Testing MCMC code

Roger B. Grosse  
Department of Computer Science  
University of Toronto  
rgrosse@cs.toronto.edu

David K. Duvenaud  
School of Engineering and Applied Sciences  
Harvard University  
dduvenaud@seas.harvard.edu

Abstract

Markov Chain Monte Carlo (MCMC) algorithms are a workhorse of probabilistic modeling and inference, but are difficult to debug, and are prone to silent failure if implemented naively. We outline several strategies for testing the correctness of MCMC algorithms. Specifically, we advocate writing code in a modular way, where conditional probability calculations are kept separate from the logic of the sampler. We discuss strategies for both unit testing and integration testing. As a running example, we show how a Python implementation of Gibbs sampling for a mixture of Gaussians model can be tested.

1 Introduction

In machine learning, we often justify the correctness of our algorithms by showing that their mathematical idealizations satisfy certain properties. However, the algorithms must ultimately be implemented in software, so the question arises: how can we check that our code correctly implements the mathematical specification of an algorithm? In this tutorial, we outline a set of techniques we have found useful for testing the correctness of one particular type of algorithm, a Markov chain Monte Carlo (MCMC) sampler. The techniques we outline are not novel, but we believe they deserve to be more widely known and practiced.

Several factors conspire to make testing of MCMC code difficult:

- The algorithms are stochastic, so there’s no single “correct” output.
- Algorithms may perform badly for reasons other than buggy implementations, such as poor modeling assumptions or slow mixing between modes.
- Good performance is often a matter of judgment: in a prediction task, if the algorithm correctly classifies 83.5% of the test examples, does that mean it’s working?

Furthermore, many machine learning algorithms have a curious property: they are robust against bugs [e.g. 6]. Since they’re designed to deal with noisy data, they can often compensate for noise caused by math mistakes as well. A buggy algorithm might still make sensible-looking predictions. This is problematic, because it means bugs can be subtle and hard to detect. The algorithm might work well in some situations, such as small toy datasets used for validation, yet completely fail in other situations – high dimensions, large numbers of training examples, noisy observations, etc. Even if unnoticed bugs hurt performance by only a few percent, that difference may be important.

For researchers in particular, there is a further reason to be concerned about bugs, even if their effect on performance is negligible. The job of a scientist isn’t simply to write an algorithm that makes good predictions, but to run experiments which yield insight into the inner workings of an algorithm.

---

1This tutorial is an adaptation of blog posts which can be found at https://hips.seas.harvard.edu/blog/2013/05/20/testing-mcmc-code-part-1-unit-tests/ and https://hips.seas.harvard.edu/blog/2013/06/10/testing-mcmc-code-part-2-integration-tests/.
Even if an algorithm performs well, implementation bugs can affect how one quantity varies as a result of changing another, for instance if some hyperparameter settings compensate for bugs better than others.

In this paper, we focus on testing MCMC samplers, partly because they are especially good illustrations of the challenges involved in testing machine learning code. The particular practices we highlight are specific to MCMC, but they also exemplify useful strategies for testing implementations of machine learning algorithms.

In software development, it is useful to distinguish two different kinds of tests: unit tests and integration tests. Unit tests are short and simple tests which check the correctness of small pieces of code, such as individual functions. The idea is for the tests to be as local as possible – ideally, a single bug should cause a single test to fail. Integration tests test the overall behavior of the system, without reference to the underlying implementation. They are more global than unit tests: they test whether different parts of the system interact correctly to produce the desired behavior. Both kinds of tests are relevant to MCMC samplers. In particular, we discuss unit tests which check that conditional distributions are consistent with the joint distribution. We then review the Geweke test [2], which we view as a form of integration testing. We present these techniques using a Gibbs sampler as a running example, and discuss how MCMC code can be written in a modular structure which enables testing.

2 Example: mixture of Gaussians

As a running example throughout this tutorial, we will implement and test a Gibbs sampler for an isotropic mixture of Gaussians model in Python (with NumPy):

\[
\begin{align*}
\pi & \sim \text{Dirichlet}(\alpha) \\
\sigma^2_{\mu} & \sim \text{InverseGamma}(a_{\mu}, b_{\mu}) \\
\sigma^2_n & \sim \text{InverseGamma}(a_n, b_n) \\
z_i | \pi & \sim \text{Multinomial}(\pi) \\
\mu_{kj} | \sigma^2_{\mu} & \sim \text{Normal}(0, \sigma^2_{\mu}) \\
x_{ij} | z_i, \mu_{z_i,j}, \sigma^2_n & \sim \text{Normal}(\mu_{z_i,j}, \sigma^2_n)
\end{align*}
\]

This is a toy model which is essentially a Bayesian analogue of K-means; however, the strategies presented here have served us well with more complex models and inference algorithms. Here are the classes which define the model and the state (i.e. the variables which are sampled):

```python
class Model:
    def __init__(self, alpha, K, sigma_sq_mu_prior, sigma_sq_n_prior):
        self.alpha = alpha  # Parameter for Dirichlet prior over mixture probabilities
        self.K = K  # Number of components
        self.sigma_sq_mu_prior = sigma_sq_mu_prior
        self.sigma_sq_n_prior = sigma_sq_n_prior

class State:
    def __init__(self, z, mu, sigma_sq_mu, sigma_sq_n, pi):
        self.z = z  # Assignments (represented as an array of integers)
        self.mu = mu  # Cluster centers
        self.sigma_sq_mu = sigma_sq_mu  # Between-cluster variance
        self.sigma_sq_n = sigma_sq_n  # Within-cluster variance
        self.pi = pi  # Mixture probabilities

class GaussianDistribution:
    def __init__(self, mu, sigma_sq):
        self.mu = mu
        self.sigma_sq = sigma_sq

    def log_p(self, x):
        return -0.5 * np.log(2*np.pi) + -0.5 * np.log(self.sigma_sq) + -0.5 * (x - self.mu)**2 / self.sigma_sq
```

As a form of modularity, we define several distribution classes which know how to generate samples and evaluate log probabilities. For instance,
The following functions compute each of the conditional probability distributions required by the Gibbs sampler:

class Model:

    def cond_pi(self, state):
        counts = np.bincount(state.z)
        counts.resize(self.K)
        return DirichletDistribution(self.alpha + counts)

    def cond_z(self, state, X):
        nax = np.newaxis
        prior = np.log(state.pi)
        evidence = GaussianDistribution(state.mu[nax, :, :], state.sigma_sq_n).log_p(X[:, nax, :]).sum(2)
        return MultinomialDistribution.from_log_odds(prior[nax, :] + evidence)

    def cond_mu(self, state, X):
        ndata, ndim = X.shape
        h = np.zeros((self.K, ndim))
        lam = np.zeros((self.K, ndim))
        for k in range(self.K):
            idxs = np.where(state.z == k)[0]
            if idxs.size > 0:
                h[k, :] = X[idxs, :].sum(0) / state.sigma_sq_n
                lam[k, :] = idxs.size / state.sigma_sq_n + 1. / state.sigma_sq_mu
            else:
                h[:, k] = 0.
                lam[k, :] = 1. / state.sigma_sq_mu
        return GaussianDistribution(h / lam, 1. / lam)

    def cond_sigma_sq_mu(self, state):
        ndim = state.mu.shape[1]
        a = self.sigma_sq_mu_prior.a + 0.5 * self.K * ndim
        b = self.sigma_sq_mu_prior.b + 0.5 * np.sum(state.mu ** 2)
        return InverseGammaDistribution(a, b)

    def cond_sigma_sq_n(self, state, X):
        ndata, ndim = X.shape
        a = self.sigma_sq_n_prior.a + 0.5 * ndata * ndim
        b = self.sigma_sq_n_prior.b + 0.5 * np.sum((X - state.mu[state.z, :]) ** 2)
        return InverseGammaDistribution(a, b)

Finally, the Gibbs sampling routine itself is a simple wrapper around the conditional probability distributions:

class Model:

    def gibbs_step(self, state, X):
        state.pi = self.cond_pi(state).sample()
        state.z = self.cond_z(state, X).sample()
        state.mu = self.cond_mu(state, X).sample()
        state.sigma_sq_mu = self.cond_sigma_sq_mu(state).sample()
        state.sigma_sq_n = self.cond_sigma_sq_n(state, X).sample()

In the next section, we will discuss our motivations for decomposing the functionality in this particular way.

3 Unit testing

Unit testing is about independently testing small chunks of code. Therefore, the code must be written in a modular way, such that different chunks are independently testable. Such a modular design doesn’t happen automatically, and it can be difficult to retrofit a code base with unit tests. (In fact, strategies for retrofitting are the subject of a whole book, Working effectively with legacy code.
which defines legacy code as “code without unit tests.”) It’s much easier to try to keep things modular and testable from the beginning.

Unfortunately, the way machine learning is typically taught encourages a programming style which is neither modular nor testable. In problem sets, students typically first derive the update rules for an iterative algorithm, and then implement the updates directly. This approach makes it easy for graders to spot differences from the correct solution, but it’s not a robust way to build real software projects. Iterative algorithms can be difficult to test as black boxes.

Fortunately, most machine learning algorithms are formulated in terms of general mathematical principles that suggest a modular organization into testable chunks. For instance, we often formulate algorithms as optimization problems which can be solved using general purpose algorithms such as gradient descent or L-BFGS [4]. From an implementation standpoint, this requires writing functions to (a) evaluate the objective function at a point, and (b) compute the gradient of the objective function with respect to the model parameters. These functions are then fed to library optimization routines. The gradients can be checked using finite difference techniques. Conveniently, most scientific computing environments provide implementations of these checks; for instance, `scipy.optimize.check_grad` (in Python).

This organization into gradient computations and general purpose optimization routines exemplifies a useful design principle for machine learning code: separate out the implementations of the model and general-purpose algorithms. Consider how this principle can be applied in the context of MCMC. Seemingly the most straightforward way to implement a Gibbs sampler would be to derive by hand the update rules for the individual variables and then write a single iterative routine using those rules. As mentioned above, such an approach can be difficult to test. However, a Gibbs sampler is defined in terms of conditional probability calculations, and these calculations can be decomposed out.

In each update, we sample a variable $x$ from its conditional distribution $p(x|z)$. It is difficult to directly test the correctness of samples from the conditional distribution: such a test would likely be slow and nondeterministic, both highly undesirable properties for a unit test to have. We instead recommend testing that the conditional distribution is consistent with the joint distribution. In particular, for any two values $x$ and $x'$, we must have that:

$$\frac{p(x'|z)}{p(x|z)} = \frac{p(x'|z)}{p(x|z)} \tag{1}$$

Importantly, this relationship must hold exactly for any two values $x$ and $x'$. For most models we use, if our formula for the conditional probability is wrong, then this relationship would likely fail for two randomly chosen values. Therefore, a simple and highly effective test for conditional probability computations is to choose random values for $x$, $x'$, and $z$, and verify the above equality to a suitable precision, such as $10^{-10}$. (As usual in probabilistic inference, we should use log probabilities rather than probabilities for numerical reasons.)

In terms of implementation, this form of testing suggests writing three separate modules (as we did in Section 2):

1. Classes representing probability distributions. These classes should know how to (a) evaluate the log probability density function (or probability mass function) at a point, and (b) generate samples.
2. A specification of the model in terms of functions which compute the probability of a joint assignment and functions which return conditional probability distributions.
3. A Gibbs sampling routine, which sweeps over the variables in the model, replacing each one with a sample from its conditional distribution.

These distribution classes require their own forms of unit testing. For instance, we may generate large numbers of samples from the distributions, and then ensure that the empirical moments are consistent with the exact moments.

This modular organization supports not just testability, but also reusability: it’s easy to reuse the distribution classes between entirely different projects, and changing the model might require modifying only a few conditional distribution routines. Sophisticated Metropolis-Hastings proposals are often defined in terms of conditional probabilities, so much of the implementation can be shared.
There are a lot of helpful software tools for managing unit tests. We use nose\(^2\) which is a simple and elegant testing framework for Python. In order to avoid clutter, we keep the tests in a separate directory whose structure parallels the main code directory.

### 3.1 Mixture of Gaussians example

In order to unit test the Gibbs sampler of Section\(^2\) we must first write one additional function which computes the joint log probability of all the variables:

```python
class Model:
    ...

    def joint_log_p(self, state, X):
        return DirichletDistribution(self.alpha * np.ones(self.K)).log_p(state.pi) + "
        self.sigma_sq_mu_prior.log_p(state.sigma_sq_mu) + "
        GaussianDistribution(0., state.sigma_sq_n).log_p(state.mu).sum() + "
        GaussianDistribution(state.mu[state.z, :]).log_p(X).sum()
```

We then test each of these conditional distributions in turn by checking the identity (\(1\)). For instance,

```python
def test_cond_mu():
    model = random_model()
    state, X = model.forward_sample(N, D)
    new_state = copy.deepcopy(state)
    new_state.mu = np.random.normal(size=(K, D))
    cond = model.cond_mu(state, X)
    assert np.allclose(cond.log_p(new_state.mu).sum() - cond.log_p(state.mu).sum(),
                       model.joint_log_p(new_state, X) - model.joint_log_p(state, X))
```

It is a good idea to sanity check our tests by introducing a small bug and verifying that the test fails. Let’s substitute 0.51 for 0.5 in our within-cluster variance computation:

```python
class Model:
    ...

    def cond_sigma_sq_n(self, state, X):
        ndata, ndim = X.shape
        a = self.sigma_sq_n_prior.a + "
        0.5 * ndata * ndim
        b = self.sigma_sq_n_prior.b + "
        0.51 * np.sum((X - state.mu[state.z, :]) ** 2)  # oops!
        return InverseGammaDistribution(a, b)
```

Sure enough, nose\(^2\) catches it. Furthermore, the only unit test which fails is the one corresponding to this function:

```bash
rgrosse:/code/testing$ nosetests
....F
FAIL: test_mog.test_cond_sigma_sq_n
----------------------------------------------------------------------
Ran 5 tests in 0.217s
FAILED (failures=1)
```

If we repair `cond_sigma_sq_n`, our tests pass:

```bash
rgrosse:/code/testing$ nosetests
.......
Ran 5 tests in 0.231s
OK
```

\(^2\)Available at [http://nose.readthedocs.org](http://nose.readthedocs.org)
4 Integration testing: the Geweke test

Most of the mistakes we’ve caught in our own code were caught by unit tests. (Naturally, we have no idea about the ones we haven’t caught.) But no matter how thoroughly we unit test, there are still subtle bugs that slip through the cracks. Integration testing is a more global approach, and tests the overall behavior of the software, which depends on the interaction of multiple components.

When testing MCMC samplers, we are interested in testing two things: whether our algorithm is mathematically correct, and whether the Markov chain has mixed. These two goals are somewhat independent of each other: a mathematically correct algorithm can get stuck and fail to find a good solution, and (counterintuitively) a mathematically incorrect algorithm can often find a good solution or at least get close. This section is about checking mathematical correctness.

One powerful technique for testing MCMC algorithms is the Geweke test [2]. The basic idea is simple: suppose we have a generative model over parameters $\theta$ and data $x$, and we want to test an MCMC sampler for the posterior $p(\theta|x)$. There are two different ways to sample from the joint distribution $p(\theta, x)$. First, we can forward sample, i.e. sample $\theta$ from $p(\theta)$, and then sample $x$ from $p(x|\theta)$. Second, we can start from a forward sample, and then run a Markov chain which alternates between

1. updating $\theta$ using one of the MCMC transition operators, which should preserve the distribution $p(\theta|x)$, and
2. resampling the data from the distribution $p(x|\theta)$.

Since each of these operations preserves the joint distribution $p(\theta, x)$, each step of this chain is a perfect sample from $p(\theta, x)$.

If the sampler is correct, then each of these two procedures should yield samples from exactly the same distribution. We can test this by comparing the distributions of a variety of statistics of the samples, e.g. the mean of $x$ or the maximum absolute value of $\theta$. No matter which statistics we choose, the two distributions should be indistinguishable.

Geweke [2] uses frequentist hypothesis tests to compare the distributions. This can be difficult, however, since one needs to account for dependencies between the samples in order to determine significance. We adopt a less principled but much simpler approach of looking at P-P plots of the statistics. Here are a few ways the plot could turn out:

- **Passes Geweke test**: The two distributions are indistinguishable, so the test passes.
- **Fails Geweke test**: The distributions are clearly different, so the test fails.
- **Unclear**: The results are noisy and unclear, so the test should be re-run with more forward samples and/or more iterations. In this third case, it may also help to reduce the number of data points. Not only does this speed up each iteration, but it also helps the chains mix faster—the fewer data points there are, the weaker the coupling between $\theta$ and $x$.

Here is a function implementing the Geweke test for the mixture of Gaussians example, where the statistic being compared is $\sigma_n^2$. (In practice, we would compare many more statistics.) Note that this
test also requires writing two additional functions to forward sample from the model and to sample from $p(x|\theta)$.

```python
def geweke(num_samples):
    model = random_model()

    forward_results = []
    for i in range(num_samples):
        state, X = model.forward_sample(N, D)
        forward_results.append(state.sigma_sq_n)

    gibbs_results = []
    for i in range(num_samples):
        model.gibbs_step(state, X)
        X = model.cond_X(state).sample()
        gibbs_results.append(state.sigma_sq_n)

    pp_plot(forward_results, gibbs_results)
```

Let’s now pretend now that we didn’t unit test the code, and therefore never caught the typo in `cond_sigma_sq_n` (where 0.5 was replaced with 0.51). In a practical setting, the effect of this bug would be to make the within-cluster variance about 2% too large. This is a subtle enough effect that we might never notice it if we simply measured the model’s performance on a task, or looked at its predictions. The beauty of the Geweke test is that it amplifies subtle bugs such as this one. After the parameters are resampled, the data are generated with a 2% larger noise variance. When the parameters are resampled yet again, the noise variance becomes 2% larger on top of that, or 4% in total. Pretty soon, the within-cluster variance explodes:

There’s a major drawback of the Geweke test, unfortunately: it gives no indication of where the bug might be. All we can do is keep staring at the code until we find the bug. Therefore, it is best to first ensure all the unit tests pass before running the Geweke test. This meshes with the general test-driven development methodology, where one gets the unit tests to pass before the integration tests.

5 Discussion

We have outlined some simple methods for testing MCMC inference code. These methods require writing the code in a modular way, so that different components can be tested independently. If this modular organization is adopted, then the additional work required for unit and integration testing is minimal: it requires writing only two short functions to forward sample from the model and evaluate joint log probabilities, as well as a handful of short testing routines.

As a running example, we discussed a mixture of Gaussians model with isotropic covariance (essentially a Bayesian analogue of k-means). While this model is simple, the testing methodology applies to more complex models and inference algorithms. For instance, some ways one might wish to extend the model and sampler include:

1. Replace the isotropic covariance with a general covariance matrix (with an inverse Wishart prior)
2. Untie the covariance between different clusters
3. Collapse out the mixture probabilities and the cluster centers in order to speed up mixing
4. Replace the finite Dirichlet mixture with a Chinese restaurant process \[\text{e.g.}[5]\]
5. Use split-merge proposals \([3]\) to speed up mixing

The first two modifications introduce no new difficulties as far as testing. Collapsing out the centers requires defining the collapsed joint probability which would be plugged into \([1]\). Furthermore, efficient implementation would require keeping track of sufficient statistics. One can define a data structure which efficiently updates the statistics, and this data structure can be tested entirely using standard testing methodology. Split-merge proposals are defined in terms of conditional probability computations, which can be unit tested the same way as our Gibbs computations; then, the Geweke test can be applied without modification. A thorough testing framework may even make it easier to add these additional features incrementally, as one can be more confident in the correctness of each modification.

References