emcee: The MCMC Hammer

Daniel Foreman-Mackey[1,2], David W. Hogg[2,3], Dustin Lang[4], Jonathan Goodman[5]

ABSTRACT

We introduce a stable, well tested Python implementation of the affine-invariant ensemble sampler for Markov chain Monte Carlo (MCMC) proposed by Goodman & Weare (2010). The code is open source and has already been used in several published projects in the Astrophysics literature. The algorithm behind emcee has several advantages over traditional MCMC sampling methods and it has excellent performance as measured by the autocorrelation time. One major advantage of the algorithm is that it requires hand-tuning of only 2 parameters compared to $\sim N^2$ for a traditional algorithm in an N-dimensional parameter space. In this document, we describe the algorithm and the details of our implementation and API. Taking advantage of the naturally parallel nature of the algorithm, emcee permits *any* user to take advantage of multiple CPUs without extra effort. This is a huge advantage over a naïve implementation of the published algorithm when applied to computationally expensive problems.

The code is available online at http://danfm.ca/emcee under the GNU General Public License v2.

Subject headings: methods: data analysis — methods: numerical — methods: statistical

1. Introduction

Probabilistic data analysis — including Bayesian inference — has transformed scientific research in the past decade. Many of the most significant gains have been due to numerical

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[1]To whom correspondence should be addressed: danfm@nyu.edu

[2]Center for Cosmology and Particle Physics, Department of Physics, New York University, 4 Washington Place, New York, NY, 10003, USA

[3]Max-Planck-Institut für Astronomie, Königstuhl 17, D-69117 Heidelberg, Germany

[4]Princeton University Observatory, Princeton, NJ, 08544, USA

[5]Courant Institute, New York University, 251 Mercer St., New York, NY 10012, United States

methods for approximate inference; especially Markov chain Monte Carlo (MCMC). Many problems in cosmology and astrophysics benefit from these advances because the observations tend to have low signal-to-noise and be incomplete.

Probabilistic data analysis procedures involve examining and operating on either the posterior probability density function (PDF) of the parameters of the model or the likelihood function. In some cases it is sufficient to just find the maximum of this function but it is often of interest to (at least approximately) measure this distribution in more detail. In particular, if we wish to propagate the effects of measurement uncertainties through the analysis to the conclusions, we must sample the PDF on sufficiently small scales. MCMC methods are designed to efficiently sample and approximate the PDF even in high dimensional parameter spaces. This has proved useful in too many research applications to list here but the results from the Wilkinson Microwave Anisotropy Probe (WMAP) mission provide a dramatic example (for example Dunkley *et al.* 2005).

Arguably the most important advantage of Bayesian data analysis is that it is possible to *marginalize* over nuisance parameters. A nuisance parameter is a component of the generative model that is of little physical interest who's value must be known in order to produce data. Marginalization is the process of integrating over all possible values of these parameters and hence propagating the effects of your uncertainty about the "true" value to the final result. The exact result of marginalization is the marginalized likelihood function $p(D|\Theta)$ of the set of observations D given the physical model parameters Θ

$$p(D|\Theta) = \int p(D|\Theta, \alpha)\, p(\alpha)\, \mathrm{d}\alpha \qquad (1)$$

where α is the set of of nuisance parameters. In general, D, Θ and α will all be lists of vectors. In some specific cases, the integral in Equation (1) is analytically tractable but in general, the likelihood function $p(D|\Theta, \alpha)$ is not a simple integrable function. In fact, in many problems, the likelihood function is actually the result of an extremely expensive numerical simulation. In this regime, the integration must be calculated numerically and it is often relatively efficient to approximate Equation (1) using MCMC sampling. If the likelihood function is expensive to calculate, it is advantageous to use a sampling algorithm that reduces the necessary number of likelihood evaluations. This also precludes the use of second order methods (such as hybrid/Hamiltonian Monte Carlo) that require the calculation of (numerical) gradients of the likelihood function.

Most uses of MCMC in the astrophysics literature are based on slight modifications to the Metropolis-Hastings (M–H) method (for example MacKay 2003). Each step in a M–H chain is proposed using a multivariate Gaussian centered on the current position of the chain. Since each term in the covariance matrix of this proposal distribution is an

unspecified parameter, this method has $N[N+1]/2$ tuning parameters (where N is the dimension of the parameter space). To make matters worse, the performance of this sampler is very sensitive to the optimality of these tuning parameters and there is no fool-proof method for choosing the values correctly. As a result, many heuristic methods have been developed to attempt to determine the optimal parameters in a data-driven way (for example Gregory 2005; Dunkley *et al.* 2005; Widrow *et al.* 2008). Unfortunately, these methods all require "burn-in" phases where shorter Markov chains are sampled and the results are used to tune the hyperparameters. This extra cost is unacceptable when the likelihood calls are computationally heavy.

The problem with traditional sampling methods can be visualized by looking at the simple but highly anisotropic density

$$p(\mathbf{x}) \propto \exp\left(-\frac{(x_1 - x_2)^2}{2\,\epsilon} - \frac{(x_1 + x_2)^2}{2}\right) \tag{2}$$

which would be considered "difficult" (in the low-ϵ regime) by standard MCMC algorithms. In principle, it is possible to tune the hyperparameters of a M–H sampler but if calculating the density in Equation (2) is computationally expensive and the covariance is not known *a priori* then the tuning procedure gets quickly intractable. Also, since the number of parameters scales as $\sim N^2$, this problem gets mush worse in higher dimensions. Equation (2) can, however, be transformed into the much easier problem of sampling an isotropic Gaussian by an *affine transformation* of the form

$$y_1 = \frac{x_1 - x_2}{\sqrt{\epsilon}}, \qquad y_2 = x_1 + x_2. \tag{3}$$

Therefore, an algorithm that is *affine invariant* will be insensitive to covariances between parameters. An affine invariant algorithm is unaffected by any transformation of the density of the form

$$\mathbf{Y} = \mathbf{A}\,\mathbf{X} + \mathbf{b}. \tag{4}$$

Extending earlier work by Christen (2007), Goodman & Weare (2010, hereafter GW10) proposed an affine invariant sampling algorithm (§2) with only two hyperparameters that can be tuned for performance. Hou *et al.* (2011) were the first group to implement this algorithm to solve a physics problem. The implementation presented here is an independent effort that has already proved effective in several projects (Lang & Hogg 2011; Bovy *et al.* 2011; Dorman *et al.* 2012, Foreman-Mackey & Widrow 2012, in prep.). In what follows, we summarize the GW algorithm and the implementation decisions made in emcee. We also describe the small changes that must be made to the algorithm to parallelize it. Finally, in §A, we outline the installation, usage and troubleshooting of the package.

2. The Algorithm

A complete discussion of MCMC methods is beyond the scope of this document. Instead, the interested reader is directed to a classic reference like MacKay (2003) and we will summarize some key concepts below.

The general goal of MCMC algorithms is to draw samples $\{\Theta_i \, \forall i = 1, \ldots, M\}$ from the joint probability distribution

$$p(\Theta, \alpha, D) = p(\Theta, \alpha) \, p(()D|\Theta, \alpha) \tag{5}$$

where the prior distribution $p(\Theta, \alpha)$ and the likelihood function $p(D|\Theta, \alpha)$ can be relatively easily (but not necessarily quickly) computed for a particular value of (Θ_i, α_i). Since the normalization $p(D)$ is independent of Θ and α, the joint distribution above is proportional to the posterior probability $p(\Theta, \alpha|D)$ given any one choice of generative model. Therefore, once the samples produced by MCMC are available, the marginalized constraints on Θ (Equation (1)) can be approximated by the histogram of the samples projected into the subspace spanned by Θ. In particular, the expectation value of a particular parameter $\phi \in \Theta$ given the samples $\{\phi_i\}$ is

$$E[\phi] = \int \phi \, p(\Theta, \alpha|D) \, \mathrm{d}\Theta \, \mathrm{d}\alpha \approx \frac{1}{M} \sum_{i=1}^{M} \phi_i. \tag{6}$$

Generating the samples Θ_i is a non-trivial process unless $p(\Theta, \alpha, D)$ is a very specific analytic distribution (for example, a Gaussian). MCMC is a procedure for generating a random walk in the parameter space the relatively efficiently draws a representative set of samples from the distribution. Each point in a Markov chain $X(t) = [\Theta(t), \alpha(t)]$ depends only on the position of the previous link $X(t-1)$.

The Metropolis-Hastings (M–H) Algorithm The simplest and most commonly used MCMC algorithm is the M–H method (Algorithm 1). The iterative procedure is as follows: (1) given a position $X(t)$ sample a proposal position Y from the transition distribution $Q(Y; X(t))$, (2) accept this proposal with probability

$$\min \left\{ 1, \frac{p(Y|D)}{p(X(t)|D)} \frac{Q(X(t); Y)}{Q(Y; X(t))} \right\}. \tag{7}$$

It is worth emphasizing that if this step is accepted $X(t+1) = Y$; Otherwise, the new position is set to the previous one $X(t+1) \leftarrow X(t)$ (in other words, the position $X(t)$ is *double counted*).

The M–H algorithm converges (as $t \to \infty$) to a stationary set of samples from the distribution but there are many algorithms with faster convergence and varying levels of

implementation difficulty (CITECITECITE). Faster convergence is preferred because of the reduction of computational cost due to the smaller number of likelihood computations necessary to obtain the equivalent level of accuracy. The efficiency of an algorithm can be measured by the autocorrelation function and more specifically, the integrated autocorrelation time (see §3). This quantity is an estimate of the number of steps needed in the chain in order to draw independent samples from the target density. Therefore, a more efficient chain will have a shorter autocorrelation time.

Algorithm 1 The procedure for a single Metropolis-Hastings MCMC step.

1: Draw a sample $Y \sim Q(Y; X(t))$
2: $q \leftarrow [p(Y) Q(X(t); Y)] / [p(X(t)) Q(Y; X(t))]$
3: $r \leftarrow R \sim [0, 1]$
4: **if** $r \geq q$ **then**
5:     $X(t+1) \leftarrow Y$
6: **else**
7:     $X(t+1) \leftarrow X(t)$
8: **end if**

The stretch move   GW10 proposed an affine invariant ensemble sampling algorithm informally called the "stretch move". For completeness and for clarity of notation, we summarize the algorithm here and refer the interested reader to the original paper for more details. This method involves simultaneously evolving an ensemble of K *walkers* $S = \{X_j, \forall j = 1, \ldots, K\}$ where the proposal distribution for one walker k is based on the current positions of the $K - 1$ walkers in the *complementary ensemble* $S_{[k]} = \{X_j, \forall j \neq k\}$. In general, each X_j is also a vector in N dimensions (the dimension of the parameter space).

To update the position of a walker at position X_k, another walker X_j with $j \neq k$ is randomly chosen and then a new position is proposed:

$$X_k(t) \rightarrow Y = X_j + Z\left[X_k(t) - X_j\right] \tag{8}$$

where Z is a random variable drawn from a distribution $g(Z = z)$. It is clear that if g satisfies

$$g(z^{-1}) = z\, g(z), \tag{9}$$

the proposal of Equation (8) is symmetric. In this case, the chain will satisfy detailed balance if the proposal is accepted with probability

$$q = \min\left\{1, Z^{n-1}\, \frac{p(Y)}{p(X_k(t))}\right\} \tag{10}$$

where n is the dimension of the parameter space. This procedure is then repeated for each walker in the ensemble *in series* following the procedure shown in Algorithm 2.

GW10 advocate for a particular form of $g(z)$, namely

$$g(z) \propto \begin{cases} \dfrac{1}{\sqrt{z}} & \text{if } z \in \left[\dfrac{1}{a}, a\right], \\ 0 & \text{otherwise} \end{cases} \tag{11}$$

where a is an adjustable scale parameter that GW10 set to 2.

Algorithm 2 A single stretch move update step from GW10 where line 5 is generally the most computationally expensive step.

1: **for** $k = 1, \ldots, K$ **do**
2:     Draw a walker X_j at random from the complementary ensemble $S_{[k]}(t)$
3:     $z \leftarrow Z \sim g(z)$, Equation (11)
4:     $Y \leftarrow X_j + z\left[X_k(t) - X_j\right]$
5:     $q \leftarrow z^{n-1} p(Y)/p(X_k(t))$
6:     $r \leftarrow R \sim [0, 1]$
7:     **if** $R \geq q$, Equation (10) **then**
8:         $X_k(t+1) \leftarrow Y$
9:     **else**
10:        $X_k(t+1) \leftarrow X_k(t)$
11:     **end if**
12: **end for**

The parallel stretch move   It is tempting to naïvely parallelize the stretch move algorithm by simultaneously advancing each walker based on the state of the ensemble instead of evolving the walkers in series. Unfortunately, this would no longer satisfy detailed balance. Instead, we must split the full ensemble into two subsets ($S^{(0)} = \{X_k \,\forall k = 1, \ldots, K/2\}$ and $S^{(1)} = \{X_k \,\forall k = K/2+1, \ldots, K\}$) and simultaneously update all the walkers in $S^{(0)}$ — using the stretch move procedure from Algorithm 2 — based *only* on the positions of the walkers in the other set ($S^{(1)}$). Then, using the new positions $S^{(0)}$, we can update $S^{(1)}$. In this case, the outcome is a valid step for all of the walkers. The pseudocode for this procedure is shown in Algorithm 3. This code appears similar to Algorithm 2 but now the computationally expensive inner loop (starting at line 2 in Algorithm 3) can be run in parallel.

The performance of this method — quantified by the autocorrelation time — is comparable to the traditional stretch move algorithm but the fact that one can now take advantage of generic parallelization makes this generalization extremely powerful.

Algorithm 3 The parallel stretch move update step

1: **for** $i \in \{0, 1\}$ **do**
2:      **for** $k = 1, \ldots, K/2$ **do**
3:          Draw a walker X_j at random from the complementary ensemble $S^{(\sim i)}(t)$
4:          $X_k \leftarrow S_k^{(i)}$
5:          $z \leftarrow Z \sim g(z)$, Equation (11)
6:          $Y \leftarrow X_j + z\left[X_k(t) - X_j\right]$
7:          $q \leftarrow z^{n-1}\, p(Y)/p(X_k(t))$
8:          $r \leftarrow R \sim [0, 1]$
9:          **if** $r \geq q$, Equation (10) **then**
10:            $X_k(t + \frac{1}{2}) \leftarrow Y$
11:          **else**
12:            $X_k(t + \frac{1}{2}) \leftarrow X_k(t)$
13:          **end if**
14:      **end for**
15:      $t \leftarrow t + \frac{1}{2}$
16: **end for**

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3. Benchmarks & Tests

Measuring the performance   A standard method of quantifying the performance of an MCMC sampler is to estimate the autocorrelation time of the sampler on several densities.

The main goal of running a Markov chain is to measure the expectation value (and variance) of a particular value (e.g. f)

$$\langle f(\mathbf{x}) \rangle = \int f(\mathbf{x})\, p(\mathbf{x})\, \mathrm{d}\mathbf{x} \tag{12}$$

which can be approximated as

$$\langle f(\mathbf{x}) \rangle \approx \frac{1}{T_s} \sum_{t=1}^{T_s} f(\mathbf{X}(t)) \tag{13}$$

where T is the length of the chain. The generalization of Equation (13) to the case of the ensemble sampler is

$$\langle f(\mathbf{x}) \rangle \approx \frac{1}{T_e} \sum_{t=1}^{T_s} \left[\frac{1}{K} \sum_{k=1}^{K} f(\mathbf{X}_k(t)) \right] \tag{14}$$

where K is the number of walkers. The autocorrelation function of the chain is then given

by

$$C(t) = \frac{1}{K^2} \lim_{t' \to \infty} \text{cov} \left[\sum_{k=1}^{K} f(\mathbf{X}_k(t + t')), \sum_{k=1}^{K} f(\mathbf{X}_k(t')) \right] \tag{15}$$

and the integrated autocorrelation time is given by

$$\tau = \sum_{t=-\infty}^{\infty} \frac{C(t)}{C(0)}. \tag{16}$$

emcee can optionally calculate the autocorrelation time using the Python module acor[1] to estimate the autocorrelation time. This module is a direct port of the original algorithm (described by GW10) and implemented by those authors in C++.[2]

Multivariate Gaussian distribution The simplest test of an MCMC sampler is its sampling performance on a highly covariant multivariate Gaussian density. For the tests in the paper, we randomly generated a 50 dimensional positive definite covariance tensor and initial conditions for each walker. Then, each sampler was tested with the same initial conditions for its performance on the density

$$\pi(\mathbf{x}) \propto \exp \left(-\frac{1}{2} \mathbf{x}^T \Sigma^{-1} \mathbf{x} \right) \tag{17}$$

for the same covariance tensor Σ in each trial.

DFM: actually do some tests here...

Rosenbrock density

4.   Discussion & Tips

The goal of this project has been to make a sampler that is a useful tool for a large class of data analysis problems—a "hammer" if you will. If development of statistical and data-analysis understanding is the key goal, a user who is new to MCMC benefits enormously by writing her or his own Metropolis–Hastings code (Algorithm 1) from scratch before downloading emcee. For typical problems, the emcee package will perform better than

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[1] http://github.com/dfm/acor

[2] http://www.math.nyu.edu/faculty/goodman/software/acor

any home-built M–H code (for all the reasons given above), but the intuitions developed by writing and tuning a self-built MCMC code cannot be replaced by reading this document and running this pre-built package. That said, once those intuitions are developed, it makes sense to switch to emcee or a similarly well engineered piece of code for performance on large problems.

Ensemble samplers like emcee require some thought for initialization. One general approach is to start the walkers at a sampling of the prior or spread out over a reasonable range in parameter space. Another general approach is to start the walkers in a very tight N-dimensional ball in parameter space around one point that is expected to be close to the maximum probability point. The first is more objective but, in practice, we find that the latter is much more effective if there is any chance of walkers getting stuck in low probability modes of a multi-modal probability landscape. A third approach would be to start from a sampling of the prior, and go through a "burn-in" phase in which the prior is transformed continuously into the posterior by increasing the "temperature". Discussion of this kind of annealing is beyond the scope of this document.

The acceptance ratio (DFM: Is there a function to display this and have you defined this concept above? If not, please do.) should be in the 0.2 to 0.5 range (there are theorems about this for specific problems; RTFL). In principle, if the acceptance ratio is too low, you can raise it by decreasing the a parameter; and if it is too high, you can reduce it by increasing the a parameter. However, in practice, we find that $a = 2$ is good in essentially all situations. That means that *if the acceptance ratio is getting very low, something is going very wrong*. Typically a low acceptance ratio means that the posterior probability is multi-modal, with the modes separated by wide, low probability "valleys". In situations like these, the best idea (though expensive of human time) is to split the space into disjoint single-mode regions and sample each one independently, combining the independently sampled regions "properly" (also expensive, and beyond the scope of this document) at the end. In previous work, we have advocated clustering methods to remove multiple modes (Hou *et al.* 2011) which work well, but only when the different modes have *very* different posterior probabilities.

In general, you want to *run with large numbers of walkers*, like hundreds. In principle, there is no reason not to go large when it comes to walker number, until you hit performance issues. Although each step takes twice as much compute time if you double the number of walkers, it also returns to you twice as many independent samples per autocorrelation time. So go large. DFM: A list of problems solved by increasing the number of walkers.

One mistake many users of MCMC methods make is to take *too many* samples! If all you want your MCMC to do is produce one- or two-dimensional error bars on two or three parameters, then you only need dozens of independent samples. With the ensemble

sampling, you get this from a *single snapshot* or single timestep, provided that you are using dozens of walkers (and we would recommend that you use hundreds in most applications). The key point is that *you should run the sampler for a few (say 10) autocorrelation times.* Once you have run that long, no matter how you initialized the walkers, the set of walkers you obtain at the end should be an independent set of samples from the distribution, of which you rarely need many.

Another common mistake, of course, is to run the sampler for *too few* steps. You can identify that you haven't run for enough steps in a couple of ways: If you plot the parameter values in the ensemble as a function of step number, you will see large-scale variations over the full run length if you have gone less than an autocorrelation time. You will also see that if you try to measure the autocorrelation time (with, say, acor), it will give you a time that is always a significant fraction of your run time; it is only when the correlation time is much shorter (say by a factor of 10) than your run time that you are sure to have run long enough. The danger of both of these methods—an unavoidable danger at present—is that you can have a huge dynamic range in contributions to the autocorrelation time; you might think it is 30 when in fact it is 30 000, but you don't "see" the 30 000 in a run that is only 300 steps long. There is not much you can do about this; it is generic when the posterior is multimodal: The autocorrelation time within each mode can be short but the mode–mode migration time can be long. See above on low acceptance ratio; in general when your acceptance ratio gets low your autocorrelation time is very, very long.

One significant limitation to the stretch move and moves like it is that they implicitly assumes that the parameters can be assembled into a vector-like object on which linear operations can be performed. This is not (trivially) true for parameters that have non-trivial constraints, like parameters that must be integer-valued or equivalent, or parameters that are subject to deterministic non-linear constraints. Sometimes these issues can be avoided by reparameterization, but in some cases, samplers like emcee will not be useful, or might require clever or interesting improvements. The emcee package is open-source software; please push us changes!

REFERENCES

Bovy, J., Rix, H.-W., Liu, C., Hogg, D. W., Beers, T. C., & Lee, Y. S., 2011, ApJ, submitted, arXiv:1111.1724 [astro-ph.GA]

Christen, J., *A general purpose scale-independent MCMC algorithm*, technical report I-07-16, CIMAT, Guanajuato, 2007.

Dorman, C., Guhathakurta, P., Fardal, M. A., Geha, M. C., Howley, K. M., Kalirai, J. S., Lang, D., Cuillandre, J., Dalcanton, J., Gilbert, K. M., Seth, A. C., Williams, B. F., & Yniguez, B., 2012, ApJ, submitted

Dunkley, J., Bucher, M., Ferreira, P. G., Moodley, K., & Skordis, C., 2005, MNRAS, 356, 925-936

Goodman, J., & Weare, J., 2010, Comm. App. Math. Comp. Sci., 5, 65

Gregory, P. C., *Bayesian Logical Data Analysis for the Physical Sciences*, Cambridge University Press, 2005

Hou, F., Goodman, J., Hogg, D. W., Weare, J., & Schwab, C., 2011, arXiv:1104.2612

Lang, D. and Hogg, D. W., 2011, arXiv:1103.6038

MacKay, D., *Information Theory, Inference, and Learning Algorithms*, Cambridge University Press, 2003

Widrow, L. M. and Pym, B. and Dubinski, J., 2008, ApJ, 679, 1239

A.   Usage

Installation   The easiest way to install emcee is using pip[3]. Running the command

```
% pip install emcee
```

at the command line of a UNIX-based system will install the package and its Python dependencies. If you would like to install for all users, you might need to run the above command

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[3]http://pypi.python.org/pypi/pip/

with superuser permissions. emcee depends on Python (> 2.7) and numpy[4] (> 1.6) and the associated `dev` headers. On some systems, you might need to install these packages separately. On most systems where Python has already been installed, this won't be necessary but if it is, you can install dependencies (on Ubuntu, for example) with the command:

```
% apt-get python python-dev numpy numpy-dev
```

An alternative installation method is to download the source code from http://danfm.ca/emcee and run

```
% python setup.py install
```

in the unzipped directory. Make sure that you have numpy installed in this case as well.

Issues & Contributions The development of emcee is being coordinated on GitHub at http://github.com/dfm/emcee and contributions are welcome. If you encounter any problems with the code, please report them at http://github.com/dfm/emcee/issues (DFM: check this url) and consider contributing a patch.

Basic usage A very simple sample problem and a common unit test for sampling code is the performance of the code on a high dimensional Gaussian density

$$p(\mathbf{x}) \propto \exp\left(-\frac{1}{2}\mathbf{x}^T\,\Sigma^{-1}\,\mathbf{x}\right). \tag{A1}$$

We will incrementally work through this example here and the source code is available online.[5]

First, import the necessary packages and define the function that calculates the logarithm of Equation (A1).

```python
import numpy as np
import emcee

def lnprobfn(x, mu, icov):
    diff = x-mu
    return -np.dot(diff,np.dot(icov,diff))/2.0
```

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[4]http://numpy.scipy.org

[5]https://github.com/dfm/emcee/blob/master/quickstart.py

Next, choose the number of dimensions to use and generate the mean vector `means` and the positive definite covariance matrix `cov` and its inverse `icov`.

```
ndim  = 10
means = np.random.rand(ndim)
cov   = 0.5-np.random.rand(ndim**2).reshape((ndim, ndim))
cov   = np.triu(cov)
cov   += cov.T - np.diag(cov.diagonal())
cov   = np.dot(cov,cov)
icov  = np.linalg.inv(cov)
```

The number of walkers to use is one of the tuning parameters of this sampler and we'll come back to some discussion of how to choose this shortly. For now, use 100 walkers and generate an initial guess for the position of each of the walkers (in a small ball centered at zero mean).

```
nwalkers = 100
p0 = [np.random.rand(ndim) for i in xrange(nwalkers)]
```

Initialize the sampler object passing the chosen hyperparameters and the generated likelihood function and it's arguments.

```
sampler = emcee.EnsembleSampler(nwalkers, ndim, lnprobfn,
                          args=[means, icov])
```

Now, run a "burn-in" chain of 500 steps. Note that each walker is advanced 500 times here so `lnprobfn` is actually be called 5×10^4 times.

```
pos, prob, state = sampler.run_mcmc(p0, 500)
```

Finally, reset the chain and sample 2000 steps starting from the final state of the burn-in chain.

```
sampler.reset()
sampler.run_mcmc(pos, 2000, rstate0=state)
```

B.   API

emcee.ensemble   emcee.`EnsembleSampler(*args, **kwargs)`

Ensemble sampling following Goodman & Weare (2010) with optional parallelization

Arguments

`k` (`int`): The number of Goodman & Weare "walkers".

`dim` (`int`): Number of dimensions in the parameter space.

`lnpostfn` (`callable`): A function that takes a vector in the parameter space as input and returns the natural logarithm of the posterior probability for that position.

Keyword Arguments

`a` (`float`): The proposal scale parameter from Equation (11). (default: `2.0`)

`args` (`list`): Optional list of extra arguments for `lnpostfn`. `lnpostfn` will be called with the sequence `lnpostfn(p, *args)`.

`postargs` (`list`): Alias of `args` for backwards compatibility.

`threads` (`int`): The number of threads to use for parallelization. If `threads == 1`, then the `multiprocessing` is not used but if `threads > 1`, then a `Pool` object is created and calls to `lnpostfn` are run in parallel following Algorithm 3. (default: `1`)

`pool` (`multiprocessing.Pool`): An alternative method of using the parallelized algorithm. If `pool is not None`, the value of `threads` is ignored and the provided `Pool` is used for all parallelization. (default: `None`)

Exceptions

`AssertionError`: If `k < 2*dim` or if `k` is not even.

Properties

`chain` (`numpy.ndarray`): A pointer to the Markov chain itself. The shape of this array is (`k, dim, iterations/resample`)

`flatchain` (`numpy.ndarray`): A shortcut for accessing `chain` flattened along the zeroth (walker) axis.

`lnprobability` (`numpy.ndarray`): A pointer to the matrix of the value of `lnprobfn` produced at each step for each walker. The shape is (`k, iterations/resample`).

`iterations` (`int`): The number of steps that have been run in the chain.

acceptance_fraction (`numpy.ndarray`): An array (length: `k`) of the fraction of steps accepted for each walker.

acor (`numpy.ndarray`): The autocorrelation time of each parameter in the chain (length: `dim`) as estimated by the `acor` module.

random_state (`tuple`): The state of the internal random number generator. In practice, it's the result of calling `get_state()` on a `numpy.random.mtrand.RandomState` object. You can try to set this property but be warned that if you do this and it fails, it will do so silently.

Methods

emcee.EnsembleSampler.sample(pos0, lnprob0=None, rstate0=None, iterations=1)

Advances the chain `iterations` steps as an iterator

Arguments

pos0 (`numpy.ndarray`):   A list of the initial positions of the walkers in the parameter space. The shape is (`k`, `dim`).

Keyword Arguments

lnprob0 (`numpy.ndarray`):   The list of log posterior probabilities for the walkers at positions given by the `p0`. If `lnprob is None`, the initial values are calculated. The shape is (`k`, `dim`).

rstate0 (`tuple`): The state of the random number generator.
See `EnsembleSampler.random_state` for details.

iterations (`int`): The number of steps to run. (default: `1`)

Yields

pos (`numpy.ndarray`):   A list of the current positions of the walkers in the parameter space. The shape is (`k`, `dim`).

lnprob (`numpy.ndarray`):   The list of log posterior probabilities for the walkers at positions given by the `pos`. The shape is (`k`, `dim`).

rstate (`tuple`): The state of the random number generator.

emcee.EnsembleSampler.run_mcmc(pos0, N, rstate0=None, lnprob0=None, **kwargs)

Iterate `sample` for `N` iterations and return the result. The parameters are passed directly to `sample` so see above for details.

Returns

> `pos` (`numpy.ndarray`): A list of the final positions of the walkers in the parameter space. The shape is `(k, dim)`.
>
> `lnprob` (`numpy.ndarray`): The list of log posterior probabilities for the walkers at positions given by the `pos`. The shape is `(k, dim)`.
>
> `rstate` (`tuple`): The final state of the random number generator.

`emcee.EnsembleSampler.reset()`

Clear `chain`, `lnprobability` and the bookkeeping parameters.

`emcee.EnsembleSampler.clear_chain()`

An alias of `reset` kept for backwards compatibility.