Mid-Project Review: C++ implementation of the Metropolis-Hasting Algorithm

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1 Introduction

Bayesian Inference is a powerful statistical method that has found a variety of applications in uncertainty quantification, decision theory, model selection and many others. These methods have been applied to diverse fields such as epidemiology, spam filters, computer vision, as well as assessments of the reliability of the readyness of the United States nuclear weapon stockpiles.

However, Bayes' Theorem, despite existing since the 18th century, has only recently become more prevalent in scientific applications. The recent dramatic growth in Bayesian methods coincides with the exponential expansion of computational power. This is because for all but a small set of models, the posterior distribution is unable to be analytically determined, and must be statistically sampled, often requiring far more samples than are humanly possible to generate.

For this project, we have developed a C++ implementation of the Metropolis-Hastings algorithm. This is a Markov Chain Monte Carlo (MCMC) method to sample from a probability distribution. These samples will be generated in order to estimate the posterior of a distribution for a Bayesian Inference problem. We will generate results for a few different models, in order to investigate the model against a known (analytic) conjugate prior, as well as more complicated (non-tracible without sampling) distributions.

The code is written in C++, and will be parallelized with openMP.

2 Methodology

Suppose we have a posterior that we want to sample from, but:

- the posterior doesn't look like any distribution we know (no conjugate model exists)
- some (or all) of the full conditionals do not look like any distributions we know (no Gibbs sampling)

In these cases, it is necessary to sample the underlying (and often quite complicted) distribution. The Metropolis-Hastings algorithm accomplishes this.

2.1 Model Document: The Metropolis Hastings Algorithm

For each Metropolis step, we begin with a guess for the starting point, ϕ_1. Afterward, we begin sampling. Each step of this so-called, "rejection sampling" involves "proposing" a new value, which if it meets a specified criterion, is accepted. The next step then begins.

Thus, we begin with a proposal step (in this case, for step two),

$$q(\tilde{\phi}_2|\phi_1) = N(\tilde{\phi}_2|\phi_1, \nu^2). \tag{1}$$

In other words, our proposal step is correlated with the previous step, in that it is drawn from a Gaussian (Normal) distribution with mean of the previous step, and standard deviation, ν. We will discuss our choice of ν more, later. In order to draw this proposal, we generate a proposal from a standard normal distribution, Z, and then transform it according to,

$$X = \phi_1 + \nu * Z. \tag{2}$$

Thus, with our new proposal $\tilde{\phi}_2$ drawn, we must evaluate whether to accept this or reject it. In order to accomplish this, we next draw from a uniform distribution, $u \sim U(0,1)$.

Now, we accept the new $\tilde{\phi}_2$ if it meets the following criterion,

$$u < \frac{\pi_n(\tilde{\phi}_2)}{\pi_n(\phi_1)}. \tag{3}$$

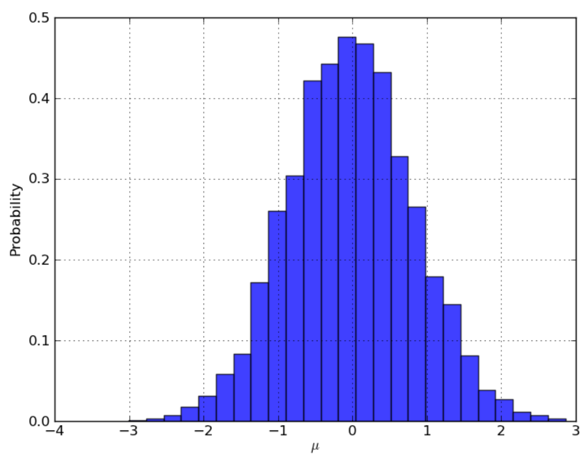
If we accept, then $\tilde{\phi}_2$ becomes ϕ_2, and we begin the next step. If we reject, then we keep our present value, e.g. $\phi_2 = \phi_1$.

Now as we proceed, you might ask, what dictates whether we accept or reject? Well, after the "burn-in" period, where we move around looking for the region where the distribution has non-zero probability, we eventually start sampling the posterior. Here, we want to "jump" around in each guess just enough that we will capture the tails of the distribution, but simultaneously, we don't want to jump so far that we move away from the areas of the distribution that has most of the probability associated with it. This is where our ν comes in. This is the variance of the proposal. If it is very large, then we will tend to make large jumps away from the mean for our proposal. These are great for finding the distribution in the first place, and they will tend to capture more of the tails, but simultaneously, too many large jumps will result in more rejections by our sampling algorithm. Therefore, we need to balance ν so that is jumps around, but not too far.

It turns out that mathematicians have shown that for various situations, an, "acceptance ratio" of right around 40% is just about right. This acceptance ratio is simply the ratio of accepted proposals to total MCMC steps we have taken. Therefore, we have tried to tune our ν parameter for each situation to have an acceptance ratio around 40%.

3 Report on Progress

The metropolis algorithm as detailed above has now been implemented in a few hundred lines of C++. Presently, we are sampling from a Gaussian distribution, in order to analytically verify that our distribution matches a known posterior. A histogram from one thousand samples is provided in figure one.



This matches quite well, and implies the basic kernel is functioning. Our next objective will be to move toward a few other distributions, with an eye on generating samples for a prior and posterior set of distributions that do not have an analytical solution.

The codebase for this project has been developed on bitbucket, with logs for each commit. A fully functioning build system (a makefile) alongside a 'make check' regression suite has been developed. At present, three regression tests are run, that perform simple checks on the distributions and sampling algorithm. The code has been tested on a local i7 quad core laptop, as well as TACC's lonestar supercomputer.

Finally, a directory, "postprocessing" contains scripts used to generate all plots. These are routines using python with numpy+scipy and matplotlib.

4 Future Work

As mentioned in the previous section, the we will expand to a few other distributions, in addition to sampling gaussians. This should not be a significant part of the work. These distributions will also be verified against conjugate priors (analytically known solution distributions) when available.

The largest remaining deliverable is to add OpenMP directives to the c++ implementation. Afterward, a detailed scaling study will be performed. Due to the nature of MCMC, each markov chain should be completely independent, and the underlying algorithm is therefore “embarassingly parallel”. As a result, and we expect the routines to scale essentially perfectly. At least, we hope so!