An adaptive Metropolis-Hastings scheme: sampling and optimization

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Abstract

We propose an adaptive Metropolis-Hastings algorithm in which sampled data are used to update the proposal distribution. We use the samples found by the algorithm at a particular step to form the information-theoretically optimal mean-field approximation to the target distribution, and update the proposal distribution to be that approximation. We employ our algorithm to sample the energy distribution for several spin-glasses and we demonstrate the superiority of our algorithm to the conventional MHI algorithm in sampling and in annealing optimization.

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Monte Carlo methods are powerful tools for evaluating integrals and simulating stochastic systems (for a recent review, see [1]), and they have proved very useful for studying thermodynamic properties of model systems with many degrees of freedom. The core of any such method is an algorithm for producing independently and identically distributed (IID) samples of a provided target probability distribution \( \pi(x \in X) \). One of the most popular methods used is the Metropolis-Hastings (MH) algorithm [2] and many of its variants [3, 4, 5, 6]. The Markov transition matrix produced by this algorithm is parameterized by a proposal distribution \( T(x, x') \). Typically \( T \) is set before the start of the Markov chain in a \( \pi \)-independent manner and fixed throughout the running of that chain. The rate at which the associated Markov chain converges to the desired IID sample is crucially dependent on the relation between \( T \) and \( \pi \) however. Since the set \( \{x(t)\} \) produced by the MH algorithm is (eventually) an IID sample of \( \pi \), one can use \( \{x(t)\} \) to produce an empirical estimate of \( \pi \) [7]. This suggests that we empirically update \( T \) along the Markov chain to be an increasingly accurate estimate of \( \pi \). An adaptive version of the MH algorithm was introduced in [13]. Here we investigate that algorithm and demonstrate its superiority through spin glass experiments. A full version of this paper can be found at http://tc.arc.nasa.gov/dlw.

1 Sampling

For many systems of interest in physics, \( X \) is high-dimensional (e.g., the number of spins in an Ising system), and for the density estimation of \( \pi \) to work well it must be restricted to producing estimates from a relatively low-dimensional space, \( Q \). Intuitively, the idea is to try to find the \( q \in Q \) that is “closest” to \( \pi \) and use that to update \( T \), presuming that this will produce the most quickly converging Markov chain. We generically call such algorithms Adaptive Metropolis Hastings (AMH). To specify an AMH algorithm one must fix the measure of closeness, the choice of \( Q \), and the precise details of the resultant density estimation algorithm. One must then specify how the estimates of \( \pi(x) \) are used to update \( T(x, x') \).

The most popular way to measure closeness between probability distributions is with the (asymmetric) Kullback-Leibler (KL) distance [8]:

\[
D(p||p') = -\sum_x p(x) \log \frac{p'(x)}{p(x)}
\]

(1)

Recent work in Probability Collectives [9] provides insight into how to do density estimation to minimize KL distance when \( Q \) is low-
dimensional. In particular, say $Q$ is the set of all product distributions over $X$, $q(x) = \prod_i q_i(x_i)$, which is equivalent to the familiar mean-field approximation \cite{11}. Then $D(q\|\pi)$ is minimized if

$$q_i(x_i) \propto e^{E(\log(\pi)|x_i)} , \forall i$$

which $E(\cdot|\cdot)$ is the expected value of the first entry conditional on the fixed second entry \cite{10}. Accordingly, $D(q\|\pi)$ is just the associated free energy of $q$ if $\pi$ is a Boltzmann distribution.

Here we instead consider $D(\pi\|q)$, which it can be argued is more appropriate, in light of the information-theoretic justification of KL distance. The product distribution minimizing this distance can be written down directly: it has the same marginals as $\pi$, i.e., the optimal $q$ obeys $q_i = \pi_i, \forall i$ \cite{10}. Now a Markov chain produced by a run of the conventional MH algorithm converges to an IID sample of $\pi$. So the $i$'th component of the elements of that chain, $\{x_i(t)\}$, become an IID sample of $\pi_i$. Accordingly, those sample-components give us an IID sample of the distribution minimizing $D(\pi\|q)$. So if the number of possible $x_i$ values is not too large, we can use simple histogramming of the elements of the Markov chain produced by the MH algorithm to form our estimate of each marginal $\pi_i$, and therefore of the $q$ minimizing $D(q\|\pi)$. This gives us a rule for updating the proposal distribution, $P(T_t | \{x(t)\})$.

There are a number of subtleties one should account for in choosing the precise details of $P(T_t | \{x(t)\})$. In practice there is almost always substantial discrepancy between $\pi$ and $q$, since $Q$ is a small subset of the set of all possible $\pi$. This means that setting $T(x, y) = q(y)$ typically results in frequent rejections of the sample points. The usual way around this problem in conventional MH (where $T$ is fixed before the Markov process starts, and therefore is typically an even worse fit to $\pi$) is to use a ($t$-independent) $T(x, y)$ that forces $x$ and $y$ to be close to one another. Intuitively, doing this means that once the Markov chain finds an $x$ with high $\pi(x)$, the $y$’s proposed by $T(x, y)$ will also have reasonable high probability (assuming $\pi$ is not too jagged). We integrate this approach into our AMH algorithm by setting $T_t(x, y)$ to be $q_t(y)$ “masked” and renormalized to force $y$ to be close to $x$.

Another important issue is that the earlier a point is on the Markov chain, the worse it serves as a sample of $\pi$. To account for this, one should not form $q_t(x_i = s)$ at time $n$ simply as the fraction of all points $t < n$ for which $x_i(t) = s$. Instead we form those estimates by geometrically aging the importance of the points before evaluating the fraction. This means that more recent points have more of an effect on our estimate of $\pi$. This aging has the additional advantage that it makes the evolution of the proposal distribution a relatively
low-dimensional Markov process, which intuitively should help speed convergence.

In [5, 6] related ideas of how to exploit online-approximations of \( \pi \) that are generated from the random walk were explored. None of that work explicitly considers information-theoretic measures of distance (like KL distance) from the approximation to \( \pi \). Nor is there any concern to “mask” the estimate of \( \pi \) in that work. The algorithms considered in that work also make no attempt to account for the fact that the early \( x(t) \) should be discounted relative to the later ones. In addition, not using product distributions, parallelization would not be as straightforward with these alternatives schemes.

Our AMH algorithm

Our proposed algorithm consists of three successive phases: the first of these is the cooling phase and the third is the data collecting phase. In both of these phases, the conventional Metropolis-Hastings algorithm is used, i.e., there is no updating on the proposal distribution. The second phase is where the proposal distribution is adaptively updated. The details are presented below:

Let \( N \) be the number of components of \( x \) and \( q^t \) the estimate of \( \pi \) at the \( t \)th step of the walk. We consider the following algorithm:

1. Set \( T^t(x, y) \) to \( q^t(y) \) masked so that \( y \) and \( x \) differ in only one component:

\[
T^t(x, y) \propto \delta \left( \sum_{i=1}^{N} \delta(x_i - y_i) - N + 1 \right) \prod_{k=1}^{N} q^t_i(y_i). \tag{3}
\]

2. As in conventional MH, sample \([0, 1]\) uniformly to produce a \( r \) and set

\[
x(t + 1) = \begin{cases} y, & \text{if } r \leq R^t(x(t), y) \\ x(t), & \text{otherwise} \end{cases} \tag{4}
\]

where

\[
R^t(x, y) = \min \left\{ 1, \frac{\pi(y)T^t(y, x)}{\pi(x)T^t(x, y)} \right\}. \tag{5}
\]

3. Only in phase 2:
   Periodically update \( q \). If \( \text{mod}_N(t + 1) = 0 \), then update the set \( \{q^t_i\} \) by the non-negative multiplier \( \alpha < 1 \):
   For all \( i, x'_i = x_i(t) \)
   \[
   q^{t+1}_i(x'_i) = \alpha(q^t_i(x'_i) - 1) + 1 \tag{6}
   \]
   otherwise
   \[
   q^{t+1}_i(x'_i) = \alpha q^t_i(x'_i) \tag{7}
   \]
If \( \text{mod}_N(t + 1) \neq 0 \), then \( q_{t+1}^i(x'_i) = q_t^i(x'_i) \). To avoid freezing the proposal distribution, \( q_i \) is not allowed to get too close to the boundary of the probability simplex (i.e., less than 0.2 \times the initial uniform distribution).

4. \( t \leftarrow t + 1 \). Repeat from step 1.

We note again that in the the first phase of the algorithm, \( T \) is uniform and step 3 is not implemented, in the second phase, all steps above are implemented and in the third phase, step 3 is not implemented. We also note that our updating method depend only on the current state and hence is much more efficient than previously proposed methods [5].

**Sampling Experiments**

Currently there is no consensus on how to quantify “how close” a set \( \{x(t)\} \) is to an IID sample of \( \pi \). One approach is to input the set into a density estimation algorithm [7]. One can then use KL distance from that estimated distribution to \( \pi \) as the desired quantification. This can be problematic in high-dimensional spaces though, where the choice of density estimation algorithm would be crucial. However say we have a contractive mapping \( F : x \in X \rightarrow y \in Y \) where \( Y \) is a low-dimensional space that captures those aspects of \( X \) that are of most interest. We can apply \( F \) to the \( \{x(t)\} \) to produce its image in \( Y \), \( \{y(t)\} \). Next one can apply something as simple and (relatively) unobjectionable as histogramming to do the density estimation translating \( \{y(t)\} \) to an associated estimate of the generating distribution over \( Y \). We can then use KL distance between that histogram and \( F(\pi) \) as the desired quantification of how good our transition matrix is. This is the approach we took here.

An important issue with KL distance is that the KL distance from (a density of) the sample points to \( \pi \) diverges if no samples are obtained in region where \( \pi \) is substantially non-zero. This is not a serious problem if the total probability, \( \epsilon \), of such regions KL divergences is negligible because the discrepancy obtained on any expected value calculations will be bound by \( \epsilon \). Figure 2 illustrates how AMH and conventional MH compare in their values of \( \epsilon \).

Our first experiment concerns the Ising spin-glass model:

\[
H(x) = \frac{1}{2} \sum_{<i,j>} J_{ij}x_i x_j + \sum_i h_i x_i
\]

where \( <i,j> \) denotes summation over all neighbours. In this function the \( J_{ij} \) and \( h_i \) are randomly generated integers in the interval \([-5, 5]\)
and the $x_i$ can take on values $-1$ and $1$. Our task is to sample the associated Boltzmann distribution:

$$\pi(x) \propto \exp\left(-\frac{H(x)}{T}\right)$$

where $T$ corresponds to the temperature in a thermodynamic setting. We have chosen spin-glasses for illustration because it is generally believed that they display salient features of complex disordered systems [12].

We have performed experiments on spin-glasses in a 1D ring formation (with 50, 75 and 100 spins shown in Figure 1). In these experiments, we firstly run, with random initial states, 5 long Markov chains ($800,000 \times N$ steps where $N$ is the number of spins and data are collected at the last quarter of chain) with the conventional MH algorithm. We then average the energy distributions obtained to form our target distribution. Its closeness to the true distribution is suggested by how small the associated KL distances to the original distributions are (the bottom three lines in Figure 1).

We then produced 100 samples of energy distributions with the MH and the adaptive MH methods, with chains of $40,000 \times N$ steps each. We note that in the adaptive MH method, $q_i(x_i)$ corresponds to the probability of spin $i$ being in state $x_i$. Data are again collected in the last quarter of each chain in both case, and we performed proposal distribution updates as detailed before in the third quarter of the chains in the adaptive M-H case (with the updating parameter $\alpha = 0.98$).

Figures 1 and 2 show the results of these experiments with the error bars being the errors on the means. We see that AMH (with $\circ$ markers) outperforms conventional MH (with * markers) in sampling, as well as in avoiding KL divergence. Similar experiments on a 2D lattice have also been performed and the adaptive M-H shows similar superior performance over conventional MH.

### Optimization Experiments

We now investigate the performance of using our algorithm for optimization rather than sampling, i.e., for minimizing energy. We consider the same problem as before, with 100 spins. In the simulation we randomly generate 20 different sets of $\{J, h\}$ for the Hamiltonian in eq. [3]. The temperature goes from 1 to 0.05 in 19 equal steps. We produce 50 samples each for the MH and AMH versions of the algorithm; the results are presented in Fig. 3.
2 Conclusion

We have proposed a new adaptive Metropolis-Hastings which, with the product distribution assumption, is easy to implement in sampling and we have shown its superiority over conventional Metropolis-Hastings with computer experiments. Compared with adaptive Metropolis-Hastings proposals [5,6], we have demonstrated the usefulness of our proposed algorithm with highly non-trivial examples, i.e., spin-glasses, which highlights the usefulness of our proposed algorithm for sampling complex distribution. With annealing in temperature, our method is also shown to be useful in hard optimization.

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Figure 1: KL distances between the random walk points and the target density . (* = MH, ◦ = AMH, + = MH with long chains. The error bars are errors on the means.) The inset plot shows the percentages of deviation with respect to the free energies found with the long chains in the 100-spin system. (Error bars are smaller than the markers.)
Figure 2: (* = MH, ◦ = AMH. The error bars are errors on the means.)
Figure 3: Results of 20 different spin-glass experiments. Constants are added to the y-axis so that the minimum energies found by AMH are zero. (* = MH, ◦ = AMH. The error bars are errors on the means.)