_i), \quad (1)$$

where $x^d = (x_1, x_2, \dots, x_d)$. It is shown that with the choice of scaling $\sigma_d^2 = \ell^2/(d-1)$ for some fixed $\ell > 0$, individual components of the resulting Markov chain converge to the solution of a stochastic differential equation (SDE). More specifically, denoting $X^d = (X_1^d, X_2^d, \dots, X_d^d)$, the first coordinate of the RWM algorithm, X_1^d , sped up by

a factor of d , i.e. $\{X_1^d(\lfloor dt \rfloor), t = 0, 1, \dots\}$, converges weakly in the usual Skorokhod topology to a limiting ergodic Langevin diffusion.

Proposition 2.1. [RGG97, Theorem 1.1] *Suppose density f satisfies that f'/f is Lipschitz continuous and*

$$\int \left[\frac{f'(x)}{f(x)} \right]^8 f(x) dx < \infty, \quad \int \left[\frac{f''(x)}{f(x)} \right]^4 f(x) dx < \infty. \quad (2)$$

Then for $U^d(t) := X_1^d(\lfloor dt \rfloor)$, as $d \rightarrow \infty$, we have

$$U^d \Rightarrow U, \quad (3)$$

where \Rightarrow denotes weak convergence in Skorokhod topology, and U satisfies the following Langevin SDE

$$dU(t) = (h(\ell))^{1/2} dB(t) + h(\ell) \frac{f'(U(t))}{2f(U(t))} dt, \quad (4)$$

with $h(\ell) := 2\ell^2 \Phi(-\ell\sqrt{I}/2)$ is the speed measure for the diffusion process, $I := \int \left[\frac{f'(x)}{f(x)} \right]^2 f(x) dx$, and Φ being the standard Gaussian cumulative density function.

This weak convergence result leads to the interpretation that, started in stationarity and applied to target measures of the i.i.d. form, the RWM algorithm will take on the order of d steps to explore the invariant measure. Furthermore, it may be shown that the value of ℓ which maximizes the speed measure $h(\ell)$ and, therefore, maximizes the speed of convergence of the limiting diffusion, leads to a universal acceptance probability, for the RWM algorithm applied to targets of i.i.d. forms, of approximately 0.234. Proposition 2.1 is proved in [RGG97] using the generator approach [EK86]. The same method of proof has also been applied to derive optimal scaling results for other types of MCMC algorithms. For example, the convergence of MALA to diffusion limits when $\sigma_d^2 = \ell^2/d^{1/3}$ (see e.g. [RR98; RR01; BPS+04; CRR05; NR+06]) with asymptotically optimal acceptance rate 0.574, and the convergence of HMC to diffusion limits when $\sigma_d^2 = \ell^2/d^{1/4}$ with asymptotically optimal acceptance rate 0.651 [BPRSS+13].

2.2. Optimal Scaling by maximizing ESJD. Another popular technique to prove optimal scaling is by maximizing expected squared jumping distance (ESJD) [PG10; ARR11; RR14], which is defined as follows.

Definition 2.2. (Expected Squared Jumping Distance)

$$\text{ESJD}(d) := \mathbb{E}_{X^d \sim \pi^d} \mathbb{E}_{Y^d} \left[\|Y^d - X^d\|^2 \left(1 \wedge \frac{\pi^d(Y^d)}{\pi^d(X^d)} \right) \right] \quad (5)$$

where the expectation over Y^d is taken for $Y^d \sim \mathcal{N}(x^d, \frac{\ell^2}{d-1})$ for given $X^d = x^d$, and $\|\cdot\|$ denotes the Euclidean distance, i.e. $\|Y^d - X^d\|^2 = \sum_{i=1}^d (Y_i - X_i)^2$.

Choosing a proposal variance to maximize ESJD is equivalent to minimizing the first-order auto-correlation of the Markov chain, and thus maximizing the efficiency if the higher order auto-correlations are monotonically increasing with respect to the first-order auto-correlation [PG10]. Furthermore, if weak convergence to a diffusion limit is established, then the ESJD converges to the quadratic variance of the diffusion limit. This suggests that maximizing the ESJD is a reasonable problem. For example, Atchadé, Roberts, and Rosenthal [ARR11] considered to maximize the ESJD to choose optimal temperature spacings for Metropolis-coupled Markov chain Monte Carlo and simulated tempering algorithms. Later, Roberts and Rosenthal [RR14] proved a diffusion limit for the simulated tempering algorithms. Using a new comparison of asymptotic variance of diffusions, Roberts and Rosenthal [RR14] showed the results in the choice of temperatures in [ARR11] does indeed minimize the asymptotic variance of all functionals.

Although establishing weak convergence of diffusion limits gives stronger guarantee than maximizing ESJD, the price to pay is to require stronger conditions on the target distribution. Maximizing ESJD instead can lead to (much) weaker conditions on the target distribution. Later in this paper, we will show that we are able to relax the restrictive product i.i.d. condition on the target distribution for both cases. In particular, the new sufficient conditions on the target distribution for maximizing ESJD are weak enough to allow target distributions arising from realistic MCMC models.

2.3. Background on Complexity Bounds. Because of the big data world, in recent years, there is much interest in the “large d , large n ” or “large d , small n ” high-dimensional regime, where d is the number of parameters and n is the sample size. Rajaratnam and Sparks [RS15] use the term convergence complexity to denote the ability of a high-dimensional MCMC scheme to draw samples from the posterior, and how the ability to do so changes as the dimension of the parameter set grows. This requires the study of computer-science-style complexity bounds [Cob65; Coo71] in terms of running time complexity order as the “size” of the problem goes to infinity. In the Markov chain context, computer scientists have been bounding convergence times of Markov chain algorithms focusing largely on spectral gap bounds for Markov chains [SJ89; LV03; Vem05; LV06; WSH09a; WSH09b]. In contrast, statisticians usually study total variation distance or other metric for MCMC algorithms. In order to bridge the gap between statistics-style convergence bounds, and computer-science-style complexity results, in one direction, Yang and Rosenthal [YR17] recently show that complexity bounds for MCMC can be obtained by quantitative bounds using a modified drift-and-minorization approach. In another direction, Roberts and

Rosenthal [RR16] connect existing results on diffusion limits of MCMC algorithm to the computer science notion of algorithm complexity. The main result in [RR16] states that any weak limit of a Markov process implies a corresponding complexity bound in an appropriate metric. More specifically, Roberts and Rosenthal [RR16] connect the diffusion limits to complexity bound using the Wasserstein metric. Let $(\mathcal{X}, \mathcal{F}, \rho)$ be a general measurable metric space, the distance of a stochastic process $\{X(t)\}$ on $(\mathcal{X}, \mathcal{F})$ to its stationary distribution π is defined by the KR distance

$$\|\mathcal{L}_x(X(t)) - \pi\|_{\text{KR}} := \sup_{g \in \text{Lip}_1^1} |\mathbb{E}[g(X(t))] - \pi(g)| \quad (6)$$

where $\pi(g) := \int g(x)\pi(dx)$ is the expected value of g with respect to π , ‘KR’ stands for ‘Kantorovich–Rubinstein’, and Lip_1^1 is the set of all functions g from \mathcal{X} to \mathbb{R} with Lipschitz constant no larger than 1 and with $|g(x)| \leq 1$ for all $x \in \mathcal{X}$, i.e.

$$\text{Lip}_1^1 := \{g : \mathcal{X} \rightarrow \mathbb{R}, |g(x) - g(y)| \leq \rho(x, y), \forall x, y \in \mathcal{X}, |g| \leq 1\}. \quad (7)$$

Note that the KR distance defined in Eq. (6) is exactly the 1-st Wasserstein metric. Then it can be shown that the π -average of the KR distance to stationarity from all initial states $X(0)$ in \mathcal{X} is non-increasing, which leads to the following complexity linking proposition.

Proposition 2.3. [RR16, Theorem 1] *Let $X^d = \{X^d(t), t \geq 0\}$ be a stochastic process on $(\mathcal{X}, \mathcal{F}, \rho)$, for each $d \in \mathbb{N}$. Suppose X^d converges weakly in the Skorokhod topology as $d \rightarrow \infty$ to a càdlàg process X^∞ . Assume these processes all have the same stationary distribution π and that X^∞ converges (either weakly or in total variation distance) to π . Then for any $\epsilon > 0$, there are $D < \infty$ and $T < \infty$ such that*

$$\mathbb{E}_{X^{d(0)} \sim \pi} \|\mathcal{L}_{X^{d(0)}}(X^d(t)) - \pi\|_{\text{KR}} < \epsilon, \quad \forall t \geq T, d \geq D. \quad (8)$$

Proposition 2.3 allows us to bound the convergence of the sequence of processes uniformly over all sufficiently large d , if the sequence of Markov processes converges weakly to a limiting ergodic process. Combining Proposition 2.3 with previously-known MCMC diffusion limit results, Roberts and Rosenthal [RR16] prove that the RWM algorithm in d dimensions takes $\mathcal{O}(d)$ iterations to converge to stationarity. However, in [RR16], the target distribution needs to be product i.i.d. with density satisfies all the assumptions of Proposition 2.1. Furthermore, the condition Eq. (2) is replaced by a stronger condition

$$\int \left[\frac{f'(x)}{f(x)} \right]^{12} f(x) dx < \infty, \quad \int \left[\frac{f''(x)}{f(x)} \right]^6 f(x) dx < \infty. \quad (9)$$

3. MAIN RESULTS

In this section, we show our main results on optimal scaling of RWM algorithms on general target distributions. We first consider optimal scaling by maximizing ESJD

in Section 3.1. We show asymptotic form of the ESJD in Theorem 3.9 under very mild conditions on the target distribution. Then we show in Theorem 3.12 that if we directly maximize the asymptotic ESJD, we can obtain 0.234 as an upper bound of the asymptotically optimal acceptance rate. Next, we show the acceptance rate 0.234 is asymptotically optimal under one more weak law of large number (WLLN) condition on the target distribution in Theorem 3.13. In Section 3.2, we consider optimal scaling via diffusion limits. We prove the new conditions for weak convergence to diffusion limits in Theorem 3.18. We then strengthen this result to consider fixed starting state in Theorem 3.20. Finally, in Section 3.3, we apply our new result on diffusion limits with fixed starting state to obtain complexity bounds for the RMW algorithm, which is given in Corollary 3.21.

Before presenting our main results, we first define a sequence of “sets of typical states”.

Definition 3.1. We call $\{F_d\}$ a sequence of “sets of typical states” if $\mathbb{P}_{X^d \sim \pi^d}(X^d \in F_d) \rightarrow 1$.

Next, we enlarge $\{F_d\}$ in different ways, which will be used later for the new conditions on the target.

Definition 3.2. For a given sequence of “sets of typical states” $\{F_d\}$, we define

$$F_d^{(i)} := \{(x_1, \dots, x_{i-1}, y, x_{i+1}, \dots, x_d) : \exists (x_1, \dots, x_d) \in F_d, \text{ and } |y - x_i| < \sqrt{\log d/d}\}. \quad (10)$$

Furthermore, we define $F_d^+ := \bigcup_{i=1}^d F_d^{(i)}$ and

$$F_d^* := \{(y_1, \dots, y_d) : \exists x^d \in F_d, |y_i - x_i| < \sqrt{\log d/d}, \forall i = 1, \dots, d\}. \quad (11)$$

Remark 3.3. It is clear from the definitions that $F_d^{(i)}$ is to enlarge the i -th coordinate of $x^d \in F_d$ by covering it with an open interval $(x_i - \sqrt{\log d/d}, x_i + \sqrt{\log d/d})$; F_d^+ is the union of $F_d^{(i)}, i = 1, \dots, d$; F_d^* is defined by covering F_d by a hypercube with radius $\sqrt{\log d/d}$. Then clearly we have $F_d \subseteq F_d^{(i)} \subseteq F_d^+ \subseteq F_d^*$. In practice, the difference between F_d^+ and F_d is usually asymptotically ignorable in high dimensions, but the difference between F_d^* and F_d can be quite large. \triangleleft

Finally, we introduce the idea of “neighborhoods” of a coordinate, which is later used to capture the correlation among different coordinates. We use \mathcal{L}_i to denote a collection of coordinates which are called “neighborhoods” of coordinate i . That is, $\mathcal{L}_i \subseteq \{1, \dots, d\} \setminus \{i\}$. Although the definition of the set \mathcal{L}_i is quite arbitrary, we expect that $j \in \mathcal{L}_i$ implies the coordinates i and j are correlated even conditional on all other coordinates. This idea of “neighborhoods” become clearer if the target distribution comes from a model which can be written as a graphical model, and

the “neighborhood” $j \in \mathcal{L}_i$ if there is an edge between nodes i and j . Clearly, in this definition for graphical models, $j \notin \mathcal{L}_i$ implies that the two coordinates i and j are conditional independent given all the other $d - 2$ coordinates.

3.1. Optimal Scaling for Maximizing ESJD. Suppose $\{F_d\}$ is a sequence of “sets of typical states” and $\{\mathcal{L}_i\}$ are collections of “neighborhoods” for each coordinate. Throughout the paper, we assume $\sup_{i \in \{1, \dots, d\}} |\mathcal{L}_i| < l_d$ where $l_d = o(d)$.

Remark 3.4. For graphical models, if we define \mathcal{L}_i as the collection of nodes that is directly connected to i by an edge, then $l_d = o(d)$ rules out “dense graphs” for which $l_d \propto d$. \triangleleft

Now we introduce the first assumption **A1** on the target π^d .

$$\begin{aligned} \sup_{(i,j):j \notin \mathcal{L}_i} \sup_{x^d \in F_d^+} \frac{\partial^2 \log \pi^d(x^d)}{\partial x_i \partial x_j} &= o(1), \\ \sup_{(i,j):j \in \mathcal{L}_i} \sup_{x^d \in F_d^+} \frac{\partial^2 \log \pi^d(x^d)}{\partial x_i \partial x_j} &= o(\sqrt{d/l_d}). \end{aligned} \quad (\text{A1})$$

Remark 3.5. For graphical models, if node i is not directly connected to node j , we always have $\frac{\partial^2 \log \pi^d(x^d)}{\partial x_i \partial x_j} = 0$. Therefore, in order to make **A1** hold, it suffices to check for each edge of the graph, say (i, j) , that $\frac{\partial^2 \log \pi^d(x^d)}{\partial x_i \partial x_j} = o(\sqrt{d/l_d})$. Since we have assumed $l_d = o(d)$, this is a very weak condition. For example, **A1** holds for all graphical models with bounded second partial derivatives. \triangleleft

Next, we denote $\pi_{i,j|-i-j} := \pi^d(x_i, x_j | x_{-i-j})$ where x_{-i-j} with $i < j$ denotes all coordinates of x^d other than the i -th, and j -th coordinates, i.e. $x_{-i-j} := (x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_{j-1}, x_{j+1}, \dots, x_d)$. Then we introduce the next assumption **A2** on the target as follows.

$$\sup_{(i,j):j \notin \mathcal{L}_i} \sup_{\{x_{-i-j}: x^d \in F_d\}} \int \frac{\partial^2 \pi_{i,j|-i-j}}{\partial x_i^2} \frac{\partial^2 \pi_{i,j|-i-j}}{\partial x_j^2} \frac{1}{\pi_{i,j|-i-j}} dx_i dx_j = o(1). \quad (\text{A2})$$

Remark 3.6. The assumption **A2** is very weak, since it is only to require that the target has a “flat tail”. To see this, consider the target distribution π^d has the special i.i.d. product form of Eq. (1), then **A2** reduces to

$$\int \frac{\partial^2 f(x_i) f(x_j)}{\partial x_i^2} \frac{\partial^2 f(x_i) f(x_j)}{\partial x_j^2} \frac{1}{f(x_i) f(x_j)} dx_i dx_j = \left(\int \frac{d^2 f(x)}{dx^2} dx \right)^2 = 0, \quad (12)$$

when f has a “flat tail” so that $\frac{df(x)}{dx} \rightarrow 0$ when $|x| \rightarrow \infty$. Similarly, for graphical models, if there is no edge between i and j , then when π^d has “flat tail” we have $\int \frac{\partial^2 \pi_{i,j|-i-j}}{\partial x_i^2} \frac{\partial^2 \pi_{i,j|-i-j}}{\partial x_j^2} \frac{1}{\pi_{i,j|-i-j}} dx_i dx_j = 0$. \triangleleft

Next assumption is about conditions on the third partial derivatives.

$$\begin{aligned} \sup_{(i,j):j \notin \mathcal{L}_i} \sup_{x^d \in F_d^*} \frac{\partial^3 \log \pi^d(x^d)}{\partial x_i^2 \partial x_j} &= o(1) \\ \sup_{(i,j):j \in \mathcal{L}_i} \sup_{x^d \in F_d^*} \frac{\partial^3 \log \pi^d(x^d)}{\partial x_i^2 \partial x_j} &= o(d/l_d), \\ \sup_{x^d \in F_d^*} \sum_{i \neq j \neq k} \left| \frac{\partial^3 \log \pi^d(x^d)}{\partial x_i \partial x_j \partial x_k} \right| &= o(d^{3/2}). \end{aligned} \tag{A3}$$

Remark 3.7. For the assumption **A3**, the first two equations are similar to **A1**. The differences include that **A3** is for third partial derivatives instead of second partial derivatives. Also the sup is taken over a slightly larger set since $F_d^+ \subseteq F_d^*$. Again, these two equations are quite weak. For example, they hold for all graphical models with bounded third partial derivatives. For graphical models, the last equation of **A3** involves the number of 3-cliques in the graph. Note that for many realistic hierarchical models, there are no 3-cliques for the corresponding graphs, which implies $\sum_{i \neq j \neq k} \left| \frac{\partial^3 \log \pi^d(x^d)}{\partial x_i \partial x_j \partial x_k} \right| = 0$. Thus, this condition is very mild. Even for the worst case, considering a graph that has d nodes and each has l_d neighbors, since there are $dl_d/2$ links, the number of 3-cliques is at most $\binom{l_d}{2}d/3 = \mathcal{O}(l_d^2 d)$. Therefore, **A3** holds for any graphical model with $l_d = o(d^{1/4})$ and bounded third partial derivatives. \triangleleft

Next assumption is the last assumption before our first main result. We first define an quantity which measures the “roughness” of $\log \pi^d$.

$$I(x^d) := \frac{1}{d} \sum_{i=1}^d \left(\frac{\partial}{\partial x_i} \log \pi^d(x^d) \right)^2. \tag{13}$$

Similarly, we can consider $I(X^d)$ where $X^d \sim \pi^d$ as a random variable. Later we will see that it turns out that $I(X^d)$ is a key quantity for optimal scaling results.

Assumption [A4](#) is as follows.

$$\begin{aligned} \sup_i \sup_{x^d \in F_d^{(i)}} \frac{\partial \log \pi^d(x^d)}{\partial x_i} &= \mathcal{O}(d^\alpha), \\ \sup_{x^d \in F_d^+} \pi^d(x^d) &= o(d^{1/2-\alpha}), \\ \sup_{x^d \in F_d^+} 1/I(x^d) &= \mathcal{O}(d^{\alpha/2}), \end{aligned} \tag{A4}$$

where there exists α with $0 < \alpha < 1/2$.

Remark 3.8. For [A4](#), the first two conditions do not even require π^d and the first partial derivative of $\log \pi^d$ to be bounded. Thus, they are quite weak. For the last condition, although the mode of π^d is ruled out from F_d^+ , the condition can hold as long as $I(X^d)$ is tight. That is $\forall 0 < \epsilon < 1$, there exists $K_\epsilon > 0$ such that $\mathbb{P}(I(X^d) > K_\epsilon) < 1 - \epsilon$. Note that $I(X^d)$ being tight is a very reasonable assumption, since if $I(X^d)$ is not tight, the target π^d becomes “flat” at almost every state x^d . \triangleleft

We are now ready to present our first main result using the assumptions [A1](#), [A2](#), [A3](#), and [A4](#). We establish the following results on asymptotic ESJD and asymptotic acceptance rate.

Theorem 3.9. (*Asymptotic ESJD and acceptance rate*) Suppose π^d satisfies [A1](#), [A2](#), [A3](#), and [A4](#), then as $d \rightarrow \infty$, we have

$$\left| \text{ESJD}(d) - 2 \frac{d\ell^2}{d-1} \mathbb{E}_{X^d \sim \pi^d} \left[\Phi \left(-\frac{\ell \sqrt{I(X^d)}}{2} \right) \right] \right| \rightarrow 0, \tag{14}$$

$$\left| \mathbb{E}_{X^d \sim \pi^d} \mathbb{E}_{Y^d} \left(1 \wedge \frac{\pi^d(Y^d)}{\pi^d(X^d)} \right) - 2 \mathbb{E}_{X^d \sim \pi^d} \left[\Phi \left(-\frac{\ell \sqrt{I(X^d)}}{2} \right) \right] \right| \rightarrow 0, \tag{15}$$

where the expectation over Y^d is taken for $Y^d \sim \mathcal{N}(x^d, \frac{\ell^2}{d-1} I)$ for given $X^d = x^d$.

Proof. See Section [5](#). □

Since the assumptions required by Theorem [3.9](#) are very mild. The result of Theorem [3.9](#) holds for a large class of realistic MCMC models. As an example, we give a class of graphical models that all conditions [A1](#), [A2](#), [A3](#), and [A4](#) hold. Therefore, the asymptotic ESJD and acceptance rate by Theorem [3.9](#) hold for this class of graphical models. We will further discuss realistic MCMC models later in Section [4.1](#) and Section [4.2](#).

Example 3.10. The asymptotic ESJD and acceptance rate results by Theorem [3.9](#) hold for any graphical model that satisfies (i) each node has at most $l_d = o(d^{1/4})$ links;

(ii) $I(X^d)$ is tight; (iii) π^d has bounded density and $\log \pi^d$ has up to the third bounded partial derivatives. \triangleleft

Note that Theorem 3.9 suggests that under mild conditions on the target distribution, the expected acceptance rate

$$\mathbb{E}_{X^d \sim \pi^d} \mathbb{E}_{Y^d} \left(1 \wedge \frac{\pi^d(Y^d)}{\pi^d(X^d)} \right) \rightarrow 2 \mathbb{E}_{X^d \sim \pi^d} \left[\Phi \left(-\frac{\ell \sqrt{I(X^d)}}{2} \right) \right]. \quad (16)$$

Therefore, we can define asymptotic acceptance rate as a function of ℓ as follows.

Definition 3.11. (Asymptotic Acceptance Rate) The asymptotic acceptance rate function is defined by

$$a(\ell) := 2 \mathbb{E}_{X^d \sim \pi^d} \left[\Phi \left(-\frac{\ell \sqrt{I(X^d)}}{2} \right) \right]. \quad (17)$$

The next theorem shows that if the target distribution satisfies A1, A2, A3 and A4, then if we maximize the asymptotic ESJD, the resulting asymptotic acceptance rate is no larger than 0.234.

Theorem 3.12. *Defining the optimal parameter for maximizing the asymptotic ESJD by $\hat{\ell}$, i.e.*

$$\hat{\ell} := \arg \max_{\ell} h(\ell), \quad h(\ell) := 2\ell^2 \mathbb{E}_{X^d \sim \pi^d} \left[\Phi \left(-\frac{\ell \sqrt{I(X^d)}}{2} \right) \right], \quad (18)$$

then we have $a(\hat{\ell}) \leq 0.234$ (to two decimal places).

Proof. We follow the arguments in [Taw17, Lemma 5.1.4]. First, it can be verified by taking the second derivatives of $h(\ell)$ with respect to ℓ that the maximum of $h(\ell)$ is achieved at ℓ such that $\frac{\partial h(\ell)}{\partial \ell} = 0$. Therefore, the optimal $\hat{\ell}$ satisfies

$$2 \mathbb{E}_{X^d \sim \pi^d} \left[\Phi \left(-\frac{\hat{\ell} \sqrt{I(X^d)}}{2} \right) \right] = \mathbb{E}_{X^d \sim \pi^d} \left[\frac{\hat{\ell} \sqrt{I(X^d)}}{2} \Phi' \left(-\frac{\hat{\ell} \sqrt{I(X^d)}}{2} \right) \right]. \quad (19)$$

Therefore, the asymptotic acceptance rate

$$a(\hat{\ell}) = \mathbb{E}_{X^d \sim \pi^d} \left[\frac{\hat{\ell} \sqrt{I(X^d)}}{2} \Phi' \left(-\frac{\hat{\ell} \sqrt{I(X^d)}}{2} \right) \right] = \mathbb{E}_{X^d \sim \pi^d} [-\Phi^{-1}(V) \Phi'(\Phi^{-1}(V))], \quad (20)$$

where $V := \Phi\left(-\frac{\hat{\ell}\sqrt{I(X^d)}}{2}\right)$. By [She06], the function $-\Phi^{-1}(x)\Phi'(\Phi^{-1}(x))$ is a concave function for any $x \in (0, 1)$. Therefore, we have

$$a(\hat{\ell}) = \mathbb{E}_{X^d \sim \pi^d} [-\Phi^{-1}(V)\Phi'(\Phi^{-1}(V))] \leq -\Phi^{-1}[\mathbb{E}_{X^d \sim \pi^d}(V)]\Phi'[\Phi^{-1}(\mathbb{E}_{X^d \sim \pi^d}(V))]. \quad (21)$$

Defining $m := -\Phi^{-1}[\mathbb{E}_{X^d \sim \pi^d}(V)]$, we can then write

$$a(\hat{\ell}) = 2\Phi(-m) \leq m\Phi'(-m). \quad (22)$$

Finally, it suffices to show that $2\Phi(-m) \leq m\Phi'(-m)$ implies $2\Phi(-m) \leq 0.234$ (to two decimal places). Note that the function $x^2\Phi(-x)$ is maximized at \hat{m} such that $2\Phi(-\hat{m}) = \hat{m}\Phi'(-\hat{m}) \approx 0.234$. By [Taw17, Lemma 5.1.4], the function $2\Phi(-x) - x\Phi'(-x)$ is positive for $x < \hat{m}$ and negative for $x > \hat{m}$. Therefore, $2\Phi(-m) \leq m\Phi'(-m)$ implies that $m > \hat{m}$. Since $\Phi(-x)$ is monotonically decreasing with x , we have

$$a(\hat{\ell}) = 2\Phi(-m) \leq 2\Phi(-\hat{m}) \approx 0.234. \quad (23)$$

□

The next result is our main result for optimal scaling by maximizing ESJD. Defining the following WLLN condition for the target π^d :

$$I(X^d) \rightarrow \bar{I}_d \quad \text{in probability} \quad (A5)$$

where $X^d \sim \pi^d$ and $\bar{I}_d := \mathbb{E}_{X^d \sim \pi^d}[I(X^d)]$, we show that if the target distribution π^d satisfies A1, A2, A3, A4, and the WLLN assumption in A5, then the acceptance rate 0.234 is asymptotically optimal.

Theorem 3.13. *(Optimal Scaling for Maximizing ESJD) Suppose the target distribution π^d satisfies A1, A2, A3, A4, and A5. Then the asymptotic optimal acceptance rate $a(\hat{\ell}) \approx 0.234$ (to two decimal places).*

Proof. By convexity of the function $\Phi(-x)$ when $x \geq 0$, we can immediately obtain a lower bound

$$\ell^2 \mathbb{E}_{X^d \sim \pi^d} \left[\Phi\left(-\frac{\ell\sqrt{I(X^d)}}{2}\right) \right] \geq \ell^2 \left[\Phi\left(-\frac{\ell\mathbb{E}_{X^d \sim \pi^d}[\sqrt{I(X^d)}]}{2}\right) \right]. \quad (24)$$

Under A5, this lower bound is asymptotically tight. Therefore, as $d \rightarrow \infty$, according to [RGG97], we have (to two decimal places)

$$\hat{\ell} \rightarrow \frac{2.38}{\mathbb{E}_{X^d \sim \pi^d}[\sqrt{I(X^d)}]}, \quad h(\hat{\ell}) \rightarrow \frac{1.3}{\left(\mathbb{E}_{X^d \sim \pi^d}[\sqrt{I(X^d)}]\right)^2}. \quad (25)$$

The acceptance rate which maximizing the asymptotic ESJD is

$$a(\hat{\ell}) = 2\mathbb{E}_{X^d \sim \pi^d} \left[\Phi \left(-\frac{\hat{\ell} \sqrt{I(X^d)}}{2} \right) \right] \rightarrow 2\Phi \left(-\frac{\hat{\ell} \mathbb{E}_{X^d \sim \pi^d} \sqrt{I(X^d)}}{2} \right) \quad (26)$$

$$\approx 2\Phi \left(-\frac{2.38}{\mathbb{E}_{X^d \sim \pi^d} [\sqrt{I(X^d)}]} \frac{\mathbb{E}_{X^d \sim \pi^d} [\sqrt{I(X^d)}]}{2} \right) \quad (27)$$

$$= 2\Phi(-1.19) \approx 0.234. \quad (28)$$

□

Remark 3.14. Comparing the results of Theorem 3.12 and Theorem 3.13, it is clear that the “roughness” of π^d , $I(X^d)$, is the key quantity which determines the optimal acceptance rate $a(\hat{\ell}) \leq 0.234$ when only the tightness of $I(X^d)$ can be verified, or $a(\hat{\ell}) \approx 0.234$ when the concentration of $I(X^d)$ as defined in A5 can be verified. We will later demonstrate how to verify A5 for some realistic MCMC models in Section 4.1 and Section 4.2. ◁

3.2. Optimal Scaling via Diffusion Limits. In this subsection, we consider sufficient conditions on π^d for establishing weak convergence of diffusion limits. As we discussed before, establishing such results gives stronger guarantee for optimal scaling than maximizing ESJD. However, it also requires stronger conditions on the target distribution. As we will see in the following, we need to strengthen assumptions A2, A3, A4, A5 and add one more assumption A6.

We first strengthen A2 to a new assumption A2+ as follows.

$$\sum_{i=1}^d \sum_{j=1}^d \sum_{k=1}^d \int \left(\frac{\partial^2 \pi^d}{\partial x_i^2} \frac{1}{\pi^d} \right) \left(\frac{\partial^2 \pi^d}{\partial x_j^2} \frac{1}{\pi^d} \right) \left(\frac{\partial^2 \pi^d}{\partial x_k^2} \frac{1}{\pi^d} \right) \pi^d dx^d = \mathcal{O}(d^{2-\delta}) \quad (\text{A2+})$$

for some $\delta > 0$.

Remark 3.15. The new assumption A2+ is stronger than A2 but is still very mild. To see this, we consider graphical models as examples. For graphical models with d nodes and $\mathcal{O}(dl_d)$ links, there are at most $\mathcal{O}(dl_d^2)$ 3-cliques. Therefore, A2+ holds for any graphical model with $l_d = o(d^{1/2-\delta})$ and bounded second partial derivatives of $\log \pi^d$. Note that this is only for the worst case, as many realistic graphical models do not have 3-cliques. ◁

Next, we slightly strengthen **A3** and **A4** to **A3+** and **A4+**.

$$\begin{aligned} \sup_{(i,j):j \notin \mathcal{L}_i} \sup_{x^d \in F_d^*} \frac{\partial^3 \log \pi^d(x^d)}{\partial x_i^2 \partial x_j} &= o(1), \\ \sup_{(i,j):j \in \mathcal{L}_i} \sup_{x^d \in F_d^*} \frac{\partial^3 \log \pi^d(x^d)}{\partial x_i^2 \partial x_j} &= o(\sqrt{d/l_d}), \\ \sup_{x^d \in F_d^*} \sum_{i \neq j \neq k} \left| \frac{\partial^3 \log \pi^d(x^d)}{\partial x_i \partial x_j \partial x_k} \right| &= o(d^{3/2}). \end{aligned} \tag{A3+}$$

Suppose exists $0 < \alpha < 1/2$ that

$$\begin{aligned} \sup_i \sup_{x^d \in F_d^{(i)}} \frac{\partial^2 \log \pi^d(x^d)}{\partial x_i^2} &= o(d^\alpha), \\ \sup_i \sup_{x^d \in F_d^{(i)}} \frac{\partial \log \pi^d(x^d)}{\partial x_i} &= \mathcal{O}(d^{\alpha/2}), \\ \sup_{x^d \in F_d^+} \pi^d(x^d) &= o(d^{1/2-\alpha}), \\ \sup_{x^d \in F_d^+} 1/I(x^d) &= \mathcal{O}(d^{\alpha/4}). \end{aligned} \tag{A4+}$$

Furthermore, we strengthen the WLLN condition **A5** to the following **A5+**.

$$\sup_{x^d \in F_d^+} |I(x^d) - \bar{I}| \rightarrow 0 \tag{A5+}$$

where $\bar{I} := \lim_{d \rightarrow \infty} \bar{I}_d$ exists.

Remark 3.16. **A3+** is only slightly stronger than **A3** on the rates. **A4+** also includes a new condition on the rate of $\frac{\partial^2 \log \pi^d(x^d)}{\partial x_i^2}$ which is quite weak. **A5+** requires any sequence $(x^1, x^2, \dots, x^d, \dots)$ where $x^i \in F_i^+$ converges to the same limit \bar{I} , so it is (slightly) stronger than WLLN condition in **A5**. It will become clear in the proof of Theorem 3.18 that **A5+** is to ensure the speed measure of the diffusion process $h(\ell)$ does not depend on the state x^d . \triangleleft

Finally, we define a new assumption **A6** on the target distribution. Roughly speaking, the new assumption is to require the first coordinate of π^d is asymptotically independent with the rest.

$$\sup_{x^d \in F_d^+} \left| \frac{d \log \pi^d(x_1 | x_{-1})}{dx_1} - \frac{d \log \tilde{\pi}_1(x_1)}{dx_1} \right| \rightarrow 0, \tag{A6}$$

where $x_{-1} := (x_2, \dots, x_d)$ and $\tilde{\pi}_1$ is a density.

Remark 3.17. Note that **A6** is a strong condition, which may not be satisfied for many realistic MCMC models. However, it might be necessary in order to get a one-dimensional diffusion limit. In the proof of the optimal scaling via diffusion limits result in Theorem 3.18, the assumption **A6** is to ensure the SDE for the first coordinate x_1 doesn't depend on the values of other coordinates. Furthermore, although we do not pursue in this paper, if in **A6** we instead assume not just the first component but a finite collection of components are asymptotically independent from the rest, a version of weak convergence to multi-dimensional diffusion limits could be obtained following similar arguments as the proof of the one-dimensional diffusion limit case in Theorem 3.18. \triangleleft

Now we are ready for the main result of optimal scaling via diffusion limits, which is given in Theorem 3.18. Comparing with the assumptions in Theorem 3.13, the new sufficient conditions for diffusion limits include strengthening **A2** to **A2+**, **A3** and **A4** to **A3+** and **A4+**, **A5** to **A5+**, and adding **A6**. We also require slightly stronger condition on the sequence of “sets of typical states” $\{F_d\}$.

Theorem 3.18. (*Optimal Scaling via Diffusion Limits*) Suppose the sequence $\{F_d\}$ satisfies $\mathbb{P}_{X^d \sim \pi^d}(X^d \notin F_d) = \mathcal{O}(d^{-1-\delta})$ for some $\delta > 0$, the target distribution π^d satisfies **A1**, **A2+**, **A3+**, **A4+**, **A5+**, and **A6**, then for $U^d(t) := X_1^d(\lfloor dt \rfloor)$, as $d \rightarrow \infty$, we have

$$U^d \Rightarrow U, \quad (29)$$

where \Rightarrow denotes weak convergence in Skorokhod topology, and U satisfies the Langevin SDE

$$dU(t) = (h(\ell))^{1/2} dB(t) + h(\ell) \frac{f'(U(t))}{2f(U(t))} dt, \quad (30)$$

where $h(\ell) := 2\ell^2 \Phi(-\ell\sqrt{I}/2)$ is the speed measure for the diffusion process.

Proof. See Appendix B. \square

Remark 3.19. Note that Theorem 3.18 allows dependent coordinates on the target distribution, which is much more general than the product i.i.d. condition. The only strong assumption is **A6** which requires the first coordinate is asymptotically independent with other coordinates. \triangleleft

Next, we present another result with slightly stronger conditions, which allows the RWM algorithm to start at a fixed state. This stronger convergence result later allows us to establish a complexity bound for the RMW algorithm in Section 3.3.

Theorem 3.20. (*Optimal Scaling via Diffusion Limits with fixed starting state*) Let $X^d = \{X^d(t), t \geq 0\}$ for $d \in \mathbb{N}$ be the RWM processes defined earlier. Without loss of generality, suppose $\{X^d, d = 1, 2, \dots\}$ are defined in a common measurable

metric space $(\mathbb{R}^\infty, \mathcal{F}, \rho)$ as independent processes. Suppose X_1^d converges weakly in the Skorokhod topology as $d \rightarrow \infty$ to a càdlàg process X_1^∞ . Moreover, assume these processes $\{X^d, d = 1, 2, \dots\}$ all have the same marginal stationary distribution π_1 for the first coordinate and that the first coordinate of X^∞ converges (either weakly or in total variation distance) to π_1 . Suppose the sequence $\{F_d\}$ satisfies $\mathbb{P}_{X^d \sim \pi^d}(X^d \notin F_d) = \mathcal{O}(d^{-2-\delta})$ for some $\delta > 0$, the target distribution π^d satisfies [A1](#), [A3+](#), [A4+](#), [A5+](#), and [A6](#). We strengthen [A2+](#) to the following condition

$$\sum_{i=2}^d \sum_{j=2}^d \sum_{k=2}^d \sum_{l=2}^d \int \left(\frac{\partial^2 \pi_{-1}}{\partial x_i^2} \frac{1}{\pi_{-1}} \right) \left(\frac{\partial^2 \pi_{-1}}{\partial x_j^2} \frac{1}{\pi_{-1}} \right) \left(\frac{\partial^2 \pi_{-1}}{\partial x_k^2} \frac{1}{\pi_{-1}} \right) \left(\frac{\partial^2 \pi_{-1}}{\partial x_l^2} \frac{1}{\pi_{-1}} \right) \pi^d dx^d = \mathcal{O}(d^{2-5\delta}). \quad (\text{A2++})$$

Then as $d \rightarrow \infty$, we have

$${}_x U^d \Rightarrow {}_x U, \quad (31)$$

where ${}_x U^d(t) := (X_1^d(\lfloor dt \rfloor) | X_1^d(0) = x)$ is the first coordinate of the RWM algorithm sped up by a factor of d , conditional on starting at the state x , and ${}_x U$ is the limiting ergodic Langevin diffusion U in [Eq. \(30\)](#) also conditional on starting at x .

Proof. See [Appendix C](#). \square

3.3. Complexity Bounds via Diffusion Limits. In the following, by combing [Theorem 3.20](#) and [Proposition 2.3](#), we present a complexity bound for the RWM algorithm which holds for much more general target distributions comparing with [\[RR16\]](#). More specifically, if the target distribution satisfies the conditions given in [Theorem 3.20](#) which allows dependent coordinates of the target distribution, the RWM algorithm in d dimensions takes $\mathcal{O}(d)$ iterations to converge to stationarity.

Corollary 3.21. (*Complexity Bound for RWM Algorithms*) Under the conditions of [Theorem 3.20](#), for any $\epsilon > 0$, there exists $D < \infty$ and $T < \infty$, such that

$$\mathbb{E}_{X^d(0) \sim \pi^d} \|\mathcal{L}_{X^d(0)}(X_1^d(\lfloor dt \rfloor)) - \pi_1\|_{KR} < \epsilon, \quad \forall t \geq T, d \geq D, \quad (32)$$

where π_1 denotes the marginal stationary distribution of the first coordinate.

Proof. The result directly comes from [Proposition 2.3](#) and [Theorem 3.20](#). \square

Remark 3.22. If we generalize the conditions in [Theorem 3.20](#) required for the first coordinate to be satisfied uniformly over the first c coordinates, then for any $\epsilon > 0$, there exists $D < \infty$ and $T < \infty$, such that

$$\mathbb{E}_{X^d(0) \sim \pi^d} \|\mathcal{L}_{X^d(0)}(X_{1:c}^d(\lfloor dt \rfloor)) - \pi_{1:c}\|_{KR} < \epsilon, \quad \forall t \geq T, d \geq D, \quad (33)$$

where $\pi_{1:c}$ denotes the marginal stationary distribution of the first c coordinates. This is because the generalization of [A6](#) to uniformly hold over any of the first c coordinates implies that the coordinates of $\pi_{1:c}$ are asymptotically independent. Then

the statement can be proved by first applying the argument in Corollary 3.21 to each of the c coordinates then combing the convergence of all c coordinates uniformly. \triangleleft

4. EXAMPLES AND APPLICATIONS

In this section, we further discuss examples and applications of the main results in Section 3. We first discuss in Section 4.1 on verifying the assumptions of Theorem 3.13 for realistic MCMC models. We have explained in Remarks 3.5 to 3.8 that A1, A2, A3, and A4 are typically very weak conditions and they hold for some classes of graphical models. However, as discussed in Remark 3.14, the assumption A5 may need to be verified case by case. Particularly, in order to satisfy A5, we may need to make additional assumptions on the observed data. Fortunately, we show by a simple Gaussian example in Example 4.1 that, in some cases, A5 can be easily verified without any further assumptions. Then, in Section 4.2, we prove that a realistic MCMC model in Example 4.5 satisfies all the assumptions required by Theorem 3.13. Thus, the acceptance rate 0.234 is indeed asymptotically optimal for this realistic MCMC model.

4.1. Discussions on Theorem 3.13. The optimal scaling result for maximizing ESJD in Theorem 3.13 requires one to verify that the target distribution satisfies A1, A2, A3, A4, and A5. We discuss how to verify the conditions on the target distribution required by Theorem 3.13 in practice. We explain that A1, A2, A3 and A4 are quite mild and usually easy to be verified. Therefore, we usually only need to focus on the WLLN condition in A5, which might be difficult to check in practice. Throughout this subsection, we demonstrate verification of all the assumptions by a simple Gaussian example, which can be seen as a simplified version of typical Bayesian hierarchical models.

Example 4.1. (A Simple Gaussian Example) Consider a simple Gaussian MCMC model

$$\begin{aligned} Y_{ij} \mid \theta_{ij} &\sim \mathcal{N}(\theta_{ij}, 1), \quad i, j \in \{1, \dots, n\} \\ \theta_{ij} \mid \mu_j &\sim \mathcal{N}(\mu_j, 1), \quad i \in \{1, \dots, n\} \\ \mu_j \mid \nu &\sim \mathcal{N}(\nu, 1) \\ \nu &\sim \text{flat prior on } \mathbb{R}, \end{aligned} \tag{34}$$

where $\{Y_{ij}\}_{i,j=1}^n$ are the observed data, and $x^d = (\nu, \{\mu_j\}_{j=1}^n, \{\theta_{ij}\}_{i,j=1}^n)$ are parameters. Note that we have the number of parameters $d = n^2 + n + 1$ in this example. The

target distribution (i.e. the posterior distribution) satisfies

$$\begin{aligned} \pi^d(x^d) &= \mathbb{P}(x^d \mid \{Y_{ij}\}_{i,j=1}^n) \\ &\propto \prod_{j=1}^n \prod_{i=1}^n \frac{1}{\sqrt{2\pi}} e^{-\frac{(\mu_j - \nu)^2}{2}} \frac{1}{\sqrt{2\pi}} e^{-\frac{(\theta_{ij} - \mu_j)^2}{2}} \frac{1}{\sqrt{2\pi}} e^{-\frac{(Y_{ij} - \theta_{ij})^2}{2}}. \end{aligned} \quad (35)$$

Note that the hyperparameters ν is conditional independent with $\{\theta_{ij}\}$. Therefore, ν is only directly dependent with n coordinates $\{\mu_j\}_{j=1}^n$. We can define the “neighborhoods” of ν using the collection of $\mu_j, j = 1, \dots, n$. Similarly, μ_j is directly dependent with ν and $\{\theta_{ij}\}_{i=1}^n$ and θ_{ij} is directly dependent with μ_j . Therefore, if we choose the directly dependent coordinates as “neighborhoods”, we have $l_d = n + 1 = \mathcal{O}(d^{1/2})$. \triangleleft

4.1.1. *Verifying A1 to A4.* First of all, the following two conditions imply asymptotically independent structure for the coordinates of the target.

$$\sup_{(i,j):j \notin \mathcal{L}_i} \sup_{x^d \in F_d^+} \frac{\partial^2 \log \pi^d(x^d)}{\partial x_i \partial x_j} = o(1), \quad \sup_{(i,j):j \notin \mathcal{L}_i} \sup_{x^d \in F_d^*} \frac{\partial^3 \log \pi^d(x^d)}{\partial x_i^2 \partial x_j} = o(1). \quad (36)$$

Therefore, each coordinate should asymptotically directly dependent with $\mathcal{O}(l_d)$ other coordinates. For graphical models, these two conditions hold trivially.

For **A2**, since the target distributions arising from realistic MCMC models usually have “flat tails”, **A2** usually holds. In particular, for graphical models, **A2** can easily be verified. In Example 4.1, the parameter ν is conditional independent with all θ_{ij} and the corresponding conditional posterior distributions all have Gaussian tails, which implies **A2** holds for any pair of coordinates (ν, θ_{ij}) . Similarly, one can easily verify the assumption holds for other pairs of parameters.

The following conditions allow π^d as well as the second and third derivatives of $\log \pi^d$ to increase to infinity at certain rates of d in F_d^+ or F_d^* .

$$\sup_{(i,j):j \in \mathcal{L}_i} \sup_{x^d \in F_d^*} \frac{\partial^3 \log \pi^d(x^d)}{\partial x_i^2 \partial x_j} = o(d/l_d), \quad \sup_{x^d \in F_d^*} \sum_{i \neq j \neq k} \left| \frac{\partial^3 \log \pi^d(x^d)}{\partial x_i \partial x_j \partial x_k} \right| = o(d^{3/2}), \quad (37)$$

$$\sup_{(i,j):j \in \mathcal{L}_i} \sup_{x^d \in F_d^+} \frac{\partial^2 \log \pi^d(x^d)}{\partial x_i \partial x_j} = o(\sqrt{d/l_d}), \quad \sup_{x^d \in F_d^+} \pi^d(x^d) = o(d^{1/2-\alpha}). \quad (38)$$

These conditions are much weaker than bounded density or bounded derivatives of $\log \pi^d$, and can hold easily by choosing the sequence of typical sets $\{F_d\}$. In Example 4.1, we have $l_d = \mathcal{O}_{\mathbb{P}}(d^{1/2})$. There is no 3-cliques, the second partial derivative is $\mathcal{O}(1)$, and the density π^d is bounded, so all the above conditions hold for Example 4.1 even without the need of choosing $\{F_d\}$.

Finally, the last two conditions are almost immediately true once [A5](#) has been verified.

$$\sup_{i \in \{1, \dots, d\}} \sup_{x^d \in F_d^+} \frac{\partial \log \pi^d(x^d)}{\partial x_i} = \mathcal{O}(d^\alpha), \quad \sup_{x^d \in F_d^+} 1/I(x^d) = \mathcal{O}(d^{\alpha/2}). \quad (39)$$

To see this, under [A5](#), we have $\frac{1}{d} \sum_{i=1}^d \left(\frac{\partial}{\partial x_i} \log \pi^d(x^d) \right)^2 \rightarrow \bar{I}_d$. If $\bar{I}_d \rightarrow \bar{I}$ and $\bar{I} > 0$, then we can select constant $K_2 > 0$ small enough such that $\bar{I} > K_2 d^{-\alpha/2} > 0$ then $\bar{I}_d > K_2 d^{-\alpha/2}$ for all large enough d . Next, by choosing the typical set F_d such that for any $x^d \in F_d^+$, we have

$$\frac{\partial \log \pi^d(x^d)}{\partial x_i} \leq K_1 d^\alpha, \quad I(x^d) \geq K_2 d^{-\alpha/2}, \quad (40)$$

where K_1 is a large enough constant. Then it suffices to check if $\{F_d\}$ is a valid sequence of typical sets such that $\mathbb{P}_{X^d \sim \pi^d}(X^d \in F_d) \rightarrow 1$. We expect this is usually true for realistic MCMC models. For [Example 4.1](#), we have $X^d = (\nu, \{\nu_j\}_{j=1}^n, \{\theta_{ij}\}_{i,j=1}^n)$. We will show later that [A5](#) holds such that under $X^d \sim \pi^d$ we have

$$\frac{1}{d} \sum_{i=1}^d \left(\frac{\partial}{\partial x_i} \log \pi^d(X^d) \right)^2 \rightarrow 3. \quad (41)$$

Therefore, we can, for example, choose $K_2 = 0.01$, $K_1 = 100$, and the typical set F_d such that for any $X^d = x^d \in F_d^+$ we have

$$I(x^d) > 0.01 n^{-\alpha}, \quad \frac{\partial \log \pi^d}{\partial \nu} = n(\bar{\mu} - \nu) \leq 100 n^{2\alpha}, \quad (42)$$

$$\frac{\partial \log \pi^d}{\partial \mu_j} = (n+1) \left(\frac{\sum_i \theta_{ij} + \nu}{n+1} - \mu_j \right) \leq 100 n^{2\alpha}, \quad (43)$$

$$\frac{\partial \log \pi^d}{\partial \theta_{ij}} = 2 \left(\frac{Y_{ij} + \mu_j}{2} - \theta_{ij} \right) \leq 100 n^{2\alpha} \quad (44)$$

where $\alpha < 1/2$ can be arbitrarily close to $1/2$. Observing that, under $X^d \sim \pi^d$, we have the following conditional distributions.

$$\begin{aligned} \theta_{ij} \mid Y_{ij}, \mu_j &\sim^{\text{indep.}} \mathcal{N} \left(\frac{\mu_j + Y_{ij}}{2}, \frac{1}{2} \right), \quad i, j \in \{1, \dots, n\}, \\ \mu_j \mid \sum_i \theta_{ij}, \nu &\sim^{\text{indep.}} \mathcal{N} \left(\frac{\sum_i \theta_{ij} + \nu}{n+1}, \frac{1}{n+1} \right), \quad i \in \{1, \dots, n\}, \\ \nu \mid \bar{\mu} &\sim \mathcal{N} \left(\bar{\mu}, \frac{1}{n} \right). \end{aligned} \quad (45)$$

Then it can be easily verified that $\mathbb{P}_{X^d \sim \pi^d}(X^d \in F_d) \rightarrow 1$.

4.1.2. *Verifying A5.* One assumption of Theorem 3.13 that could be difficult to verify in practice is A5. It requires the sequence of random variables $\{I(X^d)\}$ converge to a sequence of constants in probability. We feel this assumption has to be checked case by case and it is hard to get general sufficient condition for it to hold. For realistic MCMC models, this may require assumptions on the observed data so that the posterior distribution has certain “concentration” properties as $d \rightarrow \infty$.

Fortunately, for Example 4.1, we can verify that A5 holds without any further assumption on the observed data $\{Y_{ij}\}$. Note that in Example 4.1, we have

$$\left(\frac{\partial \log \pi^d}{\partial \nu}\right)^2 = \left(\sum_j (\mu_j - \nu)\right)^2 = n^2 (\bar{\mu} - \nu)^2, \quad (46)$$

$$\left(\frac{\partial \log \pi^d}{\partial \mu_j}\right)^2 = \left(\sum_i (\theta_{ij} - \mu_j) - (\mu_j - \nu)\right)^2 = (n+1)^2 \left(\frac{\sum_i \theta_{ij} + \nu}{n+1} - \mu_j\right)^2, \quad (47)$$

$$\left(\frac{\partial \log \pi^d}{\partial \theta_{ij}}\right)^2 = ((Y_{ij} - \theta_{ij}) - (\theta_{ij} - \mu_j))^2 = 4 \left(\frac{Y_{ij} + \mu_j}{2} - \theta_{ij}\right)^2. \quad (48)$$

Hence, it suffices to show that, under $X^d = (\nu, \{\mu_j\}_{j=1}^n, \{\theta_{ij}\}_{i,j=1}^n) \sim \pi^d$, the following three terms converges to some constants in probability or in distribution:

$$\frac{1}{d} \left(\frac{\partial \log \pi^d}{\partial \nu}\right)^2 = \frac{n^2}{n^2 + n + 1} (\bar{\mu} - \nu)^2, \quad (49)$$

$$\frac{1}{d} \sum_j \left(\frac{\partial \log \pi^d}{\partial \mu_j}\right)^2 = \frac{(n+1)^2}{n^2 + n + 1} \sum_j \left(\frac{\sum_i \theta_{ij} + \nu}{n+1} - \mu_j\right)^2, \quad (50)$$

$$\frac{1}{d} \sum_{ij} \left(\frac{\partial \log \pi^d}{\partial \theta_{ij}}\right)^2 = \frac{4}{d} \sum_{ij} \left(\frac{Y_{ij} + \mu_j}{2} - \theta_{ij}\right)^2. \quad (51)$$

We have observed that the target distribution π^d has conditional independence structure in Eq. (45), which immediately leads to

$$(\bar{\mu} - \nu)^2 \xrightarrow{\mathbb{P}} 0, \quad (52)$$

$$\sum_j \left(\frac{\sum_i \theta_{ij} + \nu}{n+1} - \mu_j\right)^2 \xrightarrow{\mathbb{P}} 1, \quad (53)$$

$$\frac{1}{d} \sum_{ij} \left(\frac{Y_{ij} + \mu_j}{2} - \theta_{ij}\right)^2 \xrightarrow{\mathbb{P}} \frac{1}{2}. \quad (54)$$

Therefore, A5 is satisfied.

Overall, we have checked all the assumptions of Theorem 3.13 for our simple Gaussian example. Therefore, by Theorem 3.13, we have the following optimal scaling result for Example 4.1.

Proposition 4.2. *The optimal scaling for Example 4.1 by maximizing ESJD is to choose (to two decimal places) $\hat{\ell} \approx \frac{2.38}{\mathbb{E}_{X^d \sim \pi^d}[\sqrt{I(X^d)}]} \rightarrow \frac{2.38}{\sqrt{3}} \approx 1.37$ and the corresponding asymptotic acceptance rate is (to two decimal places) 0.234.*

Finally, we discuss sufficient conditions for two more classes of graphical models. In Proposition 4.3, we give sufficient conditions for the first equation of A1, A2, and the first equation of A3 to hold for one particular class of graphical models. In Proposition 4.4, we give sufficient conditions for A5 to hold for one specific class of graphical models.

First, we consider the class of graphical models represented by the following factor graphs:

$$\pi^d(x^d) \propto \prod_{k=1}^{K_d} \psi_k(\{x_i : i \in C_k\}), \quad (55)$$

where C_k are cliques, ψ_k are potentials, K_d denotes the number of potentials.

Proposition 4.3. *For the class of graphical models represented by Eq. (55). Let m_d denotes the maximum number of cliques a coordinate can belong to. If all the potentials ψ_k have “flat tails” in the sense that for all k we have $\frac{\partial \psi_k}{\partial x_i} \rightarrow 0$ as $|x_i| \rightarrow \infty$ for all $i \in C_k$, and the cardinality of C_k satisfies $\sup_k |C_k| = o(d/m_d)$, then the first equation in A1, A2, and the first equation in A3 hold.*

Next, we consider Bayesian hierarchical modeling where K denotes the number of “layers” or “stages” of the model. We use $\theta^{(k)}, k = 1, \dots, K$ to denote the parameter vector with length n_k for the k -th layer, where $\theta^{(k)} := (\theta_1^{(k)}, \dots, \theta_{n_k}^{(k)})$. We consider the special structure of the graphical model such that $\theta^{(k)}$ is only connected to $\theta^{(k-1)}$ and $\theta^{(k+1)}$. Using factor graphs, let $x^d = (\theta^{(1)}, \dots, \theta^{(K)})$ we can represent the target distribution as

$$\pi^d(x^d) \propto \prod_{k=1}^K \psi_k(\theta^{(k-1)}, \theta^{(k)}), \quad (56)$$

where $d = \sum_{k=1}^K n_k$, $\{\psi_k\}$ are the potentials, and without loss of generality we assumed $\theta^{(0)}$ to be the observed data.

In the following, we show that A5 hold for the class of graphical models represented by Eq. (56) under certain conditions.

Proposition 4.4. *For the class of graphical models represented by Eq. (56), if $\theta^{(k)} = (\theta_1^{(k)}, \theta_2^{(k)}, \dots, \theta_{n_k}^{(k)})$ are independent conditional on $\theta^{(k-1)}$ and $\theta^{(k+1)}$ and this holds for all k . Moreover, if under $X^d = (\theta^{(1)}, \dots, \theta^{(K)}) \sim \pi^d$ all the potentials ψ_k satisfy*

$$\sup_{i \in \{1, \dots, n_k\}} \left| \frac{\partial \log \psi_k}{\partial \theta_i^{(k)}} \right| = \mathcal{O}_{\mathbb{P}} \left(\sqrt{d/n_k} \right), \quad \sup_{j \in \{1, \dots, n_{k-1}\}} \left| \frac{\partial \log \psi_k}{\partial \theta_j^{(k-1)}} \right| = \mathcal{O}_{\mathbb{P}} \left(\sqrt{d/n_{k-1}} \right) \quad (57)$$

then [A5](#) holds.

4.2. Optimal Scaling of a Realistic MCMC Model. In this subsection, we demonstrate a realistic MCMC model which belongs to both classes of graphical models in Eqs. (55) and (56) and show that all the assumptions for the optimal scaling result in [Theorem 3.13](#) hold for this example.

Example 4.5. (A Realistic MCMC Model) Consider a realistic MCMC model

$$\begin{aligned} Y_{ij} \mid \theta_{ij} &\sim \mathcal{N}(\theta_{ij}, W), \quad i, j \in \{1, \dots, n\} \\ \theta_{ij} \mid \mu_j &\sim \mathcal{N}(\mu_j, V), \quad i \in \{1, \dots, n\} \\ \mu_j \mid \nu &\sim \mathcal{N}(\nu, A) \\ \nu &\sim \text{flat prior on } \mathbb{R}, \\ A &\sim \mathbf{IG}(a, b), \end{aligned} \quad (58)$$

where $x^d = (\nu, A, \{\mu_j\}_{j=1}^n, \{\theta_{ij}\}_{i,j=1}^n)$ are parameters, $\{Y_{ij}\}$ are the observed data, and a, b, W, V are known constants. Note that we have the number of parameters $d = n^2 + n + 2$ in this example. The target distribution (i.e. the posterior distribution) satisfies

$$\begin{aligned} \pi^d(x^d) &= \mathbb{P}(x^d \mid \{Y_{ij}\}_{i,j=1}^n) \\ &\propto \frac{b^a}{\Gamma(a)} A^{-a-1} e^{-b/A} \prod_{j=1}^n \frac{1}{\sqrt{2\pi A}} e^{-\frac{(\mu_j - \nu)^2}{2A}} \prod_{i=1}^n \frac{1}{\sqrt{2\pi V}} e^{-\frac{(\theta_{ij} - \mu_j)^2}{2V}} \frac{1}{\sqrt{2\pi W}} e^{-\frac{(Y_{ij} - \theta_{ij})^2}{2W}}. \end{aligned} \quad (59)$$

We further assume that the observed data $\{Y_{ij}\}$ is not abnormal so that the posterior of the hyperparameter A concentrates to some unknown constant.

Assumption. *The posterior of the hyperparameter A in [Example 4.5](#) concentrates to some unknown constant $A_0 > 0$ as $n \rightarrow \infty$.*

Note that this is a very reasonable assumption which implies the MCMC model is not seriously misspecified. We do not discuss sufficient conditions on the observed data $\{Y_{ij}\}_{i,j=1}^n$ for concentration of posterior distribution of A here since it is not the focus of this paper. Next, we show that, under this assumption, the realistic MCMC model satisfies all the conditions required for optimal scaling in [Theorem 3.13](#). Therefore,

the acceptance rate 0.234 is indeed asymptotically optimal for this MCMC model in the sense of maximizing ESJD.

Clearly, this model can be represented by the graphical model in Eq. (55). It can be easily checked that the maximum number cliques any coordinate belongs to is $n + 1$ and the cardinality of cliques is bounded by constant 2, so $\sup_k |C_k| = o(d/m_d) = o(n)$. Furthermore, the target distribution clearly satisfies “flat tail” condition required by Proposition 4.3 since all the conditional distributions are standard distributions. Therefore, the first equation in A1, the first equation in A3, and A2 hold by Proposition 4.3.

Next, we verify A5 using Proposition 4.4. Note that this model can be represented by the graphical model in Eq. (56) using $K = 3$ layers. In order to check the conditions in Proposition 4.4, note that

$$\log \pi^d \propto \left(-a - 1 - \frac{n}{2}\right) \log A - \frac{b}{A} - \frac{\sum_j (\mu_j - \nu)^2}{2A} - \frac{\sum_{i,j} (\theta_{ij} - \mu_j)^2}{2V} - \frac{\sum_{i,j} (Y_{ij} - \theta_{ij})^2}{2W}. \quad (60)$$

Observing that, under $X^d = (\nu, A, \{\mu_j\}_{j=1}^n, \{\theta_{ij}\}_{i,j=1}^n) \sim \pi^d$, we have

$$\theta_{ij} \mid Y_{ij}, \mu_j \sim^{\text{indep.}} \mathcal{N} \left(\frac{W\mu_j + VY_{ij}}{W + V}, \frac{VW}{W + V} \right), \quad i, j \in \{1, \dots, n\}, \quad (61)$$

$$\mu_j \mid \sum_i \theta_{ij}, \nu, A \sim^{\text{indep.}} \mathcal{N} \left(\frac{\sum_i A\theta_{ij} + V\nu}{nA + V}, \frac{AV}{nA + V} \right), \quad i \in \{1, \dots, n\}, \quad (62)$$

$$\nu \mid \bar{\mu}, A \sim \mathcal{N} \left(\bar{\mu}, \frac{A}{n} \right), \quad (63)$$

$$A \mid \{\mu_j\}, \nu \sim \mathbf{IG} \left(a + \frac{n}{2}, b + \frac{1}{2} \sum_j (\mu_j - \nu)^2 \right). \quad (64)$$

Therefore, we have

$$\left| \frac{\partial \log \pi^d}{\partial A} \right| = \left| \frac{b + \frac{1}{2} \sum_j (\mu_j - \nu)^2}{A^2} - \frac{a + 1 + \frac{n}{2}}{A} \right| = \mathcal{O}_{\mathbb{P}}(d^{1/2}). \quad (65)$$

since $\frac{a+1+n/2}{A} \rightarrow_{\mathbb{P}} \frac{a+1+n/2}{A_0} = \mathcal{O}(d^{1/2})$ and $\sum_j (\mu_j - \nu)^2 \rightarrow_{\mathbb{P}} \sum_j (\mu_j - \bar{\mu})^2 + \frac{A_0}{n} = \mathcal{O}_{\mathbb{P}}(d^{1/2})$. Other coordinates can also be verified, which are shown as follows.

$$\left(\frac{\partial \log \pi^d}{\partial \nu}\right)^2 = \left(\frac{n(\bar{\mu} - \nu)}{A}\right)^2 = \mathcal{O}_{\mathbb{P}}\left(\frac{n}{A}\right) = \mathcal{O}_{\mathbb{P}}(d/n), \quad (66)$$

$$\left(\frac{\partial \log \pi^d}{\partial \mu_j}\right)^2 = \left(\frac{\sum_i (\theta_{ij} - \mu_j)}{V} - \frac{\mu_j - \nu}{A}\right)^2 = (nA + V)^2 \left(\frac{A \sum_i \theta_{ij} + V\nu}{nA + V} - \mu_j\right)^2 \quad (67)$$

$$= \mathcal{O}_{\mathbb{P}}\left[(nA + V)^2 \frac{AV}{nA + V}\right] = \mathcal{O}_{\mathbb{P}}(d/n), \quad (68)$$

$$\left(\frac{\partial \log \pi^d}{\partial \theta_{ij}}\right)^2 = \left(\frac{Y_{ij} - \theta_{ij}}{V} - \frac{\theta_{ij} - \mu_j}{W}\right)^2 = (W + V)^2 \left(\frac{VY_{ij} + W\mu_j}{W + V} - \theta_{ij}\right)^2 = \mathcal{O}_{\mathbb{P}}(d/n^2). \quad (69)$$

$$(70)$$

Therefore, [A5](#) holds by [Proposition 4.4](#). Finally, all the other conditions in [A1](#), [A3](#), and [A4](#) can be verified in a similar way as in [Section 4.1](#) for [Example 4.1](#). \triangleleft

Overall, since we have verified all assumptions needed for [Theorem 3.13](#), we can conclude the asymptotic optimal acceptance rate for [Example 4.5](#).

Proposition 4.6. *The optimal asymptotic acceptance rate for the realistic MCMC model in [Example 4.5](#) is (to two decimal places) 0.234.*

5. PROOF OF [THEOREM 3.9](#)

Throughout the proof, for simplicity and without loss of generality, we assume the coordinates are linear ordered. That is, we consider the “neighborhoods” of a coordinate is defined by $\mathcal{L}_i := \{j : 0 < |i - j| < l_d\}$. Therefore $\sup_{(i,j):j \in \mathcal{L}_i}$ can be simplified to $\sup_{|i-j| < l_d}$ and $\sup_{(i,j):j \notin \mathcal{L}_i}$ can be simplified to $\sup_{|i-j| \geq l_d}$. The proof for general ordering is essentially the same as the proof for linear ordering.

For [Theorem 3.9](#), we only prove

$$\left| \text{ESJD}(d) - 2 \frac{d\ell^2}{d-1} \mathbb{E}_{X^d \sim \pi^d} \left[\Phi \left(-\frac{\ell \sqrt{I(X^d)}}{2} \right) \right] \right| \rightarrow 0, \quad (71)$$

since the proof of

$$\left| \mathbb{E}_{X^d \sim \pi^d} \mathbb{E}_{Y^d} \left(1 \wedge \frac{\pi^d(Y^d)}{\pi^d(X^d)} \right) - 2 \mathbb{E}_{X^d \sim \pi^d} \left[\Phi \left(-\frac{\ell \sqrt{I(X^d)}}{2} \right) \right] \right| \rightarrow 0 \quad (72)$$

follows similarly.

First, we write ESJD as $\text{ESJD}(d) =: \sum_{i=1}^d \text{ESJD}_i(d)$, where

$$\text{ESJD}_i(d) := \mathbb{E}_{X^d \sim \pi^d} \mathbb{E}_{Y^d} \left[(Y_i - X_i)^2 \left(1 \wedge \frac{\pi^d(Y^d)}{\pi^d(X^d)} \right) \right]. \quad (73)$$

Then it suffices to show that

$$\sup_{i \in \{1, \dots, d\}} \left| \text{ESJD}_i(d) - \frac{2\ell^2}{d-1} \mathbb{E}_{X^d \sim \pi^d} \left[\Phi \left(-\frac{\ell \sqrt{I(X^d)}}{2} \right) \right] \right| = o(d^{-1}). \quad (74)$$

Writing $\text{ESJD}_i(d) = \mathbb{E}_{X^d \sim \pi^d} \mathbb{E}_{Y_i} \left[(Y_i - X_i)^2 \mathbb{E}_{Y_{-i}} \left(1 \wedge \frac{\pi^d(Y^d)}{\pi^d(X^d)} \right) \right]$, it suffices to show that uniformly over $i \in \{1, \dots, d\}$

$$\mathbb{E}_{X^d \sim \pi^d} \left| \mathbb{E}_{Y_i} \left[(Y_i - X_i)^2 \mathbb{E}_{Y_{-i}} \left(1 \wedge \frac{\pi^d(Y^d)}{\pi^d(X^d)} \right) \right] - \frac{2\ell^2}{d-1} \Phi \left(-\frac{\ell \sqrt{I(X^d)}}{2} \right) \right| \quad (75)$$

$$= \mathbb{E}_{X^d \sim \pi^d} \left| \mathbb{E}_{Y_i} \left\{ (Y_i - X_i)^2 \left[\mathbb{E}_{Y_{-i}} \left(1 \wedge \frac{\pi^d(Y^d)}{\pi^d(X^d)} \right) - 2\Phi \left(-\frac{\ell \sqrt{I(X^d)}}{2} \right) \right] \right\} \right| \quad (76)$$

$$= o(d^{-1}). \quad (77)$$

It then suffices to show

$$\sup_{x^d \in F_d} \left| \mathbb{E}_{Y_i} \left\{ (Y_i - x_i)^2 \mathbb{1}_{y^d(i) \in F_d^{(i)}} \left[\mathbb{E}_{Y_{-i}} \left(1 \wedge \frac{\pi^d(Y^d)}{\pi^d(x^d)} \right) - 2\Phi \left(-\frac{\ell \sqrt{I(x^d)}}{2} \right) \right] \right\} \right| \quad (78)$$

$$\leq \mathbb{E}_{Y_i} \left\{ (Y_i - x_i)^2 \sup_{y^d(i) \in F_d^{(i)}, x^d \in F_d} \left| \mathbb{E}_{Y_{-i}} \left(1 \wedge \frac{\pi^d(Y^d)}{\pi^d(x^d)} \right) - 2\Phi \left(-\frac{\ell \sqrt{I(x^d)}}{2} \right) \right| \right\} = o(d^{-1}), \quad (79)$$

where $y^d(i) := (x_1, \dots, x_{i-1}, Y_i, x_{i+1}, \dots, x_d)$. Defining $M_{x^d}^{(i)}(Y_i) := \mathbb{E}_{Y_{-i}} \left(1 \wedge \frac{\pi^d(Y^d)}{\pi^d(x^d)} \right)$, since

$$\log \frac{\pi^d(Y^d)}{\pi^d(x^d)} = \log \frac{\pi_i(Y_i)}{\pi_i(x_i)} + \log \frac{\pi_{-i}(Y_{-i} | Y_i)}{\pi_{-i}(x_{-i} | x_i)} \quad (80)$$

$$= \left(\log \frac{\pi_i(Y_i)}{\pi_i(x_i)} + \log \frac{\pi_{-i}(x_{-i} | Y_i)}{\pi_{-i}(x_{-i} | x_i)} \right) + \log \frac{\pi_{-i}(Y_{-i} | Y_i)}{\pi_{-i}(x_{-i} | Y_i)}, \quad (81)$$

we can write

$$M_{x^d}^{(i)}(Y_i) = \mathbb{E}_{Y_{-i}} \left[1 \wedge \frac{\pi^d(Y^d)}{\pi^d(x^d)} \right] = \mathbb{E}_{Y_{-i}} \left[1 \wedge \exp \left(\log \frac{\pi^d(Y^d)}{\pi^d(x^d)} \right) \right] \quad (82)$$

$$= \mathbb{E}_{Y_{-i}} \left[1 \wedge \exp \left(\log \frac{\pi_i(Y_i)}{\pi_i(x_i)} + \log \frac{\pi_{-i}(x_{-i} | Y_i)}{\pi_{-i}(x_{-i} | x_i)} + \log \frac{\pi_{-i}(Y_{-i} | Y_i)}{\pi_{-i}(x_{-i} | Y_i)} \right) \right]. \quad (83)$$

Note that the expectation is taken over Y_{-i} and only the last term, $\log \frac{\pi_{-i}(Y_{-i} | Y_i)}{\pi_{-i}(x_{-i} | Y_i)}$, involves Y_{-i} .

In the following, we then first focus on approximating $\log \frac{\pi_{-i}(Y_{-i} | x_i)}{\pi_{-i}(x_{-i} | x_i)}$ for given $x^d \in F_d^+$. Since $Y^d \sim \mathcal{N}(x^d, \frac{\ell^2}{d-1} I)$, we first approximate $\log \frac{\pi_{-i}(Y_{-i} | x_i)}{\pi_{-i}(x_{-i} | x_i)}$ by the first two terms of its Taylor expansion.

Define

$$m_1^{(i)}(Y_{-i}, x^d) := (\nabla \log \pi_{-i})^T (Y_{-i} - x_{-i}) + \frac{1}{2} (Y_{-i} - x_{-i})^T [\nabla^2 \log \pi_{-i}] (Y_{-i} - x_{-i}), \quad (84)$$

where

$$(\nabla \log \pi_{-i})^T (Y_{-i} - x_{-i}) := \sum_{j \in \{1, \dots, d\}, j \neq i} \frac{\partial \log \pi_{-i}(x_{-i} | x_i)}{\partial x_j} (Y_j - x_j) \quad (85)$$

and $[\nabla^2 \log \pi_{-i}]$ denotes the $(d-1) \times (d-1)$ matrix with elements

$$\left\{ \frac{\partial^2 \log \pi_{-i}(x_{-i} | x_i)}{\partial x_j \partial x_k} \right\}_{j, k \in \{1, \dots, d\}, j \neq i, k \neq i}.$$

Then, we have the following result.

Lemma 5.1. *Uniformly over $i \in \{1, \dots, d\}$, we have*

$$\sup_{x^d \in F_d^+} \mathbb{E}_{Y_{-i}} \left[\left| m_1^{(i)}(Y_{-i}, x^d) - \log \frac{\pi_{-i}(Y_{-i} | x_i)}{\pi_{-i}(x_{-i} | x_i)} \right| \right] \rightarrow 0. \quad (86)$$

Proof. See Appendix A.1. □

Next, we approximate the second order term of the Taylor approximation $\frac{1}{2} (Y_{-i} - x_{-i})^T [\nabla^2 \log \pi_{-i}] (Y_{-i} - x_{-i})$ by a non-random term $\frac{1}{2} \frac{\ell^2}{d-1} \sum_{j \neq i} \frac{\partial^2 \log \pi_{-i}}{\partial x_j^2}$.

Lemma 5.2. *Uniformly over $i \in \{1, \dots, d\}$, we have*

$$\sup_{x^d \in F_d^+} \mathbb{E}_{Y_{-i}} \left[\left| (Y_{-i} - x_{-i})^T [\nabla^2 \log \pi_{-i}] (Y_{-i} - x_{-i}) - \frac{\ell^2}{d-1} \sum_{j \neq i} \frac{\partial^2 \log \pi_{-i}}{\partial x_j^2} \right| \right] \rightarrow 0. \quad (87)$$

Proof. See Appendix A.2. □

Defining

$$m_2^{(i)}(Y_{-i}, x^d) := (\nabla \log \pi_{-i})^T (Y_{-i} - x_{-i}) + \frac{1}{2} \frac{\ell^2}{d-1} \sum_{j \neq i} \frac{\partial^2 \log \pi_{-i}}{\partial x_j^2}, \quad (88)$$

we have

$$m_2^{(i)}(Y_{-i}, x^d) \sim \mathcal{N}\left(\ell^2 S_d^{(i)}/2, \ell^2 R_d^{(i)}\right), \quad (89)$$

where

$$R_d^{(i)} := \frac{1}{d-1} \sum_{j \neq i} \left(\frac{\partial \log \pi_{-i}(x_{-i} | x_i)}{\partial x_j} \right)^2, \quad S_d^{(i)} := \frac{1}{d-1} \sum_{j \neq i} \frac{\partial^2 \log \pi_{-i}(x_{-i} | x_i)}{\partial x_j^2}. \quad (90)$$

Next, we show we can approximate $S_d^{(i)}$ by $-R_d^{(i)}$.

Lemma 5.3. *There exists a sequence of subsets of states $\{F'_d\}$, such that $\mathbb{P}_{X^d \sim \pi^d}(X^d \in F'_d) \rightarrow 1$ and*

$$\sup_{i \in \{1, \dots, d\}} \sup_{x^d \in F'_d} \left| R_d^{(i)} + S_d^{(i)} \right| \rightarrow 0. \quad (91)$$

Proof. See Appendix A.3. □

Now defining

$$m_3^{(i)}(Y_{-i}, x^d) := (\nabla \log \pi_{-i})^T(Y_{-i} - x_{-i}) + \frac{1}{2} \frac{\ell^2}{d-1} \sum_{j \neq i} \left(\frac{\partial \log \pi_{-i}(x_{-i} | x_i)}{\partial x_j} \right)^2, \quad (92)$$

we have

$$m_3^{(i)}(Y_{-i}, x^d) \sim \mathcal{N}\left(-\ell^2 R_d^{(i)}/2, \ell^2 R_d^{(i)}\right). \quad (93)$$

By triangle inequality, we can write

$$\left| m_3^{(i)}(Y_{-i}, x^d) - \log \frac{\pi_{-i}(Y_{-i} | x_i)}{\pi_{-i}(x_{-i} | x_i)} \right| \leq \left| m_1^{(i)}(Y_{-i}, x^d) - \log \frac{\pi_{-i}(Y_{-i} | x_i)}{\pi_{-i}(x_{-i} | x_i)} \right| \quad (94)$$

$$+ \left| m_2^{(i)}(Y_{-i}, x^d) - m_1^{(i)}(Y_{-i}, x^d) \right| \quad (95)$$

$$+ \left| m_3^{(i)}(Y_{-i}, x^d) - m_2^{(i)}(Y_{-i}, x^d) \right|. \quad (96)$$

Therefore, using Lemmas 5.1 to 5.3, we get

$$\sup_{i \in \{1, \dots, d\}} \sup_{x^d \in F_d^+ \cap F'_d} \mathbb{E}_{Y_{-i}} \left[\left| m_3^{(i)}(Y_{-i}, x^d) - \log \frac{\pi_{-i}(Y_{-i} | x_i)}{\pi_{-i}(x_{-i} | x_i)} \right| \right] \rightarrow 0. \quad (97)$$

Next, we abuse the notation a little bit by defining

$$R_d^{(i)}(y) := \frac{1}{d-1} \sum_{j \neq i} \left(\frac{\partial \log \pi_{-i}(x_{-i} | x_i = y)}{\partial x_j} \right)^2. \quad (98)$$

Then by the definition of $m_3^{(i)}$, we replace x^d by $y^d(i) = (x_1, \dots, x_{i-1}, Y_i, x_{i+1}, \dots, x_d)$, which yields

$$m_3^{(i)}(Y_{-i}, y^d(i)) = (\nabla \log \pi_{-i}(x_{-i} | Y_i))^T (Y_{-i} - x_{-i}) \quad (99)$$

$$+ \frac{1}{2} \frac{\ell^2}{d-1} \sum_{j \neq i} \left(\frac{\partial \log \pi_{-i}(x_{-i} | Y_i)}{\partial x_j} \right)^2. \quad (100)$$

Then, we have

$$m_3^{(i)}(Y_{-i}, y^d(i)) \sim \mathcal{N} \left(-\ell^2 R_d^{(i)}(Y_i)/2, \ell^2 R_d^{(i)}(Y_i) \right). \quad (101)$$

Recall that $M_{x^d}^{(i)}(Y_i) = \mathbb{E}_{Y_{-i}} \left[1 \wedge \exp \left(\log \frac{\pi_i(Y_i)}{\pi_i(x_i)} + \log \frac{\pi_{-i}(x_{-i} | Y_i)}{\pi_{-i}(x_{-i} | x_i)} + \log \frac{\pi_{-i}(Y_{-i} | Y_i)}{\pi_{-i}(Y_{-i} | x_i)} \right) \right]$, defining

$$\hat{M}_{x^d}^{(i)}(Y_i) = \mathbb{E}_{Y_{-i}} \left[1 \wedge \exp \left(\log \frac{\pi_i(Y_i)}{\pi_i(x_i)} + \log \frac{\pi_{-i}(x_{-i} | Y_i)}{\pi_{-i}(x_{-i} | x_i)} + m_3^{(i)}(Y_{-i}, y^d(i)) \right) \right], \quad (102)$$

we next apply the following two lemmas from [RGG97].

Lemma 5.4. ([RGG97, Proposition 2.2]) *The function $g(x) = 1 \wedge e^x$ is Lipschitz such that*

$$|g(x) - g(y)| \leq |x - y|, \quad \forall x, y. \quad (103)$$

Lemma 5.5. ([RGG97, Proposition 2.4]) *If $z \sim \mathcal{N}(\mu, \sigma^2)$ then*

$$\mathbb{E}(1 \wedge e^z) = \Phi(\mu/\sigma) + \exp(\mu + \sigma^2/2) \Phi(-\sigma - \mu/\sigma). \quad (104)$$

By Lemma 5.4 and Eq. (97), we have that uniformly over $i \in \{1, \dots, d\}$

$$\sup_{y^d(i) \in F_d^+ \cap F_d'} \left| M_{x^d}^{(i)}(Y_i) - \hat{M}_{x^d}^{(i)}(Y_i) \right| \rightarrow 0. \quad (105)$$

Applying Lemma 5.5 to $\hat{M}_{x^d}^{(i)}(Y_i)$ yields

$$\hat{M}_{x^d}^{(i)}(Y_i) = \Phi \left(R_d^{(i)}(Y_i)^{-1/2} \left(\ell^{-1} \log \frac{\pi^d(y^d(i))}{\pi^d(x^d)} - \ell R_d^{(i)}(Y_i)/2 \right) \right) \quad (106)$$

$$+ \exp \left(\log \frac{\pi^d(y^d(i))}{\pi^d(x^d)} \right) \Phi \left(-\ell R_d^{(i)}(Y_i)^{1/2}/2 - \log \frac{\pi^d(y^d(i))}{\pi^d(x^d)} R_d^{(i)}(Y_i)^{-1/2} \ell^{-1} \right). \quad (107)$$

Note that it is easy to check that $\hat{M}_{x^d}^{(i)}(x_i) = 2\Phi \left(-\frac{\ell \sqrt{R_d^{(i)}}}{2} \right)$. We then show $\hat{M}_{x^d}^{(i)}(x_i)$ converges to $2\Phi \left(-\frac{\ell \sqrt{I(x^d)}}{2} \right)$.

Lemma 5.6.

$$\sup_{i \in \{1, \dots, d\}} \sup_{x^d \in F_d^+} \left| 2\Phi \left(-\frac{\ell \sqrt{R_d^{(i)}}}{2} \right) - 2\Phi \left(-\frac{\ell \sqrt{I(x^d)}}{2} \right) \right| \rightarrow 0. \quad (108)$$

Proof. See Appendix A.4. \square

Finally, using Taylor expansion together with $\mathbb{E}_{Y_i}(Y_i - x_i)^2 = \ell^2/(d-1)$ and $\mathbb{E}_{Y_i}|Y_i - x_i|^3 = \mathcal{O}(d^{-3/2})$, we have

$$\mathbb{E}_{Y_i} \left\{ (Y_i - x_i)^2 \sup_{y^{d(i)} \in F_d^+} \left| \hat{M}_{x^d}^{(i)}(Y_i) - 2\Phi \left(-\frac{\ell \sqrt{I(x^d)}}{2} \right) \right| \right\} \quad (109)$$

$$\leq \frac{\ell^2}{d-1} \sup_{x^d \in F_d^+} \left| 2\Phi \left(-\frac{\ell \sqrt{R_d^{(i)}}}{2} \right) - 2\Phi \left(-\frac{\ell \sqrt{I(x^d)}}{2} \right) \right| \quad (110)$$

$$+ \mathcal{O}(d^{-3/2}) \sup_{y^{d(i)} \in F_d^+} \left| \frac{d\hat{M}_{x^d}^{(i)}(y_i)}{dy_i}(Y_i) \right|. \quad (111)$$

For the last term, we have the following lemma.

Lemma 5.7.

$$\sup_{i \in \{1, \dots, d\}} \sup_{y^{d(i)} \in F_d^+} \left| \frac{d\hat{M}_{x^d}^{(i)}(y_i)}{dy_i}(Y_i) \right| = o(d^{1/2}). \quad (112)$$

Proof. See Appendix A.5. \square

The proof of Theorem 3.9 is completed by applying Lemma 5.6 and Lemma 5.7.

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A. PROOF OF LEMMAS IN SECTION 5

A.1. Proof of Lemma 5.1. For $x^d \in F_d^+$, we only need to consider $Y^d \in F_d^*$. By Taylor expansion and mean value theorem, we have

$$|\log \pi_{-i}(Y_{-i} | x_i) - \log \pi_{-i}(x_{-i} | x_i) - m_1(Y_{-i}, x^d)| \quad (113)$$

$$\leq \sup_{\tilde{x}^d \in F_d^*} \left| \frac{1}{6} \sum_{j,k,l \neq i} \frac{\partial^3 \log \pi^d(\tilde{x}^d)}{\partial x_j \partial x_k \partial x_l} (Y_j - x_j)(Y_k - x_k)(Y_l - x_l) \right|. \quad (114)$$

In the above summation, the summation over the cases of $j = k = l$ equals to

$$\mathcal{O}(d\mathbb{E}|Y_j - x_j|^3) = \mathcal{O}\left(d(\sqrt{\ell^2/(d-1)})^3\right) = \mathcal{O}(d^{-1/2}) = o(1). \quad (115)$$

For the cases of $j = k \neq l$, we have

$$\sum_{j=k \neq l} \frac{\partial^3 \log \pi_{-1}(\tilde{x}^d)}{\partial x_j^2 \partial x_l} (Y_j - x_j)^2 (Y_l - x_l) = \sum_j (Y_j - x_j)^2 \sum_{l \neq k} \frac{\partial^3 \log \pi_{-1}(\tilde{x}^d)}{\partial x_j^2 \partial x_l} (Y_l - x_l). \quad (116)$$

By Assumption A3, we have $\mathbb{E} \left| \sum_{j \neq l} \frac{\partial^3 \log \pi_{-1}(\tilde{x}^d)}{\partial x_j^2 \partial x_l} (Y_l - x_l) \right| = \mathcal{O}(l_d/d) o(d/l_d) = o(1)$ since $\frac{\partial^3 \log \pi^d(\tilde{x}^d)}{\partial x_j^2 \partial x_l}$ goes to zero when $|k - i| > l_d$. Then, by $\mathbb{E}|Y_j - x_j|^2 = \mathcal{O}(1/d)$, the summation over all cases of $j = k \neq l$ equals to $d\mathcal{O}_{\mathbb{P}}(1/d) o_{\mathbb{P}}(1) = o_{\mathbb{P}}(1)$.

Finally, for $j \neq k \neq l$, it suffices to show

$$\sup_{\tilde{x}^d \in F_d^*} \left| \sum_{j \neq k \neq l \neq i} \frac{\partial^3 \log \pi_{-1}(\tilde{x}^d)}{\partial x_j \partial x_k \partial x_l} (Y_j - x_j)(Y_k - x_k)(Y_l - x_l) \right| \quad (117)$$

$$\leq \sup_{\tilde{x}^d \in F_d^*} \sum_{i \neq j \neq k \neq l} \left| \frac{\partial^3 \log \pi_{-1}(\tilde{x}^d)}{\partial x_j \partial x_k \partial x_l} \right| |(Y_j - x_j)(Y_k - x_k)(Y_l - x_l)| = o_{\mathbb{P}}(1). \quad (118)$$

Note that $|(Y_j - x_j)(Y_k - x_k)(Y_l - x_l)|$ is a random variable which doesn't depend on the values of x_j, x_k, x_l , and

$$|(Y_j - x_j)(Y_k - x_k)(Y_l - x_l)| = \mathcal{O}_{\mathbb{P}}\left(\left(\sqrt{\ell^2/(d-1)}\right)^3\right) = \mathcal{O}_{\mathbb{P}}(d^{-3/2}), \quad (119)$$

which implies the summation for cases $j \neq k \neq l$ is $o_{\mathbb{P}}(1)$ under Assumption A3. Therefore, we have proved the result for fixed i . Finally, it is easy to check the proof holds uniformly over $i \in \{1, \dots, d\}$.

A.2. Proof of Lemma 5.2.

Lemma A.1. (*Quadratic Form of Gaussian Random Vector*) If $z^d \sim \mathcal{N}_d(\mu, \Sigma)$, then

$$\mathbb{E}(z^T A z) = \text{tr}(A\Sigma) + \mu^T A \mu, \quad \text{var}(z^T A z) = 2 \text{tr}(A\Sigma A\Sigma) + 4\mu^T A \Sigma A \mu. \quad (120)$$

Note that $Y_{-i} \sim \mathcal{N}_{d-1}(x_{-i}, \frac{\ell^2}{d-1}I)$ and $(Y_{-i} - x_{-i})^T [\nabla^2 \log \pi_{-i}] (Y_{-i} - x_{-i})$ is a quadratic form of Gaussian random vector. By Lemma A.1,

$$\mathbb{E} [(Y_{-i} - x_{-i})^T [\nabla^2 \log \pi_{-i}] (Y_{-i} - x_{-i})] = \frac{\ell^2}{d-1} \sum_{j \neq i} \frac{\partial^2 \log \pi_{-i}}{\partial x_j^2}. \quad (121)$$

Therefore, it suffices to show the variance of the quadratic form goes to zero. Using the assumptions, the variance satisfies

$$\frac{2\ell^4}{(d-1)^2} \text{tr} ([\nabla^2 \log \pi_{-i}] [\nabla^2 \log \pi_{-i}]) \quad (122)$$

$$= \frac{2\ell^4}{(d-1)^2} \sum_{j \neq i} \sum_{k \neq i} \left(\frac{\partial^2 \log \pi_{-i}}{\partial x_j \partial x_k} \right)^2 \quad (123)$$

$$\leq \frac{2\ell^4}{(d-1)^2} \sum_{l=0}^{d-1} \sum_{\{j,k:|j-k|=l\}} \left(\frac{\partial^2 \log \pi^d}{\partial x_j \partial x_k} \right)^2 \quad (124)$$

$$= \frac{2\ell^4}{(d-1)^2} \sum_{l \leq l_d} \sum_{\{j,k:|j-k|=l\}} \left(\frac{\partial^2 \log \pi^d}{\partial x_i \partial x_j} \right)^2 \quad (125)$$

$$+ \frac{2\ell^4}{(d-1)^2} \sum_{l > l_d} \sum_{\{j,k:|j-k|=l\}} \left(\frac{\partial^2 \log \pi^d}{\partial x_j \partial x_k} \right)^2 \quad (126)$$

$$\leq \frac{2\ell^4}{(d-1)^2} (d-1) l_d \sup_{|j-k| \leq l_d} \sup_{x^d \in F_d^+} \left(\frac{\partial^2 \log \pi^d}{\partial x_j \partial x_k} \right)^2 \quad (127)$$

$$+ \frac{2\ell^4}{(d-1)^2} (d-1)^2 \sup_{|j-k| > l_d} \sup_{x^d \in F_d^+} \left(\frac{\partial^2 \log \pi^d}{\partial x_j \partial x_k} \right)^2 \quad (128)$$

$$= \mathcal{O}(l_d/d) o(d/l_d) + o(1) = o(1), \quad (129)$$

where we have used $\sup_{x^d \in F_d^+} \sup_{|j-k| \leq l_d} \frac{\partial^2 \log \pi^d}{\partial x_j \partial x_k} = o(\sqrt{d/l_d})$ from Assumption A1.

A.3. **Proof of Lemma 5.3.** Note that

$$R_d^{(i)} + S_d^{(i)} = \frac{1}{d-1} \sum_{j \neq i} \left(\frac{\partial \log \pi_{-i}}{\partial x_j} \right)^2 + \frac{1}{d-1} \sum_{j \neq i} \frac{\partial^2 \log \pi_{-i}}{\partial x_j^2} \quad (130)$$

$$= \frac{1}{d-1} \sum_{j \neq i} \left\{ \left(\frac{\partial \log \pi^d}{\partial x_j} \right)^2 + \frac{\partial^2 \log \pi^d}{\partial x_j^2} \right\} \quad (131)$$

$$= \frac{1}{d-1} \sum_{j \neq i} \left\{ \frac{1}{(\pi^d)^2} \left(\frac{\partial \pi^d}{\partial x_j} \right)^2 + \frac{\partial}{\partial x_j} \left(\frac{\partial \log \pi^d}{\partial x_j} \right) \right\} \quad (132)$$

$$= \frac{1}{d-1} \sum_{j \neq i} \left\{ \frac{1}{(\pi^d)^2} \left(\frac{\partial \pi^d}{\partial x_j} \right)^2 + \frac{\partial}{\partial x_j} \left(\frac{1}{\pi^d} \frac{\partial \pi^d}{\partial x_j} \right) \right\} \quad (133)$$

$$= \frac{1}{d-1} \sum_{j \neq i} \left\{ \frac{1}{(\pi^d)^2} \left(\frac{\partial \pi^d}{\partial x_j} \right)^2 + \frac{\pi^d \frac{\partial^2 \pi^d}{\partial x_j^2} - \left(\frac{\partial \pi^d}{\partial x_j} \right)^2}{(\pi^d)^2} \right\} \quad (134)$$

$$= \frac{1}{(d-1)} \sum_{j \neq i} \frac{\partial^2 \pi^d}{\partial x_j^2} \frac{1}{\pi^d}. \quad (135)$$

Next, we show $\mathbb{E} \left[\sup_i (R_d^{(i)} + S_d^{(i)})^2 \right]$ converges to 0. To prove this, consider writing $\mathbb{E} \left[\sup_i (R_d^{(i)} + S_d^{(i)})^2 \right]$ as sum of $(d-1)^2$ terms

$$\mathbb{E} \left[\sup_i (R_d^{(i)} + S_d^{(i)})^2 \right] = \frac{1}{(d-1)^2} \int \sup_i \sum_{j \neq i} \sum_{k \neq i} \left(\frac{\partial^2 \pi^d}{\partial x_j^2} \frac{1}{\pi^d} \right) \left(\frac{\partial^2 \pi^d}{\partial x_k^2} \frac{1}{\pi^d} \right) \pi^d dx^d \quad (136)$$

$$= \frac{1}{(d-1)^2} \sum_{j=1}^d \sum_{k=1}^d \int \left(\frac{\partial^2 \pi^d}{\partial x_j^2} \frac{1}{\pi^d} \right) \left(\frac{\partial^2 \pi^d}{\partial x_k^2} \frac{1}{\pi^d} \right) \pi^d dx^d - \frac{2}{(d-1)^2} \int \inf_i \sum_{j \neq i} \left(\frac{\partial^2 \pi^d}{\partial x_j^2} \frac{1}{\pi^d} \right) \pi^d dx^d \quad (137)$$

$$= \frac{1}{(d-1)^2} \sum_{j=1}^d \sum_{k=1}^d \int \left(\frac{\partial^2 \pi^d}{\partial x_j^2} \frac{1}{\pi^d} \right) \left(\frac{\partial^2 \pi^d}{\partial x_k^2} \frac{1}{\pi^d} \right) \pi^d dx^d + o(d^{-1}). \quad (138)$$

When $|j - k| \geq l_d$, by Assumption A2, we have

$$\int \left(\frac{\partial^2 \pi^d}{\partial x_j^2} \frac{1}{\pi^d} \right) \left(\frac{\partial^2 \pi^d}{\partial x_k^2} \frac{1}{\pi^d} \right) \pi^d dx^d \quad (139)$$

$$= \int \left(\frac{\partial^2 \pi^d}{\partial x_j^2} \right) \left(\frac{\partial^2 \pi^d}{\partial x_k^2} \right) \frac{1}{\pi^d} dx^d \quad (140)$$

$$= \int \left(\frac{\partial^2 \pi_{j,k|-j-k}}{\partial x_j^2} \right) \left(\frac{\partial^2 \pi_{j,k|-j-k}}{\partial x_k^2} \right) \frac{1}{\pi_{j,k|-j-k}} \pi_{-j-k} dx_{-j-k} dx_j dx_k \quad (141)$$

$$\leq \left[\sup_{x^d \in F_d} \int \left(\frac{\partial^2 \pi_{j,k|-j-k}}{\partial x_j^2} \right) \left(\frac{\partial^2 \pi_{j,k|-j-k}}{\partial x_k^2} \right) \frac{1}{\pi_{j,k|-j-k}} dx_j dx_k \right] \left(\int \pi_{-j-k} dx_{-j-k} \right) \quad (142)$$

$$\rightarrow 0. \quad (143)$$

This implies $\mathbb{E} \left[\sup_i (R_d^{(i)} + S_d^{(i)})^2 \right] = \frac{\mathcal{O}(dl_d) + (d-l_d)^2 o(1)}{(d-1)^2} + o(d^{-1}) \rightarrow 0$. Therefore, uniformly over i , $R_d^{(i)} + S_d^{(i)} \rightarrow 0$ in probability, then there exists a sequence $\{F'_d\}$ such that $\mathbb{P}(R_d^{(i)} + S_d^{(i)} \in F'_d, \forall i) \rightarrow 1$ and the following holds

$$\sup_i \sup_{x^d \in F'_d} \left| R_d^{(i)} + S_d^{(i)} \right| \rightarrow 0. \quad (144)$$

A.4. **Proof of Lemma 5.6.** Note that Assumption A4 implies

$$\sup_{i \in \{1, \dots, d\}} \sup_{x^d \in F_d^+} \frac{\partial}{\partial x_i} \log \pi^d(x^d) = o(d^{1/2}). \quad (145)$$

Then, by the definitions of $R_d^{(i)}$ and $I(x^d)$, we have

$$R_d^{(i)} - I(x^d) = \frac{1}{d-1} \sum_{j \neq i} \left(\frac{\partial \log \pi_{-i}(x_{-i} | x_i)}{\partial x_j} \right)^2 - \frac{1}{d} \sum_{j=1}^d \left(\frac{\partial}{\partial x_j} \log \pi^d(x^d) \right)^2 \quad (146)$$

$$= \frac{1}{d-1} \sum_{j \neq i} \left(\frac{\partial \log \pi^d(x^d)}{\partial x_j} \right)^2 - \frac{1}{d} \sum_{j=1}^d \left(\frac{\partial}{\partial x_j} \log \pi^d(x^d) \right)^2 \quad (147)$$

$$= \frac{1}{d} R_d^{(i)} - \frac{1}{d} \left(\frac{\partial}{\partial x_i} \log \pi^d(x^d) \right)^2 \rightarrow 0. \quad (148)$$

A.5. **Proof of Lemma 5.7.** Recall that we have shown

$$\hat{M}_{x^d}^{(i)}(Y_i) = \Phi \left(R_d^{(i)}(Y_i)^{-1/2} \left(\ell^{-1} \log \frac{\pi^d(y^d(i))}{\pi^d(x^d)} - \ell R_d^{(i)}(Y_i)/2 \right) \right) \quad (149)$$

$$+ \exp \left(\log \frac{\pi^d(y^d(i))}{\pi^d(x^d)} \right) \Phi \left(-\ell R_d^{(i)}(Y_i)^{1/2}/2 - \log \frac{\pi^d(y^d(i))}{\pi^d(x^d)} R_d^{(i)}(Y_i)^{-1/2} \ell^{-1} \right). \quad (150)$$

For notational simplicity, we omit the index i and write $R_d^{(i)}$ by R_d . To simplify the derivation, we note that $\hat{M}_{x^d}^{(i)}(y)$ has the following form

$$M(y) = \Phi \left(f(y)g(y) - \frac{1}{2}f^{-1}(y) \right) + \exp(g(y))\Phi \left(-\frac{1}{2}f^{-1}(y) - f(y)g(y) \right), \quad (151)$$

where $f^{-1}(y) := \ell R_d^{1/2}(y)$ and $g(y) = \log \pi^d(y^d(i)) - \log \pi^d(x^d)$. Taking the derivative with respect to y , we get

$$\frac{dM(y)}{dy} = \Phi'(fg - f^{-1}/2) \frac{d}{dy}(fg - f^{-1}/2) \quad (152)$$

$$+ \exp(g)\Phi'(-f^{-1}/2 - fg) \frac{d}{dy}(-fg - f^{-1}/2) \quad (153)$$

$$+ \exp(g) \left(\frac{d}{dy}g \right) \Phi(-fg - f^{-1}/2) \quad (154)$$

$$\leq \|\Phi'\|_\infty \left| \frac{df}{dy}g + \frac{dg}{dy}f - \frac{1}{2} \frac{df^{-1}}{dy} \right| \quad (155)$$

$$+ \exp(g)\|\Phi'\|_\infty \left| \frac{df}{dy}g + \frac{dg}{dy}f + \frac{1}{2} \frac{df^{-1}}{dy} \right| \quad (156)$$

$$+ \exp(g) \left| \frac{dg}{dy} \right| \|\Phi\|_\infty \quad (157)$$

Note that both Φ and Φ' are bounded functions. It then suffices to show

$$\exp(g) \left| \frac{dg}{dy} \right| = o(d^{1/2}), \quad \exp(g) \left| \frac{df}{dy}g \right| = o(d^{1/2}), \quad (158)$$

$$\exp(g) \left| \frac{dg}{dy}f \right| = o(d^{1/2}), \quad \exp(g) \left| \frac{df^{-1}}{dy} \right| = o(d^{1/2}). \quad (159)$$

Observing that $\frac{df^{-1}}{dy} = \frac{1}{2}\ell R_d'/R_d^{1/2}$ and $\frac{df}{dy} = -\frac{1}{2\ell} \frac{1}{R_d} \frac{R_d'}{R_d^{1/2}}$, if we can show

$$\sup_{i \in \{1, \dots, d\}} \frac{dR_d^{(i)}(y)}{dy} \frac{1}{[R_d^{(i)}(y)]^{1/2}} = o(1), \quad (160)$$

then we can get $\frac{df^{-1}}{dy} = o(1)$ and $\frac{df}{dy} = o(1/R_d)$. Using $R_d^{(i)} \rightarrow I(x^d)$ from Appendix A.4, it suffices to show

$$\left(\sup_{x^d \in F_d^+} \pi^d(x^d) \right) \left(\sup_i \sup_{x^d \in F_d^{(i)}} \frac{\partial \log \pi^d(x^d)}{\partial x_i} \right) = o(d^{1/2}), \quad (161)$$

$$\left(\sup_{x^d \in F_d^+} \pi^d(x^d) \right) \left(\sup_{x^d \in F_d^+} |\log(\pi^d(x^d))/I(x^d)| \right) = o(d^{1/2}), \quad (162)$$

$$\left(\sup_{x^d \in F_d^+} \pi^d(x^d) \right) \left(\sup_i \sup_{x^d \in F_d^{(i)}} \left| \frac{\partial \log \pi^d(x^d)}{\partial x_i} / \sqrt{I(x^d)} \right| \right) = o(d^{1/2}). \quad (163)$$

One can easily verify that the above equations hold under Assumption A4.

Finally, we complete the proof by showing Eq. (160). Recall that

$$R_d^{(i)}(y) = \frac{1}{d-1} \sum_{j \neq i} \left(\frac{\partial \log \pi_{-i}(x_{-i} | x_i = y)}{\partial x_j} \right)^2. \quad (164)$$

For notational simplicity, we write

$$R_d^{(i)}(y) = \frac{1}{d-1} \sum_{j \neq i} f_j^2(y), \quad (165)$$

where $f_j(y) := \frac{\partial \log \pi_{-i}(x_{-i} | x_i = y)}{\partial x_j}$. Then, by Cauchy–Schwartz inequality

$$\frac{\partial R_d^{(i)}(y)}{dy} = \frac{2}{d-1} \sum_{j \neq i} f_j(y) f_j'(y) \leq \frac{2}{d-1} \sqrt{\sum_{j \neq i} f_j^2(y) \sum_{j \neq i} |f_j'(y)|^2}. \quad (166)$$

Note that by A1, if $|i-j| > l_d$ then $f_j'(y) \leq \sup_{x^d \in F_d} \frac{\partial^2 \log \pi^d(x^d)}{\partial x_i \partial x_j} \rightarrow 0$. Hence, we have

$$\sup_{i \in \{1, \dots, d\}} \frac{dR_d^{(i)}(y)}{dy} \frac{1}{[R_d^{(i)}(y)]^{1/2}} \leq \sup_i \frac{\frac{2}{d-1} \sqrt{\sum_{j \neq i} f_j^2(y) \sum_{j \neq i} |f_j'(y)|^2}}{\sqrt{\frac{1}{d-1} \sum_{j \neq i} f_j^2(y)}} \quad (167)$$

$$= 2 \sup_i \sqrt{\frac{1}{d-1} \sum_{j \neq i} |f_j'(y)|^2} \leq 2 \sqrt{\frac{1}{d-1} \sum_{j=1}^d |f_j'(y)|^2} = o\left(\sqrt{\frac{l_d}{d} (\sqrt{d/l_d})^2}\right) = o(1). \quad (168)$$

B. PROOF OF THEOREM 3.18

Similar to Section 5, we assume the coordinates are linear ordered for simplicity. The proof follows the framework of [RGG97] using the generator approach [EK86].

Definition B.1. (“Generator” and “core”) Let C_c^∞ be the class of continuous functions with compact support such that all orders of derivatives exist. For any $f_c \in C_c^\infty$ such that $f_c(x^d) = f_c(x_1)$, define

$$(G_d f_c)(x^d) := d \mathbb{E}_{Y^d} \left\{ [f_c(Y^d) - f_c(x^d)] \left(1 \wedge \frac{\pi^d(Y^d)}{\pi^d(x^d)} \right) \right\}. \quad (169)$$

Definition B.2. (Langevin Diffusion Limits) For some fixed function $h(\ell)$ such that

$$(G f_c)(x_1) := h(\ell) \left\{ \frac{1}{2} f_c''(x_1) + \frac{1}{2} [(\log \pi_1)'(x_1)] f_c'(x_1) \right\}, \quad (170)$$

where π_1 is the marginal distribution of the first coordinate of π^d .

Note that using Assumption A2+, and the assumption $\mathbb{P}(X^d \notin F_d) = \mathcal{O}(d^{-1-\delta})$, following the arguments in the proof of Lemma 5.3 we can get a stronger version of Lemma 5.3 for $F'_d := \{x^d : \sup_i |R_d^{(i)} + S_d^{(i)}| \leq d^{-\delta}\}$. Then using a union bound yields

$$\mathbb{P}(X^d(\lfloor ds \rfloor) \notin F_d \cap F'_d, \exists 0 \leq s \leq t) \rightarrow 0. \quad (171)$$

Therefore, for any fixed t , if $d \rightarrow \infty$ then the probability of all $X^d(\lfloor ds \rfloor), 0 \leq s \leq t$ are in $F_d \cap F'_d$ goes to 1. Since $F_d \cap F'_d \subseteq F_d^+ \cap F'_d \subseteq F_d^+$, it suffices to consider $x^d \in F_d^+$.

Note that $Y^d \sim \mathcal{N}(x^d, \frac{\ell^2}{d-1}I)$, we can write

$$(G_d f_c)(x^d) = d \mathbb{E}_{Y_1} \left\{ [f_c(Y_1) - f_c(x_1)] \mathbb{E}_{Y_{-1}} \left[1 \wedge \frac{\pi^d(Y^d)}{\pi^d(x^d)} \right] \right\}, \quad (172)$$

where $\mathbb{E}_{Y_{-1}}[\cdot]$ is short for $\mathbb{E}_{Y_2, \dots, Y_d | Y_1}[\cdot]$ and π^d denotes the target distribution in d -dimension. The goal is then to prove $(G_d f_c)$ converges to $(G f_c)$.

Recall the definition Eq. (82), we omit the index to write $M_{x^d}^{(1)}$ as M_{x^d} , which is defined by

$$M_{x^d}(Y_1) = \mathbb{E}_{Y_{-1}} \left(1 \wedge \frac{\pi^d(Y^d)}{\pi^d(x^d)} \right). \quad (173)$$

Then we have previously shown in Eq. (105) that $M_{x^d}(Y_1)$ can be approximated by

$$\hat{M}_{x^d}(Y_1) = \Phi \left(R_d(Y_1)^{-1/2} \left(\ell^{-1} \log \frac{\pi^d(Y_1, x_{-1})}{\pi^d(x^d)} - \ell R_d(Y_1)/2 \right) \right) \quad (174)$$

$$+ \exp \left(\log \frac{\pi^d(Y_1, x_{-1})}{\pi^d(x^d)} \right) \Phi \left(-\ell R_d(Y_1)^{1/2}/2 - \log \frac{\pi^d(Y_1, x_{-1})}{\pi^d(x^d)} R_d(Y_1)^{-1/2} \ell^{-1} \right) \quad (175)$$

For $x^d \in F_d^+$, some properties of \hat{M}_{x^d} is given as follows.

Lemma B.3. For \hat{M}_{x^d} , we have

$$\hat{M}_{x^d}(x_1) = 2\Phi\left(-\frac{\ell R_d^{1/2}(x_1)}{2}\right), \quad (176)$$

$$\hat{M}'_{x^d}(x_1) = \Phi\left(-\frac{\ell R_d^{1/2}(x_1)}{2}\right) \frac{d[\log \pi_1(x) + \log \pi_{-1}(x_{-1}|x)]}{dx}(x_1) + o(1), \quad (177)$$

$$\hat{M}'_{x^d}(x_1) = o(d^{1/2}), \quad \sup_{x^d \in F_d^+} \hat{M}''_{x^d} = o(d^{1/2}). \quad (178)$$

Proof. See Appendix B.1. □

Since $f_c(Y_1) - f_c(x_1)$ is bounded, it suffices to show

$$\mathbb{E}_{Y_1} \left\{ d[f_c(Y_1) - f_c(x_1)] \hat{M}_{x^d}(Y_1) \right\} \rightarrow (Gf_c)(x_1). \quad (179)$$

Now using mean value theorem and Taylor expansion of $\mathbb{E}_{Y_1} \left\{ [f_c(Y_1) - f_c(x_1)] \hat{M}_{x^d}(Y_1) \right\}$ at $(Y_1 - x_1)$ yields

$$[f_c(Y_1) - f_c(x_1)] \hat{M}_{x^d}(Y_1) \quad (180)$$

$$= \left[f'_c(x_1)(Y_1 - x_1) + \frac{1}{2} f''_c(x_1)(Y_1 - x_1)^2 + K(Y_1 - x_1)^3 \right] \quad (181)$$

$$\cdot \left[\hat{M}_{x^d}(x_1) + \hat{M}'_{x^d}(x_1)(Y_1 - x_1) + \frac{1}{2} \hat{M}''_{x^d}(x')(Y_1 - x_1)^2 \right] \quad (182)$$

$$= f'_c(x_1) \hat{M}_{x^d}(x_1)(Y_1 - x_1) + \left[\frac{1}{2} f''_c(x_1) \hat{M}_{x^d}(x_1) + f'_c(x_1) \hat{M}'_{x^d}(x_1) \right] (Y_1 - x_1)^2 \quad (183)$$

$$+ \left[K \hat{M}_{x^d}(x_1) + \frac{1}{2} f''_c(x_1) \hat{M}'_{x^d}(x_1) + \frac{1}{2} \hat{M}''_{x^d}(x') f'_c(x_1) \right] (Y_1 - x_1)^3 \quad (184)$$

$$+ \left[\frac{1}{4} \hat{M}''_{x^d}(x') f''_c(x_1) + K \hat{M}'_{x^d}(x_1) \right] (Y_1 - x_1)^4 + \frac{1}{2} \hat{M}''_{x^d}(x') K (Y_1 - x_1)^5, \quad (185)$$

where K is a constant since f_c has bounded third derivative. Note that both $f'_c(x_1)$ and $f''_c(x_1)$ are bounded as well. Therefore, taking expectation over Y_1 and using $\hat{M}'_{x^d}(x_1) = o(d^{1/2})$, $\sup_{x^d} \hat{M}''_{x^d} = o(d^{1/2})$ in Lemma B.3, we have

$$\mathbb{E}_{Y_1} \left\{ [f_c(Y_1) - f_c(x_1)] \hat{M}_{x^d}(Y_1) \right\} = \left[\frac{1}{2} f''_c(x_1) \hat{M}_{x^d}(x_1) + f'_c(x_1) \hat{M}'_{x^d}(x_1) \right] \frac{\ell^2}{d-1} + o(d^{-1}). \quad (186)$$

Finally, by Assumption **A6**, we have

$$f'_c(x_1)\hat{M}'_{x^d}(x_1) + \frac{1}{2}f''_c(x_1)\hat{M}_{x^d}(x_1) \quad (187)$$

$$= 2\Phi\left(-\frac{\ell R_d^{1/2}(x_1)}{2}\right)\left(\frac{1}{2}f''_c(x_1) + \frac{1}{2}f'_c(x_1)\frac{d[\log \pi_1(x) + \log \pi_{-1}(x_{-1}|x)]}{dx}(x_1)\right) \quad (188)$$

$$= 2\Phi\left(-\frac{\ell R_d^{1/2}(x_1)}{2}\right)\left(\frac{1}{2}f''_c(x_1) + \frac{1}{2}f'_c(x_1)\frac{d \log \pi_{1|-1}(x|x_{-1})}{dx}(x_1)\right) \quad (189)$$

$$\rightarrow 2\Phi\left(-\frac{\ell I(x^d)^{1/2}}{2}\right)\left(\frac{1}{2}f''_c(x_1) + \frac{1}{2}f'_c(x_1)\frac{d \log \tilde{\pi}(x)}{dx}(x_1)\right) \quad (190)$$

$$\rightarrow 2\Phi\left(-\frac{\ell \bar{I}^{1/2}}{2}\right)\left(\frac{1}{2}f''_c(x_1) + \frac{1}{2}f'_c(x_1)\frac{d \log \tilde{\pi}(x)}{dx}(x_1)\right), \quad (191)$$

which implies that $\mathbb{E}_{Y_1}\left\{d[f_c(Y_1) - f_c(x_1)]\hat{M}_{x^d}(Y_1)\right\} \rightarrow (Gf_c)(x_1)$ where $h(\ell) := 2\ell^2\Phi(-\ell\sqrt{\bar{I}}/2)$.

B.1. Proof of Lemma **B.3.** The proof is quite tedious. In order to simplify the notations, we first introduce the following lemma.

Lemma **B.4.** *For the function $M(y)$ defined by*

$$M(y) = \Phi\left(f(y)g(y) - \frac{1}{2}f^{-1}(y)\right) + e^{g(y)}\Phi\left(-\frac{1}{2}f^{-1}(y) - f(y)g(y)\right), \quad (192)$$

we have

$$\frac{dM(y)}{dy} = \Phi'(fg - f^{-1}/2)\frac{d}{dy}(fg - f^{-1}/2) \quad (193)$$

$$+ e^g\Phi'(-f^{-1}/2 - fg)\frac{d}{dy}(-fg - f^{-1}/2) \quad (194)$$

$$+ e^g\left(\frac{d}{dy}g\right)\Phi(-fg - f^{-1}/2). \quad (195)$$

$$\frac{d^2M(y)}{dy^2} = \Phi''(fg - f^{-1}/2) \left[\frac{d}{dy}(fg - f^{-1}/2) \right]^2 + \Phi'(fg - f^{-1}/2) \frac{d^2}{dy^2}(fg - f^{-1}/2) \quad (196)$$

$$+ e^g \left(\frac{d}{dy}g \right) \Phi'(-f^{-1}/2 - fg) \frac{d}{dy}(-fg - f^{-1}/2) \quad (197)$$

$$+ e^g \left\{ \Phi''(-fg - f^{-1}/2) \left[\frac{d}{dy}(-fg - f^{-1}/2) \right]^2 + \Phi'(-fg - f^{-1}/2) \frac{d^2}{dy^2}(-fg - f^{-1}/2) \right\} \quad (198)$$

$$+ e^g \left(\frac{d}{dy}g \right) \Phi'(-fg - f^{-1}/2) \frac{d}{dy}(-fg - f^{-1}/2) \quad (199)$$

$$+ \Phi(-fg - f^{-1}/2) \left[e^g \left(\frac{d^2}{dy^2}g \right) + e^g \left(\frac{d}{dy}g \right)^2 \right]. \quad (200)$$

Furthermore, if $g(x_1) = 0$, then we have

$$\frac{dM(y)}{dy}(x_1) = \left(\Phi'(-f^{-1}/2) \frac{d}{dy}(fg - f^{-1}/2) \right) \quad (201)$$

$$+ \Phi'(-f^{-1}/2) \frac{d}{dy}(-fg - f^{-1}/2) \quad (202)$$

$$+ \left(\frac{d}{dy}g \right) \Phi(-f^{-1}/2) \Big) (x_1) \quad (203)$$

$$= \left(\Phi'(-f^{-1}/2) \frac{d}{dy}(-f^{-1}) + \left(\frac{d}{dy}g \right) \Phi(-f^{-1}/2) \right) (x_1) \quad (204)$$

$$= -\Phi' \left(-\frac{f^{-1}(x_1)}{2} \right) \frac{df^{-1}(y)}{dy}(x_1) + \frac{dg(y)}{dy}(x_1) \Phi \left(-\frac{f^{-1}(x_1)}{2} \right). \quad (205)$$

Remark B.5. Let $g(y) = \log \frac{\pi^d(y, x-1)}{\pi^d(x^d)}$ and $f^{-1}(y) = \ell R_d^{1/2}(y)$ then $\hat{M}_{x^d}(y) = M(y)$. \triangleleft

Now substituting $g(y) = \log \frac{\pi^d(y, x-1)}{\pi^d(x^d)}$ and $f^{-1}(y) = \ell R_d^{1/2}(y)$ to Lemma B.4, we have

$$\hat{M}_{x^d}(x_1) = 2\Phi \left(-\frac{\ell R_d^{1/2}(x_1)}{2} \right), \quad (206)$$

and

$$\hat{M}'_{x^d}(x_1) = \frac{d\hat{M}_{x^d}(y)}{dy}(x_1) \quad (207)$$

$$= \Phi \left(-\frac{\ell R_d^{1/2}(x_1)}{2} \right) \frac{d[\log \pi_1(x) + \log \pi_{-1}(x_{-1} | x)]}{dx}(x_1) \quad (208)$$

$$- \Phi' \left(-\frac{\ell R_d^{1/2}(x_1)}{2} \right) \frac{\ell}{2R_d^{1/2}(x_1)} R'_d(x_1). \quad (209)$$

Since Φ' is bounded and by Eq. (160), $R'_d(x_1)/R_d^{1/2}(x_1) \rightarrow 0$, therefore

$$\Phi' \left(-\frac{\ell R_d^{1/2}(x_1)}{2} \right) \frac{\ell}{2R_d^{1/2}(x_1)} R'_d(x_1) = o(1). \quad (210)$$

Also, $\hat{M}'_{x^d}(x_1) = o(d^{1/2})$ since $\frac{\partial \log \pi^d}{\partial x_i} = \mathcal{O}(d^{\alpha/2}) = o(d^{1/2})$.

Now we prove $\sup_{x^d} \hat{M}''_{x^d} = o(d^{1/2})$. For simplicity, we keep the notations of f and g (recall that $g(y) = \log \frac{\pi^d(y, x_{-1})}{\pi^d(x^d)}$ and $f^{-1}(y) = \ell R_d^{1/2}(y)$) and use the results in Appendix A.5. Since Φ, Φ', Φ'' are bounded, it suffices to bound all the following terms to be $o(d^{1/2})$:

$$\left[\frac{d}{dy}(fg - f^{-1}/2) \right]^2, \quad \frac{d^2}{dy^2}(fg - f^{-1}/2), \quad \exp(g) \left(\frac{dg}{dy} \right) \frac{d}{dy}(-fg - f^{-1}/2), \quad (211)$$

$$\exp(g) \left[\frac{d}{dy}(fg - f^{-1}/2) \right]^2, \quad \exp(g) \frac{d^2}{dy^2}(fg - f^{-1}/2), \quad \exp(g) \left(\frac{d^2 g}{dy^2} \right), \quad \exp(g) \left(\frac{dg}{dy} \right)^2. \quad (212)$$

Next, we show that most of them can be verified using Assumption A4+, and the results in Appendix A.5:

$$\left[\frac{d}{dy}(fg - f^{-1}/2) \right]^2 = \mathcal{O} \left[\left(\sup_{x^d \in F_d^+} \log \pi^d(x^d) \mathcal{O}(d^{\alpha/4}) + \sup_{x^d \in F_d^+} \frac{\partial \log \pi^d}{\partial x_1} \right)^2 \right] \quad (213)$$

$$= \mathcal{O} [(d^{\alpha/4} \log d + d^{\alpha/2})^2] = o(d^{1/2}), \quad (214)$$

$$\left| e^g \left(\frac{dg}{dy} \right) \frac{d}{dy} (-fg - f^{-1}/2) \right| = \mathcal{O} \left[\sup_{x^d \in F_d^+} \pi^d(x^d) \sup_{x^d \in F_d^+} \frac{\partial \log \pi^d}{\partial x_1} (d^{\alpha/4} \log d + d^{\alpha/2}) \right] \quad (215)$$

$$= o(d^{1/2-\alpha} d^{\alpha/2} (d^{\alpha/4} \log d + d^{\alpha/2})) = o(d^{1/2}), \quad (216)$$

$$\left| \exp(g) \left[\frac{d}{dy}(fg - f^{-1}/2) \right]^2 \right| = o(d^{1/2-\alpha} d^\alpha) = o(d^{1/2}), \quad (217)$$

$$\left| \exp(g) \left(\frac{d^2 g}{dy^2} \right) \right| = \mathcal{O} \left[\sup_{x^d \in F_d^+} \pi^d(x^d) \sup_{x^d \in F_d^+} \frac{\partial^2 \log \pi^d}{\partial x_1^2} \right] = o(d^{1/2-\alpha}) \mathcal{O}(d^\alpha) = o(d^{1/2}), \quad (218)$$

$$\left| \exp(g) \left(\frac{dg}{dy} \right)^2 \right| = \mathcal{O} \left[\sup_{x^d \in F_d^+} \pi^d(x^d) \sup_{x^d \in F_d^+} \left(\frac{\partial \log \pi^d}{\partial x_1} \right)^2 \right] = o(d^{1/2-\alpha}) \mathcal{O}(d^{\alpha/2})^2 = o(d^{1/2}). \quad (219)$$

The only terms left are $\frac{d^2}{dy^2}(fg - f^{-1}/2)$ and $\exp(g) \frac{d^2}{dy^2}(fg - f^{-1}/2)$. Therefore, it suffices to show

$$\frac{d^2}{dy^2}(fg - f^{-1}/2) = \mathcal{O}(d^\alpha). \quad (220)$$

Note that

$$\frac{d^2}{dy^2}(fg - f^{-1}/2) = \frac{d}{dy}(f'g + g'f - \frac{1}{2}df^{-1}) \quad (221)$$

$$= \frac{d}{dy} \left[\frac{1}{R_d} \frac{R'_d}{R_d^{1/2}} g + \frac{1}{R_d^{1/2}} g' - \frac{1}{2} \frac{R'_d}{R_d^{1/2}} \right] \quad (222)$$

$$= \frac{1}{R_d} \frac{R'_d}{R_d^{1/2}} g' + \left(\frac{1}{R_d} \frac{R'_d}{R_d^{1/2}} \right)' g + \frac{1}{R_d^{1/2}} g'' + \left(\frac{1}{R_d^{1/2}} \right)' g' - \frac{1}{2} \left(\frac{R'_d}{R_d^{1/2}} \right)'. \quad (223)$$

Note that we have shown $R'_d = o(R_d^{1/2})$ in Appendix A.5. Similarly, we also can show using Assumption A3+ that

$$R''_d = \frac{1}{d-1} \left(\sum_{j \neq 1} f_j f'_j \right)' = \frac{1}{d-1} \sum_{j \neq 1} (f'_j)^2 + \frac{1}{d-1} \sum_{j \neq 1} f_j f''_j \quad (224)$$

$$\leq \frac{1}{d-1} \sum_{j \neq 1} (f'_j)^2 + \sqrt{\frac{1}{d-1} \sum_{j \neq 1} f_j^2} \sqrt{\frac{1}{d-1} \sum_{j \neq 1} (f''_j)^2} \quad (225)$$

$$= \mathcal{O}(l_d/d) o((\sqrt{d/l_d})^2) + o(R_d^{1/2}) \sqrt{l_d/d (\sqrt{d/l_d})^2} = o(R_d^{1/2}), \quad (226)$$

where $f_j(x) := \frac{\partial \log \pi_{-1}(x_{-1} | x_1=x)}{\partial x_j}$. Therefore $R''_d = o(R_d^{1/2})$ as well. Finally, we can complete the proof by verifying Eq. (220) using Assumption A4+ as follows.

$$\left| \frac{1}{R_d} \frac{R'_d}{R_d^{1/2}} g' \right| = \mathcal{O} \left(\frac{1}{R_d} \right) o(1) \mathcal{O} \left(\sup_{x^d \in F_d^+} \frac{\partial \log \pi^d}{\partial x_1} \right) = \mathcal{O}(d^{\alpha/4}) o(d^{\alpha/2}) = o(d^\alpha), \quad (227)$$

$$\left| \left(\frac{1}{R_d} \frac{R'_d}{R_d^{1/2}} \right)' g \right| = \mathcal{O} \left[\frac{R''_d R_d^{3/2} + 3/2 (R'_d)^2 R_d^{1/2}}{R_d^3} g \right] = \mathcal{O} \left[\frac{1}{R_d^{3/2}} (R''_d g) \right] \quad (228)$$

$$= \mathcal{O}(d^{\alpha/4}) o(1) \mathcal{O}(d^{\alpha/2}) = o(d^\alpha), \quad (229)$$

$$\left| \frac{1}{R_d^{1/2}} g'' \right| = \mathcal{O} \left(\sup_{x^d \in F_d^+} \frac{\partial^2 \log \pi^d}{\partial x_1^2} \right) = o(d^\alpha), \quad (230)$$

$$\left| \left(\frac{1}{R_d^{1/2}} \right)' g' \right| = \mathcal{O} \left(\frac{1}{2} \frac{1}{R_d^{3/2}} R'_d g' \right) = o(1/R_d) \mathcal{O} \left(\sup_{x^d \in F_d^+} \frac{\partial \log \pi^d}{\partial x_1} \right) = \mathcal{O}(d^{\alpha/4}) o(d^{\alpha/2}) = o(d^\alpha), \quad (231)$$

$$\left| \left(\frac{R'_d}{R_d^{1/2}} \right)' \right| = \left| \frac{R''_d R_d^{1/2} - \frac{1}{2} (R'_d)^2 \frac{1}{R_d^{1/2}}}{R_d} \right| = \mathcal{O} \left(R''_d / R_d^{1/2} \right) = o(1) = o(d^\alpha). \quad (232)$$

C. PROOF OF THEOREM 3.20

We follow the same approach as in the proof of [RR16, Proposition 3]. The idea is to follow the proof of Theorem 3.18 except in the proof of Eq. (105), we need a stronger version of Lemma 5.3 to determine the sequence of “typical sets” $\{F'_d\}$.

Given fixed time t , considering the sequence of “typical sets” $\{F'_d\}$ defined by

$$F'_d := \{x^d : |R_d + S_d| \leq d^{-\delta}\}, \quad (233)$$

where $\delta > 0$ and we used R_d and S_d to denote $R_d^{(1)}$ and $S_d^{(1)}$ for simplicity. We need to guarantee that when d is large enough, we always have $X^d(\lfloor ds \rfloor) \in F_d \cap F'_d, \forall 0 \leq s \leq t$ and this happens for almost all starting state $X_1^d(0) = x$. That is, defining

$$p(d, x) := \mathbb{P}(X(\lfloor ds \rfloor) \notin F_d \cap F'_d, \exists 0 \leq s \leq t | X_1^d(0) = x), \quad (234)$$

letting π_1 denote the marginal stationary distribution for the first coordinate, we want to show that for any given $\epsilon > 0$, as $d \rightarrow \infty$

$$\mathbb{P}_{x \sim \pi_1}[p(d, x) \geq \epsilon, \text{ infinite often}] = 0. \quad (235)$$

We prove it using Borel–Cantelli Lemma. Note that the application of Borel–Cantelli lemma is valid since we have assumed all of the processes are jointly defined on the same probability space as independent processes. First, note that

$$\mathbb{E}_{x \sim \pi_1}[p(d, x)] = dt \mathbb{P}_{\pi^d}((F_d \cap F'_d)^c) = dt \mathbb{P}_{\pi^d}(F_d^c \cup (F'_d)^c) \leq dt \mathbb{P}_{\pi^d}(F_d^c) + dt \mathbb{P}_{\pi^d}((F'_d)^c). \quad (236)$$

For any given $\epsilon > 0$, we have

$$\sum_{d=2}^{\infty} \mathbb{P}(p(x, d) \geq \epsilon) \leq \sum_{d=2}^{\infty} \frac{\mathbb{E}_{x \sim \pi_1}[p(d, x)]}{\epsilon} \quad (237)$$

$$\leq \frac{dt}{\epsilon} \sum_{d=2}^{\infty} \mathbb{P}_{\pi^d}(|R_d + S_d| > d^{-\delta}) + \frac{dt}{\epsilon} \sum_{d=2}^{\infty} \mathbb{P}(X^d \notin F_d). \quad (238)$$

By $\mathbb{P}(X^d \notin F_d) = \mathcal{O}(d^{-2-\delta})$, we have $dt \sum_{d=2}^{\infty} \mathbb{P}(X^d \notin F_d) < \infty$. Now in order to use Borel–Cantelli Lemma, the condition we need is that for some number of moments m such that

$$\mathbb{P}_{\pi^d}(|R_d + S_d| > d^{-\delta}) \leq \frac{\mathbb{E}|R_d + S_d|^m}{d^{-m\delta}} = d^{m\delta} \mathbb{E}|R_d + S_d|^m = \mathcal{O}(d^{-2-\delta}), \quad (239)$$

which leads to $\sum_{d=2}^{\infty} \mathbb{P}(p(x, d) \geq \epsilon) < \infty$. In order to obtain non-trivial conditions, we let $m = 4$ and Assumption A2++ implies $\mathbb{E}|R_d + S_d|^4 = \mathcal{O}(d^{-2-5\delta})$. We can then use this sequence of typical sets $\{F'_d\}$ in the proof of Theorem 3.18 to replace the sequence of $\{F'_d\}$ used in Lemma 5.3. The residual proof follows the same as Theorem 3.18.