On the Scalability of Informed Importance Tempering

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Abstract

Informed MCMC methods have been proposed as scalable solutions to Bayesian posterior computation on high-dimensional discrete state spaces. We study a class of MCMC schemes called informed importance tempering (IIT), which combine importance sampling and informed local proposals. Spectral gap bounds for IIT estimators are obtained, which demonstrate the remarkable scalability of IIT samplers for unimodal target distributions. The theoretical insights acquired in this note provide guidance on the choice of informed proposals in model selection and the use of importance sampling in MCMC methods.

Keywords: Finite Markov chain; Importance sampling; Markov chain Monte Carlo sampling; High-dimensional model selection; Spectral gap; Tempered Gibbs sampler.

1 Introduction

Bayesian inference provides a flexible framework for modeling complex data and assessing uncertainty of model selection and parameter estimation, but these advantages often come at the cost of intensive posterior computation. In recent years, various informed Markov chain Monte Carlo (MCMC) methods have been proposed for sampling from discrete state spaces, which are particularly useful for model selection problems and have been shown numerically to scale well to high-dimensional data [Zanella and Roberts 2019, Zanella 2020]. These methods require evaluating the posterior distribution locally in each iteration so that neighboring states with larger posterior probabilities are more likely to be proposed. A theoretical guarantee for the scalability of informed MCMC samplers was obtained by [Zhou et al. 2021], who proved that their informed Metropolis-Hastings (MH) algorithm for variable selection can achieve a mixing rate that is independent of the number of variables. It was also shown in [Zhou et al. 2021] that if the informed proposal scheme is not carefully chosen, the resulting MH algorithm can be susceptible to local trapping due to exceedingly low acceptance rates.
In this note, we consider a different approach to making use of informed proposals: accept all the proposed moves and use importance weights to correct for the proposal bias. We call this scheme informed importance tempering (IIT). Since an informed proposal distribution usually has a shape similar to the local posterior landscape, a combination of informed proposals and importance sampling can sometimes be strikingly efficient. One example in the literature is the tempered Gibbs sampler (TGS) for variable selection devised by Zanella and Roberts [2019], which has largely motivated the general framework to be proposed in this work. The convergence rate of IIT estimators can be measured by the spectral gap of a continuous-time Markov chain, which enables us to use Markov chain theory to investigate the complexity of IIT schemes in general high-dimensional settings. We first consider the case where the target posterior distribution satisfies a unimodal condition and concentrates on one state, which, for model selection problems, can be interpreted as a strong notion of statistical consistency. Our theory suggests that in this “single best model” scenario, IIT schemes with locally balanced proposals, including TGS, have superior scalability. Next, we slightly modify the unimodal condition by assuming the posterior mass concentrates on two equivalent models. It turns out that then TGS may lose its advantage completely, while some other IIT samplers still perform well. Another interesting finding is that both our theory and numerical study support the use of the square root of the posterior probability as the proposal weight.

The note is structured as follows. We introduce the notation and the IIT algorithm in Section 2. Spectral gap bounds for IIT samplers are presented in Section 3. Section 4 gives an illustrative numerical example, and Section 5 concludes the note with some discussion on the implementation of IIT schemes in practice. All proofs are deferred to the appendix.

2 Informed Importance Tempering

2.1 Notation, Problem Setup and Preliminaries

Throughout this note, we use $\mathcal{X} = \mathcal{X}(p)$ to denote a finite set, where $p \in (1, \infty)$ is a parameter describing the problem size, and use $\pi$ to denote a target posterior distribution with support $\mathcal{X}$; that is, $\pi(x) > 0$ for every $x$. Our goal is to approximate $\pi$ by sampling when $\pi$ is known only up to a normalizing constant. For convenience of interpretation, we treat $\mathcal{X}$ as a set of candidate models in a model selection problem with $p$ variables, though $p$ does not have to be an integer in our theoretical results. The cardinality of a set is denoted by $|\cdot|$. We are mostly interested in the cases where $|\mathcal{X}|$ grows super-polynomially with $p$. For any function $f: \mathcal{X} \to \mathbb{R}$, let $\mathbb{E}_\pi[f] = \sum_{x \in \mathcal{X}} f(x)\pi(x)$. A stochastic matrix (i.e., transition matrix) is denoted by $P$ or $K$, which is treated as a mapping from $\mathcal{X}^2$ to $[0, 1]$. Similarly, a transition rate matrix is denoted by
a mapping $Q: \mathcal{X}^2 \to \mathbb{R}$.

Suppose that a neighborhood mapping $\mathcal{N}: \mathcal{X} \to 2^\mathcal{X}$ is given such that $x \notin \mathcal{N}(x)$ for each $x$; the set $\mathcal{N}(x)$ is referred to as the neighborhood of $x$. Let $\mathbb{M}(\mathcal{X}, \mathcal{N})$ denote the collection of all stochastic matrices $K$ with state space $\mathcal{X}$ such that $K(x, y) > 0$ if and only if $y \in \mathcal{N}(x)$. We make two assumptions on $\mathcal{N}$. First, $\mathcal{N}$ is symmetric; that is, $x \in \mathcal{N}(y)$ implies $y \in \mathcal{N}(x)$. Second, any $K \in \mathbb{M}(\mathcal{X}, \mathcal{N})$ is irreducible. The term “neighborhood” connotes that $|\mathcal{N}(\cdot)|$ tends to be much smaller than $|\mathcal{X}|$, though we will not formally impose this assumption until Section 3. In this note, we treat $\mathcal{N}$ as given and consider how to choose a proposal scheme $K$ from $\mathbb{M}(\mathcal{X}, \mathcal{N})$. If $K(x, y) = |\mathcal{N}(x)|^{-1}$ for each $y \in \mathcal{N}(x)$, $K$ becomes the usual random walk proposal and we refer to the corresponding MH algorithm as RWMH. We say $K$ is informed if the proposal probability depends on the un-normalized posterior. We assume that the time needed to evaluate $\pi(x)$ (up to a normalizing constant) for any $x \in \mathcal{X}$ is $O(1)$, which is also the complexity of one iteration of RWMH. For all the informed proposals $K$ that will be analyzed in this note, generating a sample from the distribution $K(x, \cdot)$ requires evaluating $\pi$ in the entire neighborhood $\mathcal{N}(x)$, and thus the time complexity of one informed iteration is $O(|\mathcal{N}(x)|)$.

We follow Zanella [2020] to consider informed proposals that can be written as

$$K_h(x, y) = \frac{\mathbbm{1}_{\mathcal{N}(x)}(y)}{Z_h(x)} h \left( \frac{\pi(y)}{\pi(x)} \right), \quad Z_h(x) = \sum_{y \in \mathcal{N}(x)} h \left( \frac{\pi(y)}{\pi(x)} \right),$$

(1)

where $\mathbbm{1}$ denote the indicator function and $h: \mathbb{R}_+ \to \mathbb{R}_+$ is a non-constant function ($\mathbb{R}_+$ denotes all positive real numbers). The function $h$ determines how the proposal weight of each neighboring state is calculated, and $Z_h$ is the normalizing constant. One simple choice is $h(u) = u^a$ for some $a > 0$, which forces the chain to keep climbing up. Observe that if $\pi$ is the uniform distribution on $\mathcal{X}$, no matter what $h$ is used, $K_h$ becomes identical to the random walk proposal; thus, RWMH should be used since it has a much smaller time complexity per iteration. Roughly speaking, informed MCMC methods tend to have an advantage over RWMH when the posterior mass concentrates on a small set of states (but this is exactly what we expect to happen in model selection given a sufficiently large sample size). Zanella [2020] proposed to use “locally balanced” proposals where $h$ is a “balancing function”.

**Definition 1.** We say $h: \mathbb{R}_+ \to \mathbb{R}_+$ is a balancing function if $h(u) = u h(1/u)$ for any $u \in \mathbb{R}_+$.

**Remark 1.** Three balancing functions will be considered in our analysis, which we denote by

$$h_{0.5}(u) = \sqrt{u}, \quad h_{\land 1}(u) = 1 \land u, \quad h_{+1}(u) = 1 + u.$$  

(2)

Note that $h_{+1}$ behaves just like $h(u) = 1 \lor u$, since $(1 + u)/2 \leq 1 \lor u < 1 + u$ for any $u > 0$. So $h_{+1}, h_{\land 1}$ and $h_{0.5}$ represent three very different proposal weighting strategies: $h_{\land 1}$ treats
any \( y \in \mathcal{N}(x) \) with \( \pi(y) \geq \pi(x) \) equally, while \( h_{+1} \) assigns roughly the same weight to any \( y \in \mathcal{N}(x) \) with \( \pi(y) < \pi(x) \). Only \( h_{0.5} \) always “makes full use” of the knowledge about the local posterior landscape.

### 2.2 Algorithm

Let \( x^{(1)}, x^{(2)}, \ldots, x^{(t)} \) denote \( t \) samples generated from an irreducible Markov chain with stationary distribution \( \tilde{\pi} \). Let \( \omega = \pi / \tilde{\pi} \) denote the Radon-Nikodym derivative. For any function \( f : \mathcal{X} \to \mathbb{R} \), we can estimate \( E_\pi[f] \) using the self-normalized importance sampling estimator

\[
\hat{f}(t, \omega) = \frac{\sum_{k=1}^t f(x^{(k)}) \omega(x^{(k)})}{\sum_{k=1}^t \omega(x^{(k)})},
\]

where \( \omega(x) = \pi(x)/\tilde{\pi}(x) \) is called the importance weight of the sample \( x \). Such an MCMC importance sampling scheme is commonly used with \( \tilde{\pi}(x) \propto \pi(x)^{1/T} \), where the “temperature” \( T \) can be treated as either fixed or an auxiliary random variable [Jennison 1993, Neal 1996]. Gramacy et al. [2010] called this method importance tempering (IT), and they noted that successful applications of IT schemes were surprisingly rare. Recently, Zanella and Roberts [2019] proposed the (weighted) TGS algorithm by combining IT with Gibbs sampling, which demonstrated excellent performance in high-dimensional variable selection. The great success of TGS can be mainly attributed to its “informed” choice of the coordinate to update. Though TGS was proposed as a Gibbs sampler on a product space, its main idea can be generalized to arbitrary finite state spaces by using any informed local proposal scheme.

**Algorithm 1** (Informed importance tempering). Let \( K_h \) be as given in (1) for some \( h : \mathbb{R}_+ \to \mathbb{R}_+ \). Generate samples \( x^{(1)}, \ldots, x^{(t)} \) iteratively from \( K_h \). Calculate the IIT estimator using (3) with \( \omega(x) = \pi(x)/\pi_h(x) \), where \( \pi_h \) denotes the stationary distribution of \( K_h \).

**Remark 2.** In Algorithm [1] we assume the proposal weight of \( y \in \mathcal{N}(x) \) can always be calculated by \( h(\pi(y)/\pi(x)) \). This can be generalized by assuming \( K(x, y) \propto H(x, y)1_{\mathcal{N}(x)}(y) \) for some non-negative \( H \). The generic TGS algorithm and its weighted version introduced in Zanella and Roberts [2019] are special cases of this generalized version of IIT. The TGS algorithm for variable selection considered in Zanella and Roberts [2019, Section 4.2] is an IIT scheme with \( h = h_{+1} \); see Section [AI] for details.

The name “informed importance tempering” suggests that \( h \) in Algorithm [1] should not be a constant function. Though in principle, one can apply Algorithm [1] with \( h \equiv 1 \) and \( K_h \) being a random walk proposal, such uninformed schemes rarely work well in real statistical problems since the chain \( K_h \) tends to spend most of time on the states with negligible posterior...
probabilities. Meanwhile, the function \( h \) should be chosen such that \( \pi_h \) can be easily evaluated up to a normalizing constant. The following lemma gives \( \pi_h \) for two classes of IIT schemes that are of particular interest to this work. The proof is omitted since the lemma directly follows from the detailed balance condition.

**Lemma 1.** Let \( K_h \) be as given in [1] with stationary distribution \( \pi_h \). If \( h(u) = u^a \) for some \( a \geq 0 \), then \( \pi_h \propto \pi^{2a} Z_h \). If \( h \) is a balancing function, then \( \pi_h \propto \pi Z_h \).

Since \( Z_h \) is defined as the sum of \( h(\pi(y)/\pi(x)) \) for all neighboring states \( y \), we expect that \( Z_h(x) \) does not depend much on \( \pi(x) \). Hence, Lemma [1] suggests that for “locally balanced IIT schemes” (i.e., Algorithm 1 with a balancing function \( h \)), the distribution \( \pi_h \) can be seen as a random perturbation of \( \pi \). This is an intuitive reason why locally balanced IIT schemes may work well as importance sampling tends to be most efficient when \( \pi_h \) looks similar to the target distribution \( \pi \) [Liu, 2008, Chapter 2.5].

For \( h(u) = u^a \), by Lemma [1], we have \( \omega = \pi/\pi_h \propto \pi^{1-2a} Z^{-1} \). Ignoring the term \( Z^{-1} \) (which behaves like a random noise for the reason explained above), we see that if \( a > 1/2 \), states with negligible posterior probabilities can receive exceedingly large importance weights, which can cause the estimator (3) to converge very slowly. To confirm this, we construct a toy example below.

**Example 1.** Let \( X = \{0, 1, \ldots, p\} \) and \( \pi(x) \propto r^x \) for some \( r \) such that \( r \to \infty \) as \( p \to \infty \). Let \( N(x) = \{ y \in X: |x-y| = 1 \} \). Consider Algorithm [1] with \( h(u) = u^a \) for some \( a > 0 \). Some routine calculations give \( \pi(x) \sim r^{x-p}, 2\pi_h(x) \sim r^{2(x+1-p)a} \) for \( x \leq p-1 \) and \( \pi_h(p) \sim 1/2 \), where \( \sim \) denotes asymptotic equivalence as \( p \to \infty \). Hence, \( \omega(0) = \pi(0)/\pi_h(0) \sim 2r^{(2a-1)p-2a} \). If \( a > 1/2 \), \( \omega(0) \) grows super-exponentially with \( p \), which causes the chain \( Q_h \) (to be defined in Lemma [2]) to mix slowly.

### 2.3 Measuring Rates of Convergence

Given an irreducible and reversible transition matrix \( P \), we can denote its eigenvalues by \( 1 = \lambda_1(P) > \lambda_2(P) \geq \cdots \geq \lambda_{|X|}(P) \geq -1 \), and define its spectral gap by \( \text{Gap}(P) = 1 - \lambda_2(P) \). If \( P \) is aperiodic, \( \text{Gap}(P) \) is the asymptotic rate of convergence to the stationary distribution, and \( 1/\text{Gap}(P) \) can be interpreted as the “average-case mixing time” [Aldous and Fill, 2002, Page 114]. If \( Q \) is the transition rate matrix of an irreducible and reversible continuous-time Markov chain, it has eigenvalues \( 0 = \lambda_1(Q) > \lambda_2(Q) \geq \cdots \geq \lambda_{|X|}(Q) \), and we define its spectral gap by \( \text{Gap}(Q) = -\lambda_2(Q) \). The interpretations of \( \text{Gap}(Q) \) are essentially the same as those of \( \text{Gap}(P) \).
Though the performance of the IIT estimator partially depends on the mixing rate of $K_h$, $\text{Gap}(K_h)$ does not reflect the overall efficiency of IIT since it does not take into account the importance weights. But if we replace $\omega(x^{(k)})$ in (3) with an exponential random variable with mean $\omega(x^{(k)})$, we obtain the (unweighted) time average of a continuous-time Markov chain. This motivates us to use the spectral gap of this new chain, which we denote by $Q_h$, to measure the “convergence rate” of IIT. The importance weight of state $x$, $\omega(x)$, becomes the average holding time at state $x$ of the chain $Q_h$. The following result was proved in Zanella and Roberts [2019, Lemma 2] for TGS by using a variational characterization of the asymptotic variance [Andrieu and Vihola, 2016]. We give a different proof in the appendix.

**Lemma 2.** Consider the setting of Algorithm 1. Define a transition rate matrix $Q_h$ by

$$Q_h(x, y) = \begin{cases} 
K_h(x, y)/\omega(x), & \text{if } x \neq y, \\
-\sum_{x' \neq x} Q_h(x, x'), & \text{if } x = y,
\end{cases}$$

(4)

where $\omega = \pi/\pi_h$. Let $x^{(1)}, \ldots, x^{(t)}$ be samples generated from $K_h$. Consider the estimator $\hat{f}(t, \omega)$ defined in (3) for some function $f$ such that $E_{\pi}[f] = 0$. Then, $\sqrt{\hat{f}(t, \omega)} \xrightarrow{D} N(0, \sigma^2)$ where $D$ denotes the convergence in distribution and $\sigma^2 \leq 2E_{\pi}[f^2]/\text{Gap}(Q_h)$.

**Remark 3.** We call $\sigma^2$ the asymptotic variance of the estimator $\hat{f}(t, \omega)$. Analogously, the asymptotic variance of an unweighted time average of a discrete-time Markov chain $P$ can be bounded by $E_{\pi}[f^2]/\text{Gap}(P)$ [Rosenthal, 2003, Proposition 1]. So henceforth, we use $\text{Gap}(Q_h)$ to measure the convergence rate of Algorithm 1 and similarly, the convergence rate of RWMH is measured by the spectral gap of its transition matrix.

## 3 Spectral gap bounds for informed importance tempering

### 3.1 Scenario I: Single Best Model

Sampling from continuous unimodal distributions has been extensively studied in the literature; see, for example, Jarner and Yuen [2004], Mangoubi and Smith [2017], Johndrow and Smith [2018] for results related to MCMC algorithms and Saumard and Wellner [2014, Section 9.10] for more references on sampling from log-concave distributions (log-concavity can be seen as a stronger notion of unimodality). In our setting, the state space $\mathcal{X}$ is finite, and thus “unimodal” means that there exists a point $x^* \in \mathcal{X}$ such that for any $x \neq x^*$, we have $\max_{y \in \mathcal{N}(x)} \pi(y) > \pi(x)$. Consider the following unimodal scenario.

**Assumption 1.** Let $|\mathcal{X}| < \infty$, $\pi(x) > 0$ for each $x$, and $\mathcal{N}$ be a symmetric neighborhood mapping such that $\max_{x \in \mathcal{X}} |\mathcal{N}(x)| \leq p^\alpha$ for some $\alpha > 0$ and $p > 1$. There exist a point
Let \( x^* \in X \), an operator \( T: X \to X \) and some constant \( \nu > \alpha \) such that \( T(x) \in \mathcal{N}(x) \) and \( \pi(T(x)) \geq p^\nu \pi(x) \) for each \( x \neq x^* \).

For high-dimensional model selection problems, \(|X| \) usually grows super-polynomially with \( p \), but most MCMC samplers used in practice are “local” in the sense that the neighborhood size grows only polynomially with \( p \). The state \( x^* \) represents the “true” model (more precisely, \( x^* \) is often defined as the model that contains all the signals that exceed some threshold). We expect that Assumption 1 can be established asymptotically under certain mild conditions if the “true” model can be defined uniquely (\( \alpha, \nu \) are treated as universal constants independent of \( p \)), and the state \( T(x) \) is typically chosen such that it looks “more similar” to \( x^* \) than \( x \) does. Thus, Assumption 1 can be seen as a consistency property of the model selection procedure. It was verified in [Yang et al., 2016] for variable selection and in [Zhou and Chang, 2021] for sparse structure learning. Distributions that satisfy Assumption 1 can still look very irregular due to the dependence among the \( p \) variables.

It is known that when the unique mode is “sufficiently sharp”, we can bound the spectral gap of a reversible Markov chain using “canonical paths” [Sinclair, 1992]. Lemma 3 below is a slight improvement on the bound given in [Zhou and Chang, 2021, Theorem 1] (see also [Yang et al., 2016]). It can be used to quickly find spectral gap bounds for some locally balanced IIT schemes.

**Lemma 3.** Suppose Assumption 1 holds. For any transition matrix \( P \) or transition rate matrix \( Q \) that is irreducible and reversible with respect to \( \pi \), we have

\[
\text{Gap}(P) \geq \kappa(p, \alpha, \nu) \min_{x \neq x^*} P(x, T(x)), \quad \text{where} \quad \kappa(p, \alpha, \nu) = \frac{1}{2} \left\{ 1 - p^{-1} \right\}^{\frac{3}{2}},
\]

and \( \text{Gap}(Q) \geq \kappa(p, \alpha, \nu) \min_{x \neq x^*} Q(x, T(x)) \).

**Remark 4.** Lemma 3 is non-asymptotic. For high-dimensional model selection problems, we can consider the asymptotic regime where \( p \to \infty \) and \( \nu > \alpha \) are fixed constants. Then, by Lemma 3, the convergence rate of an MCMC algorithm has the same order as the minimum transition probability/rate from \( x \) to \( T(x) \). For RWMH, one can use Lemma 3 to show that its convergence rate is \( O(p^{-\alpha}) \). Since each IIT iteration has complexity \( O(p^\alpha) \), we need \( Q_h(x, T(x)) \geq c \) for some universal constant \( c \) so that the “real-time convergence rate” of IIT is at least as fast as that of RWMH.

**Theorem 1.** Suppose Assumption 1 holds and let \( \kappa(p, \alpha, \nu) \) be as given in Lemma 3. For Algorithm 2 with some non-decreasing balancing function \( h \), we have

\[
\text{Gap}(Q_h) \geq \kappa(p, \alpha, \nu) \frac{h(p^\nu)}{E_{\pi}[Z_h]}.
\]
where $Q_h$ is as defined in (4). Further, for the three balancing functions defined in (2), we have

\[
\frac{2\text{Gap}(Q_h)}{\kappa(p, \alpha, \nu)} \geq \begin{cases} 
    p^{\nu - \alpha}, & \text{if } h = h_{+1}, \\
    p^{\nu - 2\alpha}, & \text{if } h = h_{\land 1}, \\
    p^{\nu/2} / (p^{2\alpha - \nu} + p^{\alpha - \nu/2}), & \text{if } h = h_{0.5}.
\end{cases}
\]

Theorem 1 provides the theoretical guarantee for the scalability of IIT schemes when the posterior mass concentrates on just one model $x^*$. Consider $h_{+1}$ for example, which was used by the TGS algorithm for variable selection proposed in [Zanella and Roberts 2019, Section 4.2]. Theorem 1 suggests that the real-time convergence rate of TGS is $O(p^{\nu - 2\alpha})$ under Assumption 1, which is always faster than that of RWMH by Remark 4. This result partly explains why it was observed in [Zanella and Roberts 2019] that TGS can have significantly better performance than RWMH (for variable selection). If $\nu > 2\alpha$ (which can easily happen if the sample size is sufficiently large), $h_{0.5}$ is as efficient as $h_{+1}$.

One may find Theorem 1 to be counter-intuitive. If $\nu > 2\alpha$, our bound implies that the IIT scheme $h_{+1}$ converges even faster (in real time) for larger $p$. To gain insights into this surprising phenomenon, recall that for locally balanced IIT schemes the importance weight $\pi_h / \pi \propto Z_h^{-1}$.

For $h = h_{+1}$, under Assumption 1, $Z_h(x) \geq p^\nu$ for any $x \neq x^*$ while $Z_h(x^*) \approx p^{\alpha}$; that is, $x^*$ receives a much larger importance weight than any other state. Consequently, the estimator $\hat{f}(t, \pi_h)$ defined in (3) becomes almost a constant (i.e., variance gets reduced to almost zero) once the chain visits $x^*$, which should happen quickly due to the use of informed proposals. Essentially, when $\nu$ is sufficiently large, an IIT sampler can behave just like a single best model selection procedure due to the importance weighting.

3.2 Scenario II: Two Best Models

The excellent scalability of IIT demonstrated by Theorem 1 needs to be taken with a grain of salt. If the posterior mass concentrates on more than one “good” models, IIT has to visit all those good models many times in order to reduce the variance of the estimator $\hat{f}$ given in (3); as a result, importance weighting can no longer boost the sampler’s efficiency as significantly as under Assumption 1. Consider the following setting which differs from Assumption 1 only in that now we have two equivalent “true” models $x^*_1$ and $x^*_2$; assume they are also neighbors. This happens, for example in structure learning, when there are equivalent models that cannot be distinguished by the data likelihood.

**Assumption 2.** Let $\mathcal{X}, \pi, \mathcal{N}$ be as given in Assumption 1. There exist two points $x^*_1 \in \mathcal{X}$ and $x^*_2 \in \mathcal{N}(x^*_1)$ with $\pi(x^*_1) = \pi(x^*_2)$, an operator $T : \mathcal{X} \to \mathcal{X}$ and some constant $\nu > \alpha$ such that $T(x) \in \mathcal{N}(x)$ and $\pi(T(x)) \geq p^\nu \pi(x)$ for each $x \in \mathcal{X} \setminus \{x^*_1, x^*_2\}$. 

Remark 5. One can extend Assumption 1 and Lemma 3 to more general settings where the posterior mass concentrates on a set of states using “state decomposition” [Madras and Randall, 2002; Guan and Krone, 2007]. Assumption 2 is used here mainly for convenience of presentation. As we see in Theorem 2 below, though Assumption 2 does not appear to be a much more challenging setting than Assumption 1, it changes the spectral gap bounds for locally balanced IIT schemes drastically.

Theorem 2. Suppose Assumption 2 holds and let $\kappa'(p, \alpha, \nu) = (1 - 4p^{-(\nu-\alpha)/2})/4$. Consider Algorithm 1 and $Q_h$ defined in (4). For the three balancing functions defined in (2), we have

$$\frac{\text{Gap}(Q_h)}{\kappa'(p, \alpha, \nu)} \geq \begin{cases} p^{-\alpha}, & \text{if } h = h_{+1}, \\ (4p^{2\alpha-\nu} + 1)^{-1}, & \text{if } h = h_{\Lambda 1}, \\ (2p^{2\alpha-\nu} + 2p^{\nu}/2 + 1)^{-1}, & \text{if } h = h_{0.5}. \end{cases}$$

Interestingly, in Theorem 1, $h_{+1}$ is the most efficient among the three balancing functions considered, while in Theorem 2 it is the worst. The problem of this proposal in the setting of Assumption 2 is that the chain cannot move quickly between $x_1^*$ and $x_2^*$. When $h = h_{+1}$, we have $K_h(x_1^*, x_2^*) \approx 2/p^{2\alpha}$, and thus $\text{Gap}(Q_h)$ may have the same order as the spectral gap of RWMH, which suggests that RWMH would perform much better in reality since each iteration of RWMH runs much faster. For the other two choices $h_{\Lambda 1}$ and $h_{0.5}$, we have $\text{Gap}(Q_h) \gtrsim c$ for some universal constant $c$ if Assumption 2 holds for some $\nu > 2\alpha$. So Theorem 2 suggests that when the posterior mass concentrates on more than one models, the IIT schemes $h_{\Lambda 1}$ and $h_{0.5}$ tend to have better scalability than the scheme $h_{+1}$.

4 A numerical example

We present a simulation study which helps illustrate the key points of our theory. Let $\mathcal{X}$ be the collection of all possible permutations of $\{1, \ldots, p\}$. For each $\tau \in \mathcal{X}$, let $\tau(i)$ be the index of the variable that has the $i$-th position in $\tau$ and $\tau^{-1}(k)$ be the ranking of the $k$-th variable. Assume that $\pi(\tau) \propto \prod_{k=1}^{p} W(k, \tau^{-1}(k))$, where $W: \mathcal{X}^2 \to \mathbb{R}_+$ is a positive matrix. This problem was called “weighted permutations” in Zanella [2020]. For applications in statistics, we can think of $\pi$ as an approximate representation of the target posterior distribution of order-based MCMC methods in structure learning [Friedman and Koller, 2003; Agrawal et al., 2018]. We assume that

$$\log W(k, j) = -\eta \phi_k |j - \mu_k| \log p, \quad \forall j, k \in \{1, \ldots, p\},$$

for some $\eta > 0$, $\phi_k > 0$ and $\mu_k \in [1, p]$. We interpret $\eta$ as the signal-to-noise ratio (SNR). Let $\mathcal{N}(\tau)$ be the set of all permutations that can be obtained from $\tau$ by a transposition; thus,
$|\mathcal{N}(\tau)| = p(p-1)/2$. We consider two scenarios where $\pi$ has one unique mode at $\tau^* = (1,\ldots,p)$. In the first “strongly unimodal” scenario, we draw $\mu_k \sim \text{Unif}(k-0.1, k+0.1)$ and $\phi_k \sim \text{Unif}(0.5, 1)$. In the second “weakly unimodal” scenario, we draw $\mu_k \sim \text{Unif}(k-0.5, k+0.5)$ and $\phi_k \sim \text{Unif}(0.1, 1)$ so that $\pi$ is “flatter” and states in $\mathcal{N}(\tau^*)$ can have posterior probabilities comparable to $\pi(\tau^*)$. We choose $p = 100$, and for each scenario, we generate two instances of $\pi$, one with $\eta = 1$ and the other with $\eta = 2$.

We use simulation to compare the performance of six samplers, including RWMH and Algorithm 1, with the following five choices of $h$: $h_{+1}, h_{\wedge 1}, h_{0.5}, h_{0.3}(u) = u^{0.3}$ and $h_{0.4}(u) = u^{0.4}$. For each choice of $h$, the stationary distribution of the IIT chain, $\pi_h$, can be calculated by Lemma 1. Let $f_k(\tau) = \tau^{-1}(k)$ and consider the estimator $\hat{f}_k(t, \omega)$ defined in (3) for each $k \in \{1,\ldots,p\}$ (for RWMH, $\omega \equiv 1$, and for IIT samplers, $\omega = \pi/\pi_h$). The number of iterations $t$ is chosen to be $7 \times 10^5$ for RWMH and $10^3$ for each IIT sampler so that the wall time used by each algorithm is about the same (the code is written in R). For each instance of $\pi$, we run each sampler 100 times and then calculate the variance of $\hat{f}_k$ for each $k$. Boxplots for $\{\text{Var}(\hat{f}_k)\}_{k=1}^p$ are shown in Figure 1. As is consistent with our theory, the IIT scheme $h_{+1}$ is most sensitive to the unimodality of $\pi$. It is worse than RWMH when the posterior mass does not concentrate on $\tau^*$ alone. For all the IIT schemes considered, their performance is better when $\pi$ has a sharper mode. In the weakly unimodal case with SNR = 1, only the IIT scheme $h_{0.5}$ is arguably slightly better than RWMH, and the IIT schemes $h_{+1}, h_{\wedge 1}$ and $h_{0.3}$ are clearly less efficient than RWMH. But when SNR increases to 2, IIT schemes $h_{0.3}, h_{0.4}, h_{0.5}$ all perform significantly better than RWMH. In the strongly unimodal settings, the advantage of IIT schemes is overwhelming.

Figure 1: Each plot corresponds to one instance of $\pi$ for the “weighted permutation” problem with $p = 100$. Each box gives the empirical distribution of $\{\text{Var}(\hat{f}_k)\}_{k=1}^p$ for one sampler, where $\text{Var}(\hat{f}_k)$ is calculated from 100 independent runs of the algorithm. Each RWMH run has $7 \times 10^5$ iterations, which takes about 10.3 seconds; each IIT run has $10^3$ iterations, which takes about 10.1 seconds.
5 Discussion

Overall, the theory developed in this note advocates the use of informed MCMC methods for model selection problems. When one has enough parallel computing resources, informed samplers are even more appealing since the time complexity of each informed iteration can be greatly reduced by parallelizing the evaluation of $\pi$ for neighboring states. IIT has two main advantages over other informed MCMC methods or MCMC importance sampling algorithms. First, the chain $K_h$ often mixes quickly since it is informed, and it never gets stuck at a single state. In contrast, the performance of an informed MH algorithm largely depends on the acceptance rate, which can be very difficult to control [Zhou et al., 2021]; the same concern applies to other importance sampling schemes built on MH chains [Geyer and Thompson, 1995, Rudolf and Sprungk, 2020, Schuster and Klebanov, 2020]. Second, if the informed proposal is chosen properly, the distribution $\pi_h$ looks similar to $\pi$, making the importance weighting scheme efficient.

From Theorems 1 and 2 and the simulation study, we see that the balancing function $h_{0.5}$ appears to be the best choice. We offer two intuitive explanations. First, consider a state $x$ and some $y \in \mathcal{N}(x)$ such that $\pi(y) \gg \pi(x')$ for any other $x' \in \mathcal{N}(x)$. Then, neither $h_{+1}$ nor $h_{-1}$ can ensure that the proposal probability $K_h(x, y)$ is always sufficiently large, while $h_{0.5}$ does (recall Remark 1). Second, among the class of informed proposals with $h(u) = u^a$, the choice $a = 0.5$ tends to yield the most efficient importance weighting. The problem of the choice $a > 0.5$ was discussed in Example 1. We tried $h(u) = u^{0.6}$ in the simulation study, but the result was too poor and thus not shown in Section 4. If $a < 0.5$, the informed proposal explores posterior modes less efficiently than that with $a = 0.5$ (in the extreme case $a = 0$, $K_h$ becomes the random walk proposal). The theory developed in a recent work of Gagnon and Maire [2020] may be used to obtain some “optimality” result regarding the choice of $h$. Finally, we want to emphasize that in order to design a scalable sampler for a specific statistical problem, a theoretical understanding about how the posterior looks like is perhaps most important. It can help us choose the neighborhood function, determine whether an advanced sampling algorithm is necessary (e.g. if the posterior is very flat, RWMH may be good enough), and tweak an existing sampler to maximize its efficiency. For example, Zanella and Roberts [2019] improved the performance of TGS substantially by devising a coordinate-weighting scheme specific to the variable selection problem.
Appendix

A1 Tempered Gibbs samplers

We first review the generic TGS algorithm introduced in Zanella and Roberts [2019] Section 2. Let $\mathcal{X} = \mathcal{X}_1 \times \cdots \times \mathcal{X}_p$ be a product space. For convenience, we still assume $|\mathcal{X}| < \infty$. Define $\mathcal{N}(x) = \bigcup_{i=1}^{p} \mathcal{N}_i(x)$ where $\mathcal{N}_i(x) = \{y \in \mathcal{X}: y_j = x_j, \forall j \neq i\}$. That is, $\mathcal{N}_i(x)$ is the set of all states which can only differ from $x$ at the $i$-th coordinate. (Note that this definition is slightly different from the setting considered in the main text in that we assume $x \in \mathcal{N}_i(x)$ here.) Let $\pi(x_i | x_{-i})$ denote the conditional density of the $i$-th coordinate given $x_{-i} = (x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_p)$. For each $i$ and each possible value of $x_{-i}$, let $g(x_i | x_{-i})$ denote a conditional "proposal" distribution for the $i$-th coordinate with support $\mathcal{N}_i(x)$. TGS is a Markov chain with transition matrix $K_{TGS}(x, y) = 0$ if $y \notin \mathcal{N}(x)$, and

$$K_{TGS}(x, y) \propto \frac{g(x_i | x_{-i})g(y_i | x_{-i})}{\pi(x_i | x_{-i})}, \quad \forall y \in \mathcal{N}_i(x).$$

In Zanella and Roberts [2019] Section 3.6, TGS was further generalized by introducing coordinate weight functions $\xi_i(x_{-i})$ for each $(i, x_{-i})$. The transition matrix of the weighted TGS scheme is given by

$$K_{WTGS}(x, y) \propto \xi_i(x_{-i})\frac{g(x_i | x_{-i})g(y_i | x_{-i})}{\pi(x_i | x_{-i})}, \quad \forall y \in \mathcal{N}_i(x).$$

Denote the right-hand side of the above equation by $H(x, y)$. One can check that $\pi(x)H(x, y) = \pi(y)H(y, x)$. It follows that $K_{WTGS}$ is reversible w.r.t. $\pi Z$ where $Z(x) = \sum_{y \in \mathcal{N}(x)} H(x, y)$, and $Z^{-1}(x)$ is the importance weight associated with $x$.

Consider the variable selection problem where $\mathcal{X} = \{0, 1\}^p$, and define

$$y^{(i)}(x) = (x_1, \ldots, x_{i-1}, 1 - x_i, x_{i+1}, \ldots, x_p), \quad i = 1, \ldots, p. \quad (5)$$

Redefine the neighborhood of $x$ by $\mathcal{N}(x) = \{y^{(1)}(x), \ldots, y^{(p)}(x)\}$ which does not include $x$. Suppose that the proposal $g(x_i | x_{-i})$ can be written as $g'(\pi(x_i | x_{-i}))$ for some function $g': \mathbb{R}_+ \to \mathbb{R}_+$. Observe that $\pi(x_i | x_{-i}) = \pi(x)/[\pi(x) + \pi(y^{(i)}(x))]$. Consider a balancing function

$$h(u) = (1 + u)g'(1/(1 + u))g'(u/(1 + u)),$$

and let $K_h$ be as given in (1). Then, for $y = y^{(i)}(x)$, we have

$$K_h(x, y) \propto \left(1 + \frac{\pi(y)}{\pi(x)}\right)g'\left(\frac{\pi(x)}{\pi(x) + \pi(y)}\right)g'\left(\frac{\pi(y)}{\pi(x) + \pi(y)}\right) = \frac{g(x_i | x_{-i})g(y_i | x_{-i})}{\pi(x_i | x_{-i})},$$

which is a TGS scheme. Zanella and Roberts [2019] Section 4.2] used the above transition matrix $K_h$ with $g' \equiv 1$ (that is, $h(u) = 1 + u$).
A2 Proof of Lemma 2

Proof. Without loss of generality, we can assume that \( x^{(0)} \) is generated from \( \pi_h \), since the limiting distribution of the estimator \([\text{Douc et al., 2018}, \text{Chapter 22.5}]\) does not depend on the initial distribution. Let \( W^{(0)}, W^{(1)}, \ldots, W^{(t)} \) denote random variables such that given \( x^{(k)} \), \( W^{(k)} \) is an exponential random variable with mean \( \omega(x^{(k)}) \) and independent of everything else. Define

\[
\hat{f}_Q(T_m) = \sum_{k=0}^{m} \frac{f(x^{(k)})W^{(k)}}{T_m}, \quad \text{where} \quad T_m = \sum_{k=0}^{m} W^{(k)}.
\]

Now one can see that Proposition 5 of [Deligiannidis and Lee, 2018] differs from our setting only in that the former assumes each \( W^{(k)} \) is geometrically distributed [c.f. Doucet et al., 2015, Proposition 2]. So, we can apply their argument. Since \( \omega = \frac{\pi}{\pi_h} \), by the law of large numbers and central limit theorem for ergodic Markov chains [Haggström and Rosenthal, 2007, Corollary 6],

\[
\frac{1}{t} \sum_{k=1}^{t} \omega(x^{(k)}) \overset{a.s.}{\rightarrow} \mathbb{E}_{\pi_h}[\omega] = 1, \quad \frac{1}{\sqrt{t}} \sum_{k=1}^{t} f(x^{(k)})\omega(x^{(k)}) \overset{D}{\rightarrow} N(0, \sigma^2),
\]

where

\[
\sigma^2 = \lim_{t \to \infty} t^{-1} \text{Var} \left( \sum_{k=1}^{t} f(x^{(k)})\omega(x^{(k)}) \right).
\]

It then follows from Slutsky’s theorem that \( \sqrt{t} \hat{f}(t, \omega) \overset{D}{\rightarrow} N(0, \sigma^2) \). Similarly, by a standard conditioning argument and treating \((f(x^{(k)}), W^{(k)})\) as a bivariate Markov chain, we obtain that \( \sqrt{T_m} \hat{f}_Q(T_m) \overset{D}{\rightarrow} N(0, \sigma^2_c) \) as \( m \to \infty \), where

\[
\sigma^2_c = \lim_{t \to \infty} t^{-1} \text{Var} \left( \sum_{k=1}^{t} f(x^{(k)})W^{(k)} \right).
\]

But \( \hat{f}_Q(T_m) \) is just the time average of the continuous-time Markov chain \( Q_h \) at time \( T_m \). Thus, by standard results (see, for example, Aldous and Fill [2002, Proposition 4.29]),

\[
\sigma^2_c \leq \frac{\mathbb{E}_\pi[f^2]}{\text{Gap}(Q_h)}.
\]
So it only remains to compare \( \sigma^2 \) with \( \sigma_c^2 \). A direct calculation using conditioning yields that
\[
\mathbb{E}_{\pi_h} \left[ \sum_{k=1}^{t} f(x^{(k)})W^{(k)} - \mathbb{E}_{\pi_h} \left[ \sum_{k=1}^{t} f(x^{(k)})\omega(x^{(k)}) \right]^2 \right] = t \mathbb{E}_{\pi_h} \left[ f(X)^2W^2 - f(X)^2\omega(X)^2 \right] - \mathbb{E}_{\pi} [f^2\omega],
\]
Hence, \( \sigma^2 = \sigma_c^2 - \mathbb{E}_{\pi} [f^2\omega] \), from which the result follows. \( \square \)

### A3 Proof of Lemma 3

**Proof.** We first show that it suffices to prove the claim for \( Gap(P) \). Let \( b = \max_{x \in \mathcal{X}} Q(x, x) \), which is finite since \( |\mathcal{X}| < \infty \). Then \( P = b^{-1}Q + I \) is the transition matrix of a discrete-time Markov chain such that \( Gap(Q) = b Gap(P) \), which is still irreducible and reversible w.r.t. \( \pi \). Since \( x \neq T(x) \), we have \( P(x, T(x)) = b^{-1}Q(x, T(x)) \). Thus, if \( Gap(P) \geq \kappa(p, \alpha, \nu) \min_{x \neq x^*} P(x, T(x)) \), the same bound holds for \( Gap(Q) \) with \( P \) replaced by \( Q \).

Our proof for \( Gap(P) \) is conceptually similar to the analysis of the birth-death chain given in [Kahale 1997, Section 3]. Without loss of generality, we can assume that \( P(x, T(x)) > 0 \), since otherwise the spectral gap bound holds trivially. Set \( T(x^*) = x^* \) to avoid ambiguity.

Let \( (\mathcal{X}, T) \) be the bidirected graph with node set \( \mathcal{X} \) and edge set \( \mathcal{E}(T) = \{(x, y) \in \mathcal{X}^2 : x \neq y, \text{ and } y = T(x) \text{ or } x = T(y)\} \), which implies \((x, y) \in \mathcal{E}(T)\) if and only if \((y, x) \in \mathcal{E}(T)\).

Observe that \((\mathcal{X}, T)\) is a tree, and thus for any \( x \neq y \), there exists one unique directed path without repeated edges that starts at \( x \) and ends at \( y \); denote this path by \( \gamma(x, y) \). We use the notation \( e \in \gamma \) to mean that the path \( \gamma \) traverses the edge \( e \).

Given an edge \( e = (z, w) \in \mathcal{E}(T) \), we define its load by
\[
\rho(e) = \pi(z)P(z, w) = \pi(w)P(w, z).
\]
The second equality holds since \( P \) is reversible. Define the “length” of this edge by
\[
\ell(e) = \{\pi(z) \wedge \pi(w)\}^{-q}, \quad q = \frac{\nu - \alpha}{2\nu}.
\]
(7)

For any directed path \( \gamma \), let \( |\gamma|_\ell = \sum_{e \in \gamma} \ell(e) \) denote the “length” of the path. Note that for any \( x \neq x^* \), there exists some \( d = d(x) < \infty \) such that \( \gamma(x, x^*) = (x, T(x), \ldots, T^{d(x)}) \). It follows that
\[
|\gamma(x, x^*)|_\ell = \sum_{e \in \gamma(x, x^*)} \ell(e) = \sum_{k=0}^{d-1} \pi(T^k(x))^{-q} \leq \sum_{k=0}^{d-1} \pi(x)^{-q} p^{-kq} \leq \frac{\pi(x)^{-q}}{1 - p^{-\nu q}},
\]
where $T^0(x)$ denotes $x$ itself. For any $x \neq y$, we can bound the length of $\gamma(x, y)$ by

$$|\gamma(x, y)|_\ell \leq |\gamma(x, x^*)|_\ell + |\gamma(y, x^*)|_\ell \leq \frac{\pi(x)^{-q} + \pi(y)^{-q}}{1 - p^{-\nu q}}.$$  \hspace{1cm} (8)

By Saloff-Coste [1997, Theorem 3.2.3],

$$\text{Gap}(P)^{-1} \leq \max_{e \in \mathcal{E}(T)} \left\{ \frac{1}{p(e)\ell(e)} \sum_{(x,y): e \in \gamma(x,y)} \pi(x)\pi(y)|\gamma(x,y)|_\ell \right\}.$$  \hspace{1cm} (9)

The rest of the argument is similar to the proof of Theorem 1 of Zhou and Chang [2021]. To bound the right-hand side of the above inequality, by symmetry, it suffices to consider edges $e = (z, w)$ such that $w = T(z)$. Fix an arbitrary $z \neq x^*$ and let $w = T(z)$. Let $\mathcal{A}(z) = \{x \in \mathcal{X} : T^k(x) = z \text{ for some } k \geq 0 \}$ denote all the “ancestors” of $z$ (including $z$ itself). Recalling that $(\mathcal{X}, T)$ is a tree, one can show that $e = (z, w) \in \gamma(x, y)$ only if $x \in \mathcal{A}(z)$ and $y \notin \mathcal{A}(z)$. Hence, by (8),

$$\sum_{(x,y) : e \in \gamma(x,y)} \pi(x)\pi(y)|\gamma(x,y)|_\ell \leq \frac{1}{1 - p^{-\nu q}} \sum_{x \in \mathcal{A}(z)} \sum_{y \notin \mathcal{A}(z)} \left\{ \pi(x)^{1-q}\pi(y) + \pi(x)\pi(y)^{1-q} \right\}$$

$$\leq \frac{2}{1 - p^{-\nu q}} \sum_{x \in \mathcal{A}(z)} \sum_{y \notin \mathcal{A}(z)} \pi(x)^{1-q}\pi(y)^{1-q}.$$

The assumption $|\mathcal{N}(x)| \leq p^a$ and the reversibility of $P$ imply that $|\{y \in \mathcal{X} : T(y) = x\}| \leq p^a$. Thus,

$$\sum_{x \in \mathcal{A}(z)} \pi(x)^{1-q} \leq \sum_{h=0}^{\infty} \pi(z)^{1-q}p^{(\alpha - \nu(1-q))k} \leq \frac{\pi(z)^{1-q}}{1 - p^{a-\nu(1-q)}} = \frac{\pi(z)^{1-q}}{1 - p^{-(\nu-\alpha)/2}}.$$  \hspace{1cm} (10)

Plugging these inequalities into (9), we obtain that

$$\text{Gap}(P)^{-1} \leq \max_{z \neq x^*} \frac{2}{\{1 - p^{-(\nu-\alpha)/2}\}^2} P(z, T(z))^{-1},$$

which yields the asserted spectral gap bound. \hfill \Box

### A4 Proof of Theorem 1

**Proof.** From Lemma 1 we know that for a balancing function $h$, we have $\pi_h \propto \pi Z_h$, which can be equivalently expressed as $\pi_h(x) = \pi(x) Z_h(x)/\mathbb{E}_\pi[Z_h]$. Hence, for any $y \neq x$,

$$Q_h(x,y) = \frac{\pi_h(x) h(\pi(y)/\pi(x))}{\pi(x) Z_h(x)} = \frac{h(\pi(y)/\pi(x))}{\mathbb{E}_\pi[Z_h]}.$$  \hspace{1cm} (11)

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If \( h \) is non-decreasing, we have \( Q_h(x,T(x)) \geq h(p^\alpha)/E_{\pi}[Z_h] \) under Assumption 1. Let \( I_h(x,y) = \pi(x)h(\pi(y)/\pi(x)) = I_h(y,x) \). Then,
\[
E_{\pi}[Z_h] = \sum_{x \in \mathcal{X}} \pi(x)Z_h(x) = \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{N}(x)} I_h(x,y). \tag{12}
\]

Since \( \mathcal{N} \) is symmetric, \( E_{\pi}[Z_h] \) is twice the sum of \( I_h(x,y) \) over all unordered pairs of neighbors. Now we bound \( E_{\pi}[Z_h] \) for the three choices of \( h \) separately, from which the asserted bounds on \( \text{Gap}(Q_h) \) follow.

**Case 1:** \( h(u) = 1+u \). We have \( I_h(x,y) = \pi(x) + \pi(y) \). Since each \( x \) has at most \( p^\alpha \) neighbors,
\[
E_{\pi}[Z_h] = 2 \sum_{x \in \mathcal{X}} |\mathcal{N}(x)|\pi(x) \leq 2p^\alpha.
\]

**Case 2:** \( h(u) = 1 \wedge u \). We have \( I_h(x,y) = \pi(x) \wedge \pi(y) \). For any \( x \neq x^* \), \( \pi(x) \) can appear in the summation in (12) at most \( 2|\mathcal{N}(x)| \) times. But \( \pi(x^*) \) cannot appear in the summation since \( x^* \) is the mode. By a calculation similar to (10), we find that \( \pi(x^*) \geq 1 - p^{\alpha-\nu} \) under Assumption 1. Thus,
\[
E_{\pi}[Z_h] \leq 2 \sum_{x \neq x^*} |\mathcal{N}(x)|\pi(x) \leq 2p^\alpha(1 - \pi(x^*)) \leq 2p^{2\alpha-\nu}.
\]

**Case 3:** \( h(u) = \sqrt{u} \). We have \( I_h(x,y) = \sqrt{\pi(x)\pi(y)} \leq (\pi(x) + \pi(y))/2 \). Applying this inequality to any pair of neighbors that does not involve \( x^* \), we obtain from (12) that
\[
E_{\pi}[Z_h] \leq 2 \sum_{x \neq x^*} |\mathcal{N}(x)|\pi(x) + 2 \sum_{y \in \mathcal{N}(x^*)} \sqrt{\pi(x)\pi(y)}.
\]

Since for any \( x \neq x^* \), \( \pi(x) \leq p^{-\nu} \) under Assumption 1 we have
\[
E_{\pi}[Z_h] \leq 2p^{2\alpha-\nu} + 2p^{\alpha-\nu/2},
\]
which completes the proof. \( \square \)

### A5 Proof of Theorem 2

We first prove an auxiliary lemma.

**Lemma A1.** Suppose Assumption 2 holds. For any transition matrix \( P \) or transition rate matrix \( Q \) that is irreducible and reversible with respect to \( \pi \), we have
\[
\text{Gap}(P) \geq \kappa'(p,\alpha,\nu) \min_{x \neq x^*} P(x,T(x)), \quad \text{where} \quad \kappa'(p,\alpha,\nu) = \frac{1 - 4p^{-(\nu-\alpha)/2}}{4},
\]
and \( \text{Gap}(Q) \geq \kappa(p,\alpha,\nu) \min_{x \neq x^*} Q(x,T(x)) \).
Proof. Define $T(x_1^*) = x_2^*$ and $T(x_2^*) = x_2^*$; that is, we treat $x_2^*$ as the central state, which plays the same role as $x^*$ in the proof of Lemma [3]. Then apply the path argument used to prove Lemma [3] with the same length function $\ell$. Note that we can bound $|\gamma(x, x_2^*)|_\ell$ by

$$|\gamma(x, x_2^*)|_\ell \leq \frac{\pi(x)^{-q}}{1 - 2p^{-\nu q}},$$

which takes into account the fact that $\gamma(x, x_2^*)$ may traverse the edge $(x_1^*, x_2^*)$. Another inequality which needs to be modified concerns $\sum_y \pi(y)^{1-q}$. Now we have

$$\sum_{y \in \mathcal{A}} \pi(y)^{1-q} \leq \pi(x_2^*)^{1-q} + \sum_{x \in A(x_1^*)} \pi(x)^{1-q} \leq \frac{\pi(x_2^*)^{1-q}}{1 - p^{-(\nu - \alpha)/2}} \leq \frac{2}{1 - p^{-(\nu - \alpha)/2}}.$$

Using the above two displayed inequalities, we obtain that

$$\sum_{(x, y): e \in \gamma(x, y)} \pi(x)\pi(y)|\gamma(x, y)|_\ell \leq \frac{2}{1 - 2p^{-\nu q}} \sum_{x \in A(x)} \sum_{y \in A(x^*)} \pi(x)^{1-q}\pi(y)^{1-q} \leq \frac{4\pi(z)^{1-q}}{(1 - 2p^{-(\nu - \alpha)/2})(1 - p^{-(\nu - \alpha)/2})^2}.$$

Let $p^{-(\nu - \alpha)/2} = \delta \in (0, 1)$. The result then follows from the inequality $(1 - 2\delta)(1 - \delta)^2 \geq 1 - 4\delta$. 

Proof of Theorem [2] Under Assumption [2]

$$Q_h(x, T(x)) = \frac{\pi_h(x) h(\pi(T(x))/\pi(x))}{Z_h(x)} \geq \frac{h(1)}{E_\pi[Z_h]}$$

for any non-decreasing balancing function $h$. The inequality is attained at $x = x_1^*$. We still bound $E_\pi[Z_h]$ using (12). Let $\mathcal{X}_0 = \mathcal{X} \setminus \{x_1^*, x_2^*\}$. By a calculation similar to (10), one can use Assumption [2] to show that $\pi(x_1^*) \geq (1 - 2p^{\alpha - \nu})/2$, which implies $\pi(\mathcal{X}_0) \leq 2p^{\alpha - \nu}$.

Case 1: $h(u) = 1 + u$. The same bound $E_\pi[Z_h] \leq 2p^\alpha$ holds.

Case 2: $h(u) = 1 \wedge u$. Observe that $I_h(x, y) = \pi(x_1^*) = \pi(x_2^*)$ only when both $x, y \in \{x_1^*, x_2^*\}$, which happens twice in the summation in (12). Hence,

$$E_\pi[Z_h] \leq 2 \sum_{x \in \mathcal{X}_0} |\mathcal{N}(x)|\pi(x) + 2\pi(x_1^*) \leq 4p^{2\alpha - \nu} + 1.$$
Case 3: \( h(u) = \sqrt{u} \). To bound \( I_h(x,y) = \sqrt{\pi(x)\pi(y)} \), we consider three subcases according to whether \( x \) and \( y \) are in \( \mathcal{X}_0 \). First, using \( \sqrt{\pi(x)\pi(y)} \leq (\pi(x) + \pi(y))/2 \), we find that

\[
\sum_{(x,y) \in \mathcal{X}_0^2 : y \in \mathcal{N}(x)} \sqrt{\pi(x)\pi(y)} \leq \sum_{x \in \mathcal{X}_0} |\mathcal{N}(x)|\pi(x) \leq 2p^{2\alpha-\nu}.
\]

If \( x = x_1^* \) or \( x_2^* \) and \( y \in \mathcal{X}_0 \), we have \( \pi(y) \leq p^{-\nu}\pi(x) \). Hence,

\[
\sum_{x \in \mathcal{X} \setminus \mathcal{X}_0, y \in \mathcal{N}(x)} \sqrt{\pi(x)\pi(y)} \leq \sum_{x \in \mathcal{X} \setminus \mathcal{X}_0, y \in \mathcal{N}(x)} \pi(x)p^{-\nu/2} \leq p^{\alpha-\nu/2}.
\]

Using \( \sqrt{\pi(x_1^*)\pi(x_2^*)} \leq 1/2 \), we finally obtain that

\[
\mathbb{E}_\pi[Z_h] \leq 2p^{2\alpha-\nu} + 2p^{\alpha-\nu/2} + 1.
\]

The claim then follows from Lemma [A1].

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