Fast Doubly-Adaptive MCMC to Estimate the Gibbs Partition Function with Weak Mixing Time Bounds

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Abstract

We present a novel method for reducing the computational complexity of rigorously estimating the partition functions (normalizing constants) of Gibbs (Boltzmann) distributions, which arise ubiquitously in probabilistic graphical models. A major obstacle to practical applications of Gibbs distributions is the need to estimate their partition functions. The state of the art in addressing this problem is multi-stage algorithms, which consist of a cooling schedule, and a mean estimator in each step of the schedule. While the cooling schedule in these algorithms is adaptive, the mean estimation computations use MCMC as a black-box to draw approximate samples. We develop a doubly adaptive approach, combining the adaptive cooling schedule with an adaptive MCMC mean estimator, whose number of Markov chain steps adapts dynamically to the underlying chain. Through rigorous theoretical analysis, we prove that our method outperforms the state of the art algorithms in several factors: (1) The computational complexity of our method is smaller; (2) Our method is less sensitive to loose bounds on mixing times, an inherent component in these algorithms; and (3) The improvement obtained by our method is particularly significant in the most challenging regime of high-precision estimation. We demonstrate the advantage of our method in experiments run on classic factor graphs, such as voting models and Ising models.

1 Introduction

The Gibbs (Boltzmann) distribution is a family of probability distributions of exponential form. First introduced in the context of statistical mechanics [26], Gibbs distributions are now ubiquitous in a variety of other disciplines, such as chemistry [32, 25], economics [56, 1] and machine learning. Gibbs distributions are typically used to model the global state of a system as a function of a collection of interdependent random variables, each representing local states in the system. The dependencies in the system are modeled by a Hamiltonian function, and the probability distribution is inversely proportional to exponent of the Hamiltonian scaled by the temperature (see eq. (1) § 1.1).

Gibbs distributions provide potent statistical inference tools in many machine learning applications. They appear in probabilistic graphical models [42, 51, 52], including restricted Boltzmann machines [68, 44], Markov random fields [11, 49], and Bayes networks [33], and are applied in the analysis of images and graphical data [67, 43, 24, 21], topic modeling (LDA) [28, 59, 55, 64], and more [13, 58, 2, 18, 17, 70, 27, 31, 50, 60].

A major obstacle in applying the Gibbs distribution in practice is the need to compute, or estimate, its partition function (normalizing constant), henceforth written GPF. The partition function is defined over the Cartesian product of supports of a (typically large) number of variables, making exact computation intractable. Furthermore, due to interdependence of variables, exact sampling is not practically feasible, thus Markov-chain Monte-Carlo (MCMC) solutions for this problem have been extensively studied [51, 38, 23, 69, 65, 33, 6, 43, 30, 40].
Like other MCMC methods, here various heuristics are used. The most well-known heuristics are the annealed importance sampling \[54, 60, 40\] or convergence diagnostics methods \[20, 11, 10, 63\]. Unfortunately, these methods are often error-prone, as their correctness is only proven asymptotically, without rigorous mathematical analysis to bound their estimation error with finite samples. In fact, theoretical findings have shown that with no prior knowledge of relevant measures, such as the variance of importance weights in annealed importance sampling, or upper bounds on mixing or relaxation times for diagnostic methods, these methods are either unreliable or computationally intractable (see \[54\] section 4 or \[7, 34\]).

On the other hand, theoreticians study this problem by designing Fully Polynomial Randomized Approximation Schemes (FPRAS) (see problem 1). The state of the art FPRAS for estimating the GPF is a multi-stage algorithm involving a sequence of functions at various temperatures, such that the expectation of the product of these functions, or the product of the expectations of said functions, is the GPF. FPRAS's are proven to produce (approximate) solutions w.h.p., but their performance guarantees rely on available upper-bounds on various measures such as variances of estimators or mixing times of Markov chains. In static algorithms, these upper-bounds are given a priori, and adaptive algorithms estimate them dynamically, while increasing the sample size until desired properties are mathematically guaranteed. Thus, adaptive algorithms are less sensitive to looseness of known upper-bounds, more robust, often faster, and more easily applied to various settings.

Most of the research on designing FPRAS's for the GPF is focused on designing adaptive algorithms to produce sequences (cooling schedules) with minimum length while keeping the variances of estimators small (thus removing the need to have a-priori known bounds on variances). In contrast, the computation of the sequence of mean estimates, which dominates the total computation cost, is done by black-box MCMC estimators, with a priori known upper bounds on the mixing times of the chains. These upper bounds are often loose, and improving them for particular models is a challenging active area of research \[5, 65, 9, 12, 4, 29\]. In order to complement the adaptive cooling schedule and reduce dependence on a priori bounds on Markov chains' mixing times, it seems necessary to design an adaptive procedure with theoretical guarantees for MCMC-mean estimation.

In this work we develop a doubly adaptive FPRAS, combining the adaptive cooling schedule with adaptive MCMC mean estimator that dynamically adapts the number of Markov chain steps to the observed underlying chain. Through rigorous theoretical analysis, we prove that our method outperforms the state of the art algorithms in several factors: (1) The computational complexity of our method is smaller; (2) Our method is less sensitive to loose bounds on mixing times, an inherent component in these algorithms; and (3) The improvement obtained by our method is particularly significant in the most challenging regime of high precision estimates. We demonstrate the advantage of our method in experiments run on classic factor graphs, such as voting and Ising models \[15, 5, 8\].

1.1 Preliminaries and Prior Work

Assume a sample space \(\Omega\), Hamiltonian function \(H: \Omega \rightarrow \{0\} \cup [1, \infty)\), and inverse temperature parameter \(\beta \in \mathbb{R}\), referred to as inverse temperature. The Gibbs distribution on \(\Omega\), \(H(\cdot)\), and \(\beta\) is then characterized by probability law

\[
\forall x \in \Omega : \pi_\beta(x) = \frac{1}{Z(\beta)} \exp(-\beta H(x)) .
\]

Here \(Z(\beta)\) is the normalizing constant or Gibbs partition function (GPF) of the distribution, with

\[
Z(\beta) = \sum_{x \in \Omega} \exp(-\beta H(x)) .
\]

Estimating the GPF \(Z(\beta)\), is computationally challenging, since typically the size of \(\Omega\) is exponential in the number of variables, and the values of random terms in the sum have large variance (due to the exponential). The following problem has been extensively studied, and is the focus of this paper.

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1The usage of the word “adaptive” here refers to algorithms which draw samples progressively and adapt their sample complexity based on empirical estimates until desired conditions are met, as it has been used in \[35, 143\] (see § 1.1), and should not confused with the work of \[62\].
Problem 1. Given a domain $\Omega$, a Hamiltonian function $H$, and a parameter $\beta$, design a Fully Polynomial Randomized Approximation Scheme (FPRAS) for estimating the partition function $Z(\beta) \doteq \sum_{x \in \Omega} \exp(-\beta H(x))$. In other words, for user-supplied $\epsilon$, the task is to produce an estimate $\hat{Z}(\beta)$, such that with probability at least $1 - \delta$, we have $(1 - \epsilon)Z(\beta) \leq \hat{Z}(\beta) \leq (1 + \epsilon)Z(\beta)$, in time polynomial in $1/\epsilon$, $\ln(1/\delta)$, and all other problem parameters (e.g., the number of vertices in an Ising model, or neurons in an RBM).

All known scalable solutions to this problem rely on Monte-Carlo Markov-chain (MCMC) methods, and their execution cost is dominated by the total number of Markov chain steps they execute. We therefore follow past work, and analyze our algorithms in terms of number of the Markov chain steps.

TPA-Based Adaptive Cooling Schedules Building on extensive earlier work [23, 6, 69, 6], the current state of the art is due to Huber and Schott [36], with Kolmogorov’s sharper analysis [43]. They introduce the paired product estimator (PPE), see definition 1.1 and apply the tootsie-pop algorithm (TPA) to adaptively compute a near-optimal cooling schedule, i.e., a sequence of inverse temperatures $\beta_0 < \beta_1 < \cdots < \beta_{\ell-1} < \beta_{\ell}$ satisfying $\beta_{\ell} = \beta$, and that $Z(\beta_0)$ is easy to compute, e.g., $\beta_0 = 0$ is often convenient, since $Z(0) = |\Omega|$. We thus define $Q = Z(\beta)/Z(\beta_0)$ and estimate it using the paired product estimator.

Definition 1.1 (PPE [35]). Assume a cooling schedule $\beta_0, \beta_1, \ldots, \beta_{\ell}$. For each pair $(\beta_i, \beta_{i+1})$ in the schedule, we define two random variables, $X_i \sim \pi_{\beta_i}$ and $Y_i \sim \pi_{\beta_{i+1}}$, all independent, and we then define $f_{\beta_i, \beta_{i+1}} \doteq \exp(-\frac{\beta_i - \beta_{i+1}}{2} H(X_i))$ and $g_{\beta_i, \beta_{i+1}} \doteq \exp(-\frac{\beta_i - \beta_{i+1}}{2} H(Y_i))$. It is easy to verify that $E[f_{\beta_i, \beta_{i+1}}] = Z(\beta_i, \beta_{i+1})/Z(\beta_i)$, and $E[g_{\beta_i, \beta_{i+1}}] = Z(\beta_i, \beta_{i+1})/Z(\beta_{i+1})$. We then define $F = \prod_{i=1}^{\ell} f_{\beta_i, \beta_{i+1}}, G = \prod_{i=1}^{\ell} g_{\beta_i, \beta_{i+1}}$, Letting $\hat{\mu}$ and $\hat{\nu}$ denote empirical estimates of $E[F]$ and $E[G]$, respectively, the paired product estimator (PPE) is $\hat{Q} = \hat{\mu}/\hat{\nu}$.

Denote by $\mathbb{V}_{\text{rel}}[X] \doteq \mathbb{E}[X^2]/\mathbb{E}[X]^2 - 1 = \mathbb{V}[X]/\mathbb{E}[X]^2$ the relative variance of a random variable $X$. The TPA schedule [37, 38] is generated by an adaptive algorithm, which, by a proper setting of parameters, outputs a cooling schedule guaranteeing constant $\mathbb{V}_{\text{rel}}[F]$ and $\mathbb{V}_{\text{rel}}[G]$ (see alg. 3 in the supplementary material). Kolmogorov [38] presents a tighter analysis of Huber’s TPA method, and proves that with slight modifications (see alg. 4 in the Appendix) the schedule has a shorter length, while preserving constant relative variance for the paired product estimators (see thm. 1.1). In this paper, we use Kolmogorov’s algorithm, and we denote it by Tpa$(k, d)$. For completeness, both of Huber’s and Kolmogorov’s versions of TPA are presented in the Appendix.

We will use the following result in our analysis:

Theorem 1.1 (22). Let $H_{\text{max}} \doteq \max_{x \in \Omega} H(x)$, using TPa$(k, d)$, $k = \Theta(\log H_{\text{max}})$ and $d = 16$ to generate cooling schedule $(\beta_0, \beta_1, \ldots, \beta_{\ell})$. W.h.p., we have $\ell = \Theta(\log(Q) \log(H_{\text{max}}))$ and $\mathbb{V}_{\text{rel}}[F] + 1 = \prod_{i=1}^{\ell} \mathbb{V}_{\text{rel}}[f_{\beta_i, \beta_{i+1}} + 1] = \Theta(1)$ and $\mathbb{V}_{\text{rel}}[G] + 1 = \prod_{i=1}^{\ell} \mathbb{V}_{\text{rel}}[g_{\beta_i, \beta_{i+1}} + 1] = \Theta(1)$.

Kolmogorov [43] nearly matches known lower bounds when given oracle access to near-independent samples, but leaves open the possibility of better use of the dependent sequence of samples generated by MCMC chains. This fertile ground is ill-explored, since if an approximate sampling oracle draws samples by running a chain for $T$ steps, there is a factor $T$ potential improvement.

MCMC Mean-Estimator Huber and Schott [36] assume unit-cost for exact sampling from each $\pi_{\beta_i}$, and Kolmogorov [43] extends their analysis to include the complexity of generating approximate samples with standard MCMC processes, assuming a priori upper-bounds on their mixing times. The main contribution of our paper is a specialized, adaptive, multiplicative MCMC-mean estimator for the TPA-based PPE. Our method is significantly more efficient than using standard black-box MCMC sampling for this problem, thus we improve the best-known algorithm for estimating the GPF.

Let $M$ be an ergodic Markov chain with state space $S$ and stationary distribution $\pi$. Let $\tau_{\text{mix}}(\epsilon)$ denote the $\epsilon$-mixing time of $M$, and define $\tau_{\text{mix}} \doteq \tau_{\text{mix}}(1/4)$. Letting $\lambda$ denote the second largest absolute eigenvalue of $M$’s transition matrix, the relaxation time of $M$ is $\tau_{\text{rx}} \doteq (1 - \lambda)^{-1}$, and it is related to the mixing time $\tau_{\text{mix}}$, by $(\tau_{\text{rx}}(M) - 1) \ln(2) \leq \tau_{\text{mix}}(M) \leq \left[\tau_{\text{rx}}(M) \ln(2/\sqrt{\tau_{\text{mix}}})\right]$ [47]. Let $T$ be an upper bound on $\max\{\tau_{\text{rx}}(M), \tau_{\text{mix}}(M)\}$.
Consider any i.i.d. sampling concentration bound like Chebyshev’s, Hoeffding’s, or Bernstein’s inequalities [52], with, say, sample complexity \(m_x\). Using MCMC as a black-box sampling tool, we obtain the same precision estimation guarantees, with a computational cost of \(m_x \cdot \tau_{\text{mix}}(\varepsilon/m_x)\), which is equal to \(m_x \log(m_x \cdot \varepsilon^{-1}) \cdot T\) in the absence of exact values for \(\tau_{\text{mix}}\).

Other concentration bounds compute the average over the entire trace of a Markov chain, and their complexity is dependent on known upper-bounds on the relaxation time [57], [52], [48], [14], [39], or function specific mixing time [51]. Note that since \(\log(\frac{1}{\varepsilon})/\tau_{\text{rel}} - 1 \leq \tau_{\text{mix}}(\varepsilon) \leq \log(\frac{1}{\varepsilon})\tau_{\text{rel}}\), using these bounds is often more efficient, saving at least \(\log(m_x)\) steps.

Recently, Cousins et al. [16] introduce a novel Markov chain statistical measure, the inter-trace variance. The inter-trace variance depends on both the function being estimated and the dependency structure between nearby samples in the chain, and unlike the mixing time, it can be efficiently estimated from data. By using progressive sampling, Cousins et al. show an additive MCMC mean estimator whose complexity is proved in terms of inter-trace variance and they show it it less sensitive to prior knowledge of the input parameters, such as relaxation time and trace variance. Unfortunately due to a few technical problems, their result can not directly be used with the TP\(\Delta\) method. Thus, in order to obtain a doubly adaptive algorithm for problem 1, we tailor their techniques to our setting, which requires developing new algorithms and analysis tools.

### 1.2 Our Main Contributions

- We present a specialized mean estimator method that significantly improves the state of the art computational complexity of computing the partition function of Gibbs distribution.
- While all rigorous MCMC-based estimates depend on some a priori knowledge of the Markov chain properties (such as bounds on its mixing or relaxation time), the complexity of our method is less dependent on these a priori bounds, and decays gracefully as they become looser.
- The improvement of our method is particularly significant in the more challenging high precision regime, where the goal is to compute estimates with very small multiplicative error.
- Our method improves the computational cost of prior work by replacing standard black-box MCMC mean estimators with an adaptive MCMC mean estimator, specially tailored to this problem.
- The analysis of our method relies on a novel notion of sample variance in a sequence of observations obtained by Markov chains runs, which we term the relative trace variance.
- We demonstrate the practicality of our method through experiments on Ising and voting models.

### 2 Algorithms

In this section, we develop two doubly-adaptive fully polynomial randomized approximation schemes providing more efficient algorithmic solutions to problem 1. The proof of all of the lemmas and theorems are presented fully in the supplementary material.

#### Notation and Setting Parameters
We use the following notation throughout: We use capital letters to denote upper-bounds, e.g., \(T\) denotes an upper-bound on \(\max(\tau_{\text{mix}}, \tau_{\text{rel}})\), and \(\Lambda\) denotes a upper-bound on the second absolute eigenvalue \(\lambda\). We use \(G_{H,\beta}\) to denote any Markov chain with Gibbs stationary distribution \(\pi_\beta\), eq. [1]. Having the Hamiltonian \(H\), we denote its maximum and minimum values as \(H_{\text{max}}\) and \(H_{\text{min}}\), i.e., \(H_{\text{max}} = \max_{x \in \Omega} \{H(x)\}\) and \(H_{\text{min}} = \min_{x \in \Omega} \{H(x)\}\). Having a schedule \((\beta_0, \beta_1, \ldots, \beta_\ell)\), the paired product estimators \(f_{\beta_0,\beta_\ell}, g_{\beta_0,\beta_\ell}\), \(F = \bigotimes_{i=1}^\ell f_{\beta_i,\beta_{i+1}}\) and \(G = \bigotimes_{i=1}^\ell g_{\beta_i,\beta_{i+1}}\) are as in definition [1]. When writing \((\beta_0, \beta_1, \ldots, \beta_\ell) = \text{TPA}(k, d)\), we mean the cooling schedule is obtained from running alg. 4 in the Appendix, and we always set \(k = \log H_{\text{max}}\) and \(d = 64\), as these parameters are shown to produce a near-optimal schedule w.h.p. [18].

We first introduce a novel MCMC-based multiplicative mean estimation procedure \textsc{RelMeanEst} (see alg. [2]), and analyze its computational complexity in terms of a new quantity, which we coin the relative trace variance (see definition 2.1). \textsc{RelMeanEst} receives as input a Markov chain \(\mathcal{M}\), a function \(f\), and precision parameters \(\varepsilon\) and \(\delta\), and it outputs a multiplicative estimate of the expected value of the function w.r.t. the stationary distribution of the Markov chain. For simplicity, we may refer to it as \textsc{RelMeanEst}(\(\mathcal{M}, f\)), leaving out the precision parameters.
Letting \((\beta_0, \beta_1, \ldots, \beta_k) = \text{TPA}(k, d)\), we first present \textsc{ParallelTraceGibbs}, in which we invoke both \textsc{RelMeanEst}(G_{H, \beta_i}, f_{\beta_1, \beta_{i+1}}) and \textsc{RelMeanEst}(G_{H, \beta_i}, g_{\beta_1, \beta_{i+1}}) for each \(i = 1, 2, \ldots, \ell - 1\). We then present an often-more-efficient algorithm, \textsc{SuperChainTraceGibbs}, which invokes \textsc{RelMeanEst} once each on \(F\) and \(G\) on a “super” product chain (see definition 2.2). We prove correctness of both \textsc{ParallelTraceGibbs} and \textsc{SuperChainTraceGibbs}, and bound their complexity in terms of the relative trace variance of the estimators. Furthermore, we prove \textsc{SuperChainTraceGibbs} improves the computational complexity of the state of the art \cite{13} (thm. 2.4 and corollary 2.6). Both of these algorithms have low dependence on tightness of mixing time: They receive as input an upper-bound on mixing or relaxation time \(T\), but we show for \(\varepsilon \geq \varepsilon_0\) their computation complexity is dominated by the true relaxation time \(\tau_{\text{rel}}\) (of each Gibbs chain or the product chain).

### 2.1 Relative trace variance and RelMeanEst

In this section we introduce a new variance notion, the relative trace variance, which captures the computational complexity of MCMC-mean estimation with multiplicative precision guarantees. The relative trace variance depends on both the chain \(\mathcal{M}\) and the function \(f\), and it generalizes the relative variance, defined as \(\mathbb{V}_{\text{rel}}[f] = \frac{\mathbb{V}[f(\bar{X}_{1:\tau})]}{\mathbb{V}[f(X_{1:\tau})]}\), which depends only on \(f\), and is used in i.i.d. regimes.

**Definition 2.1 (Relative Trace Variance).** For arbitrary \(T\), consider a trace of length \(\tau\) of a Markov chain \(\mathcal{M}\), and a real-valued function \(f\). On \(\mathcal{M}\), we define the relative trace variance of \(f\) as

\[
\text{Reltrv}_{\mathcal{M}}[f] = \frac{\mathbb{E}[f(\bar{X}_{1:\tau})]^2}{(\mathbb{E}[f(X_{1:\tau})])^2} - 1,
\]

where \(\bar{X}_{1:\tau} = X_1, X_2, \ldots, X_\tau\) is a trace of length \(\tau\) of \(\mathcal{M}\), and \(f(\bar{X}_{1:\tau}) = (\frac{1}{\tau}) \sum_{i=1}^{\tau} f(X_i)\). We may drop the subscript when the chain is clear from the context.

The above definition is similar to what Cousins et al. coined as the inter-trace variance, denoted by \text{trv}(\tau)(\mathcal{M}, f)\), which they showed it captures MCMC-mean estimation with additive precision guarantees \cite{10}. In fact, the two terms are related as

\[
\text{Reltrv}_{\mathcal{M}}[f] = \frac{\text{trv}(\tau)(\mathcal{M}, f)}{(\mathbb{E}[f(X_{1:\tau})])^2}.
\]

Note that the two terms are not easily convertible without knowing the mean, \(\mathbb{E}[f(\bar{X}_{1:\tau})]\).

**Lemma 2.1.** For any \(\tau\) we have

\[
\text{Reltrv}_{\mathcal{M}}^\tau[f] \leq \mathbb{V}_{\text{rel}}[f].
\]

Furthermore, for \(\tau \geq \tau_{\text{rel}}(\mathcal{M})\) we have,

\[
\text{Reltrv}_{\mathcal{M}}[f] = O\left(\frac{\tau_{\text{rel}}(\mathcal{M})}{\tau} \text{Reltrv}_{\mathcal{M}}^\tau[f]\right).
\]

Lemma 2.1 enables us to compare the computational complexity of our algorithms with the state of the art \cite{13}. In particular, using \cite{3}, we show our results improve the state of the art (which is in terms of \(\mathbb{V}_{\text{rel}}\), and using \cite{1}, we show that for high-precision estimations, the sample complexity of our algorithms only depends on \(\tau_{\text{rel}}\), which improves the state of the art (which is in terms of \(T\)).

The relative trace variance is a better analysis tool for estimating the GPF, because, unlike the inter-trace variance, it leads directly to relative error bounds, rather than absolute error bounds. We now present some definitions which can also be found in standard MCMC textbooks, e.g., \cite{47}.

**Definition 2.2 (Product Chain and Tensor Product Function).** Consider \(k\) Markov chains \(\{\mathcal{M}_i\}_{i=1}^k\) each defined on state space \(S_i\) and assume real valued functions \(\{f_i : S_i \to \mathbb{R}\}_{i=1}^k\). The product chain \(\mathcal{M}_{\otimes}^k\) is defined on the Cartesian product of \(S_i\) as follows: at any step \(\mathcal{M}_{\otimes}^k\) chooses \(i\) with probability \(\omega_i\) (thus \(\sum_{i=1}^k \omega_i = 1\)), and moves from \((x_1, x_2, \ldots, x_i, \ldots, x_k)\) to \((x_1, x_2, \ldots, y_i, \ldots, x_k)\), with the transition probability of moving from \(x_i\) to \(y_i\) in \(\mathcal{M}_i\). The tensor product of \(\{f_i\}_{i=1}^k\), denoted by \(\otimes_{1:k} f_i\), is defined as \((\otimes_{1:k} f_i)(x_1, x_2, \ldots, x_k) = \prod_{i=1}^k f_i(x_i)\).
RelMeanEst Let $T$ denote an upper bound on the relaxation time of a Markov chain $\mathcal{M}$. RelMeanEst receives $T$, $\mathcal{M}$, $f$ and precision parameters $\varepsilon$ and $\delta$ as input. Before it starts collecting samples, it runs the chain for a warm start ($\S 4$ of alg. 3). Starting from a minimum sample size $m_0$, it runs $\mathcal{M}$ for $T \cdot m$ steps, and collect samples $X_1, X_2, \ldots, X_T, m$. It then computes for $j = 1, 2, \ldots, m$, $\hat{f}_j = \frac{1}{T} \sum_{i=1}^{T} j f(X_i)$; using them, it calculates an empirical estimate of the mean, $\hat{\mu}$, and an empirical estimation for the trace variance of $\mathcal{M}$ and $f$, $\hat{\varepsilon}$. Based on these estimates, we derive an upper-bound on the current trace variance $u_i$ and relative error $\hat{\varepsilon}_i^2$, and check whether is smaller than the user-specified error $\varepsilon$ (lines 18–19). If so, we return the current mean estimate, otherwise we double the sample size and repeat.

Algorithm 1 RelMeanEst

1. procedure RelMeanEst
2. Input: Markov chain $\mathcal{M}$, upper-bound on relaxation time $T$, real-valued function $f$ with range $[a, b]$, letting $R = b - a$, multiplicative precision $\varepsilon$, error probability $\delta$.
3. Output: Multiplicative approximation $\hat{\mu}$ of $\mu = E_x[f]$.
4. $T \leftarrow \left\lceil \frac{1}{\varepsilon^2} \ln \sqrt{7T} \right\rceil$; $\mathcal{N} \leftarrow \mathcal{N}^T$  

\[ T \leftarrow \left\lceil \frac{1}{\varepsilon^2} \ln \sqrt{7T} \right\rceil \n \n \text{\textbullet\ Choose } T \text{~} \text{to be an upperbound on relaxation time} \]

5. $I \leftarrow 1 \vee \log_2 \left( \frac{\mathcal{N}^T}{\varepsilon^2 \ln \sqrt{7T}} \right)$; $\alpha \leftarrow (1 + \lambda) R H \frac{2}{\varepsilon^2 \ln \sqrt{7T}}$; $m_0 \leftarrow 0$  

\[ I \leftarrow 1 \vee \log_2 \left( \frac{\mathcal{N}^T}{\varepsilon^2 \ln \sqrt{7T}} \right) \n \n \text{\textbullet\ Initialize sampling schedule} \]

6. $T_{\text{ unfair}} \leftarrow \left\lceil \frac{T \cdot \ln(1/\varepsilon_0)}{\varepsilon_0} \right\rceil$; $(\hat{\mathcal{X}}_{0.1}, \hat{\mathcal{X}}_{0.2}) \leftarrow \mathcal{M}_{T_{\text{ unfair}}}((\perp))$  

\[ T_{\text{ unfair}} \leftarrow \left\lceil \frac{T \cdot \ln(1/\varepsilon_0)}{\varepsilon_0} \right\rceil \n \n \text{\textbullet\ Warm-start two chains for } T_{\text{ unfair}} \text{ steps from arbitrary } \perp \in \Omega \]

7. for $i \in 1, 2, \ldots, I$ do  

\[ \text{\textbullet\ Total sample count at iteration } i; \text{~} r \text{~ is the geometric ratio (constant, usually 2) size} \]

8. $m_i \leftarrow \lceil ar^i \rceil$  

9. for $j \in (m_{i-1} + 1), \ldots, m_i$ do  

\[ \text{\textbullet\ Run two independent copies of } \mathcal{M} \text{ for } T \text{ steps} \]

10. $(\hat{\mathcal{X}}_{i,1}, \hat{\mathcal{X}}_{i,2}) \leftarrow (T \text{ steps of } \mathcal{M} \text{ starting at } \hat{\mathcal{X}}_{i-1,1}, \hat{\mathcal{X}}_{i-1,2})$  

\[ \text{\textbullet\ Average } f \text{ over } T \text{-traces} \]

11. $\hat{f}(\hat{\mathcal{X}}_{i,1}) \leftarrow \frac{1}{T} \sum_{t=1}^{T} f(\hat{\mathcal{X}}_{i,1}(t))$; $\hat{f}(\hat{\mathcal{X}}_{i,2}) \leftarrow \frac{1}{T} \sum_{t=1}^{T} f(\hat{\mathcal{X}}_{i,2}(t))$  

\[ \text{\textbullet\ Compute empirical mean; trace variance} \]

12. $\hat{\mu}_i \leftarrow \frac{1}{2m_i} \sum_{t=1}^{m_i} (f(\hat{\mathcal{X}}_{1,t}) + f(\hat{\mathcal{X}}_{2,t}))$; $\hat{\varepsilon}_i \leftarrow \frac{1}{2m_i} \sum_{t=1}^{m_i} (f(\hat{\mathcal{X}}_{1,t}) - f(\hat{\mathcal{X}}_{2,t}))$  

\[ \text{\textbullet\ Variance upper bound} \]

13. $u_i \leftarrow \frac{10 R \ln \frac{\mathcal{N}}{\varepsilon^2}}{(1 - \lambda)m_i} + \frac{1}{(1 + \lambda)m_i} \ln \frac{\mathcal{N}}{\varepsilon^2}$  

\[ \text{\textbullet\ Apply Bernstein bound} \]

14. $\hat{\mu}_i^2 \leftarrow \frac{(\hat{\mu}_i - \hat{\varepsilon}_i^2)}{2} \vee a + (\hat{\mu}_i + \hat{\varepsilon}_i^2) \wedge b$  

\[ \text{\textbullet\ Optimal mean estimate} \]

15. $\hat{\varepsilon}_i^2 \leftarrow \frac{(\hat{\mu}_i - \hat{\varepsilon}_i^2)}{2 \hat{\mu}_i^2} \vee b - (\hat{\mu}_i - \hat{\varepsilon}_i^2) \vee a$  

\[ \text{\textbullet\ Empirical relative error bound} \]

16. if $(\hat{\mu}_i - \hat{\varepsilon}_i^2 \leq \varepsilon)$ then  

\[ \text{\textbullet\ Terminate if accuracy guarantee is met} \]

17. return $\hat{\mu}_i$  

18. end if  

19. end for  

20. end procedure

The following theorem shows the correctness of RelMeanEst and bounds its complexity.

Theorem 2.2 (Efficiency and Correctness of RelMeanEst). With probability at least $1 - \delta$, RelMeanEst will output $\hat{\mu}$ satisfying $(1 - \varepsilon) \mu \leq \hat{\mu} \leq (1 + \varepsilon) \mu$. Furthermore, with probability at least $1 - \frac{\delta}{4T}$, the total Markov chain steps of RelMeanEst, $\hat{m}$, obeys

$$
\hat{m} \in \mathcal{O} \left( \ln \frac{\ln \frac{\mathcal{N}}{\varepsilon^2}}{\delta} \left( \frac{T \cdot R}{\mu \varepsilon} + \frac{\tau_R \text{Reltrv}^7 \tau_R}{\varepsilon^2} \right) \right). 
$$

2.2 Doubly adaptive algorithms: SuperChainTraceGibbs and ParallelTraceGibbs

Let $(\beta_0, \beta_1, \ldots, \beta_1) = \text{Tpa}(k,d)$, and consider a family of Gibbs chains $\mathcal{G}_{H,\beta}$, each corresponding to some $\beta_i$, and the paired product estimators $F = \bigotimes_{i=1}^{T} f_{\beta_i,\beta_{i+1}}$; $G = \bigotimes_{i=1}^{T} g_{\beta_i,\beta_{i+1}}$. The Tpa method is designed to ensure $\mathbb{V}_{\text{rel}}$ of the estimators are bounded, which can be employed by concentration bounds (e.g., Chebyshev’s bound) to guarantee the multiplicative error is bounded with high probability for a given sample size.

In order to generalize the same machinery for samples generated from a Markov chain using RelMeanEst, we need to bound the two terms appearing in eq. (5), which dominate the computational complexity of
We refer to the first term, $T \cdot R / \mu$, as the range term, and to the term $\tau_{\text{prx}} \cdot \text{Reltrv}^{\tau_{\text{prx}}}$ as the trace variance term. Note that as $\varepsilon$ becomes smaller, the trace variance term dominates the sample complexity of $\text{RelMeanEst}$, thus dependence on loose bounds $T$ and $R$ is dominated by dependence on true and a priori unknown values $\tau_{\text{prx}}$ and $\text{Reltrv}^{\tau_{\text{prx}}}$.

In order to ensure that the ranges of estimators are small, we prove that the length of each inverse-temperature interval in the $\text{TPA}$ schedule is w.h.p. small. Having a schedule $(\beta_0, \beta_1, \ldots, \beta_\ell)$ we define and use the following notation: for $0 \leq i < \ell - 1$, interval length $\Delta_i \equiv \beta_{i+1} - \beta_i$, maximum interval length $\Delta_{\text{max}} \equiv \max_i \Delta_i$, and total length $\Delta = \beta_{\ell} - \beta_0$.

**Lemma 2.3.** Let $z(\beta) \equiv \ln \left( \frac{z(\beta_i)}{z(\beta_{i+1})} \right)$, and let $\beta_i, \beta_{i+1}$ be two consecutive points generated by $\text{TPA}(k, d)$. For arbitrary $\varepsilon > 0$, we have:

1. $P(z(\beta_i) - z(\beta_{i+1}) \leq \varepsilon) \geq (1 - \exp(-\varepsilon k/d))^d$.
2. $P \left( \Delta_i \geq \tau / \mathbb{E}[H(x)] \right) \leq d \exp(-\varepsilon k/d)$, where $\mathbb{E}[H(x)]$ is taken w.r.t. $x \sim \pi_{\beta_{i+1}}$.

**SuperChainTraceGibbs** Let $\mathcal{G}^\otimes$ the product of $\mathcal{G}_{\beta_i}$’s with uniform weights i.e., $\omega_i = \frac{1}{\mathcal{V}}$, $\forall i$ (see definition 2.2). **SuperChainTraceGibbs** calls $\text{RelMeanEst}(\mathcal{G}^\otimes, F)$ and $\text{RelMeanEst}(\mathcal{G}^\otimes, G)$, with appropriate parameters, and simply outputs the ratio of the two estimates (see alg. 4 left).

**Algorithm 2 SuperChainTraceGibbs and ParallelTraceGibbs**

1: procedure SuperChainTraceGibbs(...) 
2: $(\beta_0, \beta_1, \ldots, \beta_\ell) \leftarrow \text{TPA}(k, d)$ 
3: $\varepsilon' \leftarrow \frac{\varepsilon}{\mathcal{V} \cdot \varepsilon^2}$ 
4: for $i \in [1, \ell]$ do 
5: $f_i(x) \leftarrow \exp(\varepsilon_{i+1} - \frac{\beta_{i+1} - \beta_i}{2} H(x))$ 
6: $g_i(x) \leftarrow \exp(\varepsilon_i - \frac{\beta_i - \beta_{i-1}}{2} H(x))$ 
7: for $i \in [1, \ell]$ do 
8: $F = \bigotimes_{i=1}^{i} f_i; G = \bigotimes_{i=1}^{i} g_i$ 
9: $\mathcal{G}^\otimes \leftarrow \bigotimes_{i=1}^{i} \mathcal{G}_{\beta_i}$, with $\omega_i = \frac{1}{\mathcal{V}}, \forall i$ 
10: $R_i \leftarrow \exp(-\frac{\beta_{i+1} - \beta_i}{2} \mathbb{H}_{\beta_i}) - \exp(-\frac{\beta_i - \beta_{i-1}}{2} \mathbb{H}_{\beta_i})$ 
11: $R_i' \leftarrow \exp(-\varepsilon_{i+1}) \mathbb{H}_{\beta_i} - \exp(-\varepsilon_i) \mathbb{H}_{\beta_i}$ 
12: $\mu^{'} \leftarrow \text{RelMeanEst}(\mathcal{G}^\otimes, R_i, T, F, \varepsilon', \varepsilon')$ 
13: $\nu^{'} \leftarrow \text{RelMeanEst}(\mathcal{G}^\otimes, R_i, T, G, \varepsilon', \varepsilon')$ 
14: return $\tilde{Z} \leftarrow \frac{F}{G}$ 
15: end procedure

$^{a}k = \Theta(\log H_{\text{max}})$ and $d = 64$ as in [19].

We now show the correctness and efficiency of **SuperChainTraceGibbs**. Let $\tau_{\text{prx}}$ denote $\mathcal{G}^\otimes$’s true (and unknown) relaxation time and $T$ a known upper-bound on it ($T \geq \tau_{\text{prx}}$), $\varepsilon$ and $\delta$ are user specified precision parameters. For simplicity of presentation we use the following notation to refer to relative ranges: $\text{relR} = \text{Range}(F)/\mu - \text{Range}(G)/\nu$, where $\mu = \mathbb{E}[F]$ and $\nu = \mathbb{E}[G]$.

**Theorem 2.4.** With probability at least $1 - \delta$, it holds that the total number $n$ of Markov chain steps taken by **SuperChainTraceGibbs** is upper-bounded by

$$\tilde{O}\left(\ln\left(\frac{1}{\delta}\right) \left( T \cdot \text{relR} + \frac{\tau_{\text{prx}} \cdot (\text{Reltrv}^{\tau_{\text{prx}}}(F) + \text{Reltrv}^{\tau_{\text{prx}}}(G))}{\varepsilon^2}\right)\right).$$

**Lemma 2.5.** Defining $\alpha_1 = \sqrt{\frac{Z(\beta_0)}{Z(\beta_0 - \Delta_{\text{max}})}}$, we have:

$$\frac{\text{Range}(F)}{\mu} \leq \alpha_1 \sqrt{\frac{Q}{\exp(\Delta H_{\text{min}})}}$$

and

$$\frac{\text{Range}(G)}{\nu} \leq \alpha_1 \sqrt{\frac{Q}{\exp(\Delta H_{\text{max}})}}.$$
Table 1: Comparison of the number of Markov chain steps, when $\varepsilon$ is adequately small. In all columns, a multiplicative factor of $1/\varepsilon^2$ is omitted to ease presentation, and $q = \ln Q$. Note that computational complexity of both ParallelTraceGibbs and SuperChainTraceGibbs only depends on true relaxation times, denoted by $\tau_i$, and the TPA + PPE method’s complexity is dependent on their upper bounds, denoted by $T_i$.

**ParallelTraceGibbs** For $i = 1, 2, \ldots, \ell - 1$, ParallelTraceGibbs (alg. 3 right) runs RelMeanEst($G_{H, \beta_i, f_{\beta_i, \beta_{i+1}}}$) and RelMeanEst($G_{H, \beta_i, g_{\beta_i, \beta_{i+1}}}$) independently. We show the computational complexity of ParallelTraceGibbs in thm. 2.7.

For $i = 1, 2, \ldots, \ell$, assume $\tau_i$ is the true (unknown) relaxation time of $G_{H, \beta_i}$ and $T_i$ is a known bound on it. For simplicity of presentation we use the following notations: $\text{relR}_i = \text{Range}(f_{\beta_i, \beta_{i+1}})/\mu_i + \text{Range}(g_{\beta_{i-1}, \beta_i})/\nu_i$, where $\mu_i = \mathbb{E}(f_{\beta_i, \beta_{i+1}})$ and $\nu_i = \mathbb{E}(g_{\beta_i, \beta_{i+1}})$.

**Theorem 2.7 (Efficiency of ParallelTraceGibbs).** With probability at least $1 - \delta$, it holds that the total number $m_i$ of Markov chain steps taken by ParallelTraceGibbs is upper-bounded by

$$O\left(\log\left(\frac{\ell}{\delta}\right) \sum_{i=1}^{\ell} \left(\frac{\ell \cdot T_i \cdot \text{relR}_i}{\varepsilon} + \frac{\ell^2}{\varepsilon^2} \tau_i \cdot \left(\text{Reltrv}_{G_{H, \beta_i}}^{\alpha_{\beta_i}}(f_{\beta_i, \beta_{i+1}}) + \text{Reltrv}_{G_{H, \beta_i}}^{\alpha_{\beta_i}}(g_{\beta_{i-1}, \beta_i})\right)\right)\right).$$

Furthermore, for all $1 \leq i \leq \ell$, $\text{Range}(f_{\beta_i, \beta_{i+1}})/\mu_i \leq \ell^4/\log(n)$ and $\text{Range}(g_{\beta_{i-1}, \beta_i})/\nu_i \leq \ell^{\alpha_0(i)}/\log n$, where $\alpha_0(i) = (H_{\text{max}}/2\mathbb{E}(H(x))) - 1$, for $x \sim \pi_{\beta_i}$.

ParallelTraceGibbs and SuperChainTraceGibbs make different computational complexity tradeoffs. ParallelTraceGibbs is usually slower than SuperChainTraceGibbs, because in each iteration $i = 1, 2, \ldots, \ell$, the mean estimator must acquire a higher-precision estimate so that all estimators together achieve an $\varepsilon$-relative-error guarantee. Relaxation times (true values and their upper-bounds) appear in a sum in the complexity of ParallelTraceGibbs, whereas they appear in a maximum in SuperChainTraceGibbs ($\sum_{i=1}^{\ell} \tau_i$ vs. $\max_{t=1,\ldots,\ell} \tau_t$). Furthermore, dominance of the trace variance terms in both of these algorithms occur at different values of $\varepsilon$. A comparison of the complexity of these algorithms, in the high-precision regime, with Kolmogorov’s TPA + PPE (which uses MCMC as a black box) is presented in table 1.

### 3 Experimental Results

In this section we report our experiment results, comparing the performance of the two versions of our *doubly adaptive* method (alg. 2), to the performance of the state of the art algorithm in [44].

**Setup.** We run the experiments using the single site Gibbs sampler (known also as the Glauber dynamics) on two different factor graph models:

**A) The Ising model on 2D lattices.** Having a 2-dimension lattice of size $n \times n$, the Hamiltonian is defined on $n^2$ random variables having values $\pm 1$ and their dependency is represented by the Hamiltonian: $H(x) = -\sum_{(i,j) \in E} \mathbb{I}(x(i) = x(j))$. We run the algorithms on lattices of sizes $2 \times 2, 3 \times 3, 4 \times 4, 6 \times 6$. For each lattice, the parameter $\beta \geq 0$ is chosen below the critical inverse temperature at which it undergoes a phase transition. We use known mixing time bounds for high temperature Ising models [33] (see fig. 1 and A.6 of supplementary material).

**B) The logical voting model.** For a parameter $n$, we have $2n + 1$ random variables: the query variable $Q \in \{-1, 1\}$, and the voter variables $T_1, T_2, \ldots, T_n$ and $F_1, F_2, \ldots, F_n$ all in $\{0, 1\}$. The factors have $2n + 1$ weights, $\omega, \omega_{T_1}, \omega_{F_1}, i = 1, \ldots, n$. The Hamiltonian is:
\[ H(Q, T, F) = \omega Q \max_{i} T_i - \omega Q \max_{i} F_i + \sum_{i=1}^{n} \omega_{T_i} T_i + \sum_{i=1}^{n} \omega_{F_i} F_i, \]

where \( \omega, \omega_{T_i}, \omega_{F_i} \in [-1, 1] \).

The parameters are reported in fig. 2. We follow De Sa et al. [19] and use hierarchy width to derive upper bounds on mixing times. To make a fair comparison, we always run the TPA algorithms once, and with the parameters given in [23]. At each iteration of RELMEANEST, the sample size is extended with geometric ratio 1.1 (see alg. 3 line 8). All code is available at https://github.com/zysophia/Doubly_Adaptive_MCMC.

Results: Our experiments demonstrate the practical advantages of our doubly adaptive method, validating our theoretical analysis.

1. We first compare the complexity of our algorithms to Kolmogorov’s algorithm. Our experiments show the superiority of both versions of our methods on different models and various sets of parameters. Figure 1 demonstrates the superiority of our methods on the Ising model for various sets of parameters, and in figs. 2a and 2c for the voting model, when \( \varepsilon \) is fixed and \( Z(\beta) \) is varying (fig. 2c), and when \( Z \) is fixed and \( \varepsilon \) is varying (fig. 2a). All of these hold while the precision of our algorithms beats [43] as \( \varepsilon \to 0 \) (fig. 1c).

2. To demonstrate the advantage of using the relative trace variance, in contrast to the relative variance, we run both of our algorithms using a simpler mean estimator which only uses progressive sampling, and we compare the results. This is done by setting \( T \leftarrow 1 \) in line 4 of RELMEANEST. In Figure 2b, we show the effectiveness of trace averaging, since both SUPERCHAINTRACEGIBBS and PARALLELTRACEGIBBS beat their simplified versions (\( T \leftarrow 1 \)) after \( 1/\varepsilon \) passes a certain threshold. This is consistent for different parameters of the voting model.

3. Comparing the performance of SUPERCHAINTRACEGIBBS and PARALLELTRACEGIBBS, we observe that in all of our experiments SUPERCHAINTRACEGIBBS has better performance than PARALLELTRACEGIBBS. In fig. 2b we show the trace variance term PARALLELTRACEGIBBS becomes dominant earlier as \( 1/\varepsilon \) grows, thus it performs better in this perspective. This is consistent with our theoretical findings, because the ranges of estimators in PARALLELTRACEGIBBS are smaller than the ranges used in SUPERCHAINTRACEGIBBS.

4 Conclusions: advantages and limitations of proposed algorithms

We develop a doubly-adaptive MCMC-based estimator for the partition function of Gibbs distributions, which resolves a major impediment of prior methods that use MCMC as a black-box sampler. We show, both theoretically and experimentally, that our method requires substantially fewer MCMC steps than the state-of-the-art method. The better performance is due to several factors, which all stem from the use of an adaptive MCMC mean estimator instead of a standard "black-box" MCMC estimate. The complexity of the adaptive MCMC process depends on the (smaller) trace, rather than stationary, relative variances, and on relaxation times instead of mixing times. It is also less sensitive to weak upper-bounds on mixing and relaxation times.
In particular, Kolmogorov’s method requires $\Theta(\ell/\varepsilon^2)$ approximately independent samples, where $\ell$ is the length of cooling schedule. This requires tight convergence (total variance distance of $O(\varepsilon^2/\ell)$ from stationary) for each sample, which adds a multiplicative $\ln \frac{1}{\varepsilon^2}$, with $\ell = \Theta(\ln Q \ln H_{\max})$, to its complexity (see column 3 of table 1 and [43], theorem 9). In contrast, our doubly adaptive method only depends on relaxation times, which do not depend on $\varepsilon$.

**Limitations.** While significantly improving the state of the art, our methods suffer from several limitations. In SuperChainTraceGibbs, the major limitation is the dependence on the relative ranges of $F$ and $G$, which can be large, especially when the Hamiltonian range is large. Another issue is that the product chain’s mixing time is dominated by $\ell \max\{\tau_i\}_{i=1}^\ell$, as opposed to $\sum_{i=1}^\ell \tau_i$. While ParallelTraceGibbs circumvents these issues by estimating each factor of the telescoping product independently, it fails to beat SuperChainTraceGibbs’s efficiency in general, due both to the union bound and the higher-precision guarantees required for each subproblem. Improving performance further will likely require new estimators with smaller ranges and relative trace variances.

**Statement of Broader Impact.** While probabilistic graphical models as other machine learning methods that rely on MCMC estimations continue to grow in importance and popularity. But running the MCMC to theoretical convergence guarantees is often prohibitively expensive, while running it to apparent convergence is methodologically unsound, particularly in the modern context, where public confidence in machine learning systems is continuously eroded by ethical, accuracy, and safety failures. Our work attempts to bridge the gap between the definite, elegant and theoretically sound analytic methods, and efficiency-focused practical utility, as we seek to reduce proof-burden, while maintaining theoretical guarantees of accuracy, with adaptive methods that bound efficiency in terms of (potentially unknown) convergence rate metrics and variances.

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Algorithm 3 RelMeanEst

1. procedure RelMeanEst
2. Input: Markov chain $M$, upper-bound on relaxation time $T$, real-valued function $f$ with range $[a, b]$, letting $R = b - a$, multiplicative precision $\varepsilon$, error probability $\delta$.
3. Output: Multiplicative approximation $\hat{\mu}$ of $\mu = \mathbb{E}_x[f]$.
4. $T \leftarrow \left[ \frac{1}{\varepsilon \ln \sqrt{T}} \right] / \alpha \leftarrow \sqrt{T}$ \quad \triangleright \text{Choose } T \text{ to be an upperbound on relaxation time}
5. $I \leftarrow 1 \lor \log_2 \left( \frac{\log_2 \left( \frac{\log_2 (\frac{1}{1 + \frac{\varepsilon}{\delta}})}{\log_2 (\frac{\log_2 (\frac{1}{1 + \frac{\varepsilon}{\delta}}))} \right)} {\log_2 (\frac{\log_2 (\frac{1}{1 + \frac{\varepsilon}{\delta}}))} \right)$ \quad \triangleright \text{Initialize sampling schedule}
6. $T_{\text{init}} \leftarrow \left[ T \cdot \log(n_{\text{init}}) \right]$; $(\bar{X}_{0.1}, \bar{X}_{0.2}) \leftarrow \mathcal{M}^{T_{\text{init}}}(\perp)$ \quad \triangleright \text{Warm-start two chains for } T_{\text{init}} \text{ steps from arbitrary } \perp \in \Omega
7. for $i = 1, 2, \ldots, I$ do
8. $m_i \leftarrow \left| \alpha r^i \right|$ \quad \triangleright \text{Total sample count at iteration } \hat{i} \text{ is the geometric ratio (constant, usually 2)} size
9. for $j \in (m_{i-1} + 1), \ldots, m_i$ do
10. $(\bar{X}_{j,1}, \bar{X}_{j,2}) \leftarrow (T \text{ steps of } M \text{ starting at } \bar{X}_{j-1,1}, \bar{X}_{j-1,2})$
11. $f(\bar{X}_{j,1}) \leftarrow \frac{1}{T} \sum_{t=1}^{T} f(\bar{X}_{j,1}(t)); f(\bar{X}_{j,2}) \leftarrow \frac{1}{T} \sum_{t=1}^{T} f(\bar{X}_{j,2}(t))$ \quad \triangleright \text{Run two independent copies of } M \text{ for } T \text{ steps}
12. end for
13. $\bar{\mu}_i \leftarrow \frac{1}{2m_i} \sum_{j=1}^{m_i} (f(\bar{X}_{j,1}) + f(\bar{X}_{j,2})); \hat{\varepsilon}_i \leftarrow \frac{1}{2m_i} \sum_{j=1}^{m_i} (f(\bar{X}_{j,1}) - f(\bar{X}_{j,2}))$ \quad \triangleright \text{Compute empirical mean; trace variance}
14. $u_i \leftarrow \hat{\varepsilon}_i + (11 \sqrt{T} (1 + \Delta) R^2 \ln \frac{2}{\delta}) (1 + \Delta) m_i$ \quad \triangleright \text{Variance upper bound}
15. $\hat{\mu}_i \leftarrow 10 R \ln \frac{2}{(1 - \Delta) m_i} \quad \triangleright \text{Apply Bernstein bound}
16. $\mu_i \leftarrow (\hat{\mu}_i - \hat{\varepsilon}_i) \lor a + (\hat{\mu}_i + \hat{\varepsilon}_i) \land b$ \quad \triangleright \text{Optimal mean estimate}
17. $\hat{\mu}_i^* \leftarrow 2(b - (\hat{\mu}_i - \hat{\varepsilon}_i)) \lor a$ \quad \triangleright \text{Empirical relative error bound}
18. if $(i = I) \lor (\hat{\mu}_i^* \leq \varepsilon)$ then
19. return $\hat{\mu}_i^*$
20. end if
21. end for
22. end procedure

A

A.1 Algorithms used in the literature

A.1.1 The Tpa method [37, 43]

We refer to Huber and Schott’s algorithm as the original TPA, and Kolmogorov’s, which is used in our algorithms and referred to as TPA($k, d$) in the main manuscript, as the TPA method.

A.1.2 Single site Gibbs sampler (Glauber dynamics chain)

Consider $\beta$ and $H$ defined as above. Let $X = (X_1, X_2, \ldots, X_n)$ be the set of all variables in the Gibbs distribution with inverse temperature $\beta$ and Hamiltonian $H$, thus, the domain of $H$ is $\Omega = \Omega_1 \times \Omega_2 \times \ldots \Omega_n$, and each $\Omega_i$ is the range of random variable $X_i$. At each time step $t$, assume the current state is $x^{(t)} = (x_1, x_2, \ldots, x_n)$. Take $i \sim 1, \ldots, n$ uniformly at random. Sample $y$ from the following distribution:

$$
\pi_\beta(y|x^{(t)}) = \frac{\exp(-\beta H(x^{(t)}; x_i \leftarrow y))}{\sum_{\omega \in \Omega_i} \exp(-\beta H(x^{(t)}; x_i \leftarrow \omega))},
$$

(6)

where for an arbitrary $\omega \in \Omega_i$ we define $(x^{(t)}; x_i \leftarrow \omega)$ be the vector in which all the elements except the ith element are equal to $x_i$ and the ith element is replaced with $\omega$.

In other words, for any arbitrary vectors $x^{(t)}$ and $x^{(t+1)}$, the transition probability is:
Algorithm 4 SuperChainTraceGibbs and ParallelTraceGibbs

1: procedure SuperChainTraceGibbs(...) 
2: \((\beta_0, \beta_1, \ldots, \beta_t) \leftarrow \text{TPa}(k, d)\) 
3: \(z' \leftarrow \frac{z'}{2}; \delta' \leftarrow \frac{\delta}{2}\) 
4: for \(i \in 1, 2, \ldots, t\) do 
5: \(f_i(x) \equiv \exp(- \frac{\beta_{i+1} - \beta_i}{2} H(x))\) 
6: \(g_i(x) \equiv \exp(\beta_{i+1} - \beta_i H(x))\) 
7: end for 
8: \(F \equiv \bigotimes_{i=1}^{t} f_i; G \equiv \bigotimes_{i=1}^{t} g_i\) 
9: \(\mathcal{G}^\circ \equiv \bigotimes_{i=1}^{t} \mathcal{G}_{H, \beta_i}\); with \(\omega_i = \frac{1}{t}\) for all \(i\) 
10: \(R_f \leftarrow \exp(- \frac{\beta_{i+1} - \beta_i}{2} H_{\min}) - \exp(- \frac{\beta_{i+1} - \beta_0}{2} H_{\max})\) 
11: \(R_g \leftarrow \exp(\beta_{i+1} - \beta_0 H_{\max}) - \exp(\beta_{i+1} - \beta_0 H_{\min})\) 
12: \(\mu \leftarrow \text{RelMeanEst}(\mathcal{G}^\circ, R_f, T, F, \epsilon', \delta')\) 
13: \(\nu \leftarrow \text{RelMeanEst}(\mathcal{G}^\circ, R_g, T, G, \epsilon', \delta')\) 
14: return \(\hat{Z} \leftarrow \frac{\mu}{\nu}\) 
15: end procedure 

Algorithm 5 The Original TPA-method

1: output a schedule \((\beta_1, \ldots, \beta_t)\) of values in the interval \([\beta_{\min}, \beta_{\max}]\). 
2: \(\beta_0 \leftarrow \beta_{\min}\) 
3: for \(i = 0 : \infty\) do 
4: sample \(X \sim \pi_{\beta_i}\) draw \(U \in [0, 1]\) uniformly, \(\beta_{i+1} = \beta_i - \log U / H(X)\) (or +\(\infty\) if \(H(X) = 0\).) 
5: if \(\beta_{i+1} \notin [\beta_{\min}, \beta_{\max}]\) then Terminate 
6: end if 
7: end for 

\[
\mathcal{G}_{H, \beta}(x^{(t)}, x^{(t+1)}) = \begin{cases} 
\frac{(1/\pi_{\beta}) (y | x^{(t)}_i)}{\sum_{i=1}^{n} (1/\pi_{\beta}) (x_i | x^{(t)}_i)} & \exists y, i \text{ such that } x_i \neq y \text{ and } x^{(t+1)} = (x^{(t)}; x_i \leftarrow y), \\
0 & \text{if } x^{(t)} = x^{(t+1)}, \\
\text{otherwise}. & 
\end{cases}
\]

A.2 Missing proofs: TPA and relative trace variance properties

Lemma A.1. Let \(z(\beta) \equiv \log( Z(\beta) )\), \(d\) and \(k\) the parameters of the TPA method, and \(\beta_i\) and \(\beta_{i+1}\) two consecutive points generated by \(\text{TPa}(k, d)\), we have:
1. For any \(\varepsilon \geq 0\), we have \(\mathbb{P}(z(\beta_i) - z(\beta_{i+1}) \leq \varepsilon) \geq 1 - \exp( - \varepsilon / k d)\)
2. For any \(\varepsilon \geq 0\), \(\mathbb{P}(\Delta_j \geq \varepsilon / \mathbb{E}(\Pi(x))) \leq d \exp( - \varepsilon / k d)\)

Proof of lemma A.1. Note that \(\text{TPa}(k, d)\) of (33) consists of \(k\) parallel runs of the original TPa of (37) and outputting a sub-sequence of elements which are \(d\) apart.

Let \((b_i)\) be the sequence generated by \(k\) parallel copies of the original TPa, thus \(\Delta_j = \beta_{j+1} - \beta_j = b_{j+d} - b_j\).

We first show item 1 by bounding \(\mathbb{P}(z(b_j) - z(b_{j+d}) \geq \varepsilon)\), and using
\[
\mathbb{P}(b_{j+d} - b_j < \varepsilon) \geq \prod_{i=1}^{d} \mathbb{P}(b_{j+i} - b_{j+i-1} < \varepsilon / d).
\]

With the definition of the PPP, and using (30) we have \(z(b_i) - z(b_{i+1})\) follows the exponential distribution with mean \(1/k\), thus \(\mathbb{P}(z(b_i) - z(b_{i+1}) \geq \varepsilon / d) = \exp(- \varepsilon / k d)\). Therefore,
\[
\mathbb{P}(z(b_{j+d}) - z(b_j) \geq \varepsilon) \geq \prod_{i=1}^{d} \mathbb{P}(z(b_{j+i}) - z(b_{j+i-1}) < \varepsilon / d) = (1 - \exp(- \varepsilon / k d))^d.
\]
To see item 2 of the Lemma let \( z'(\beta) \) be the derivative of \( z(\cdot) \) with respect to \( \beta \), which is \( z'(\beta) = \sum_{x \in \Omega} -H(x) \exp(-\beta H(x))/Z(\beta) \), thus \( z'(\beta) \leq 0 \). Using the Cauchy–Schwarz inequality we have \( z''(\beta) = (\sum_{x \in \Omega} H^2(x) \exp(-\beta H(x))) \sum_{x \in \Omega} \exp(-\beta H(x)) - (\sum_{x \in \Omega} -H(x) \exp(-\beta H(x))^2)/Z^2(\beta) \geq 0 \). Therefore,

\[
    z'(\beta_i) < \frac{z(\beta_{i+1}) - z(\beta_i)}{\beta_{i+1} - \beta_i} < z'(\beta_{i+1}),
\]

Thus, \( \beta_{i+1} - \beta_i < \frac{z(\beta_i) - z(\beta_{i+1})}{z'(\beta_i)} \). Note that \( -z'(\beta_i) = E[H(x)], x \sim \pi_{\beta_i} \). Therefore, we have:

\[
    \Pr \left( \Delta_i \leq \frac{\epsilon}{E[H]} \right) \geq \Pr \left( \frac{z(\beta_i) - z(\beta_{i+1})}{z'(\beta_{i+1})} \leq \frac{\epsilon}{E[H]} \right) = \Pr \left( z(\beta_i) - z(\beta_{i+1}) \leq \epsilon \right) \geq (1 - \exp(-\epsilon k/d))^d
\]

Thus \( \Pr \left( \Delta_i \geq \frac{\epsilon}{E[H]} \right) \geq 1 - (1 - \exp(-\epsilon k/d))^d \approx d \exp(-\epsilon k/d) \).

\[\square\]

**Proof of Lemma 2.1.** Note that by Thm 3.1. of \([57]\) we have, \( E[(\bar{f}(X_{1:rx}) - E(f))^2] \leq \frac{2\tau_{rx} \lambda}{2} \). Dividing both sides by \( (E(f))^2 \) we get the second part of the premise. The first part concludes from setting \( \tau = \tau_{rx} \).

\[\square\]

### A.3 RelMeanEst

**RelMeanEst in summary** To employ progressive sampling, we start by a small sample size and calculate the empirical estimation of the variance at each iteration. We estimate an upper bound on the trace variance based on its empirical estimation, and using that we check a termination condition.

Our variance estimator is what Cousins et al. introduced, and is based on running two independent chains. Each sample is obtained by taking a trace of length \( T \) (given upper-bound on relaxation time) and taking the average over all observed values on that trace. Thus, half the square difference of the averages on the two chains is an unbiased estimate of the trace variance.

Before showing the result, we state two key theorems from the literature, which describe how our tail bounds work.

**Theorem A.2** (Hoeffding-Type Bounds for Mixing Processes, (see Thm. 2.1 of \([22]\))). For any \( \delta \in (0, 1) \), we have

\[
    \Pr \left( |\hat{\mu} - \mu| \geq \sqrt{\frac{2(1 + \lambda)(\frac{R^2}{2}) \ln(\frac{2}{\delta})}{(1 - \lambda)m}} \right) \leq \delta. \tag{7}
\]

This implies sample complexity

\[
    m_H(\lambda, R, \varepsilon, \delta) = \frac{1 + \lambda}{1 - \lambda} \frac{R^2}{2\varepsilon^2} \in \Theta \left( \tau_{rx} \ln(\frac{1}{\varepsilon}) \frac{R^2}{\varepsilon^2} \right).
\]
Theorem A.3 (Bernstein-Type Bound for Mixing Process [39 Thm. 1.2]). For any $\delta \in (0, 1)$, we have

$$
\mathbb{P} \left( |\hat{\mu} - \mu| \geq 10R \ln \left( \frac{\lambda}{2(1 - \lambda)} \right) + \sqrt{\frac{2(1 + \lambda)\nu_\pi \ln \left( \frac{\lambda}{2(1 - \lambda)} \right)}{(1 - \lambda)m}} \right) \leq \delta .
$$

This implies sample complexity

$$
m_B(\lambda, R, v, \varepsilon, \delta) = \frac{2}{1 - \lambda} \ln \left( \frac{\lambda}{2} \right) + \left( \frac{1 + \lambda}{2} \right) \ln \left( \frac{\lambda}{2} \right) \in \Theta \left( \eta_{\pi} \ln \left( \frac{1}{2} \right) \left( \frac{R}{\varepsilon} + \frac{\nu_\pi}{\varepsilon^2} \right) \right).
$$

We now show the main result.

Proof of Theorem 2.2. Suppose confidence interval $[a, b]$. The interval endpoints, multiplicative error $\varepsilon_x$, and additive error $\varepsilon_\pi$ are related as $2\varepsilon_\pi = a + \varepsilon_x$ and $b - a = \frac{2\varepsilon_\pi}{1 - \varepsilon_x}$, depicted graphically below.

We derive a geometric progressive sampling schedule such that the algorithm draws sample sizes, ranging between optimistic and pessimistic (over unknown variance and mean) upper and lower bounds on the sufficient sample size.

Using the Markov chain Bennett inequality [39], the best-case complexity, assuming maximal expectation, and minimal variance, is

$$
m^+ \geq m_B(\Lambda, R, 0, \varepsilon_+, \frac{2\delta}{3I}) \geq \frac{(1 + \Lambda)R \ln \left( \frac{\lambda}{2} \right)}{(1 - \Lambda)\varepsilon_+} + \frac{(1 + \Lambda)R \ln \left( \frac{\lambda}{2} \right)}{b(1 - \Lambda)\varepsilon_x}.
$$

The worst-case complexity, then assuming minimal expectation, and maximal variance, is

$$
m^- \geq m_H(\Lambda, R, \varepsilon_+, \frac{2\delta}{3I}) \geq \frac{(1 + \Lambda)R^2 \ln \left( \frac{\lambda}{2} \right)}{2(1 - \Lambda)\varepsilon_+^2} \geq \frac{(1 + \Lambda)R^2 \ln \left( \frac{\lambda}{2} \right)}{2(1 - \Lambda)\varepsilon_x^2}.
$$

via the Markov chain Hoeffding’s inequality [40].

Consequently, a doubling schedule requires $I = \left\lceil \log_2 \left( \frac{m^-}{m^+} \right) \right\rceil = \left\lceil \log_2 \left( \frac{bR}{2R} \right) \right\rceil$ steps.

All tail bounds on variances and means are hold simultaneously with probability at least $1 - \delta$ (by union bound), and the doubling schedule never overshoots the sufficient sample size by more than a constant factor, which yields the stated guarantees.

The proof consists of two parts, in both we make derive our new bounds by writing an $\varepsilon_x$-multiplicative approximation in terms of an $\varepsilon_\pi$-additive approximation.

In the worst-case, we underestimate the true mean $\mu$ by a factor $(1 - \varepsilon_x)$, and thus require a radius $\varepsilon_+ = \varepsilon_x (1 - \varepsilon_x) \mu$ additive confidence interval.

We first show the correctness guarantee.

Observe that the sampling schedule is selected such that the final iteration $I$ of the algorithm will draw a sufficiently large sample (size $m^+$) such that the Hoeffding inequality will yield such a confidence interval, even for worst-case (minimal) $\mu$. Now observe that over the course of the algorithm, in each iteration, 3 tail bounds are applied; one to upper-bound the variance, and then two to upper and lower bound the mean in terms of the variance bound) as in [10]. By union bound, all $3I$ tail-bounds hold simultaneously with probability at least $1 - \delta$, thus when the algorithm terminates, it produces a correct answer with at least said probability.
We now show the efficiency guarantee. Suppose we get \( \hat{\mu} \) from \textsc{RelMeanEst}, by guarantee of correctness of the algorithm, we have a lower bound on \( \hat{\mu} \), \( \hat{\mu} \geq \mu(1 - \varepsilon \times \epsilon) \) with probability at least \( 1 - \delta \).

Furthermore, we have \( \varepsilon_+ = \mu \varepsilon \times \epsilon \) and \( \text{trv}^{(\tau_{rx})} = (\text{Reltrv}^{\tau_{rx}} - 1) \times \hat{\mu}^2 \geq (\text{Reltrv}^{\tau_{rx}} - 1)\mu^2(1 - \varepsilon \times \epsilon)^2 \). For this \( \varepsilon_+ \), we have via the Bernstein inequality that

\[
m^* \in O \left( \log \left( \frac{\log(R/\mu \varepsilon \times \epsilon)}{\delta} \right) \left( \frac{R/\mu}{(1 - \Lambda)\varepsilon \times \epsilon} + \frac{\tau_{rx} (\text{Reltrv}^{\tau_{rx}} - 1)}{\varepsilon \times \epsilon} \right) \right)
\]

would be a sufficient sample size if (1) the algorithm were to draw a sample of this size, and (2) we were to use the true trace variance instead of the estimated upper-bound on trace variance.

Fortunately, correcting for (1) adds a constant factor to the sample complexity, as the first sample size \( \alpha \) is selected to be twice the minimal sufficient sample size \( m \) (i.e., the sample size such that no smaller sample size would be sufficient), and at each iteration the sample size selected is double the previous (line 8). In other words, this geometric grid will never overshoot any sample size by more than a factor 2.

Resolving (2) is a bit more subtle, but we now show that there is no asymptotic change in replacing the variance with the estimated variance upper bound (w.h.p.). First, note that the Bernstein bound is bidirectional, so it can just as well be used to upper-bound empirical variance with true variance as to upper-bound true variance with empirical variance. We bound true variance in terms of empirical variance on line 14, and note that here we have

\[
v \leq u \in \hat{v} + O \left( \frac{R^2 \ln \frac{4}{3}}{m} + \sqrt{\frac{R^2 \hat{v} \ln \frac{4}{3}}{m}} \right) .
\]

Fortunately, the latter terms are negligible, as in line 15, we bound

\[
\varepsilon_+ \in O \left( \frac{R \ln \frac{4}{3}}{m} + \sqrt{\frac{u \ln \frac{4}{3}}{m}} \right)
\]

\[
= O \left( \frac{R \ln \frac{4}{3}}{m} + \sqrt{\frac{v + O \left( \frac{R \ln \frac{4}{3}}{m} + \sqrt{\frac{u \ln \frac{4}{3}}{m}} \right) \ln \frac{4}{3}}{m}} \right)
\]

\[
= O \left( \frac{R \ln \frac{4}{3}}{m} + \sqrt{\frac{v + O \left( \frac{R \ln \frac{4}{3}}{m} + \sqrt{\frac{u \ln \frac{4}{3}}{m}} \right) \ln \frac{4}{3}}{m}} \right) \quad \text{(w.h.p.)}
\]

Putting these together, we thus have that, w.h.p., sample consumption is bounded as

\[
\hat{m} \in 2O(m^*) = O \left( \log \left( \frac{\log(R/\mu \varepsilon \times \epsilon)}{\delta} \right) \left( \frac{R/\mu}{(1 - \Lambda)\varepsilon \times \epsilon} + \frac{\tau_{rx} (\text{Reltrv}^{\tau_{rx}} - 1)}{\varepsilon \times \epsilon} \right) \right) .
\]

To conclude, we need only relate \( T(\text{Reltrv}^T - 1) \) and \( \tau_{rx}(\text{Reltrv}^{\tau_{rx}} - 1) \). Letting \( T \) as in line ???, note that since \( T \geq \tau_{rx} \), it holds that \( T(\text{Reltrv}^T - 1) \geq \tau_{rx}(\text{Reltrv}^{\tau_{rx}} - 1) \), by the trace variance inequalities, which yields the result.
A.4 Missing proofs from analysis of SuperChainTraceGibbs

Proof of thm 2.4. Follows immediately from thm. 2.2 and plugging in the values for paired product estimators and the product chain. \( \square \)

Full Proof of Lemma 2.8. Let \( \bar{\beta}_{i,i+1} = \frac{\beta_i + \beta_{i+1}}{2} \), we have \( \mu_i = \frac{Z(\bar{\beta}_{i,i+1})}{Z(\beta_i)} \) and \( \nu_i = \frac{Z(\bar{\beta}_{i,i+1})}{Z(\beta_{i+1})} \). Thus we have

\[
\nu = \prod_{i=1}^{\ell-1} \frac{Z(\bar{\beta}_{i,i+1})}{Z(\beta_{i+1})} > 1, \mu = \prod_{i=1}^{\ell-1} \frac{Z(\bar{\beta}_{i,i+1})}{Z(\beta_i)} < 1.
\]

Note that \( \nu = \mu \frac{Z(\beta_i)}{Z(\bar{\beta}^{\text{max}})} \), thus we proceed by bounding \( \mu \).

\[
\log \prod_{i=1}^{\ell-1} Z(\bar{\beta}_{i,i+1}) = \sum_{i=1}^{\ell-1} z(\bar{\beta}_{i,i+1}) \quad \text{TAKING log}
\]

\[
\geq \sum_{i=1}^{\ell-1} z(\beta_i) - \frac{\Delta_i}{2} \mathbb{E}_{x \sim \pi_{\beta_i}} [H(x)] \quad \text{TAYLOR EXPANSION & THAT} \quad \frac{\partial^2}{\partial \beta^2} z(\beta) > 0
\]

Thus, by taking exponents we get:

\[
\prod_{i=1}^{\ell-1} Z(\bar{\beta}_{i,i+1}) \geq \exp \left( \sum_{i=1}^{\ell-1} z(\beta_i) - \frac{\Delta_i}{2} \mathbb{E}_{x \sim \pi_{\beta_{i+1}}} [H(x)] \right) \geq \left( \prod_{i=1}^{\ell-1} Z(\beta_i) \right) \exp \left( - \sum_{i=1}^{\ell-1} \frac{\Delta_i}{2} \mathbb{E}_{x \sim \pi_{\beta_i}} [H(x)] \right)
\]

Therefore, \( \mu = \prod_{i=1}^{\ell-1} \frac{Z(\bar{\beta}_{i,i+1})}{Z(\beta_i)} \geq \exp \left( - \sum_{i=1}^{\ell-1} \frac{\Delta_i}{2} \mathbb{E}_{x \sim \pi_{\beta_i}} [H(x)] \right) \). Using this form, we now employ the fundamental theorem of calculus to prove the premise:

Let \( \Delta_{\text{max}} = \max_i \Delta_i \).

\[
\mu \geq \exp \left( - \sum_{i=1}^{\ell-1} \frac{\Delta_i}{2} \mathbb{E}_{x \sim \pi_{\beta_i}} [H(x)] \right)
\]

\[
= \exp \left( - \sum_{i=1}^{\ell-1} \frac{\Delta_i}{2} \mathbb{E}_{x \sim \pi_{\beta_i}} [H(x)] \right)
\]

\[
\geq \exp \left( \frac{1}{2} \int_{\beta_{\text{max}} - \Delta_{\text{max}}}^{\beta_{\text{min}} - \Delta_{\text{max}}} - \mathbb{E}_{x \sim \pi_{\beta}} [H(x)] \, d\beta \right) \quad \text{INCORPORATING INTEGRAND}
\]

\[
= \exp \left( \frac{1}{2} \left( z(\beta_{\text{max}} - \Delta_{\text{max}}) - z(\beta_{\text{min}} - \Delta_{\text{max}}) \right) \right) \quad \text{FTOC AND THAT} \quad z'(\beta) = \mathbb{E}_{x \sim \pi_{\beta}} H \quad \text{AND} \quad z \text{ IS DECREASING}
\]

\[
= \exp \left( \frac{1}{2} \left( z(\beta_{\text{max}}) - z(\beta_{\text{min}}) + z(\beta_{\text{min}} - \Delta_{\text{max}}) \right) \right)
\]

\[
\geq Q^{-\frac{1}{2}} \sqrt{\frac{Z(\beta_{\text{min}})}{Z(\beta_{\text{min}} - \Delta_{\text{max}})}}.
\]
From the above we also conclude that $\nu \geq Q^{1/2} \sqrt{\frac{Z(\beta_{\min})}{Z(\beta_{\min} - \Delta_{\text{max}})}}$. Note that $\text{Range}(f) = \exp(-\frac{H}{2} \beta_{\min}) - \exp(-\frac{H}{2} \beta_{\max}) \leq \sqrt{\exp(-\Delta H_{\text{min}})}$ and $\text{Range}(g) = \exp(\frac{H}{2} \beta_{\max}) - \exp(\frac{H}{2} \beta_{\min}) \leq \sqrt{\exp(\Delta H_{\text{max}})}$. Thus the lemma is concluded.

Proof of Corollary 2.6. The corollary follows from thm 2.2 plugging in $R$ from lemma 2.5 and setting $\tau_{\text{prx}} = \ell \max_{i=1}^\ell \tau_i$ (see, e.g., [17]).

A.5 Analysis of ParallelTraceGibbs

Let $(\beta_0, \beta_1, \ldots, \beta_i)$ be a cooling schedule generated by $\text{TPA}(k, d)$, where $k$ and $d$ are chosen as in [15]. For each $i$ let $f_{\beta_i, \beta_{i+1}}, g_{\beta_{i-1}, \beta_i}$ be the paired estimators corresponding to this schedule, and $\mu_i = \mathbb{E}[f_{\beta_i, \beta_{i+1}}], \nu_i = \mathbb{E}[g_{\beta_{i-1}, \beta_i}]$. $\text{PARALLELTraceGibbs}$ estimates $Q$ by running $\text{RELMEANEston}$ each $G_{H, \beta_i}$, to estimate $\mu_i$ and $\nu_i$s each with precision $\epsilon$.

Let $z = \exp(\Delta H_{\text{max}})/\sqrt{\ell}$, $\Delta$ the first and second derivative of $z$ with respect to $\beta$. Note that $z'(\beta) = \mathbb{E}_{x \sim \pi_\beta}[-H(x)]$. Since $z'' \geq 0$ we have:

$$z'(\beta_i) < \frac{z(\beta_i + \Delta_i/2) - z(\beta_i)}{\Delta_i/2} < z'(\beta_i + \Delta_i/2)$$
and
\[ z'(\beta_{i+1} - \Delta_i/2) < \frac{z(\beta_{i+1}) - z(\beta_{i+1} - \Delta_i/2)}{\Delta_i/2} < z'(\beta_{i+1}). \]
Which are equivalent to
\[ \frac{1}{z'(\beta_{i+1} - \Delta_i/2)} \leq \frac{\Delta_i/2}{z(\beta_{i+1}) - z(\beta_{i+1} - \Delta_i/2)} \leq \frac{1}{z'(\beta_{i+1})} \]
and
\[ \frac{1}{z'(\beta_{i+1} - \Delta_i/2)} \leq \frac{\Delta_i/2}{z(\beta_{i+1}) - z(\beta_{i+1} - \Delta_i/2)} \leq \frac{\Delta_i/2}{z(\beta_{i+1}) - z(\beta_{i+1} - \Delta_i/2)} \leq \frac{1}{z'(\beta_{i+1})}. \]
Therefore,
\[
\frac{\text{Range}(f_i)}{\mu_i} \leq \exp \left( (z(\beta_i + \Delta_i/2) - z(\beta_i)) \left( \frac{-\min_x H(x)}{2} \frac{1}{z'(\beta_i)} - 1 \right) \right)
\]
\[= \exp \left( (z(\beta_i + \Delta_i/2) - z(\beta_i)) \left( \frac{\min_x H(x)}{2} \frac{1}{\mathbb{E}[H]} - 1 \right) \right) \]
\[\leq \exp \left( (z(\beta_i) - z(\beta_i + \Delta_i/2)) \right) \]
(10)
Similarly for range of \( g_i \)s we have:
\[
\frac{\text{Range}(g_i)}{\nu_i} \leq \exp \left( (z(\beta_{i+1} - \Delta_i/2) - z(\beta_{i+1})) \left( \frac{-\max_x H(x)}{2} \frac{1}{z'(\beta_{i+1})} - 1 \right) \right)
\]
\[\leq \exp \left( (z(\beta_{i+1} - \Delta_i/2) - z(\beta_{i+1})) \left( \frac{\max_x H(x)}{2\mathbb{E}_{\pi_{\beta_i}}[H(X)]} - 1 \right) \right) \]
(14)
We now use [10] together with lemma A.1 Setting \( d = 1 \) we have,
\[
P \left( z(\beta_i) - z(\beta_{i+1}) > \frac{\log(3l/4)}{\log n} \right) = \exp(- \frac{\log(3l/4)}{\log n} \cdot k) = (3/4) \exp(- l/ \log n) = (3/4)(1/l).
\]
Using union bound over all \( 1 \leq i \leq l \) and that \( z(\beta_i) - z(\beta_{i+1}) \geq z(\beta_i) - z(\beta_i + \Delta_i/2) \), we conclude that with probability at least \( 3/4 \) we have that for all \( f_i \), \( \text{Range}(f_i)/\mu_i \leq \ell^{1/\log(n)} \).
Similarly using [13], the union bound, lemma A.1 and that \( z(\beta_i) - z(\beta_{i+1}) \geq z(\beta_i - \Delta_i/2) - z(\beta_{i+1}) \), we can show that with constant probability all \( g_i \)s generated by the Tpa schedule obey: \( \forall g_i; 1 \leq i \leq l \), \( \text{Range}(g_i)/\nu_i \leq \exp \left( (\log l/ \log n) \cdot (\alpha) \right) = \ell^{\alpha_0/\log n} \), where \( \alpha_0 = \frac{\max_x H(x)}{2\mathbb{E}_{\pi_{\beta_i}}[H(X)]} - 1 \).

The following corollary is concluded from lemma A.4 and relative trace variance bounds:

**Corollary A.5.** When \( \varepsilon \leq \ell^{1/\log(n)} \left( 1 + \ell^{\alpha_0(i)} \cdot \frac{\tau_{\beta_i}}{(1-\lambda_i)} \right) \), RELMEANEst invoked on the ith iteration will stop using sample consumption of \( \tilde{O}(\ell^2 \tau_i \text{Reltrv}_i) \) note that this is improvement over classic bounds which are \( \tilde{O} ((1 - \lambda_i)^{-1} \text{Reltrv}_i) \). In total the sample complexity of PARALLELTRACEGIBBS for \( \varepsilon \leq \ell^{1/\log(n)} \min_i (1 + \ell^{\alpha_0(i)} \cdot \frac{\tau_{\beta_i}}{(1-\lambda_i)}) \) is dominated by \( \tilde{O} \left( \ell^2 \sum_{i=1}^{l} \tau_i \text{Reltrv}_i \right) \).

**A.6 Further experimental results**

**References**

[1] Permit allocation in emissions trading using the Boltzmann distribution. Physica, A 391:4883–4890, 2012.

[2] H. Afshar, S. Sanner, and C. Webers. Closed-form Gibbs sampling for graphical models with algebraic constraints. In AAAI, 2016.
Figure 3: Comparison of sample complexity on Ising models.

[3] D. Aldous, G. R. Grimmett, C. D. Howard, F. Martinelli, J. M. Steele, and L. Saloff-Coste. Probability on discrete structures, volume 110. Springer Science & Business Media, 2013.

[4] Y. Alimohammadi, N. Anari, K. Shiragur, and T. Vuong. Fractionally log-concave and sector-stable polynomials: Counting planar matchings and more. ArXiv, abs/2102.02708, 2021.

[5] N. Anari, K. Liu, and S. O. Gharan. Spectral independence in high-dimensional expanders and applications to the hardcore model. SIAM Journal on Computing, (0):FOCS20–1, 2021.

[6] I. Bezáková, D. Stefankovic, V. Vazirani, and E. Vigoda. Accelerating simulated annealing for the permanent and combinatorial counting problems. In SODA 2006, 2006.

[7] N. Bhatnagar, A. Bogdanov, and E. Mossel. The computational complexity of estimating MCMC convergence time. In Approximation, Randomization, and Combinatorial Optimization. Algorithms and Techniques, pages 424–435. Springer, 2011.

[8] N. Bhatnagar, A. Sly, and P. Tetali. Reconstruction threshold for the hardcore model. In Approximation, Randomization, and Combinatorial Optimization. Algorithms and Techniques, pages 434–447. Springer, 2010.

[9] A. Blanca, P. Caputo, Z. Chen, D. Parisi, D. Stefankovic, and E. Vigoda. On mixing of Markov chains: Coupling, spectral independence, and entropy factorization. ArXiv, abs/2103.07459, 2021.
10] S. P. Brooks and A. Gelman. General methods for monitoring convergence of iterative simulations. *Journal of computational and graphical statistics*, 7(4):434–455, 1998.

[11] S. P. Brooks and G. O. Roberts. Assessing convergence of Markov chain Monte Carlo algorithms. *Statistics and Computing*, 8(4):319–335, 1998.

[12] Z. Chen, A. Galanis, D. Štefanković, and E. Vigoda. Rapid mixing for colorings via spectral independence. In *Proceedings of the 2021 ACM-SIAM Symposium on Discrete Algorithms (SODA)*, pages 1548–1557. SIAM, 2021.

[13] H. Cheng, L. Qu, D. Garrick, and R. Fernando. A fast and efficient Gibbs sampler for BayesB in whole-genome analyses. *Genetics, Selection, Evolution : GSE*, 47, 2015.

[14] K.-M. Chung, H. Lam, Z. Liu, and M. Mitzenmacher. Chernoff-Hoeffding bounds for Markov chains: Generalized and simplified. *arXiv:1201.0559*, 2012.

[15] B. A. Cipra. An introduction to the Ising model. *The American Mathematical Monthly*, 94(10):937–959, 1987.

[16] C. Cousins, S. Haddadan, and E. Upfal. Making mean-estimation more efficient using an MCMC trace variance approach: DynaMITE. *CoRR*, abs/2011.11129, 2020.

[17] C. De Sa, V. Chen, and W. Wong. Minibatch Gibbs sampling on large graphical models. In *Proceedings of the 35th International Conference on Machine Learning*, volume 80 of *Proceedings of Machine Learning Research*, pages 1165–1173. PMLR, 10–15 Jul 2018.

[18] C. De Sa, K. Olukotun, and C. Ré. Ensuring rapid mixing and low bias for asynchronous Gibbs sampling. In *Proceedings of the 33rd International Conference on International Conference on Machine Learning - Volume 48*, ICML’16, pages 1567–1576, 2016.

[19] C. De Sa, C. Zhang, K. Olukotun, and C. Ré. Rapidly mixing Gibbs sampling for a class of factor graphs using hierarchy width. *Advances in neural information processing systems*, 28:3079–3087, 2015.

[20] A. Dixit and V. Roy. MCMC diagnostics for higher dimensions using Kullback Leibler divergence. *Journal of Statistical Computation and Simulation*, 87(13):2622–2638, 2017.

[21] H. Elliott, H. Derin, R. Cristi, and D. Geman. Application of the Gibbs distribution to image segmentation. 9:678–681, 1984.

[22] J. Fan, B. Jiang, and Q. Sun. Hoeffding’s lemma for Markov chains and its applications to statistical learning. *arXiv:1802.00211*, 2018.

[23] G. S. Fishman. Choosing sample path length and number of sample paths when starting in steady state. *Oper. Res. Lett.*, 16:209–219, 1994.

[24] S. Geman and D. Geman. Stochastic relaxation, Gibbs distributions, and the Bayesian restoration of images. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, PAMI-6(6):721–741, 1984.

[25] C. R. Gibbs. Characterization and application of ferrozine iron reagent as a ferrous iron indicator. *Analytical Chemistry*, 48(8):1197–1201, 1976.

[26] J. W. Gibbs. *Elementary Principles in Statistical Mechanics*. Scribner, 1902.

[27] J. Gonzalez, Y. Low, A. Gretton, and C. Guestrin. Parallel Gibbs sampling: From colored fields to thin junction trees. In G. Gordon, D. Dunson, and M. Dudík, editors, *Proceedings of the Fourteenth International Conference on Artificial Intelligence and Statistics*, volume 15 of *Proceedings of Machine Learning Research*, pages 324–332, Fort Lauderdale, FL, USA, 11–13 Apr 2011. PMLR.

[28] T. Griffiths. Gibbs sampling in the generative model of latent Dirichlet allocation. Technical report, 2002.
[29] S. Haddadan and P. Winkler. Mixing of permutations by biased transpositions. *Theory of Computing Systems*, 63(5):1068–1088, 2019.

[30] D. G. Harris and V. Kolmogorov. Parameter estimation for Gibbs distributions. *CoRR*, abs/2007.10824, 2020.

[31] B. He, C. De Sa, I. Mitliagkas, and C. Ré. Scan order in Gibbs sampling: Models in which it matters and bounds on how much. *Advances in neural information processing systems*, 29, 2016.

[32] A. Hellweg and F. Eckert. Brick by brick computation of the Gibbs free energy of reaction in solution using quantum chemistry and COSMO-RS. *AIChE Journal*, 63(9):3944–3954, 2017.

[33] T. Hrycej. Gibbs sampling in Bayesian networks. *Artificial Intelligence*, 46(3):351–363, 1990.

[34] D. Hsu, A. Kontorovich, D. A. Levin, Y. Peres, C. Szepesvári, and G. Wolfer. Mixing time estimation in reversible Markov chains from a single sample path. *The Annals of Applied Probability*, 29(4):2439–2480, 2019.

[35] M. Huber. Approximation algorithms for the normalizing constant of Gibbs distributions. *The Annals of Applied Probability*, 25(2):974–985, 2015.

[36] M. Huber and S. Schott. Random construction of interpolating sets for high-dimensional integration. *Journal of Applied Probability*, 51(1):92–105, 2014.

[37] M. Huber, S. Schott, et al. Using TPA for Bayesian inference. *Bayesian Statistics*, 9:257–282, 2010.

[38] M. Jerrum, L. G. Valiant, and V. V. Vazirani. Random generation of combinatorial structures from a uniform distribution. *Theoretical Computer Science*, 43:169–188, 1986.

[39] B. Jiang, Q. Sun, and J. Fan. Bernstein’s inequality for general Markov chains. *arXiv:1805.10721*, 2018.

[40] G. Karagiannis and C. Andrieu. Annealed importance sampling reversible jump MCMC algorithms. *Journal of Computational and Graphical Statistics*, 22(3):623–648, 2013.

[41] J. G. Kemeny, J. L. Snell, and A. W. Knapp. *Denumerable Markov chains: with a chapter of Markov random fields by David Griffeath*, volume 40. Springer Science & Business Media, 2012.

[42] D. Koller and N. Friedman. *Probabilistic Graphical Models: Principles and Techniques - Adaptive Computation and Machine Learning*. The MIT Press, 2009.

[43] V. Kolmogorov. A faster approximation algorithm for the Gibbs partition function. In *Conference On Learning Theory*, pages 228–249. PMLR, 2018.

[44] O. Krause, A. Fischer, and C. Igel. Algorithms for estimating the partition function of restricted Boltzmann machines. *Artificial Intelligence*, 278:103–195, 10 2019.

[45] P. S. La Rosa, T. L. Brooks, E. Deych, B. Shands, F. Prior, L. J. Larson-Prior, and W. D. Shannon. Gibbs distribution for statistical analysis of graphical data with a sample application to fcmri brain images. *Statistics in medicine*, 35(4):566–580, February 2016.

[46] C. Leon and F. Perron. Optimal Hoeffding bounds for discrete reversible Markov chains. *The Annals of Applied Probability*, 14, 05 2004.

[47] D. A. Levin and Y. Peres. *Markov chains and mixing times*, volume 107. American Mathematical Soc., 2017.

[48] P. Lezaud. Chernoff-type bound for finite Markov chains. *The Annals of Applied Probability*, 8, 08 1998.

[49] X. Liu and J. Domke. Projecting Markov random field parameters for fast mixing. *NIPS’14, pages 1377–1385, Cambridge, MA, USA, 2014. MIT Press.*
[50] D. Lunn, D. Spiegelhalter, A. Thomas, and N. Best. The BUGS project: Evolution, critique and future directions. *Stat Med.*, 28(25):3049-67, 2009 Nov 10.

[51] A. McCallum, K. Schultz, and S. Singh. FACTORIE: Probabilistic programming via imperatively defined factor graphs. In *Advances in Neural Information Processing Systems*, volume 22. Curran Associates, Inc., 2009.

[52] M. Mitzenmacher and E. Upfal. *Probability and computing: Randomization and probabilistic techniques in algorithms and data analysis*. Cambridge university press, 2017.

[53] J. M. Mooij and S. Ong. *libDAI: A free/open source C++ library for discrete approximate inference methods*, 2008.

[54] R. M. Neal. Annealed importance sampling. *Statistics and computing*, 11(2):125–139, 2001.

[55] D. Newman, P. Smyth, M. Welling, and A. Asuncion. Distributed inference for latent Dirichlet allocation. In *Advances in Neural Information Processing Systems*, volume 20. Curran Associates, Inc., 2008.

[56] M. Patriarca, A. Chakraborti, and K. Kaski. Gibbs versus non-gibbs distributions in money dynamics. *Physica A: Statistical Mechanics and its Applications*, 340(1):334–339, 2004. News and Expectations in Thermostatistics.

[57] D. Paulin. Concentration inequalities for Markov chains by Marton couplings and spectral methods. *Electron. J. Probab.*, 20, 2015.

[58] M. Plummer. JAGS: A program for analysis of Bayesian graphical models using Gibbs sampling. 2003.

[59] I. Porteous, D. Newman, A. Ihler, A. Asuncion, P. Smyth, and M. Welling. Fast collapsed Gibbs sampling for latent Dirichlet allocation. In *Proceedings of the 14th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, KDD ’08, pages 569–577, New York, NY, USA, 2008. Association for Computing Machinery.

[60] A. Prasad, V. Srinivasan, S. Balakrishnan, and P. Ravikumar. On learning Ising models under Huber’s contamination model. *Advances in neural information processing systems*, 33, 2020.

[61] M. Rabinovich, A. Ramdas, M. Jordan, and M. Wainwright. Function-specific mixing times and concentration away from equilibrium. *Bayesian Analysis*, 15, 05 2016.

[62] G. O. Roberts and J. S. Rosenthal. Examples of adaptive MCMC. *Journal of computational and graphical statistics*, 18(2):349–367, 2009.

[63] J. Rosenthal et al. Quantitative convergence rates of Markov chains: A simple account. *Electronic Communications in Probability*, 7:123–128, 2002.

[64] A. Smola and S. Narayananamurthy. An architecture for parallel topic models. *Proceedings of the VLDB Endowment*, 3(1–2):703–710, Sept. 2010.

[65] D. Stefankovic, S. Vempala, and E. Vigoda. Adaptive simulated annealing: A near-optimal connection between sampling and counting. In *48th Annual IEEE Symposium on Foundations of Computer Science (FOCS’07)*, pages 183–193, 2007.

[66] A. S. Stordal and A. H. Elsheikh. Iterative ensemble smoothers in the annealed importance sampling framework. *Advances in Water Resources*, 86:231–239, 2015.

[67] L. Theis, J. Sohl-Dickstein, and M. Bethge. Training sparse natural image models with a fast Gibbs sampler of an extended state space. In *Proceedings of the 25th International Conference on Neural Information Processing Systems - Volume 1*, NIPS’12, pages 1124–1132, Red Hook, NY, USA, 2012. Curran Associates Inc.

[68] C. Tosh. Mixing rates for the alternating Gibbs sampler over restricted Boltzmann machines and friends. In *ICML*, 2016.
[69] D. Štefankovič, S. Vempala, and E. Vigoda. Adaptive simulated annealing: A near-optimal connection between sampling and counting. *J. ACM*, 56(3), May 2009.

[70] R. Zhang and C. De Sa. Poisson-minibatching for Gibbs sampling with convergence rate guarantees. In *NeurIPS*, 2019.