Adaptive MCMC via Combining Local Samplers

Kiarash Shaloudegi
1Department of Electrical and Electronic Engineering
Imperial College London, London, UK
k.shaloudegi16@imperial.ac.uk

András György2,1
1DeepMind
London, UK
agyorgy@google.com

Abstract

Markov chain Monte Carlo (MCMC) methods are widely used in machine learning. One of the major problems with MCMC is the question of how to design chains that mix fast over the whole space; in particular, how to select the parameters of an MCMC algorithm. Here we take a different approach and, instead of trying to find a single chain to sample from the whole distribution, we combine samples from several chains run in parallel, each exploring only a few modes. The chains are prioritized based on Stein discrepancy, which provides a good measure of performance locally. We present a new method, based on estimating the Rényi entropy of subsets of the samples, to combine the samples coming from the different samplers. The resulting algorithm is asymptotically consistent and may lead to significant speedups, especially for multimodal target functions, as demonstrated by our experiments.

1 Introduction

We consider the problem of computing expectations $\mathbb{E}_P[f(X)] = \int_X f(x)p(x)dx$ for some complicated target distribution $P$ with density $p$ over a set $X \subset \mathbb{R}^d$. Such expectations often arise in Bayesian inference and maximum likelihood estimation (Andrieu et al., 2003; Brooks et al., 2011). Often times, $p$ has a closed form, but it is only known up to a normalization constant, making the computation of the integral especially challenging (Andrieu et al., 2003).1 Markov chain Monte Carlo (MCMC) methods are a family of numerical estimation methods, which are successfully applied to estimate the aforementioned expectations, especially in high-dimensional problems. MCMC algorithms take random samples from an ergodic Markov chain with stationary distribution $P$, and approximate the expectation via averaging over the produced sample.

The challenging problem in designing MCMC methods is to ensure that the distribution of the samples converge to $P$ fast, and, in practice, some domain specific knowledge has to be used in the design of their proposal distributions to have achieve fast convergence (Andrieu et al., 2003). This need for specialized design led to the development of dozens of methods for each problem, each of which has their own tunable parameters (Neufeld et al., 2014). Consequently, choosing the right method with corresponding parameters to achieve fast convergence is quite difficult and requires considerable time and effort.

To address this difficulty, a large body of work has been done: some of them proposed ways for optimal parameter-setting, for instance optimal tuning of the Metropolis-Hasting algorithms was discussed in (Roberts & Rosenthal, 2001; Bédard, 2008; Roberts et al., 1997; Atchadé et al., 2011) (Brooks et al., 2011, Chapter 4). The problem with this line of research is that they rely on some Markov chain parameters (stationary distribution) that are typically unknown (Łatuszyński et al., 2013).

1In most of real world applications finding this normalization constant is as hard as solving the original expectation under $P$. 

Preprint. Work in progress.
A more promising line of research to address the parameter setting issue is based on adaptive MCMC methods. In this framework, the MCMC samples are used to learn about the target distribution, and the algorithm adjust the parameters as the MCMC progresses (Łatuszyński et al., 2013). To do so, they rely on optimizing some objective functions such as expected squared jumping distance (Wang et al., 2013; Pasarica & Gelman, 2010), the area under the autocorrelation function up to some specific lag (Mahendran et al., 2012), the difference between the proposal covariance matrix and its empirical estimation (Mbalawata et al., 2015; Haario et al., 2001, 2006; Sejdinovic et al., 2014), and the difference between the optimal acceptance rate and its empirical estimation (the authors used some practical recommendations instead of the true optimal values) (Yang & Zhang, 2011). Also, an adaptive strategy for finding the optimal step size in Hamiltonian Monte Carlo (HMC) has been developed through monitoring the sample-trajectories in (Hoffman & Gelman, 2014) which is called NUTS. Such adaptive schemes are only useful if they can ensure ergodicity; therefore, they need more elaborate theoretical analysis to make sure the resulting sample sequence converges to the true distribution (Łatuszyński et al., 2013) (for more details about adaptive MCMC methods, see Andrieu & Thoms, 2008).

In this paper we will propose a novel adaptive MCMC method via bandit allocation. Our general strategy is the following: Instead of trying to find a single very good sampler that approximates the target distribution well on its whole domain, we are going to run several samplers and select which sampler to use at any given time in a sequential manner, based on all the samples obtained before.

1.1 Approach and challenges

The simpler case is when all MCMC samplers mix well on the whole domain, and then our goal is to select the best sampler (which mixes the fastest) most of the time. This is very similar to the case of running several unbiased MC samplers. For the latter, Neufeld et al. (2014) showed that scheduling which samplers to use when is equivalent to a stochastic multi-armed bandit problem Bubeck & Cesa-Bianchi (2012). This allows the straightforward application of bandit algorithms to choose which sampler to use for the next sample, and the decision depends on the overall performance of the samplers so far, measured by the variance for each sampler. Extending the same idea to the MCMC case is not trivial, since measuring the quality of MCMC samplers is a much harder task. In fact, until recently, there has not been any empirical measure that can monitor the sample convergence. Indeed, common MCMC diagnostics such as effective sample size, trace and mean plots, and asymptotic variance assume the chain asymptotically convergences to the target distribution, so they cannot detect asymptotic bias (Gorham & Mackey, 2015). To address the issue, Gorham & Mackey (2015) developed an empirical sample quality measure that can detect non-convergence/bias based on Stein’s method. We are going to use a kernelized version of this measure, called kernel Stein discrepancy (KSD) to compare the quality of different samplers (Liu et al., 2016; Chwialkowski et al., 2016; Gorham & Mackey, 2017).

On the negative side, KSD is not able to detect underfitting if the target distribution has well-separated modes (with a distance that is large relative to the kernel width), so it cannot distinguish, between two samplers such that one samples only one mode while the other samples both modes, and the samples are equally good locally (Liu et al., 2016; Chwialkowski et al., 2016; Gorham & Mackey, 2017). This brings us to the next problem: namely, MCMC methods usually fail to explore the whole domain if the support has reasonably high-probability regions separated by low probability regions (of course, such notion of separation depends on the actual sampler used). Setting the parameters of the samplers to deal with this issue and, more importantly, detecting its presence is extremely hard, and to our knowledge no practical algorithm can deal with it. To alleviate this problem, we change our requirement for the samplers, and only expect that they provide good samples locally. Then, running several samplers in parallel, we hope that the multiple instances will explore the space sufficiently, finding all the important regions of the support. Then, in the end, we combine all the samples (from all the samplers) to approximate the target distribution. This is again challenging due to two reasons: (i) it is not straightforward how the samples from different samplers should be weighted, and (ii) we do not want to waste resources to run several samplers exploring the same region of the domain. For (ii), following the approach of Neufeld et al. (2014) for combining MC samplers, we will use a bandit-based racing method, developed for the case of mixing samplers (as locally these samplers do mix in the sense that the empirical distribution they generate is close to the true distribution restricted to the given area). To address (i), we develop a method to estimate the probability of the region a set of samples cover based on Rényi-entropy estimates (Pál et al., 2010), and use these to weight the samples.
In the rest of the paper we develop each ingredient of the above plan, and end up with a final sampling algorithm. We demonstrate, through a number of experiments, that our method is competitive with state-of-the-art adaptive MCMC methods, such as the no-U-turn sampler NUTS (Hoffman & Gelman, 2014) or the recent sample reweighting method of Liu & Lee (2016) on simpler cases when the distribution is concentrated on a single “connected” region, while significantly outperforming the competitors on more challenging cases where high-probability regions are separated with areas of low-probability.

2 Measuring sample quality

As mentioned in Section 1.1, measuring the quality of samples produced by an MCMC algorithm is crucial in our approach. To this end we are going to use the recently introduced kernel Stein discrepancy (KSD) (Liu et al., 2016; Chwialkowski et al., 2016; Gorham & Mackey, 2017).

To measure the quality of a set of samples, we want to quantify how well a probability distribution \( Q_n \) over \( \mathbb{R}^d \) can approximate the target distribution \( P \). Oftentimes, \( Q_n \) is given by a weighted sample \( \{(x_i, q_i)\}_{i \in [n]}^2 \) where \( x_i \in \mathbb{R}^d \) and \( Q_n(x_i) = q_i \) with \( \sum_{i \in [n]} q_i = 1 \). One way to do this is to measure the maximum expectation error over a class of real-valued test functions \( \mathcal{H} \subset \{ f : \mathbb{R}^d \to \mathbb{R} \} \):

\[
\mathcal{D}_\mathcal{H}(Q_n, P) \define \sup_{h \in \mathcal{H}} |E_{Q_n}[h(Z)] - E_P[h(X)]| ,
\]

where, in case of a weighted sample, \( E_{Q_n}[h(Z)] = \sum_{i=1}^n q_i h(x_i) \) (we use \( Z \) to distinguish the sample from \( X \)). If the class of test functions \( \mathcal{H} \) is big enough, for any sequence of probability measures \( (Q_n)_{n \geq 1} \), the convergence of \( \mathcal{D}_\mathcal{H}(Q_n, P) \) to zero implies that \( Q_n \) converges weakly to \( P \). One advantage of using this formulation is that we can recover different metrics in the form (1) by changing the class of test functions \( \mathcal{H} \) (Gorham & Mackey, 2015); for example, using \( \mathcal{H} \define \{ h : \mathcal{X} \to \mathbb{R} | \sup_{x \in X} |h(x)| \leq 1 \} \), the measure in (1) becomes the total variation distance, while using \( \mathcal{H} \define \{ h : \mathcal{X} \to \mathbb{R} | \sup_{x \neq y \in \mathcal{X}} \frac{|h(x) - h(y)|}{\|x - y\|_2} \} \) recovers the Wasserstein distance. Note that typically finding the exact solution in (1) is impossible since calculating \( E_P[h(X)] \) is intractable; however, if we can find an operator \( T \) such that \( E_P[(Th)(X)] = 0 \) for any function \( h(\cdot) \), we can avoid this problem.

Let \( k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R} \) be a positive definite kernel, \( \mathcal{K} \) be its associated reproducing kernel Hilbert space (RKHS), \( \| \cdot \|_{\mathcal{K}} \) be the induced norm from the inner product in \( \mathcal{K} \), and \( \| \cdot \|_{\mathcal{K}}^* \) be its dual norm. Then, for \( x \in \mathbb{R}^d, f \in \mathcal{K}, \) and \( k(x, \cdot) \in \mathcal{K} \), we have \( f(x) = \langle f, k(x, \cdot) \rangle \). Given this kernel, Gorham & Mackey (2017) defined a kernel Stein set as

\[
\mathcal{F}_k,\| \cdot \|_k^* \define \{ f \in \mathcal{K} | \| f \|_{\mathcal{K}}^* \leq 1 \},
\]

and a Stein operator as

\[
(T_p,f)(x) \define \frac{1}{p(x)} \nabla_x (p(x)f(x)) = \nabla_x \log p(x) f(x) + \nabla_x f(x).
\]

Gorham & Mackey (2017) showed that if \( k(x,y) \) is twice differentiable and \( \nabla_x \nabla_y k(x, y) \) are continuous, both are uniformly bounded, and \( E_P[\|\nabla_x \log p(X)\|_2] < \infty \), then \( E_P[(T_p f)(X)] = 0 \) for all \( f \in \mathcal{F}_k \). Thus, with \( \mathcal{H} = T_p \mathcal{F}_k \), \( P \) cancels from the definition of (1) reducing it to

\[
S(Q_n) = \mathcal{D}_{T_p \mathcal{F}_k}(Q_n, P) = \sup_{h \in T_p \mathcal{F}_k} |E_{Q_n}[h(Z)]| \]

(2)

where we suppressed the dependence on \( P, T_p, \) and \( \mathcal{F}_k \) in the notation \( S(Q_n) \). This makes it possible to compute the optimum in the definition. Indeed, defining \( s_p(\cdot) \define \nabla \log p(x) \) and

\[
k_p(x, x') \define s_p(x)^\top k(x, x') s_p(x') + s_p(x')^\top \nabla_x k(x, x') + s_p(x')^\top \nabla_x s_p(x') k(x, x'),
\]

the resulting maximum becomes

\[
S(Q_n) = \sqrt{E_{Q_n \times Q_n}[k_p(Z, Z')]} \]

(3)

\(^2\)For a positive integer \( n \), \([n]\) denotes the set \( \{1, \ldots, n\} \).
if $E_{\mu}[k_p(X, X)^{1/2}] < \infty$. We call $S(Q_n)$ the kernel Stein discrepancy. Note that $S(Q_n)$ can be computed with our information about $p$, since it only depends on $p$ through $s_p(\cdot) = \nabla \log p(x)$, which cancels the effect of the unknown normalization constant.

It is known that under some technical conditions, for unimodal distributions $P$, the KSD measure goes to 0 if and only if $Q_n$ converges weakly to $P$. However, the discriminative power of KSD weakens for multi-modal distributions, particularly when the modes are well-separated: Gorham et al. (2016) demonstrated that for a one-dimensional Gauss-mixture target function (with two components), the KSD measure fails to distinguish between two sets of samples for reasonable sample sizes, one drawn independently from one mode and the other drawn independently from the target distribution, and it requires even more samples to distinguish between the two cases as the modes’ distance increases, see Section 6.1 of Gorham et al. (2016) for more details. Another issue is that the complexity of computing the KSD for an empirical distribution is quadratic in the sample size, which quickly becomes infeasible as the sample size grows.

3 Sequential selection of samplers

In this section we present several strategies to select from a pool of MCMC samplers in a sequential manner. In all of our algorithms the selection of the sampler to be used next depends on the quality of the samples generated by the different samplers, where the quality will be measured by the KSD measure (or its approximations). Formally, assume we have access to $M$ MCMC samplers (e.g., multiple sampling methods and/or multiple instances of the same sampling algorithm with different parameters, such as starting point or step size), and denote the set of samplers by $[M]$. At every step of the algorithm, we select one of the samplers and use it to produce the next sample (or the next batch of samples).

3.1 Mixing samplers

First we consider the case when each sampler is asymptotically unbiased, that is, it generates samples with an empirical distribution converging weakly to the target $P$ (this is usually satisfied for any standard MCMC sampler when $P$ is unimodal). Our task is to sequentially allocate calls among the $M$ samplers to minimize the Stein discrepancy of the set of samples we collect. The goal is to design an algorithm which gives preference to samplers where the convergence is faster. This setup is similar to the one considered by Neufeld et al. (2014), who designed sequential sampling strategies for MC samplers generating independent and identically distributed (i.i.d.) samples, based on multi-armed bandit algorithms. In this section we generalize their method to MCMC samplers. Our overall goal is to produce samples such that the total KSD measure (cf. Eq. 3) of the samples is small. However, as mentioned in Section 2, computing the Stein discrepancy even for relatively small sample sizes is computationally infeasible (also note that any computation we spend on selecting samplers could also be used for sampling). Therefore, we are going to approximate the KSD measure as the average KSD over smaller blocks of samples.

For a sampler with total sampling budget $n$, we break the sampling process into $T$ rounds: At each round the sampler takes a batch of samples of size $n_b$. Let $S_i$ be the KSD measure of samples from the $t$th round; then we will approximate $\hat{S}_n$, the KSD of the full sample of size $n$ with the average $(1/T) \sum_{t=1}^T S_i$. We will call this the block-diagonal approximation, as it corresponds to a block-diagonal approximation of the kernel matrix in (3). To quantify the accuracy of the approximation, we assume that there exists a function $g(t, n_b)$ such that $\lim_{n_b \to \infty} g(t, n_b) = 0$ and $\frac{1}{2} \sum_{t=1}^T E[S_i] - E[\hat{S}_n] \leq g(t, n_b)$. Using the block-diagonal approximation, our goal is to compete with a sampler with the smallest average approximate block-KSD measure $(1/T) \sum_{t=1}^T S_{i,t}$, where $S_{i,t}$ is the KSD measure of the $n_b$ samples generated by sampler $i$ when it is called the $t$th time. Experimental results presented in Section 5.1 indicate that the block-diagonal approximation mostly preserves the ranking of the samplers (as defined by the true KSD measure), hence we pay very little price for the computational advantage we get.
Algorithm 1 KSD-UCB1

for $i \in \{1, \ldots, M\}$ do
- Use sampler $i$ to generate $n_b$ samples; observe $S_{i,1}$; set $\bar{\mu}_{i,1} = S_{i,1}$ and $T_{i}(1) = 1$
end for

for $t \in \{M + 1, M + 2, \ldots, n\}$ do
- Play arm $i$ that minimizes $\bar{\mu}_{i,t-1} - \sqrt{\frac{2 \log t}{T_{i}(t-1)}}$,
- Set $T_{i}(t) = T_{i}(t-1) + 1$ and $T_{j}(t) = T_{j}(t-1)$ for $j \neq i$,
- Observer $S_{i,T_{i}(t)}$, and compute $\hat{\mu}_{i,t} = (1 - \frac{1}{T_{i}(t)}) \bar{\mu}_{i,t-1} + \frac{S_{i,T_{i}(t)}}{T_{i}(t)}$
end for

Furthermore, solving this problem is well-suited for any bandit algorithm (Bubeck & Cesa-Bianchi, 2012); here we adapt the UCB1 method of Auer et al. (2002), given in Algorithm 1.\(^3\) In short, the algorithm keeps track of an optimistic estimate of the average approximate KSD value for each sampler, and selects a sampler whose performance is estimated to be the best possible (with high probability).

If the KSD values $S_{i,1}, \ldots, S_{i,T}$ were i.i.d., the standard bandit regret bound (Bubeck & Cesa-Bianchi, 2012) would yield $\sum_{t=1}^{T} \mathbb{E}[S_{i}] - \min_{i} \mathbb{E}[S_{i}] \sum_{t=1}^{T} \mathbb{E}[S_{i,t}] = O(\log(T))$. Using our assumption and the convexity of the KSD measure (which follows since it is defined as the supremum of linear functions, see Section 2), this would imply that after $T$ rounds of sampling,

$$\mathbb{E}[\tilde{S}_{T,n_b}] - \min_{i} \mathbb{E}[S_{i,T,n_b}] \leq \frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[S_{i}] - \min_{i} \mathbb{E}[S_{i,t}] + \frac{g(T,n_b)}{T} + g(T,n_b)$$

This shows that increasing $T$ and $n_b$, the performance of KSD-UCB1 would be close to using the best sampler. However, in our case, the $S_{i,t}$ are not i.i.d. Assuming that the samplers mix (which is reasonable for a single mode distribution), the $S_{i,t}$ are getting closer and closer to be sampled i.i.d. as $n_b$ increases. Also, as mentioned above, the effect of the block-diagonal approximation (and hence that of $g(T,n_b)$) is small in practice (see also Section 5.1).

3.2 Locally mixing samplers

In practice, if the target distribution is multi-modal and the modes are far from each other, MCMC methods often get stuck in some of the modes and fail to explore all the regions where $P$ is supported; while eventually all asymptotically consistent methods reach each mode, this may not happen after any practically reasonable time. To model this situation, we assume that the support of $P$ is partitioned into sets $A_1, \ldots, A_K$ with $P(A_j) > 0$ for all $j \in [K]$ (the $A_j$ are pairwise disjoint and their union is the support of $P$) such that the empirical distribution of the samples generated by sampler $i \in [M]$ converges weakly to $P(|A_j)$ for some $j \in [K]$, where $P(|A)$ is the conditional distribution of $P$ over $A$. We will refer to the sets $A_j$ as regions, and a sampler satisfying the above condition a locally mixing sampler.

For simplicity we first consider the case where there is one sampler in each region (consequently $M = K$). This setup is similar to stratified sampling, which is a variance reduction technique for MC. The idea is to partition the domain into non-overlapping regions (a.k.a. strata), draw samples from each region, and combine the final samples to estimate $\mu = \mathbb{E}[f(X)]$ (Owen, 2013). The problem in stratified sampling is to find the optimal number of samples that need to be taken from each stratum in order to reduce the variance of Monte Carlo integration error. Carpenter et al. (2015) showed that an optimal strategy for minimizing the mean squared error (MSE) is to sample each stratum $n_j = \frac{\sigma_j P(A_j)}{\sum_{i=1}^{K} \sigma_i P(A_i)} n$ times, where $\sigma_i$ is the conditional standard deviation of $f(X)$ given that $X$ falls into the $i$th region. They also gave an adaptive sampling algorithm, based on a reduction to multiarmed bandit problems, for the case when the weights and standard deviations are unknown.

One can immediately see that the setup we consider in this subsection is very similar to the last case with the important differences that our samplers are not i.i.d., and we do not minimize the squared

\(^3\)The algorithm assumes that $S_{i,t} \in [0, 1]$, which can be achieved by rescaling the KSD measures. In practice, a reasonable estimate for the range can be obtained from $S_{i,1}$ for each sampler $i$. 

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error but the KSD measure. Denoting the distribution of samples from region \( A_i \) by \( Q_{n,i} \) after taking \( n \) samples in total, let \( w_i \) denote the weight of sampler \( i \) generating these samples (recall that here, by assumption, we have one sampler in each region). Then our total weighted sample distribution becomes

\[
Q_n = \sum_{i=1}^{M} w_i Q_{n,i}.
\]

Since according to our assumptions, \( Q_{n,i} \) converges weakly to \( P(A_i) \) for all \( i \), we need to have \( w_i \to P(A_i) \) for all \( i \) in \([M]\) to ensure that \( Q_n \) converges to \( P \) weakly (we will refer to this as the \( w_i \) being asymptotically consistent). A procedure for estimating \( w_i \) this way will be given in the next section. Assuming for a moment that \( w_i = P(A_i) \), using the form (2), we can bound the KSD as

\[
\tilde{S}_n = \sup_{f \in F_k} ||E_{Q_n} [(T_p f)(Z)]|| = \sup_{f \in F_k} \left| \sum_{i=1}^{M} w_i E_{Q_{n,i}} [(T_p f)(Z)] \right| \leq \sum_{i=1}^{M} w_i \sum_{i=1}^{M} w_i S(Q_{n,i}) = \sum_{i=1}^{M} w_i \tilde{S}_{i,n},
\]

where, as before, \( \tilde{S}_n \) and \( \tilde{S}_{i,n} \) denote the KSD measure of the whole sample and, resp., that of sampler \( i \) (with number of samples \( n_i \) from obtained by sampler \( i \)). Based on this inequality, we could aim for minimizing \( \sum_{i=1}^{M} w_i \tilde{S}_{i,n} \) and use the ideas from adaptive stratified sampling (Carpentier et al., 2015); however, multiple challenges preclude us to do it: (i) \( w_i \) is not known in advance; (ii) the stratified sampling algorithm is based on the known concentration of the variance, but we do not know how fast \( \tilde{S}_{i,n} \) approaches zero (as a function of \( n_i = w_i n \)); and (iii) the computational complexity of calculating \( \tilde{S}_{i,n} \) is \( O(n_i^2) \). To handle (i), we will address the problem of estimating \( w_i \) in Section 3.3. For (ii), a conservative approach is to uniformly minimize \( w_i \tilde{S}_{i,n} \), hence selecting sampler \( i \) for which this quantity is the largest. For (iii), we will again use a block-diagonal approximation to \( \tilde{S}_{i,n} \), which causes problems with (ii), since the estimate does not converge to 0 for a fixed block size. In Section 5.3 we present experiments with different strategies under different setups, but the strategies considered seem to perform rather similarly. The simplest strategy considered is to select regions uniformly at random. Another approach is to minimize the maximum \( \tilde{S}_{i,n} \), that is, choosing \( i = \arg\max \tilde{S}_{i,n} \), which does not require the knowledge of the weights \( w_i \), while we also test strategies selecting regions based on their estimated weights or, similarly to stratified sampling, based on their estimated variance.

Unfortunately, we cannot guarantee that we start samplers in such a way that we have a single sampler for each region. If we know which sampler belongs to which region, we can combine the region selection strategies described above with the bandit method described in Section 3.1 in a straightforward way: in each region, run an instance of KSD-UCB1 over the samplers exploring this region, and use it as a locally mixing sampler above. We will refer to this sampling algorithm as KSD-UCB1-M (M stands for Multiple regions); the pseudocode of the algorithm is given in Algorithm 2. Clearly, since the bandit algorithms sample each arm infinitely often, we have the following consistency result:

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**Algorithm 2 KSD-UCB1-M**

**Given:** (Unnormalized) density \( \hat{p} \); partition of the domain \( A_1, \ldots, A_K \); \( M \) samplers in \( K \) classes: samplers in \( A_i \) sample from \( p(A_i) \) for all \( i \in [K], \cup_{i \in [K]} A_i = [M]; \) total number of rounds: \( T \); batch size: \( n_b \).

**Initialize:** Draw a batch of samples from each sampler \( i \), observe \( S_{i,1} \) and set \( \hat{\mu}_{i,1} = S_{i,1} \) and \( T_i(1) = 1 \) for \( i \in [M] \) for all \( i \in [M] \)

for \( i \in \{M+1, \ldots, T\} \) do

- Select a region \( I_i \).
- Draw a batch of samples from arm \( i_t = \arg \min_{i \in A_{I_i}} \left( \hat{\mu}_{i,t-1} - \sqrt{\frac{8 \log T}{T_i(t-1)}} \right) \).
- Set \( T_i(t) = T_i(t-1) + 1 \) and \( T_j(t) = T_j(t-1) \) for \( j \neq i \).
- Observer \( S_{i,T_i(t)} \), and compute \( \hat{\mu}_{i,t} = \left( 1 - \frac{1}{T_i(t)} \right) \hat{\mu}_{i,t-1} + \frac{S_{i,T_i(t)}}{T_i(t)} \).
end for

- Reweight the samples of each mode proportional to its weight, \( w_k \).

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Under the local mixing assumption made at the beginning of this section, the final weighted sample (4) obtained by KSD-UCB1-M is asymptotically unbiased as long as the weight estimates \( w_i \) are asymptotically unbiased.

Thus, we need to find some asymptotically unbiased estimates of the probabilities of the regions \( A_i \).

### 3.3 Weight estimation

In this section we consider the problem of finding the weights \( w_i \) in (4). As discussed after the equation, this amounts to finding the probability of the region the samples cover, which is again challenging since we have access only to an unnormalized density function. This problem is faced by every algorithm which tries to speed up MCMC methods by running parallel chains. As an example, in big-data scenarios it is common to split the data and try to run an MCMC sampler on each subset to combine the final samples. To our knowledge, most work in the literature solves this problem by estimating the density of each batch of samples separately (Angelino et al., 2016; Nemeth & Sherlock, 2018), using typically either a Gaussian approximation (Scott et al., 2016) or some kernel-density estimation method (Neiswanger et al., 2014). According to Nemeth & Sherlock (2018), the first approach works well in practice, in spite of not having any theory; while the second, kernel based estimation scales poorly with the dimension \( d \).

Here we take a different approach and rather than estimating the density of the sample batches, we directly estimate the probabilities \( P(A_i) \) via the Rényi entropy.

Formally, suppose the domain of \( P \) is partitioned into non-overlapping regions \( A_1, \ldots, A_K \), and from each region \( A_i \) we have a set of samples \( X^{(A_i)} \). The Rényi entropy of order \( \alpha \neq 1 \) for a density \( p \) is defined as \( R_\alpha(p) = \frac{1}{1-\alpha} \log \int P^\alpha(x) \, dx \). The conditional density of \( P \) restricted to a set \( A \) is denoted as \( p(x|A) = \frac{p(x)}{\int_{x \in A} p(x) \, dx} \), and its Rényi entropy is \( R_\alpha(p|A) = \frac{1}{1-\alpha} \log \int_A \left( \frac{p(x)}{\int_{x \in A} p(x) \, dx} \right)^\alpha \, dx \).

From this definition it trivially follows that \( \log P(A) = R_\alpha(p|A) - \frac{1}{1-\alpha} \log \mathbb{E} [p(X)^{\alpha-1} | X \in A] \).

In our case, instead of \( p \) we only have access to \( \hat{p} = cp \) for some \( c > 0 \). Replacing \( p \) with \( \hat{p} \) in the integral, we obtain \( \log P(A)c = R_\alpha(p|A) - \frac{1}{1-\alpha} \log \mathbb{E} [\hat{p}(X)^{\alpha-1} | X \in A] \). Thus, we can estimate \( P(A) \) by estimating the two terms above.

Given a sample \( X^{(A)} \) taken i.i.d. from \( p(|A) \), the second term can be estimated by the empirical average \( \hat{R}_\alpha(X^{(A)}) = \frac{1}{|X^{(A)}|} \sum_{x \in X^{(A)}} \hat{p}(x)^{\alpha-1} \), while for the first term we can use a graph-based estimate (Hero & Michel, 1999). In particular, we are going to use the estimator \( \hat{R}_\alpha(X^{(A)}) \) of Pál et al. (2010), which is based on generalized k-nearest neighbor graphs of the sample \( X^{(A)} \), and it converges to \( R_\alpha(p|A) \), for any \( \alpha \in (0, 1) \) as the sample size grows to infinity. Thus, we obtain that \( \beta(X^{(A)}) = \hat{R}_\alpha(X^{(A)}) - \hat{B}_\alpha(X^{(A)}) \) is an asymptotically unbiased estimate of \( \log(P(A)c) \).

Therefore, given that we have a partition \( A_1, \ldots, A_K \),

\[
P(A_i) \approx w_i = \frac{e^{\beta(A_i)}}{\sum_{j \in [K]} e^{\beta(A_j)}}.
\]

### 4 The final algorithm

So far we have discussed how to solve our problem if we have either local mixing or all the samplers mix. While the latter is the case asymptotically for all the MCMC samplers used in practice, the mixing may be too slow to be observed for any practical number of samples. However, the problem does not simplify to the local mixing scenario, since–even if well-separated regions are actually present–, the chains often jump from one region to another even if they do not cover the whole domain.

To be able to adapt our KSD-UCB1-M algorithm, we need to group the samplers covering the same region together (even though what a region is is not clearly defined in this scenario). The problem is especially hard since the grouping of the samplers is non-stationary, and we should also be able to track when a sampler leaves or joins a region (equivalently, group). Furthermore, if the groups are too large, we do not explore the whole domain, while if they are too small, we waste resources by running multiple samplers for the same region.

To solve this issue, we propose a simple heuristic to identify samplers that are close together: In each round of the sampling, we take all the samples from the last batch of each sampler, and for each
Algorithm 3 KSD-MCMC-WR

Given: (Unnormalized) distribution \( p(x) \); \( M \) samplers; total number of rounds \( T \); batch size \( n_b \); number \( N \) of nearest neighbors for clustering; the order \( \alpha \) of the Rényi entropy.

Initialize: For each \( i \in [M] \), draw \( n_b \) samples from the \( i \)th sampler with random initialization; compute \( S_{i,1} \) and set \( \bar{\mu}_{i,1} = S_{i,1} \) and \( T_i(1) = 1 \).

for \( t \in \{M+1, \ldots, T\} \) do
  - Cluster the samplers by clustering the samples from their last batches:
    - Initially, the last batch of samples from each sampler forms a cluster.
    - Merge two clusters if any point of one cluster has a point from the other cluster among its \( N \) nearest neighbors.
    - Find the number of clusters \( n_c \).
    - Define \( A_i \subset [M] \) for \( i \in [n_c] \) as the set of samplers belonging to cluster \( i \) (i.e., \( A_i \cap A_j = \emptyset \) for \( i \neq j \)).
    - Choose a cluster \( I_t \) (e.g., sampled from the probability distribution \( \{w_i\} \) computed as the estimated weight of each cluster of samples computed above).
  - Draw a batch of samples of size \( n_b \) from sampler \( i_t = \arg \min_{i \in A_{I_t}} \left( \bar{\mu}_{i,T_i(t-1)} - \sqrt{\frac{8 \log T}{T_i(t-1)}} \right) \).
  - Set \( T_i(t) = T_i(t-1) + 1 \) and \( T_j(t) = T_j(t-1) \) for \( j \neq i \).
  - Observer \( S_{i,T_i(t)} \), and compute \( \bar{\mu}_{i,T_i(t)} = (1 - \frac{1}{T_i(t)})\bar{\mu}_{i,T_i(t-1)} + \frac{S_{i,T_i(t)}}{T_i(t)} \).
end for

- Cluster all the samples into \( M \) clusters by k-means clustering; for each cluster calculate its estimated probability \( w_i \) using (6) and output the reweighted samples with weight \( w_i/n_i \) where \( n_i \) is the total number of samples in cluster \( i \in [M] \).

5 Experiments

In this section we empirically evaluate our choices in the algorithm design process and the final algorithm on several synthetic problems and compare the results with different competitor algorithms from the literature.

We use three different base sampling methods: Metropolis-Hastings (MH), the Metropolis-adjusted Langevin algorithm (MALA) of Roberts & Rosenthal (2002), and the no-u-turn sampler (NUTS) of Hoffman & Gelman (2014). For the latter, which is a state-of-the-art sampling method (Wang et al., 2013; Liu & Lee, 2016), we used the implementation provided in the pymc3 package (Salvatier et al., 2016) which, on top of the original NUTS, also includes several modifications recommended in the literature for boosting the performance (see the pymc3 package website for more details). Beside the initial point, MH and MALA have a single step size parameter (for MALA the preconditioning matrix is always the identity), while for NUTS we used the default setting (the performance was insensitive to the choice of its parameters). In our experiments, when a MH or MALA sampler is chosen randomly, the step size is selected uniformly at random from \([0.1, 5]\) (the initial points are selected uniformly at random “not too far” from the modes of the underlying distribution).

We present one set of experiments for each component of our algorithm. Throughout this section, to compute the KSD measure, we use the inverse multiquadratic kernel \( k(x, y) = (1 + \|x - y\|^2/h)^\gamma \) suggested by Gorham & Mackey (2017) with \( h = 1 \) and \( \gamma = -0.5 \). Section 5.1 analyzes the effect of using the block-diagonal approximation of the KSD measure. The performance of our bandit-based samplers for unimodal target distributions are considered in Section 5.2. Multimodal densities with separated modes and one sampler in each mode are considered in Section 5.3. Lastly,
in Section 5.4, our final algorithm KSD-MCMC-WR is tested in the general setting of a multimodal target distribution with an unknown number of modes.

5.1 Block-diagonal approximation of the KSD measure

The intuition behind our bandit MCMC method is that we can identify the best sampler among a group of samplers from the average KSD for small batch sizes instead of making the decision based on the KSD computed over a large set of samples. To verify this hypothesis, we need to check if the average approximate KSD computed on small blocks preserves the order of two samplers as defined by the true KSD measure. In order to do so, we compared the average block-KSD measure of two samplers for different block sizes. We drew $n = 100000$ samples from each sampler for a non-isotropic two-dimensional independent Gaussian distribution and computed the average block-KSD measure for these samples with block sizes $10, 25, 50, 100, 250, 500, 2000$ (the parameters of the samplers and the distribution were selected randomly). Formally, for each sampler $i$ with block size $n_b$ and total sample size $n$, we compute the average block-KSD as $ar{S}_{i,n_b} = \frac{n_b}{n} \sum_{b=1}^{n/n_b} S_{i,b}$, where $S_{i,b}$ is the average block-KSD computed on the $b$th block of data, and for a given block size $n_b$, $\arg\max_i \bar{S}_{i,n_b}$ is declared to be the better sampler according to the measurements.

Table 1 shows in what percentage did the average block-KSD result in the same ordering of the samplers as the ordering obtained for block size 2000 (which is treated as the ground truth), both for MH and MALA as base samplers. We can observe that the ordering obtained from the average block-KSD measures is most of the time the same as the “ground truth,” justifying its use for measuring sample quality. Scatter plots of average block-KSD differences ($\bar{S}_{1,n_b} - \bar{S}_{2,n_b}$) for different block sizes, given in Figure 1 for the MH algorithm, show that in cases of incorrect ordering, the average block-KSD values of the samplers are really close for both block sizes, thus the two samplers considered are of approximately the same quality according to both measures (thus, practically it does not matter which of them is used for sampling).

| Batch Size | 10 | 25 | 50 | 100 | 250 | 500 | 2000 |
|------------|----|----|----|-----|-----|-----|------|
| MH         | 93%| 95%| 94%| 94% | 96% | 97% | 100% |
| MALA       | 93%| 92%| 93%| 91% | 93% | 94% | 100% |

Table 1: The percentage of times that the ranking of samplers based on the empirical expectation of small batch sizes can rank the samplers in the correct order.

Figure 1: Block-diagonal approximation of the KSD measure.

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Throughout this section we choose the variance of the components of a Gaussian distribution uniformly from $[0.1, 3]$
5.2 Unimodal target distributions with multiple samplers

In this section we consider sampling from a standard normal Gaussian distribution, where the samplers have access to the unnormalized density $p(x) = e^{-x^T x/2}$. The goal of the samplers is to estimate the mean of the distribution with respect to the mean squared error. We consider 5 different MH and, resp. MALA, samplers (with step size parameters 0.1, 0.2, 0.5, 1, 2, resp.) and run our proposed algorithm KSD-UCB1 (Algorithm 1) on top of them. We compare its performance with multiple combination methods:

- Uniform: This algorithm distributes the computational budget equally among the samplers, and in the end takes all the samples generated from all samplers with equal weights.
- KSD-opt: This method again takes the same number of samples from each sampler, but reweights them using the method of Liu & Lee (2016). This reweighting can be very effective, but it is computationally quite demanding.
- $\varepsilon$-greedy: This method is a variant of KSD-UCB1, but is based on the $\varepsilon$-greedy bandit algorithm (Bubeck & Cesa-Bianchi, 2012) instead of UCB1. That is, in every round, with probability $1 - \varepsilon$, the sampler with the smallest approximate block-KSD measure is selected, while with probability $\varepsilon$, a sampler is selected uniformly at random. In the experiments $\varepsilon = \frac{0.05}{\sqrt{t}}$ in round $t$.

We also compare the performance with that of NUTS. Figures 3 and 4 show the results for MH base samplers with $d = 2$ and as a function of $d$, respectively. One can observe that both bandit-based algorithms (i.e., KSD-UCB1 and KSD-$\varepsilon$-greedy) perform similarly, almost achieving the performance of the best base sampler. Interestingly, there is no significant difference between the two methods, and $\varepsilon$-greedy, which is an inferior bandit algorithm, seems to perform slightly better. This might indicate, that in our case less exploration could be preferable. Also, it is interesting to note that the bandit method with the smaller batch size of 10 outperformed the one with bigger batch size of 100; since we have already observed that the ordering of the samplers is not really affected by the batch size, this improved performance is most likely due to the increased number of decision points, which allows better adaptation. Note that given that the computational complexity of calculating the KSD measure is quadratic in the number of samples, smaller batch sizes have a huge advantage compared to bigger ones; in particular, in our experiment, the computational cost for batch size 10 is about two orders of magnitude smaller than for batch size 100. The running time of the different KSD computations are shown in Figure 2.

On the other hand, although our methods are competitive with the MH samplers, one can observe that NUTS significantly outperforms all of them, hence also their combinations. Furthermore, the reweighting mechanism of KSD-opt can provide a significant boost in performance for lower dimensions.

The performance of the aggregating sampling algorithm can be significantly improved by changing the base samplers. This is shown in Figures 5 and 6, where MH is replaced with the much better MALA samplers, making the best sampler and our bandit-based sampling method competitive with NUTS. Interestingly, due to the better quality samples, in this case KSD-opt outperforms MALA for the whole range of dimensions (up to $d = 22$) we consider, although the performance difference vanishes as $d$ increases, and indicates (as expected) that NUTS will be better for large values of $d$.

5.3 Separated modes with one sampler for each mode

In this section we consider the case of a multimodal target density (Gauss mixture) with separated modes, where we have one sampler for each mode. Here we run several versions of KSD-UCB1-M,
Figure 3: Unimodal case, Gaussian target distribution: MSE for different sample sizes with MH samplers in 2-dimensions (d = 2) with batch size 10 (left) and batch size 100 (right). The dashed lines without labels show the performance of the different MH samplers. The total number of samples is 5000 in each case.

Figure 4: Unimodal case, Gaussian target distribution: MSE versus dimension d with MH samplers and batch size 10(left) and batch size 100 (right). The dashed lines without labels show the performance of the different MH samplers. The total number of samples is 5000 in each case.

which differ in how the region (mode) \( I_t \) is selected in the algorithm. In particular, we consider the following methods for selecting \( I_t \):

- Uniformly at random (this is called "Equal probability" in the figures).
- Random, proportionally to the estimated weights \( w_i \) (or, equivalently, the estimated probability of the corresponding region), as described in Section 3.3 (\( w \)). In all the experiments, we used the Information Theoretical Estimators package of Szabó (2014) to calculate estimates of the Rényi entropy.
- \( I_t \) is selected as the sampler (region) with the largest average block-KSD measure (KSD).
- \( I_t \) is selected randomly with probability proportional to \( w_i \hat{S}_{i,n} \), as suggested by (5) (KSD.\( w \)).
- \( I_t \) based on the stratified sampling idea of (Carpentier et al., 2015), with probability proportional to \( \hat{\sigma}_i w_i \), where \( w_i \) is the estimated weight and \( \hat{\sigma}_i \) is the estimated standard deviation of the samples (\( \sigma.w \)).

For completeness, for the last reweighting step we conducted experiments with both the true weights and also with estimated weights.

We ran experiments for a target distribution with three separated modes, where the goal again was to estimate the mean of the distribution with respect to the mean squared error. We selected one sampler for each mode (with random parameters). The experiment were repeated 100 times, both for MH and
MALA base samplers, with different random initializations for the MCMC chains. Finally, the whole process was repeated 20 times, drawing different parameters for the samplers. Figure 7 shows the results for one of the 20 settings with MH samplers (the results for all the 20 settings followed the same pattern); both with and without the a priori knowledge of the weights. The results with MALA instead of MH are presented in Figure 8. One can observe that, for known weights, the best method for selecting $I_t$ in both experiments is the random choice with probability proportional to $w_i S_i n_i$. On the other hand, when the weights are needed to be estimated, the performance of our more informed methods (i.e., all except for the uniform random selection) is approximately the same, which is due to the unavoidable errors in estimating the weights (this effect is more visible for small sample sizes).

A crucial step in the aggregation of the samples coming from different samplers is to estimate the weight of each mode. To this end, we repeated the same experiment with a uniformly random choice of $I_t$, but considering different methods for the final weight estimation. In particular, we compare the Rényi-entropy-based estimates with different $\alpha$ parameters and the natural weight estimates for Gaussian mixtures based on estimating the covariance matrix for each mode (Scott et al., 2016). The results presented in Figure 9 show that the weight estimation is not really sensitive to the choice of $\alpha$ (the recommendation of Szabó, 2014 is to use values close to 1). Interestingly, in case of MALA base samplers, the Rényi-entropy-based methods outperform the ones designed specifically for the Gaussian distribution, which is indeed the underlying distribution in our case.
Figure 7: Multimodal distributions (Gauss mixtures): MSE for different sample sizes when the samplers are MH when the weight of each mode is known in advance (left) and when the weights are estimated with our proposed weight estimation method based on Rényi entropy with $\alpha = 0.95$ (right). The samples are taken from the following unnormalized distribution $p(x) = \sum_{i=1}^{3} \beta_i \exp \left\{ (x - \mu_i)^\top \Sigma_i^{-1} (x - \mu_i) \right\}$ where $\beta = [0.5, 0.3, 0.2]$, $\Sigma_i = \sigma_i I$ with $\sigma = [0.9, 0.4, 0.5]$ and $\mu_1 = [6, 6]^\top$, $\mu_2 = [-6, 6]$ and $\mu_3 = [0, -6]$. After a sharp decline the error slightly goes up for all the method which is due to a chain that visited some areas of low probability that affect the weight estimation. Also, it can be seen that the error starts to decline again which means that the chain goes back to a high probability area.

Figure 8: Multimodal distributions (Gauss mixtures): MSE for different sample sizes with MALA base samplers when the weight of each mode is known in advance (left) and when the weights are estimated with our proposed weight estimation method based on Rényi entropy with $\alpha = 0.95$ (right).

5.4 The general case: unknown number of modes with multiple chains

In this section, we consider a realistic situation where we have access to an unnormalized distribution but we don’t know how many separated regions/modes it has. Again, the goal is to estimate the mean of the distribution. Here we cannot guarantee that any MCMC chain used will only sample one; on the contrary, chains will usually move among different regions. We consider a Gaussian mixture model with 5 modes of random parameters, and run 10 base samplers whose parameters are also chosen randomly. We compare several combination methods discussed before: (i) each sampler is used to generate the same number of samples (Uniform); (ii) the same as the previous, but the final clustering and reweighting step of KSD-MCMC-WR (Algorithm 3) is used in the end (Uniform+clustering); finally, four versions of KSD-MCMC-WR are considered where the bandit method is $\varepsilon$-greedy or UCB1, and the selection of $I_t$ is uniform at random (Equal probability) or random with probabilities proportional to $w_i \tilde{S}_{i,n_t}$. For clustering, we used the "Kmean" method of the scikit-learn package (Pedregosa et al., 2011).

After randomly choosing the distribution and the samplers, we considered them fixed and ran 100 experiments; in each one the sampling methods are started from random initial points. The whole process was then repeated for 20 different sets of distributions and samplers. Figure 10 shows the results for two representative cases (out of 20) when MH is used as the base sampler. The top row
Figure 9: Multimodal distributions (Gauss mixtures): Mean squared error of different weight estimation methods for the setup in Section 5.3 when the samplers receive equal budget. “Gaussian” refers to considering a Gaussian distribution for each mode and calculating its weight by estimating its covariance matrix, while “Rényi” refers to our proposed weight-estimation method based on the Rényi entropy. Results for MH base samplers are shown on the left, while for MALA samplers on the right.

Figure 10: Unknown number of modes: MSE for different sample sizes when combining 10 randomly initialized MH samplers. The samples are taken from a 2-dimensional Gaussian mixture model with 5 isotropic modes. The mean of each mode is selected uniformly at randomly from $[-5, 5]^2$ and the variance of each component is selected randomly from $[0.2, 1]$. Two representative cases are shown: in the top row the modes are far from each other, in the bottom row the modes are close. The left column corresponds to batch size 10, while it is 100 for the right column. The Rényi entropy with $\alpha = 0.99$ is used for weight estimation.

 corresponds to a situation when the modes are far from each other; in this case our proposed method significantly outperforms NUTS and also unweighted uniform usage of the samplers. The bottom row depicts a case when the modes are really close together, in which case NUTS performs the best. Interestingly, in these experiments the application of any bandit algorithm is not really beneficial as the best combination algorithm is essentially using the samplers uniformly and then reweighting the samples via our clustering method.

On the other hand, if the MH samplers are replaced with NUTS samplers, a more careful selection of which sampler to use becomes important. This is because these samplers explore individual modes efficiently, thus using multiple samplers for the same mode is really wasteful. Figure 11
Figure 11: MSE for different sample sizes with separated modes: KSD-MCMC-WR with 10 randomly initialized NUTS samplers for an unknown number of modes. The batch size on the left figure is 10 and on the right figure is 100. The dashed green lines show the results for the individual NUTS samplers. Rényi entropy with $\alpha = 0.99$ is used for weight estimation. The problem setup is the same as the one in Figure 10.

Figure 12: Running KSD-MCMC-WR for a multivariate standard normal distribution with 10 NUTS instances started with different (random) initialization. The batch size is 10 on the left and 100 on the right. shows the results for another representative example out of the 20 cases that we used in the previous experiment. The results indicate that our combination method (with various choices for the details) significantly outperform NUTS. Also, as mentioned before, using bandit algorithms to select from the base samplers is much better than just choosing them uniformly.

Although the previous experiment demonstrated that the KSD-MCMC-WR is preferable to NUTS when the modes of the distribution are separated, it is not sufficient to argue that KSD-MCMC-WR is preferable to NUTS. In order to be able to make such a claim, we should also look at cases in favor of NUTS; the most favorable being the case of a unimodal distribution. To this end, we compared the performance of NUTS and KSD-MCMC-WR when sampling from a multivariate standard normal distribution. Figure 12 shows that running KSD-MCMC-WR is competitive with the individual NUTS instances.

These results suggest that one should always run KSD-MCMC-WR with NUTS base samplers, as it provides significant improvements form multimodal distributions while remains a safe choice for the easier, unimodal cases.

6 Conclusion

Selecting the best MCMC method and its best parameter setting for a given problem is a hard task. Even if the parameters are selected correctly, in case of multi-modal distribution, MCMC chains can easily get trapped in different modes for a long time, which may lead to biased results. To solve these issues, in this paper we proposed an adaptive MCMC method that runs several chains in parallel,
measures the quality of samples from each mode locally via kernel Stein discrepancy, and decides sequentially how to allocate the sampling budget among the different samplers. The final step of our algorithm is to combine the samples obtained by the different samplers: for this we developed a novel weighting scheme based on Rényi-entropy estimation, which might be of independent interest. Extensive experiments on several setups demonstrated that our proposed algorithm works well in both unimodal and multimodal problems, and it can particularly perform well when used in combination with NUTS as its base sampler.

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