# Random construction of interpolating sets for high dimensional integration

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#### Mark L. Huber

Claremont McKenna College mhuber@cmc.edu

#### Sarah Schott

Duke University schott@math.duke.edu

#### **Abstract**

Many high dimensional integrals can be reduced to the problem of finding the relative measures of two sets. Often one set will be exponentially larger than the other, making it difficult to compare the sizes. A standard method of dealing with this problem is to interpolate between the sets with a sequence of nested sets where neighboring sets have relative measures bounded above by a constant. Choosing such a well balanced sequence can be very difficult in practice. Here a new approach that automatically creates such sets is presented. These well balanced sets allow for faster approximation algorithms for integrals and sums, and better tempering and annealing Markov chains for generating random samples. Applications such as finding the partition function of the Ising model and normalizing constants for posterior distributions in Bayesian methods are discussed.

## 1 Introduction

Monte Carlo methods for numerical integration can have enormous variance for the types of high dimensional problems that arise in statistics and combinatorial optimization applications. Consider a state space  $\Omega$  with measure  $\mu$ , and  $B \subset \Omega$  with finite measure. Then the problem considered here is approximating

$$Z = \int_{x \in B} d\mu(x). \tag{1.1}$$

The classical Monte Carlo approach is to create a random variable X such that E(X) = Z where X has variance as small as possible. Unfortunately, it is often not possible to know the variance of X ahead of time, and this must be

estimated as well. How good the estimate of the variance is depends on even higher moments which are even more difficult to estimate.

The method presented here creates an estimate of Z of the form  $e^{X/k}$ , where k is a known constant and X is a Poisson random variable with mean  $k \ln(Z)$ . Because the mean and variance for a Poisson random variable are the same, we simultaneously obtain our estimate of Z and knowledge of the variance of our estimate.

In fact, the output from our method does the following:

- Estimate Z to within a specified relative error with a specified failure probability in time  $O(\ln(Z)^2)$ .
- Create a well balanced sequence of nested sets useful in building annealing and tempering Markov chains that can be used to generate Monte Carlo samples.
- Develop an omnithermal approximation for partition functions arising from spatial point processes and Gibbs distributions.

**Previous work** The new method presented here follows a long line of work using interpolating sets. For instance, Valleau and Card [18] introduced what they called *multistage sampling* where an intermediate distribution was added to make estimation more effective. Jerrum, Valiant and Vazirani [8] used a similar idea of *self-reducibility*, and carefully analyzed the computational complexity of the resulting approximation method.

Suppose we are given two finite sets B' and B such that  $B' \subset B$  and #B (the number of elements of B), is known. One way of viewing self-reducibility, is that it effectively requires a sequence of sets  $B = B_0 \supset B_1 \supset B_2 \supset \cdots \supset B_\ell = B'$  such that the relative sizes of the sets  $\#B_{i+1}/\#B_i \geq \alpha$  for a fixed constant  $\alpha \in (0,1)$ . Then an unbiased estimate  $\hat{b}_i$  of  $\#B_{i+1}/\#B_i$  is created for each i. The product of these estimates will then be an unbiased estimator for #B'/#B, and multiplying by #B gives the final estimate of #B.

For fixed  $\alpha \in (0,1)$ , it is easy to estimate  $\#B_{i+1}/\#B_i$  with small relative error simply by drawing samples from  $\#B_i$  and counting the percentage that fall in  $\#B_{i+1}$ . The relative standard deviation of a Bernoulli random variable with parameter  $\alpha$  is  $(1-\alpha)/\alpha$ , so it is important not to make  $\alpha$  too small. On the other hand, if  $\alpha$  is too large, then the nested sets are not shrinking much at each step, and it will require a lengthy sequence of such sets. To be precise, the number of sets  $\ell$  must satisfy  $\ell \geq \ln_{\alpha}(\#B'/\#B) = \ln(\#B/\#B')/\ln(\alpha^{-1})$  which goes to infinity as  $\alpha$  goes to 1. Balancing these two considerations leads to a optimal  $\alpha$  value of about 0.2031.

The difficulty in applying self-reducibility is finding a sequence of sets such that  $\#B_{i+1}/\#B_i$  is provably at least  $\alpha$ , but not so close to 1 that the sequence of sets is too long. Ideally,  $\#B_{i+1}/\#B_i$  would equal  $\alpha$  for every i, or at least be very close. For fixed constants  $\alpha_1$  and  $\alpha_2$ , refer to a sequence of sets where the ratios  $\#B_{i+1}/\#B_i$  fall in  $[\alpha_1, \alpha_2]$  for all i as well-balanced.

Well-balanced sequences have other uses as well. Methods of designing Markov chains such as simulated annealing [10], simulated tempering, and parallel tempering [16, 5, 11] all require such a sequence of well-balanced sets in order to mix rapidly (see [19, 20].)

Now consider the special case of (1.1) where Z is the normalizing constant of a posterior distribution of a Bayesian analysis. Skilling [15] introduced nested sampling as a way of generating a random sequence of nested sets. The advantage this method has over self-reducibility is that there is no need to have the sequence of sets in hand ahead of time. Instead, it builds up sets from scratch at random according to a well-defined procedure.

The disadvantage is that it loses the property of self-reducible algorithms that the variance of the output could be bounded prior to running the algorithm. Because deterministic numerical integration was used in the method, the variance can be determined only up to a factor that depends upon the derivatives of a function that is difficult to compute. Therefore, nested sampling falls in the class of methods where the variance must be estimated, rather than bounded ahead of time as with self-reducibility.

The Tootsie Pop Algorithm The method presented here is called *The Tootsie Pop Algorithm* (TPA), and combines the tight analysis of self-reducibility by adding features similar to nested sampling. Like self-reducibility, it is very general, working over a wide variety of problems. This includes the nested sampling domain of Bayesian posterior normalization, but also includes many other problems where self-reducibility has been applied such as the Ising model. Portions of this work were presented at the Ninth Valencia International Meetings on Bayesian Statistics, and also appears in the conference proceedings [7] with a discussion.

The name is somewhat unusual, and references an advertising campaign run for Tootsie Pop candies. A Tootsie Pop is a chocolate chewy center surrounded by a candy shell. The ad campaign asked "How many licks does it take to get to the center of a Tootsie Pop?". Our algorithm operates in a similar fashion. Our set B is slowly whittled away until the center B' is reached. The number of steps taken to move from B to B' will be Poisson with mean  $\ln(\mu(B)/\mu(B'))$ , thereby allowing approximation of  $\mu(B)/\mu(B')$ . Therefore, the "number of licks" is exactly what is needed to form our estimate!

#### 1.1 Organization

Section 2 describes the TPA procedure in detail, then Section 3 shows some applications. Section 4 then analyzes the expected running time of the method, and introduces a two phase approach to TPA. Section 5 describes how TPA can be used to build well-balanced nested sets for tempering. Section 6 shows how to create an approximation that simultaneously works for all members of a continuous family of sets at once. Finally, Section 7 discusses further areas of exploration with TPA techniques.

## 2 The Tootsie Pop Algorithm

The TPA method has four general ingredients:

- 1. A measure space  $(\Omega, \mathcal{F}, \mu)$
- 2. Two finite measurable sets B and B' satisfying  $B' \subset B$  and  $\mu(B') > 0$ . The set B' is the *center* and B is the *shell*.
- 3. A family of nested sets  $\{A(\beta): \beta \in \mathbf{R} \cup \{\infty\}\}$  such that  $\beta' < \beta$  implies  $A(\beta') \subseteq A(\beta)$ ,  $\mu(A(\beta))$  is a continuous function of  $\beta$ , and the limit of  $\mu(A(\beta))$  as  $\beta$  goes to  $-\infty$  is 0.
- 4. Special values  $\beta_B$  and  $\beta_{B'}$  that satisfy  $A(\beta_B) = B$  and  $A(\beta_{B'}) = B'$ .

With these ingredients, the TPA method is very simple to describe.

- 1. Start with i = 0 and  $\beta_i = \beta_B$ .
- 2. Draw a random sample Y from  $\mu$  conditioned to lie in  $A(\beta_i)$ .
- 3. Let  $\beta_{i+1} = \inf\{\beta : Y \in A(\beta)\}.$
- 4. If  $Y \in B'$  stop and output i.
- 5. Else set i to be i + 1 and go back to step 2.

Another way of describing the draw in Step 2 is that for measurable D,  $P(Y \in D) = \mu(D \cap A(\beta_i))/\mu(A(\beta_i))$ . At each step, the set  $A(\beta_i)$  shrinks with probability 1, and so is slowly worn away until the sample falls into the region B'.

Line 2 above deserves special attention. Drawing a random sample Y from  $\mu$  conditioned to lie in  $A(\beta_i)$  is in general a very difficult problem. The good news is that the importance of this problem means that a vast literature for solving this problem exists. Markov chain Monte Carlo (MCMC) methods are critical to obtaining these samples, and variations on the early methods have blossomed over the last fifty years. Readers are referred to [14, 13, 3] and the references therein for more information.

Of course, any other method for turning samples into approximations either implicitly or explicitly depend on the ability to execute some variant of line 2 as well, so our algorithm is not actually demanding anything above and beyond what others require. The algorithm is easily modified to handle different methods of simulating random variables. For instance, nested sampling [15] draws several such Y variables at once, and TPA can be written to do so as well.

The key fact about this process is the following:

**Theorem 2.1.** At any step of the algorithm, let

$$E_i = \ln(\mu(A(\beta_i))) - \ln(\mu(A(\beta_{i+1}))).$$

Then the  $E_i$  are independent, identically distributed exponential random variables with mean 1.

*Proof.* To simplify the notation, let  $m(b) = \mu(A(b))$ . Begin by showing that each  $U_i = m(\beta_{i+1})/m(\beta_i)$  is uniform over [0,1]. Fix  $\beta_i \geq \beta_{B'}$  and let  $a \in (0,1)$ . Then since m(b) is a continuous function in b with  $\lim_{b\to -\infty} m(b) = 0$ , there exists a  $b \in (-\infty, \beta_i]$  such that  $m(b)/m(\beta_i) = a$ . Call this value  $\beta_a$ .

Let  $0 < \epsilon < m(\beta_B) - a$ . Then by the same reasoning there is a value  $\beta_{a+\epsilon} \le \beta_B$  such that  $m(\beta_{a+\epsilon})/\mu(\beta_i) = a + \epsilon$ . Now consider Y drawn from  $\mu$  conditioned to lie in  $A(\beta_i)$ . Then  $\beta_{i+1} = \inf\{b : Y \in A(b)\}$ .

Moreover,  $\{U_i \leq a\} \Rightarrow \{Y \in A(\beta_a)\}$ , an event which occurs with probability  $m(\beta_a)/m(\beta_i) = a$ . So  $P(U_i \leq a) \geq a$ .

On the other hand,  $Y \notin A(\beta_{a+\epsilon})$  implies  $\beta_{i+1} \geq \beta_{a+\epsilon}$  which means that  $U_i = m(\beta_{i+1})/m(\beta_i) \geq a + \epsilon$ . In other words,  $P(U_1 < a + \epsilon) \leq P(Y \in A(\beta_{a+\epsilon})) = a + \epsilon$ . This holds for  $\epsilon$  arbitrarily small, hence by dominated convergence  $P(U_i \leq a) \leq a$ . Therefore,  $P(U_i \leq a)$  is at least and at most a, so  $P(U_i \leq a) = a$ , which shows that  $U_i$  is uniform on [0, 1].

Observing that the negative of the natural log of a uniform number of [0,1] is an exponential with mean 1 completes the proof.

For  $t(b) = \ln(\mu(A(b)))$ , the theorem says the points  $t(\beta_0), t(\beta_1), \dots, t(\beta_i)$  in a run of TPA are separated by exponential random variables of mean 1, in other words, these points form a homogeneous Poisson point process on  $[t(\beta_{B'}), t(\beta_B)]$  of rate 1.

#### 2.1 Taking advantage of Poisson point processes

The first application of this is to describe the total number of points used by a run of TPA, that is, the value of i at the end of the algorithm. Because the  $t(\beta_i)$  values form a Poisson point process, the distribution of i is Poisson with mean  $t(\beta_B) - t(\beta_{B'}) = \ln(\mu(B)/\mu(B'))$ .

Furthermore, the union of k independent Poisson point processes of rate 1 is also a Poisson point process of rate k. That means that after k runs of TPA, the distribution of the total number of samples used is Poisson with mean  $k \ln(\mu(B)/\mu(B'))$ .

## 3 Applications

The following examples illustrate some of the uses for TPA.

#### 3.1 The Ising model

The Ising model is an example of a Gibbs distribution, where a function  $H : \Omega \to \mathbf{R}$  gives rise to a distribution on  $\Omega$ :

$$\pi(x) = \frac{1}{Z(\beta)} \exp(-\beta H(x)). \tag{3.1}$$

From applications in statistical physics,  $\beta \geq 0$  is known as the inverse temperature, and  $Z(\beta)$  is called the partition function.

In the Ising model, each node of a graph G=(V,E) is assigned one of two values. There are many ways to represent the model. In the form considered here, each node is either 0 or 1, and for  $x \in \{0,1\}^V$ , -H(x) is one plus the number of edges  $e \in E$  such that the endpoints of the edge have the same value in x. This can be written as  $H(x) = -[1 + \sum_{\{i,j\} \in E} (1 - x(i) - x(j) + 2x(i)x(j))]$ .

In order to embed this problem in the framework of TPA, add an auxiliary dimension to the configuration x. The auxiliary state space is

$$\Omega_{\text{aux}}(\beta) = \{(x, y) : x \in \{0, 1\}^V, y \in [0, \exp(-\beta H(x))\}.$$

Some notes on  $\Omega_{\rm aux}(\beta)$ :

- The total length of the line segments in  $\Omega_{\text{aux}}(\beta)$  is just  $Z(\beta)$ . That is to say,  $\mu(\Omega_{\text{aux}}(\beta)) = Z(\beta)$  where  $\mu$  is the one dimensional Lebesgue measure of the union of the line segments.
- Let  $\beta' < \beta$ . Then since -H(x) > 0,  $\Omega_{\text{aux}}(\beta') \subset \Omega_{\text{aux}}(\beta)$ . Moreover,  $Z(\beta)$  is a continuous function that goes to 0 as  $\beta \to -\infty$ . Therefore Condition 2 of the TPA ingredients is satisfied.
- For  $\beta = 0, y \in [0, 1]$  for all  $x \in \{0, 1\}$ . That means  $Z(0) = 2^V$ .
- Let  $\beta > 0$ . Then  $\Omega_{\text{aux}}(\beta)$  is the shell, and  $\Omega_{\text{aux}}(0)$  is the center.

With this in mind, the TPA algorithm works as follows.

- 1. Start with i = 0 and  $\beta_i = \beta$ .
- 2. Draw a random sample X from  $\pi_{\beta_i}$ , then draw Y (given X) uniformly from  $[0, \exp(-\beta_i H(X))]$ .
- 3. Let  $\beta_{i+1} = \ln(Y)/(-H(X))$
- 4. If  $\beta_{i+1} \leq 0$  stop and output i.
- 5. Else set i to be i + 1 and go back to step 2.

One run of TPA will require on average  $1 + \ln(Z(\beta)/Z(0)) = 1 + \ln(Z(\beta)) - \#V \ln(2)$  samples from various values of  $\beta$ , where #V is the number of vertices of the graph.

This method of adding an auxiliary variable allows TPA to be used on a variety of discrete distributions by changing the measure to one that varies continuously in the index.

#### 3.2 Posterior distributions

In Bayesian analysis, often it is necessary to find the normalizing constant of a posterior distribution. This is known as the *evidence* for a model, and can be written:

$$Z = \int_{x \in \Omega} f(x) \ dx,$$

where f(x) is a nonnegative density (the product of the prior density and the likelihood of the data) and  $\Omega \subseteq \mathbf{R}^n$ .

For a point  $c \in \Omega$  and  $\epsilon > 0$ , let  $B^1_{\epsilon}(c)$  be the points within  $L_1$  distance  $\epsilon$  of c. Suppose that for a particular c and  $\epsilon$ ,  $B^1_{\epsilon}(c) \subset \Omega$  and there is a known M such that  $(1/2)M \leq f(x) \leq M$  for all  $x \in B^1_{\epsilon}(c)$ .

Then to estimate  $Z(\epsilon) = \int_{x \in B^1_{\epsilon}(c)} f(x) dx$ , draw N iid samples  $X_1, \ldots, X_N$  uniformly from  $B_{\epsilon}(c)$ , and let the estimate be  $\hat{Z}(\epsilon) = (2\epsilon)^{-n} \sum_i f(X_i)/N$ . Then  $\hat{Z}(\epsilon)$  is an unbiased estimate for  $Z(\epsilon)$  with standard deviation bounded above by  $Z(\epsilon)/\sqrt{k}$ .

Now the connection to TPA can be made. The family of sets will be  $\{A(\beta) = B_{\beta}^{1}(c) \cap \Omega\}$ , and the measure is  $\mu(A(\beta)) = \int_{x \in A(\beta)} f(x) dx$ . The shell will be  $A(\infty)$  (so  $Z = \mu(A(\infty))$ ) and the center  $A(\epsilon)$  (with measure  $Z(\epsilon)$ .) TPA can then be used to estimate  $Z/Z(\epsilon)$ , and the estimate of  $Z(\epsilon)$  can then finish the job.

## 4 Running time of TPA

Suppose that TPA is run k times, and the k values of the i variable at the end of each run are summed together. Call this sum N. Then N has a Poisson distribution with mean  $k \ln(\mu(B)/\mu(B'))$ . This makes N/k an unbiased estimate of  $\ln(\mu(B)/\mu(B'))$ . The variance of N/k is  $\ln(\mu(B)/\mu(B'))/k$ .

Let W be a normal random variable of mean 0 and variance 1, and  $W_{\alpha}$  be the inverse cdf of W so that  $\Pr(W \leq W_{\alpha}) = \alpha$ . Then the normal approximation to the Poisson gives

$$\left\lceil (N/k) - W_{\alpha/2} \sqrt{N/k}, (N/k) + W_{\alpha/2} \sqrt{N/k} \right\rceil \tag{4.1}$$

as an approximately  $1 - \alpha$  level confidence interval for  $\ln(\mu(B)/\mu(B'))$ . Exponentiating then gives the  $1 - \alpha$  level for  $\mu(B)/\mu(B')$ .

For a specific output, it is also possible to build an exact confidence interval for  $\mu(B)/\mu(B')$  since the distribution of the output is known exactly.

Similarly, it is easy to perform a Bayesian analysis and find a credible interval given a prior on  $\ln(\mu(B)/\mu(B'))$ .

Lastly, consider how to build an  $(\epsilon, \delta)$  randomized approximation scheme (RAS) whose output  $\hat{A}$  satisfies:

$$\Pr\left((1+\epsilon)^{-1} \le \frac{\hat{A}}{\mu(B)/\mu(B')} < 1+\epsilon\right) > 1-\delta.$$

For simplicity, assume that  $\mu(B)/\mu(B') \ge e$ . Note that when  $\mu(B)/\mu(B') < e$ , then simple acceptance rejection can be used to obtain an  $(\epsilon, \delta)$ -RAS in  $\Theta(\epsilon^{-2} \ln(\delta^{-1}))$  time. See [4] for a description of this method.

The following lemma gives a bound on the tails of the Poisson distribution.

**Lemma 4.1.** Let  $\tilde{\epsilon} > 0$  and N be a Poisson random variable with mean  $k\lambda$ , where  $\tilde{\epsilon}/\lambda \leq 2.3$ . Then

$$Pr\left(\left|\frac{N}{k} - \lambda\right| \ge \tilde{\epsilon}\right) \le 2\exp\left(-\frac{k\tilde{\epsilon}^2}{2\lambda}\left(1 - \frac{\tilde{\epsilon}}{\lambda}\right)\right).$$

(This result is a special case of Theorem 6.1 shown later.)

To obtain our  $(\epsilon, \delta)$ -RAS, it is sufficient to make  $\tilde{\epsilon} = \ln(1+\epsilon)$ , and to choose k so that  $2\exp(-k\tilde{\epsilon}^2(1-\tilde{\epsilon}/\lambda)/[2\lambda]) \leq \delta$ , where  $\lambda = \ln(\mu(B)/\mu(B'))$ . This is made more difficult by the fact that  $\lambda$  is unknown at the start of the algorithm!

There are many ways around this difficulty, perhaps the simplest is to use a two phase method. First get a rough estimate of  $\lambda$ , then refine this estimate to the level demanded by  $\epsilon$ .

**Phase I** Let  $\epsilon_a = \ln(1+\epsilon)$  and  $k_1 = 2\epsilon_a^{-2}(1-\epsilon_a)^{-1}\ln(2\delta^{-1})$ . Then let  $N_1$  be the sum of the outputs from  $k_1$  runs of TPA.

**Phase II** Set  $k_2 = N_1(1 - \epsilon_a)^{-1}$ . Let  $N_2$  be the sum of the outputs from  $k_2$  runs of TPA. The final estimate is  $\exp(N_2/k_2)$ .

Phase I estimates  $\lambda$  to within an additive error  $\epsilon_a \lambda$ . Phase II uses the Phase I estimate of  $\lambda$  to create a better estimate of  $\lambda$  to within an additive error of  $\epsilon_a$ . Note that  $\epsilon_a \approx \epsilon$  in the sense that  $\lim_{\epsilon \to 0} \epsilon_a / \epsilon = 1$ .

**Theorem 4.1.** The output  $\hat{A}$  of the above procedure is an  $(\epsilon, \delta)$  randomized approximation scheme for  $\mu(B)/\mu(B')$ . The running time is random, with an expected running time that is  $\Theta((\ln(\mu(B)/\mu(B')))^2\epsilon^{-2}\ln(\delta^{-1}))$ .

*Proof.* Call Phase I a success if  $N_1/k_1$  is within distance  $\epsilon_a \lambda$  of  $\lambda$ . From Lemma 4.1 with  $\tilde{\epsilon} = \epsilon_a \lambda$ :

$$\Pr\left(\left|\frac{N_1}{k_1} - \lambda\right| \ge \epsilon_a \lambda\right) = 2 \exp\left(-k_1(\lambda \epsilon_a^2)(1 - \epsilon_a)\right) \le \delta/2$$

since  $\lambda \geq 1$  and  $k_1 = \epsilon_a^{-2} (1 - \epsilon_a)^{-1} \ln(2\delta^{-1})$ . Therefore, the probability that Phase I is a failure is at most  $\delta/2$ .

When Phase I is a success,  $(1 - \epsilon_a)\lambda k_1 \leq N_1$ . In this event  $k_2 = N_1(1 - \epsilon_a)^{-1} \geq \lambda k_1 = \lambda \epsilon_a^{-2} (1 - \epsilon_a)^{-1} \ln(2\delta^{-1})$ . Plugging this in to Lemma 4.1 yields:

$$\Pr\left(\left|\frac{N_2}{k_2} - \lambda\right| \ge \epsilon_a \lambda\right) \le 2 \exp\left(-\frac{\lambda \epsilon_a^{-2} (1 - \epsilon_a)^{-1} \ln(2\delta^{-1}) \epsilon_a^2}{2\lambda} \left(1 - \frac{\epsilon_a}{\lambda}\right)\right).$$

Using  $\lambda \geq 1$ , the right hand side is at most  $2\delta$ .

The chance of failure in either Phase is at most  $\delta/2 + \delta/2 = \delta$ , so altogether  $|(N_2/k_2) - \lambda| \le \epsilon_a$  with probability at least  $1 - \delta$ . Exponentiating then gives

$$(1+\epsilon)^{-1} = e^{-\epsilon_a} \le \exp(N_2/k_2)/\lambda \le e^{\epsilon_a} = 1+\epsilon$$

with probability at least  $1 - \delta$ .

The expected number of samples needed in Phase I is  $k_1\lambda$ , while the expected number needed in Phase II is:

$$E(N_2) = E(E(N_2|N_1)) = E((1 - \epsilon_a)^{-1} N_1 \lambda) = 2(1 - \epsilon_a)^{-2} \epsilon_a^{-2} \ln(2\delta^{-1}) \lambda^2.$$

Since  $\epsilon_a = \Theta(\epsilon)$ , the proof is complete.

#### 5 Well-balanced nested sets

Consider running TPA k times, and collecting all the values of  $\beta_i$  generated during these runs. Let P denote this set of values, then P forms a Poisson point process of rate k on  $[\beta_{B'}, \beta_B]$ .

Call  $\beta_B = \alpha_0 > \alpha_1 > \cdots > \alpha_\ell = \beta_{B'}$  a well-balanced cooling schedule if  $\mu(A(\alpha_{i+1}))/\mu(A(\alpha_i))$  is close to 1/e for all i from 0 to  $\ell-1$ .

Given P, finding such a well-balanced set is easy: simply order the  $\beta$  values in P, and set  $\alpha_i = \beta_{(ik)}$ . The value of  $\ln(\mu(A(\alpha_{i+1})/A(\alpha_i)))$  will have distribution equal to the sum of k iid exponential random variables with mean 1/k. So  $\ln(\mu(A(\alpha_{i+1})/\mu(A(\alpha_i))))$  will be gamma distributed with mean 1 and standard deviation 1/k.

# 6 Omnithermal approximation

Suppose instead of just a single value of interest  $\mu(B)/\mu(B')$ , it is necessary to create an approximation of  $\mu(A(\beta))/\mu(B')$  that is valid for all values  $\beta \in [\beta_{B'}, \beta_B]$  simultaneously. Call this an *omnithermal approximation*. These problems appear in what are called doubly intractable posterior distributions arising in Bayesian analyses involving spatial point processes. They are usually dealt with indirectly using Markov chain Monte Carlo with auxiliary variables [12], but omnithermal approximation allows for a more direct approach.

In the last section the Poisson point process P formed from the  $\beta_i$  values collected from k runs of TPA was introduced. To move from P to a Poisson process, set

$$N_P(t) = \#\{b \in P : b \ge \beta_B - t\}.$$

As t advances from 0 to  $\beta_B - \beta_{B'}$ ,  $N_P(t)$  increases by 1 whenever it hits a  $\beta$  value. By the theory of Poisson point processes, this happens at intervals that will be independent exponential random variables with rate k.

Given  $N_P(t)$ , approximate  $\mu(B)/\mu(A(\beta))$  by  $\exp(N_P(\beta_B - \beta)/k)$ . When  $\beta = \beta_{B'}$ , this is just the approximation given earlier, so this generalizes the description of TPA from before.

The key fact is that  $N_P(t)-kt$  is a right continuous martingale. To bound the error in  $\exp(N_P(t)/k)$ , it is necessary to bound the probability that  $N_P(t)-kt$  has drifted too far away from 0.

**Theorem 6.1.** Let  $\tilde{\epsilon} > 0$ . Then for  $N_P(\cdot)$  a rate k Poisson process on  $[0, \lambda]$ , where  $\tilde{\epsilon}/\lambda \leq 2.3$ :

$$Pr\left(\sup_{t\in[0,\lambda]}\left|\frac{N_P(t)}{k}-t\right|\geq \tilde{\epsilon}\right)\leq 2\exp\left(-\frac{k\tilde{\epsilon}^2}{2\lambda}\left(1-\frac{\tilde{\epsilon}}{\lambda}\right)\right).$$

*Proof.* The approach will be similar to finding a Chernoff bound [2]. Since  $\exp(\alpha x)$  is convex for any positive constant  $\alpha$ , and  $N_P(t)$  is a right continuous martingale,  $\exp(\alpha N_P(t))$  is a right continuous submartingale.

Let  $A_U$  denote the event that  $(N_P(t)/k) - t > \epsilon$  for some  $t \in [0, \lambda]$ . Then for all  $\alpha > 0$ :

$$\Pr(A_U) = \Pr\left(\sup_{t \in [0,\lambda]} \exp(\alpha N_P(t)) \ge \exp(\alpha kt + \alpha k\epsilon)\right).$$

It follows from basic Markov-type inequalities on right continuous submartingales (p. 13 of [9]) that this probability can be upper bounded as

$$\Pr(A_U) \le \mathbb{E}(\alpha \exp(N_P(\lambda)) / \exp(\alpha k \lambda + \alpha k \tilde{\epsilon})).$$

Using the moment generating function for a Poisson with parameter  $k\lambda$ :

$$E[\exp(\alpha N_P(\lambda))] = \exp(k\lambda(\exp(\alpha) - 1)),$$

which means

$$\Pr(A_U) \le \exp(\lambda(e^{\alpha} - 1 - \alpha) + \alpha\tilde{\epsilon})^k$$
.

A Taylor series expansion shows that  $e^{\alpha} - 1 - \alpha \leq (\alpha^2/2)(1 + \alpha)$  as long as  $\alpha \in [0, 2.31858...]$ . Set  $\alpha = \tilde{\epsilon}/\lambda$ . Simplifying the resulting upper bound yields

$$\Pr(A_U) \le \exp\left(-\frac{k\tilde{\epsilon}^2}{2\lambda}\left(1 - \frac{\tilde{\epsilon}}{\lambda}\right)\right).$$

The other tail can be dealt with in a similar fashion, yielding a bound

$$\Pr\left(\sup_{t\in[0,\lambda]} [N_P(\alpha)/k] - t < \tilde{\epsilon}\right) \le \exp\left(-\frac{k\tilde{\epsilon}^2}{2\lambda}\right).$$

The union bound on the two tails then yields the theorem.

**Corollary 6.1.** For  $\epsilon \in (0, 0.3)$ ,  $\delta \in (0, 1)$ , and  $\ln(\mu(B)/\mu(B')) > 1$ , after

$$k = 2(\ln(\mu(B)/\mu(B'))(3\epsilon^{-1} + \epsilon^{-2})\ln(2/\delta)$$

runs of TPA, the points obtained can be used to build an  $(\epsilon, \delta)$  omnithermal approximation.

Proof. In order for the final approximation to be within a multiplicative factor of  $1 + \epsilon$  of the true result, the log of the approximation must be accurate to an additive term of  $\ln(1+\epsilon)$ . Let  $\lambda = \ln(\mu(B)/\mu(B'))$ , so  $k = 2\lambda(3\epsilon^{-1} + \epsilon^{-2})\ln(2/\delta)$ . To prove the corollary from the theorem, it suffices to show that  $2\exp(-2\lambda(3\epsilon^{-1} + \epsilon^{-2}\ln(2/\delta)[\ln(1+\epsilon)]^2(1-\epsilon/\lambda)/(2\lambda)) < \delta$ . After canceling the factors of  $\lambda$ , and noting that when  $\lambda > 1$ ,  $1 - \epsilon/\lambda < 1 - \epsilon$ , it suffices to show that  $(3\epsilon^{-1} + \epsilon^{-2})(1-\epsilon)[\ln(1+\epsilon)]^2 > 1$ . This can be shown for  $\epsilon \in (0,0.3)$  by a Taylor series expansion.

### 6.1 Example: Omnithermal approximation for the Ising model

Consider the following model. The value of  $\beta$  is drawn from a prior density  $f_{\text{prior}}(\cdot)$  on  $[0, \infty)$ , and then the data (conditioned on  $\beta$ ) is drawn from the Ising model. This was used by Besag [1] as a model for agriculture wherein soil quality of adjacent plots was more likely to be similar.

Given the data X, the posterior in the Bayesian analysis is the following density on  $\beta$  :

$$f_{\text{post}}(b) \propto f_{\text{prior}}(b) \frac{\exp(bH(X))}{Z(b)}.$$
 (6.1)

The evidence for the model is the integral of the right hand side of (6.1) as b runs from 0 to  $\infty$ . This is only a one-dimensional integration, and so should be straightforward from a numerical perspective, except that Z(b) is unknown.

Here is where the omnithermal approximation comes in: it gives an approximation for Z(b) that is valid for *all* values of b at once. Any numerical integration technique can be used, and the final value for the evidence (not including error arising from the numerical method) will be within a factor of  $1+\epsilon$  of the true answer.

Figure 1 presents two omnithermal approximations for  $\log Z_{\beta}$  generated using this method on a small  $4\times 4$  square lattice. The top graph is the result of a single run of TPA from  $\beta=2$  down to  $\beta=0$ . At each  $\beta$  value returned by TPA, the approximation drops by 1. The bottom graph is the result of  $\lceil \ln(4\cdot 10^6) \rceil = 16$  runs of TPA. This run told us that  $Z_2 \leq 217$  with confidence  $1-10^{-6}/2$ . Therefore, using  $\epsilon=0.1$ , and  $\delta=10^6/2$  in Theorem 6.1 shows that r=330000 samples suffice for a  $(0.1,10^{-6})$  omnithermal approximation.

#### 7 Conclusions and further work

The strength of TPA is the generality of the procedure, but that same generality means that it is possible to do better in restricted circumstances. For instance, when f(x) falls into the class of Gibbs distributions, Štefankovič et al. [17] were able to give an  $\tilde{O}(\ln(Z))$  algorithm for approximating Z, but the high constants involved in their algorithm make it solely of theoretical interest. (Here the  $\tilde{O}$  notation hides logarithmic factors.) TPA can be used in conjunction with their

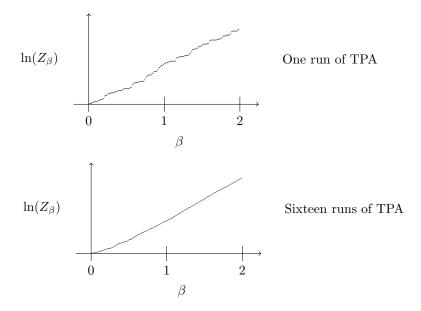


Figure 1: Omnithermal approximations for the partition function of the Ising model on a  $4 \times 4$  lattice

algorithm [6] to build an  $O(\ln(Z)\ln(\ln(Z)))$  algorithm, and work continues to bring this running time down to  $O(\ln(Z))$ .

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