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Asymptotically Efficient Simulation and Modeling of Rare Binary Images

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Abstract

Modeling and simulation of rare events is a problem that has been largely ignored by the image processing community, but is of great interest in many areas of science. Rare events in physical systems are responsible for many failure modes, and as such must be precisely understood. We propose a novel method for simulating and modeling rare images using asymptotically efficient importance sampling, and apply it to binary images of interest in statistical mechanics and materials science. These rare images correspond to the occurrence of rare events in systems modeled by Gibbs distributions, more commonly known as Markov random fields (MRFs) in image processing. We will first give a precise definition of a rare event, in terms of a rare event statistic and a rare event region. The rare event statistic of interest here will be the per-site magnetization of a ferromagnet under the Ising model, but this could be replaced by many other statistics for other problems, such as boundary length in two-phase material microstructures, for example. For the given rare event statistic, we estimate the asymptotically efficient importance sampling (AEIS) distribution, which is based on a large deviation principle (LDP); draw samples of rare binary images from this AEIS distribution; and estimate rare event probabilities for several different rare event regions. Theoretically, the AEIS sampling distribution gives an unbiased estimator with the lowest variance asymptotically from a class of importance sampling distributions that are practically feasible for Monte Carlo Markov chain simulation. Finally, we fit large deviations rate functions from simulations using several rare event regions. This allows us to compute probability estimates associated with a given rare event statistic for any rare event region of interest without requiring further simulations.

Introduction

Many important rare events occur in systems that are characterized using image data. A few examples include the growth of an abnormally large grain in a polycrystalline material [1, 2], tumor growth in humans or animals [3, 4], and abnormal clustering of particles in certain metal alloys [5].

Estimating probabilities of rare events in images is often of critical importance. One reason for this is that the expected number of occurrences of a rare event in a given number of samples depends on the probability of the rare event. Is the event expected to occur on the order of once in 100 samples? Once in 10,000 samples? Once in 100,000 samples? This is important when manufacturing defects are considered, for example. Estimating rare event probabilities is also important for "grounding" a rare event simulation in reality. If in simulation, our estimated probability of a certain event is extremely small, there can be two possible causes. First, the real probability of that event is indeed tiny. In this case, the likelihood of observing the event in the real world is so small that we do not need to model it. Second, it may arise from an inaccurate or incomplete model, such as an energy expression in the Gibbs distribution that is not sufficiently precise to accurately capture the tail behavior of the probability measure.

To the best of our knowledge, there has been no published work that simulates rare images and then uses those images to estimate probabilities of associated rare events. We present a novel method that performs asymptotically efficient importance sampling of images modeled by Gibbs distributions, or equivalently Markov random fields, and estimates rare event probabilities, providing unprecedented capabilities for characterizing rare events in images.

Simulation of images is often performed using Monte Carlo Markov chain (MCMC) sampling, but drawing from the system distribution is extremely unlikely to generate images that are rare under that distribution. There have been many efforts to draw rare samples of images using MCMC, with a biasing energy term to drive the simulation into certain desired regions [6, 7]. These methods effectively use importance sampling (IS) (although it is not identified as such in published papers), but they do not consider optimal IS, nor do they estimate associated rare probabilities. In fact, they do not even frame the rare event as an event in a probability space, so it is not clear how probabilities would be precisely defined in those approaches. We address these limitations by using a mathematically precise, practically useful definition of rare events, performing asymptotically efficient importance sampling based on results from large deviations, and estimating the optimal rare event probabilities from the sampled images.

The novelty of our proposed approach, which is based on theoretical results from large deviations (LD), includes

- precise definition of a rare event, in terms of a rare event statistic, computed from the appropriate rare images, and a rare event region;
- use of an asymptotically efficient importance sampling distribution;
- estimation of an optimal value of the IS biasing parameter;
- estimation of rare event probabilities from simulated images;
- estimation of the large deviation rate function for a given rare event statistic.

There are two advances in probability theory that have enabled our work. The first is a large deviations result for Gibbs distributions that was proved in the 1980s [8], and the second is the introduction of the AEIS distribution for Gibbs distributions in 1993 [9]. The problem with these results is that they do not admit closed-form solutions, so we have developed estimation procedures to approximate the theoretically correct results.

Before moving on, it should be noted that importance sampling methods based on large deviation theory have been used to compute rare event probabilities in high dimensions. In [10] rare event probabilities are estimated for high-dimensional Gaussian random variables, for a 1D diffusion problem, and for 1D tsunami characterization. However, only Gaussian random variables and one dimensional random processes were characterized in [10]. The problem of simulating rare images and estimating probabilities from the simulated images provides different challenges. A solution to this problem would allow domain experts to evaluate rare event probabilities with associated images that help visually validate that the expected rare event has actually occurred in the simulation.

Methods

Mathematical definition of a rare event characterized by image data

The first step is to set up the rare event for which we wish to find a probability. Consider three elements:

- A random image X defined on a lattice S, with some probability distribution p (either a probability density or a probability mass function) for X. We assume a Gibbs distribution p for X, and focus on the case where X is a binary image in this paper.
- A random vector $T(X) \in \mathbb{R}^d$, which is a statistic computed from the image X, for some $d \geq 1$. Note that we do not need to know the probability measure P of T to estimate the probability of the rare event. As will be seen, it is enough to know p and the mean $E[T(X)]$, which we can estimate from samples of X. In this paper, we consider the case $d = 1$ only.
- A region $A \subset \mathbb{R}^d$, which does not contain the mean vector $E[T(X)]$. When $d = 1$, A will usually be a tail interval.

With these definitions in hand, we say that the rare event of interest occurs whenever $T(X) \in A$. We refer to the vector T as the *rare event statistic* and the set A as the *rare event region*. Intuitively, the farther A is (in some sense) from the mean of T, the more rare the event, but all that is required of the set A is that it not include the mean behavior of the system, as represented by the mean vector of T.

Importance sampling for estimation of rare event probabilities in images

There are a couple of problems that arise in the practical application of our definition of a rare event $T(X) \in A$. First, it is infeasible to draw samples of the image X under distribution p directly. This problem is addressed by using well-established MCMC methods, such as the Metropolis-Hastings algorithm, which we have used for the results in this paper, and the Gibbs sampler. The second problem we face is that samples drawn from the distribution p will not include sufficient occurrences of the rare event of interest to allow effective characterization, unless the event is not actually very rare (which can happen when the rare event region A contains points that are close to the mean of rare event statistic $T(X)$). Thus we turn to importance sampling, which draws samples instead from an *importance sampling distribution* q, and estimates the probability $P(T(X) \in A)$ under p from those samples, as described next.

Consider N image samples $\left\{X^{(k)}\right\}_{k=1}^{N}$ drawn from some selected IS distribution function q by MCMC simulations. Then, an unbiased estimate on the probability of the rare event of interest under p is given as follow:

$$\hat{P}_n(T(X_n) \in A) = \frac{1}{N} \sum_{k=1}^{N} \mathbb{1}_{\{A\}}(T(X_n^{(k)})) \frac{p_n\left(X_n^{(k)}\right)}{q_n\left(X_n^{(k)}\right)} \tag{1}$$

for some large n, where n is the number of lattice sites, X_n^k is the kth sample image, and P_n is the measure of $T(X_n)$. Here we assume that the Markov chain is ergodic. It gives that for large n, the expectation of the per-site quantity T can be approximated by the average of T from a large amount of image samples X_n.

Selecting an IS distribution

Now we address the question of which IS distribution function q we should use. The right side of (1) is an unbiased estimator of $P_n(T(X_n) \in A)$ for any sequence of distributions q_n, so long as q_n is not zero anywhere, but we also want an estimator whose variance is as low as possible.

It turns out that we cannot minimize the variance of the estimator of (1) for any finite n, so instead the optimality criterion we use is the minimization of the asymptotic variance as $n \to \infty$ [16].

Now that we have defined the selection of the IS distribution q as a minimization problem, namely minimization of the asymptotic variance of the rare event probability estimator in (1), we have only to perform the optimization. But commonly-used optimization methods cannot be used here. Since LDP provides a mathematical framework for rare events, we turn to it to address this problem.

More specifically, we rely on two results from LD, beginning with the result that a sequence of empirical Gibbs distributions satisfies a *large deviations principle* (LDP) [8]. The mathematical definition of an LDP, and more formal statements of the relevant Gibbs LDP results, are given in that reference, but there are two important implications for our purposes.

Optimal IS distribution

The first implication of the LDP for Gibbs distributions actually gives us a solution to our question of which IS distribution to use [9]. First, we write the Gibbs distribution p as

$$p(x) = \frac{1}{Z^U} \exp(-\beta U(x)), \tag{2}$$

where β is the inverse temperature and Z^U is the normalizing constant (also known as the partition function) associated with Gibbs energy function U.

Then the result derived by Baldi, for the case where T is single-variate and $A = [u, \infty)$ for some $u > E[T]$ for simplicity, can be summarized as

- the AEIS distribution q_n at MCMC step n has the form

$$q_n(x) = \frac{1}{Z^{U_q}} \exp\left(-\beta\left(U_q(x)\right)\right), \tag{3}$$

- where $U_q(x) = U(x) - tnT(x)$ is the IS energy function. It can be seen from this form for q_n that the AEIS distribution is another Gibbs distribution, where the system energy function $U(x)$ has been shifted with a biasing energy based on the statistic T,

and

- the value of the biasing parameter t must satisfy $E_{q_n}[T] \to u$ as $n \to \infty$.

This sequence of sampling distributions q_n, with the optimal value of t, guarantees an optimal estimator of the probability of our rare event in the sense of being unbiased and having the lowest variance asymptotically from a class of practically feasible importance sampling distributions.

Large deviation rate function for rare event probability

The second implication of the LDP for Gibbs distributions is that, under certain mild conditions, the sequence of rare event statistics T also satisfies an LDP (based on what is known as the large deviation contraction principle). This means that for some large deviation rate function I

$$\hat{P}_n(T(X_n) \in A) \asymp \exp(-nI(A))) \quad (4)$$

for large n. This is potentially a very useful result, because it means that if we can find the large deviation rate function I associated with a rare event statistic T, then we can obtain an optimal estimate of the rare event $T(X) \in A$ for any A without needing to draw more rare images.

Application examples

Spontaneous magnetization of a ferromagnet

Our approach

In this example, the rare event of interest is the spontaneous magnetization of a ferromagnet, without an external magnetic field. The statistic T is per-site magnetization and the region A is the interval $[u, \infty)$ for some real number u. This choice of A is made because the expected per-site magnetization with no external field is zero, so we consider a magnetization per-site of $T > u > 0$ to correspond to a rare event.

The Gibbs distribution that describes the spin-spin interactions of a ferromagnetic metal is called the Ising model. Under no external magnetic field, the potential term is

$$U(x) = -J \sum_{\langle i,j \rangle} x_i x_j, \quad (5)$$

where i and j are site locations in the ferromagnet (e.g., the lattice S), J is the coupling coefficient between neighboring sites, and x_i is the spin value at site i. Each spin value x_i can be either $+1$ or -1. The summation is over all pairs of neighbors in the lattice. In theory, the configuration x is defined on an infinite lattice, but we use a finite lattice with periodic boundary conditions (See [9] for a discussion of this issue).

As given in the previous section, for a given cutoff value u, we first generate samples $\left\{X^{(k)}\right\}_{k=1}^{N}$ from the sequence of distributions q_n given in (3), using an estimate of the optimal t.

The simulated microstructure images are shown in Fig .1. From the expression of U_q, we know that as the optimal biasing parameter t increases, the behavior of the sampled system becomes farther away from the normal of the original system, described by probability measure p. Hence, as t goes up, the areas of black pixels and with pixels differ more, as illustrated in Fig. 1. In addition, higher coupling coefficient J indicates stronger interaction between neighbors. Thus, larger magnetic domains are observed in the simulated images with larger J.

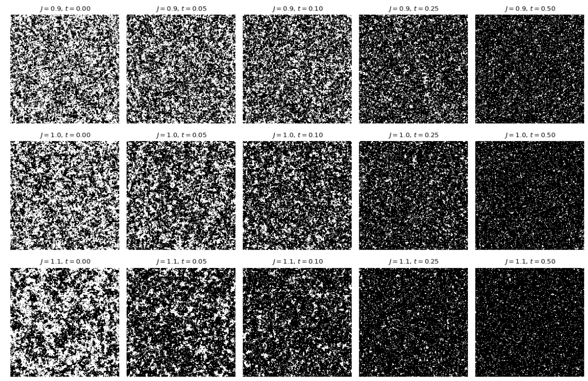


Figure 1: Sample images for multiple values of t and J. Lattice size 240×240 was used. From left to right, t increases from 0 to 0.5. From top to bottom, J increases from 0.9 to 1.1. The inverse temperature β was set to be 0.35. Note that here we only consider the cases when Ising model simulations are above critical temperature.

Then, with those simulated images, the probability of rare event $T(X) \in A$ is estimated by

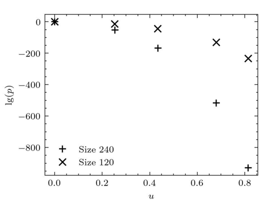
$$\hat{P}_n(T(X) \in A) = \frac{Z^{U-tG}}{NZ^U} \sum_{k=1}^{N} \mathbb{1}_{[u,\infty)}(T(X^k)) \exp\left(-\beta tnT\left(X^{(k)}\right)\right). \quad (6)$$

Note that (6) requires estimation of the normalizing constant ratio, Z^{U-tG} / Z^U. We have tested three different estimation methods: Numerical Integration (NI), Annealing Importance Sampling (AIS) [17] and the Cumulant Expansion Method (CEM) [18]. Results are shown in Table 1. From the table, we notice that results given from NI and AIS are similar. However, results from CEM deviate from those two methods, especially when t grows larger. That is due to the perturbation nature of CEM. Hence, here we used normalizing constant ratio from NI for probability estimation.

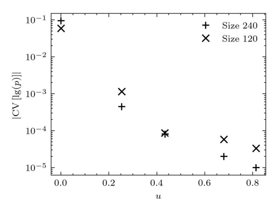
Table 1: Estimations of normalizing constant ratio

t			0.00	0.05	0.10	0.25	0.50
u			0.0004 ± 0.0011	0.2539 ± 0.0107	0.4339 ± 0.0314	0.6796 ± 0.0770	0.8141 ± 0.1105
$\ln\left(Z^{U-tG}/Z^U\right)$	NI		0.0	139.2	419.6	2238.5	6069.1
	AIS		NA	159.1 ± 1.8	511.2 ± 2.5	2262.7 ± 4.7	6084.9 ± 5.3
	CEM	$t_1 > 0$	NA	131.7	525.8	3282.5	13124.8
		$t_1 = 0$	NA	136.4	448.6	1833.5	3680.6

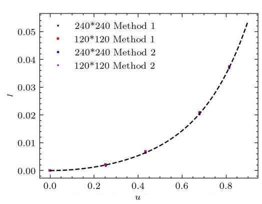
Now we have the estimates for all the terms in (6) to compute the probabilities. The results are shown in Fig. 2. When the cutoff value u increases, the rare event becomes smaller and hence its probability decreases. Since AEIS and LDP characterize asymptotical behaviors of the system, we did simulations on lattices of two large sizes. That enables us to test if the lattice size of use is large enough to be described by those theories. As shown in Fig. 2c, the rate function estimations given by simulations on the two kinds of lattice show a high consistency. Thus, we conclude that the sizes of the simulated lattices are sufficiently large to apply those two theories. Additionally, the coefficient of variations (CV) are significantly smaller than 1, which indicates precise estimations. We also estimated the rate function values using two methods, the results of which are highly consistent.



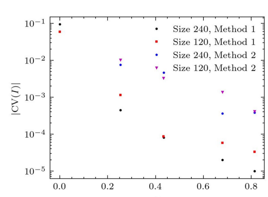
(a) Estimations of probabilities of several rare event regions.



(b) Coefficient of variation of the probability estimations.



(c) Estimations of rate function values.



(d) Coefficient of variation of the rate function values.

Figure 2: Estimation results of rare event probabilities p and rate function I values. The coupling coefficient was set to be 1. Simulations were conducted on square images in two sizes for comparison and validation, edge 120 and edge 240. Fifteen individual MCs were run for each setting. Results here are averages from those simulated data. Two approaches were used to estimate rate function values. For Method 1, rate function values were computed from estimated probabilities. For Method 2, they were obtained by Gibbs variational principle in theoretical physics.

Ising model can also be used for binary image restoration, in which J values correspond to penalty of the violation of smoothness [32]. Here, results from three J assignments are presented in Fig. 3. As shown in Fig. 1, larger coupling coefficient lead to higher magnetization with nonzero t. As J decreases, probabilities drop faster. That can be explained as follows. Larger J indicates stronger interaction between one site and its neighbors, which makes the energy cost for obtaining an outlier higher. Hence, for larger J, it is less likely to deviate a lot from the normal behavior.

Validation and comparison

Here we used four approaches to validate our results.

First, we compared estimations from our results to those from direct sampling for events of small deviations. The results are shown in Fig. 4. The black data points are given by directly sampling the distribution of the system, while the red data points are from our proposed sampling approach. As discussed above, we had zero hit in the very rare event regions in these simulations, when the event's probability was lower than 10^{-5}. Hence, direct

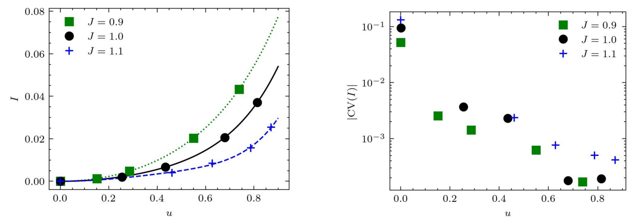


Figure 3: Estimations of rate function values for different coupling coefficients. The fitted curve of rate function for $J = 1.0$ is $y = \left(456.3x^6 + 49.8x^4 + 326.9x^2\right)/10000$ with R-squared 0.9999, for $J = 1.1$ is $y = \left(697.2x^6 - 441.5x^4 + 267.0x^2\right)/10000$ with R-squared 0.9985, for $J = 0.9$ is $y = \left(216.3x^6 - 318.0x^4 + 556.9x^2\right)/10000$ with R-squared 0.9999.

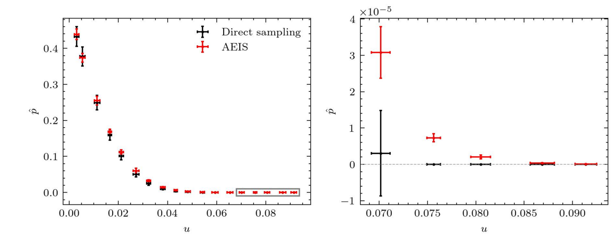


Figure 4: Fifteen Markov chains were generated for each $t(u)$. The figure on the right is a zoomed-in view of the region highlighted by the gray box in the figure on the left. Note that as the cutoff u increases, the event of interest becomes rarer. For tiny u, estimations from the two methods were on the same order. Except for the second smallest u, estimations by AEIS were always higher than those by Direct sampling. That is due to the positively skewness property of binomial distribution with success rate less than 0.5. Hence, in rare event regions, for direct sampling, there is a higher probability to get underestimation then overestimation.

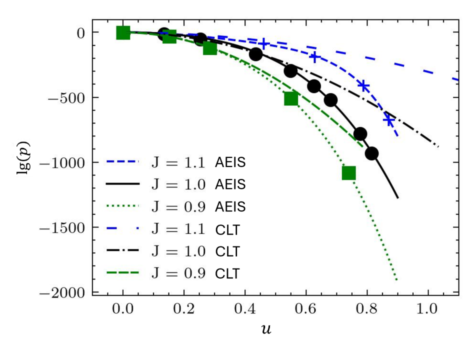


Figure 5: Comparison of estimates from the AEIS and CLT. Estimations of rare event probabilities are shown in this figure. Three values of the coupling coefficient J were tested: 0.9, 1.0, 1.1. Data points shown are estimations from simulations, with curves fitted to those points. The other three curves are the approximations resulting from the CLT.

sampling does not give reliable estimations for events of large deviations.

Another straightforward approach to probability estimation is the Central Limit Theorem (CLT) approximation. As shown in Fig. 5, we compared estimates of rare event probabilities from the CLT approximation and the proposed approach AEIS, for different coupling coefficient J. The CLT estimations deviate from the data more as events become rarer. That is due to the nature of low order approximation of CLT. For CLT, only the first two cumulants are taken into account, but the characterization of the tail of a probability distribution requires the information from high-order cumulants. Thus, we can only obtain a poor estimation on the rare event probabilities for a non-Gaussian probability distribution.

Additionally, we consider two numerical ways of estimating the rate function values on lattices in different sizes, as illustrated in Fig. 2a. Nearly overlapping data points indicate high precision of estimations.

Conclusions

In this work, we have developed a novel approach, grounded in mathematical rigor, to characterize rare events in images, and demonstrate it for a commonly used binary image model, the Ising model. Here, we first give a mathematical definition of rare events in terms of a statistic and a set. Then we use an optimal sampling distribution for the simulation. We simulate the event that the material becomes magnetized in the absence of an external magnetic field. Computation results illustrate that AEIS with optimal t gives smaller variance than direct sampling and IS with other t values. For CLT, although around the expectation, the estimated event probability by our proposed methods is in the same order of that by CLT, our proposed methods give a more accurate estimations in extremely rare region. Reliable estimations on the rate function in LDP are obtained, validated by a high consistency using two methods. We also show the possibility of applying this proposed approach to another binary model, Strauss model, which has been used for super-alloy modeling in material science.

Our approach has the potential to be useful in domains where Gibbs distributions are used to model image data. Some examples include materials science [23] and astronomy [25]. One popular Gibbs distribution is the Potts model, which is basically a multiclass extension of the Ising model. We are currently investigating the use of our method to characterize the rare event of abnormal grain growth in a polycrystalline material. This occurs when one or more of the grains becomes abnormally large at the expense of other grains. Also, we want to note that for a given rare event statistic T, selection of a rare event region A is generally straightforward if T is single-variate, since A can simply be an interval, or possibly a union of disjoint intervals. However, if T is multivariate, the region A can be more complicated. For some regular events, they can have similar form of AEIS and the optimal vector t to be found is dominating point [16, 29].

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