Release 2.0

PyMC

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January 5, 2009

CONTENTS

CHAPTER
ONE

Introduction

1.1 Purpose

PyMC is a python module that implements Bayesian statistical models and fitting algorithms, including Markov chain Monte Carlo. Its flexibility makes it applicable to a large suite of problems as well as easily extensible. Along with core sampling functionality, PyMC includes methods for summarizing output, plotting, goodness-of-fit and convergence diagnostics.

1.2 Features

- Fits Bayesian statistical models you create with Markov chain Monte Carlo and other algorithms.
- Large suite of well-documented statistical distributions.
- Gaussian processes.
- Sampling loops can be paused and tuned manually, or saved and restarted later.
- Creates summaries including tables and plots.
- Traces can be saved to the disk as plain text, Python pickles, SQLite or MySQL database, or hdf5 archives.
- Convergence diagnostics.
- Extensible: easily incorporates custom step methods and unusual probability distributions.
- MCMC loops can be embedded in larger programs, and results can be analyzed with the full power of Python.

1.3 What's new in 2.0

- New flexible object model and syntax (not backward-compatible).
- Reduced redundant computations: only relevant log-probability terms are computed, and these are cached.
- Optimized probability distributions.
- New adaptive blocked Metropolis step method.
- Much more!

1.4 Usage

First, define your model in a file, say mymodel.py (with comments, of course!):

```
# Import relevant modules
import pymc
import numpy as np

# Some data
n = 5*np.ones(4,dtype=int)
x = np.array([-.86,-.3,-.05,.73])

# Priors on unknown parameters
alpha = pymc.Normal('alpha',mu=0,tau=.01)
beta = pymc.Normal('beta',mu=0,tau=.01)

# Arbitrary deterministic function of parameters
@pymc.deterministic
def theta(a=alpha, b=beta):
    """theta = logit^{-1}(a+b)"""
    return pymc.invlogit(a+b*x)

# Binomial likelihood for data
d = pymc.Binomial('d', n=n, p=theta, value=np.array([0.,1.,3.,5.]),
                  \observed=True)
```

Save this file, then from a python shell (or another filein the same directory), call:

```
import pymc
import mymodel

S = pymc.MCMC(mymodel, db='pickle')
S.sample(iter=10000, burn=5000, thin=2)
pymc.Matplot.plot(S)
```

This will generate 10000 posterior samples, thinned by a factor of 2, with the first half discarded as burn-in. The sample is stored in a Python serialization (pickle) database.

1.5 History

PyMC began development in 2003, as an effort to generalize the process of building Metropolis-Hastings samplers, with an aim to making Markov chain Monte Carlo (MCMC) more accessible to non-statisticians (particularly ecologists). The choice to develop PyMC as a python module, rather than a standalone application, allowed the use MCMC methods in a larger modeling framework. By 2005, PyMC was reliable enough for version 1.0 to be released to the public. A small group of regular users, most associated with the University of Georgia, provided much of the feedback necessary for the refinement of PyMC to a usable state.

In 2006, David Huard and Anand Patil joined Chris Fonnesbeck on the development team for PyMC 2.0. This iteration of the software strives for more flexibility, better performance and a better end-user experience than any previous version of PyMC.

1.6 Getting started

This user guide provides all the information needed to install PyMC, code a Bayesian statistical model, run the sampler, save and analyze the results. In addition, the appendix contains a chapter on MCMC theory as well as the list of the available statistical distributions. More examples of usage as well as tutorials are available from the PyMC web site.

CHAPTER TWO

Installation

PyMC is known to run on Mac OS X, Linux and Windows, but in theory should be able to work on just about any platform for which Python, a Fortran compiler and the NumPy module are available. However, installing some extra depencies can greatly improve PyMC's performance and versatility. The following describes the required and optional dependencies and takes you through the installation process.

2.1 Dependencies

PyMC requires some prerequisite packages to be present on the system. Fortunately, there are currently only a few dependencies, and all are freely available online.

- Python version 2.5.
- NumPy (1.2 or newer): The fundamental scientific programming package, it provides a multidimensional array type and many useful functions for numerical analysis.
- Matplotlib (optional): 2D plotting library which produces publication quality figures in a variety of image formats and interactive environments
- pyTables (optional): Package for managing hierarchical datasets and designed to efficiently and easily cope with extremely large amounts of data. Requires the HDF5 library.
- pydot (optional): Python interface to Graphviz's Dot language, it allows PyMC to create both directed and non-directed graphical representations of models. Requires the Graphviz library.
- SciPy (optional): Library of algorithms for mathematics, science and engineering.
- IPython (optional): An enhanced interactive Python shell and an architecture for interactive parallel computing.
- nose (optional): A test discovery-based unittest extension (required to run the test suite).

There are prebuilt distributions that include all required dependencies. For Mac OSX users, we recommend the MacPython distribution, the Enthought Python Distribution, or Python 2.5.1 that ships with OSX 10.5 (Leopard). Windows users should download and install the Enthought Python Distribution. The Enthought Python Distribution comes bundled with these prerequisites. Note that depending on the currency of these distributions, some packages may need to be updated manually.

If instead of installing the prebuilt binaries you prefer (or have) to build `pymc` yourself, make sure you have a Fortran and a C compiler. There are free compilers (gfortran, gcc) available on all platforms. Other compilers have not been tested with PyMC but may work nonetheless.

2.2 Installation using EasyInstall

The easiest way to install PyMC is to type in a terminal:

```
easy_install pymc
```

Provided EasyInstall (part of the setuptools module) is installed and in your path, this should fetch and install the package from the Python Package Index. Make sure you have the appropriate administrative privileges to install software on your computer.

2.3 Installing from pre-built binaries

Pre-built binaries are available for Windows XP and Mac OS X. There are at least two ways to install these:

1. Download the installer for your platform from PyPI.
2. Double-click the executable installation package, then follow the on-screen instructions.

For other platforms, you will need to build the package yourself from source. Fortunately, this should be relatively straightforward.

2.4 Compiling the source code

First download the source code tarball from PyPI and unpack it. Then move into the unpacked directory and follow the platform specific instructions.

Windows

One way to compile PyMC on Windows is to install MinGW and MSYS. MinGW is the GNU Compiler Collection (GCC) augmented with Windows specific headers and libraries. MSYS is a POSIX-like console (bash) with UNIX command line tools. Download the Automated MinGW Installer and double-click on it to launch the installation process. You will be asked to select which components are to be installed: make sure the g77 compiler is selected and proceed with the instructions. Then download and install MSYS-1.0.exe, launch it and again follow the on-screen instructions.

Once this is done, launch the MSYS console, change into the PyMC directory and type:

```
python setup.py install
```

This will build the C and Fortran extension and copy the libraries and python modules in the C:/Python25/Lib/site-packages/pymc directory.

Mac OS X or Linux

In a terminal, type:

```
python setup.py build
sudo python setup.py install
```

The *sudo* command is required to install PyMC into the Python `site-packages` directory if it has restricted privileges. You will be prompted for a password, and provided you have superuser privileges, the installation will proceed.

2.5 Development version

You can check out the bleeding edge version of the code from the subversion repository:

```
svn checkout http://pymc.googlecode.com/svn/trunk/ pymc
```

Previous versions are available in the `/tags` directory.

2.6 Running the test suite

`pymc` comes with a set of tests that verify that the critical components of the code work as expected. To run these tests, users must have nose installed. The tests are launched from a python shell:

```
import pymc
pymc.test()
```

In case of failures, messages detailing the nature of these failures will appear. In case this happens (it shouldn't), please report the problems on the issue tracker, specifying the version you are using and the environment.

2.7 Bugs and feature requests

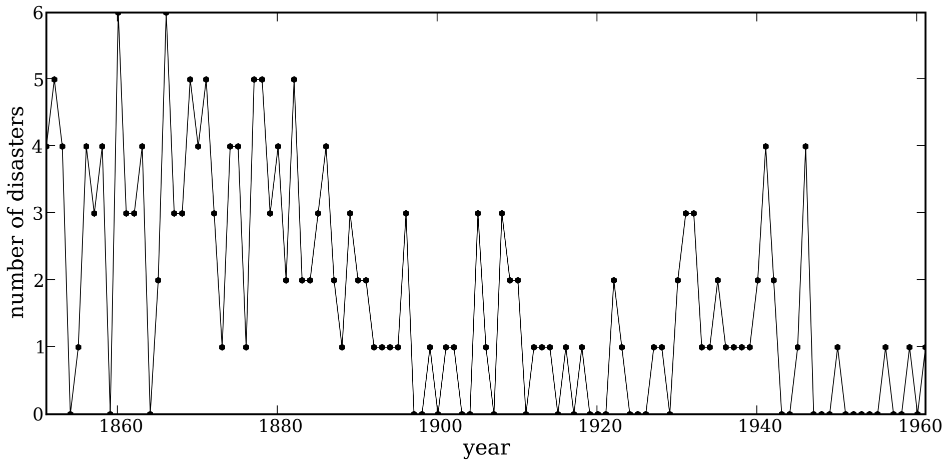
Report problems with the installation, bugs in the code or feature request at the issue tracker. Comments and questions are welcome and should be addressed to PyMC's mailing list.

CHAPTER
THREE

Tutorial

3.1 An example statistical model

Consider the following dataset, which is a time series of recorded coal mining disasters in the UK from 1851 to 1962 [Jarrett, 1979].



Occurrences of disasters in the time series is thought to be derived from a Poisson process with a large rate parameter in the early part of the time series, and from one with a smaller rate in the later part. We are interested in locating the change point in the series, which perhaps is related to changes in mining safety regulations.

We represent our conceptual model formally as a statistical model:

$$\begin{aligned}(D_t|s,e,l) &\sim \text{Poisson}\left(r_t\right), \quad r_t = \begin{cases} e & \text{if} \quad t < s \\ l & \text{if} \quad t \geq s \end{cases}, \quad t \in [t_l, t_h] \\ s &\sim \text{Discrete Uniform}(t_l, t_h) \\ e &\sim \text{Exponential}(r_e) \\ l &\sim \text{Exponential}(r_l)\end{aligned} \tag{3.1}$$

The symbols are defined as:

D_t: The number of disasters in year t.

r_t: The rate parameter of the Poisson distribution of disasters in year t.

s: The year in which the rate parameter changes (the switchpoint).

e: The rate parameter before the switchpoint s.

l: The rate parameter after the switchpoint s.

t_l, t_h: The lower and upper boundaries of year t.

r_e, r_l: The rate parameters of the priors of the early and late rates, respectively.

Because we have defined D by its dependence on s, e and l, the latter three are known as the 'parents' of D and D is called their 'child'. Similarly, the parents of s are t_l and t_h, and s is the child of t_l and t_h.

3.2 Two types of variables

At the model-specification stage (before the data are observed), D, s, e, r and l are all random variables. Bayesian 'random' variables have not necessarily arisen from a physical random process. The Bayesian interpretation of probability is *epistemic*, meaning random variable x's probability distribution $p(x)$ represents our knowledge and uncertainty about x's value. Candidate values of x for which $p(x)$ is high are relatively more probable, given what we know. Random variables are represented in PyMC by the classes `Stochastic` and `Deterministic`.

The only `Deterministic` in the model is r. If we knew the values of r's parents (s, l and e), we could compute the value of r exactly. A `Deterministic` like r is defined by a mathematical function that returns its value given values for its parents. The nomenclature is a bit confusing, because these objects usually represent random variables; since the parents of r are random, r is random also. A more descriptive (though more awkward) name for this class would be `DeterminedByValuesOfParents`.

On the other hand, even if the values of the parents of variables s, D (before observing the data), e or l were known, we would still be uncertain of their values. These variables are characterized by probability distributions that express how plausible their candidate values are, given values for their parents. The `Stochastic` class represents these variables. A more descriptive name for these objects might be `RandomEvenGivenValuesOfParents`.

We can represent model 3.1 in a file called `DisasterModel.py` as follows. First, we import the PyMC and NumPy namespaces:

```
from pymc import DiscreteUniform, Exponential, deterministic, Poisson, Uniform
import numpy as np
```

Notice that from `pymc` we have only imported a select few objects that are needed for this particular model, whereas the entire `numpy` namespace has been imported, and conveniently given a shorter name. Objects from NumPy are subsequently accessed by prefixing `np.` to the name. Either approach is acceptable.

Next, we enter the actual data values into an array:

```
disasters_array =   np.array([ 4, 5, 4, 0, 1, 4, 3, 4, 0, 6, 3, 3, 4, 0, 2, 6,
                   3, 3, 5, 4, 5, 3, 1, 4, 4, 1, 5, 5, 3, 4, 2, 5,
                   2, 2, 3, 4, 2, 1, 3, 2, 2, 1, 1, 1, 1, 3, 0, 0,
                   1, 0, 1, 1, 0, 0, 3, 1, 0, 3, 2, 2, 0, 1, 1, 1,
                   0, 1, 0, 1, 0, 0, 0, 2, 1, 0, 0, 0, 1, 1, 0, 2,
                   3, 3, 1, 1, 2, 1, 1, 1, 1, 2, 4, 2, 0, 0, 1, 4,
                   0, 0, 0, 1, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0, 1])
```

Next, we create the switchpoint variable s:

```
s = DiscreteUniform('s', lower=0, upper=110, doc='Switchpoint[year]')
```

`DiscreteUniform` is a subclass of `Stochastic` that represents uniformly-distributed discrete variables. Use of this distribution suggests that we have no preference *a priori* regarding the location of the switchpoint; all values are equally likely. Now we create the exponentially-distributed variables e and l for the early and late Poisson rates, respectively:

```
e = Exponential('e', beta=1)
l = Exponential('l', beta=1)
```

Next, we define the variable r, which selects the early rate e for times before s and the late rate l for times after s. We create r using the `deterministic` decorator, which converts the ordinary Python function r into a `Deterministic` object.

```
@deterministic(plot=False)
def r(s=s, e=e, l=l):
""" Concatenate Poisson means """
    out = np.empty(len(disasters_array))
    out[:s] = e
    out[s:] = l
    return out
```

The last step is to define the number of disasters D. This is a stochastic variable, but unlike s, e and l we have observed its value. To express this, we set the argument `observed` to `True` (it is set to `False` by default). This tells PyMC that this object's value should not be changed:

```
D = Poisson('D', mu=r, value=disasters_array, observed=True)
```

Why are data and unknown variables represented by the same object?

Since its represented by a `Stochastic` object, D is defined by its dependence on its parent r even though its value is fixed. This isn't just a quirk of PyMC's syntax; Bayesian hierarchical notation itself makes no distinction between random variables and data. The reason is simple: to use Bayes' theorem to compute the posterior $p(e,s,l|D)$ of model 3.1, we require the likelihood $p(D|e,s,l) = p(D|r)$. Even though D's value is known and fixed, we need to formally assign it a probability distribution as if it were a random variable. Remember, the likelihood and the probability function are essentially the same, except that the former is regarded as a function of the parameters and the latter as a function of the data.

This point can be counterintuitive at first, as many peoples' instinct is to regard data as fixed a priori and unknown variables as dependent on the data. One way to understand this is to think of statistical models like (3.1) as predictive models for data, or as models of the processes that gave rise to data. Before observing the value of D, we could have sampled from its prior predictive distribution $p(D)$ (*i.e.* the marginal distribution of the data) as follows:

1. Sample e, s and l from their priors.
2. Sample D conditional on these values.

Even after we observe the value of *D*, we need to use this process model to make inferences about *e*, *s* and *l* because its the only information we have about how the variables are related.

3.3 Parents and children

We have above created a PyMC probability model, which is simply a linked collection of variables. To see the nature of the links, import or run `DisasterModel.py` and examine *s*'s `parents` attribute from the Python prompt:

```
>>> s.parents
>>> {'lower': 0, 'upper': 110}
```

The `parents` dictionary shows us the distributional parameters of *s*, which are constants. Now let's examinine *D*'s parents:

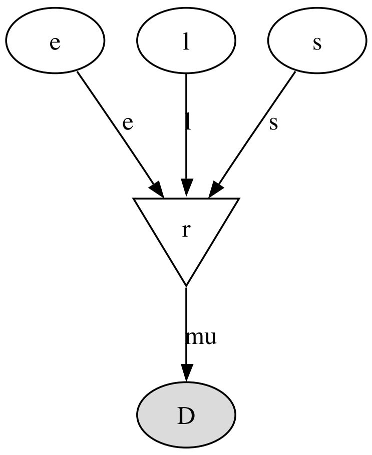
```
>>> D.parents
>>> {'mu': <pymc.PyMCObjects.Deterministic 'r' at 0x3e51a70>}
```

We are using *r* as a distributional parameter of *D* (*i.e.* *r* is *D*'s parent). *D* internally labels *r* as `mu`, meaning *r* plays the role of the rate parameter in *D*'s Poisson distribution. Now examine *r*'s `children` attribute:

```
>>> r.children
>>> set([<pymc.distributions.Poisson 'D' at 0x3e51290>])
```

Because *D* considers *r* its parent, *r* considers *D* its child. Unlike `parents`, `children` is a set (an unordered collection of objects); variables do not associate their children with any particular distributional role. Try examining the `parents` and `children` attributes of the other parameters in the model.

The following 'directed acyclic graph' is a visualization of the parent-child relationships in the model. Unobserved stochastic variables *s*, *e* and *l* are open ellipses, observed stochastic variable *D* is a filled ellipse and deterministic variable *r* is a triangle. Arrows point from parent to child and display the label that the child assigns to the parent. See section 4.6 for more details.



3.4 Variables' values and log-probabilities

All PyMC variables have an attribute called `value` that stores the current value of that variable. Try examining *D*'s value, and you'll see the initial value we provided for it:

```
>>> D.value
>>>
array([4, 5, 4, 0, 1, 4, 3, 4, 0, 6, 3, 3, 4, 0, 2, 6, 3, 3, 5, 4, 5, 3, 1,
       4, 4, 1, 5, 5, 3, 4, 2, 5, 2, 2, 3, 4, 2, 1, 3, 2, 2, 1, 1, 1, 1, 3,
       0, 0, 1, 0, 1, 1, 0, 0, 3, 1, 0, 3, 2, 2, 0, 1, 1, 1, 0, 1, 0, 1, 0,
       0, 0, 2, 1, 0, 0, 0, 1, 1, 0, 2, 3, 3, 1, 1, 2, 1, 1, 1, 1, 2, 4, 2,
       0, 0, 1, 4, 0, 0, 0, 1, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0, 1])
```

If you check *e*'s, *s*'s and *l*'s values, you'll see random initial values generated by PyMC:

```
>>> s.value
>>> 44

>>> e.value
>>> 0.33464706250079584

>>> l.value
>>> 2.6491936762267811
```

Of course, since these are `Stochastic` elements, your values will be different than these. If you check *r*'s value, you'll see an array whose first *s* elements are *e* (here 0.33464706), and whose remaining elements are *l* (here 2.64919368):

```
>>> r.value
>>>
array([ 0.33464706,  0.33464706,  0.33464706,  0.33464706,  0.33464706,
        0.33464706,  0.33464706,  0.33464706,  0.33464706,  0.33464706,
        0.33464706,  0.33464706,  0.33464706,  0.33464706,  0.33464706,
        0.33464706,  0.33464706,  0.33464706,  0.33464706,  0.33464706,
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        0.33464706,  0.33464706,  0.33464706,  0.33464706,  2.64919368,
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        2.64919368,  2.64919368,  2.64919368,  2.64919368,  2.64919368,
        2.64919368,  2.64919368,  2.64919368,  2.64919368,  2.64919368])
```

To compute its value, r calls the funtion we used to create it, passing in the values of its parents.

`Stochastic` objects can evaluate their probability mass or density functions at their current values given the values of their parents. The logarithm of a stochastic object's probability mass or density can be accessed via the `logp` attribute. For vector-valued variables like D, the `logp` attribute returns the sum of the logarithms of the joint probability or density of all elements of the value. Try examining s's and D's log-probabilities and e's and l's log-densities:

```
>>> s.logp
>>> -4.7095302013123339

>>> D.logp
>>> -1080.5149888046033

>>> e.logp
>>> -0.33464706250079584

>>> l.logp
>>> -2.6491936762267811
```

`Stochastic` objects need to call an internal function to compute their `logp` attributes, as r needed to call an internal function to compute its value. Just as we created r by decorating a function that computes its value, it's possible to create custom `Stochastic` objects by decorating functions that compute their log-probabilities or densities (see chapter 4). Users are thus not limited to the set of of statistical distributions provided by PyMC.

Using `Variables` as parents of other `Variables`

Let's take a closer look at our definition of r:

```
@deterministic(plot=False)
def r(s=s, e=e, l=l):
    """ Concatenate Poisson means """
    out = np.empty(len(disasters_array))
    out[:s] = e
    out[s:] = l
    return out
```

The arguments s, e and l are `Stochastic` objects, not numbers. Why aren't errors raised when we attempt to slice array `out` up to a `Stochastic` object?

Whenever a variable is used as a parent for a child variable, PyMC replaces it with its `value` attribute when the child's value or log-probability is computed. When r's value is recomputed, `s.value` is passed to the function as argument `s`. To see the values of the parents of r all together, look at `r.parents.value`.

3.5 Fitting the model with MCMC

PyMC provides several objects that fit probability models (linked collections of variables) like ours. The primary such object, `MCMC`, fits models with the Markov chain Monte Carlo algorithm. See appendix A for an introduction to the algorithm itself. To create an `MCMC` object to handle our model, import `DisasterModel.py` and use it as an argument for `MCMC`:

```
import DisasterModel
from pymc import MCMC
M = MCMC(DisasterModel)
```

In this case `M` will expose variables `s`, `e`, `l`, `r` and `D` as attributes; that is, `M.s` will be the same object as `DisasterModel.s`.

To run the sampler, call the MCMC object's `isample()` (or `sample()`) method with arguments for the number of iterations, burn-in length, and thinning interval (if desired):

```
M.isample(iter=10000, burn=1000, thin=10)
```

After a few seconds, you should see that sampling has finished normally. The model has been fitted.

What does it mean to fit a model?

'Fitting' a model means characterizing its posterior distribution somehow. In this case, we are trying to represent the posterior $p(s, e, l|D)$ by a set of joint samples from it. To produce these samples, the MCMC sampler randomly updates the values of s, e and l according to the Metropolis-Hastings algorithm (Gelman et al. [2004]) for `iter` iterations.

After a sufficiently large number of iterations, the current values of s, e and l can be considered a sample from the posterior. PyMC assumes that the `burn` parameter specifies a 'sufficiently large' number of iterations for convergence of the algorithm, so it is up to the user to verify that this is the case (see chapter 7). Consecutive values sampled from s, e and l are necessarily dependent on the previous sample, since it is a Markov chain. However, MCMC often results in strong autocorrelation among samples that can result in imprecise posterior inference. To circumvent this, it is often effective to thin the sample by only retaining every kth sample, where k is an integer value. This thinning interval is passed to the sampler via the `thin` argument.

If you are not sure ahead of time what values to choose for the `burn` and `thin` parameters, you may want to retain all the MCMC samples, that is to set `burn=0` and `thin=1`, and then discard the 'burnin period' and thin the samples after examining the traces (the series of samples). See Gelman et al. [2004] for general guidance.

Accessing the samples

The output of the MCMC algorithm is a 'trace', the sequence of retained samples for each variable in the model. These traces can be accessed using the `trace(name, chain=-1)` method. For example:

```
>>> M.trace('s')[:]
array([41, 40, 40, ..., 43, 44, 44])
```

The trace slice `[start:stop:step]` works just like the NumPy array slice. By default, the returned trace array contains the samples from the last call to `sample`, that is, `chain=-1`, but the trace from previous sampling runs can be retrieved by specifying the correspondent chain index. To return the trace from all chains, simply use `chain=None`.[1]

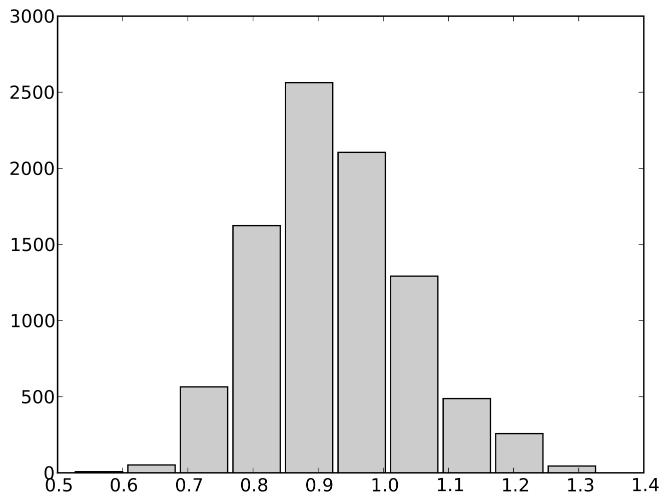
Sampling output

You can examine the marginal posterior of any variable by plotting a histogram of its trace:

```
>>> from pylab import hist, show
>>> hist(M.trace('l')[:])
>>>
(array([   8,   52,  565, 1624, 2563, 2105, 1292,  488,  258,   45]),
 array([ 0.52721865,  0.60788251,  0.68854637,  0.76921023,  0.84987409,
        0.93053795,  1.01120181,  1.09186567,  1.17252953,  1.25319339]),
 <a list of 10 Patch objects>)
>>> show()
```

You should see something like this:

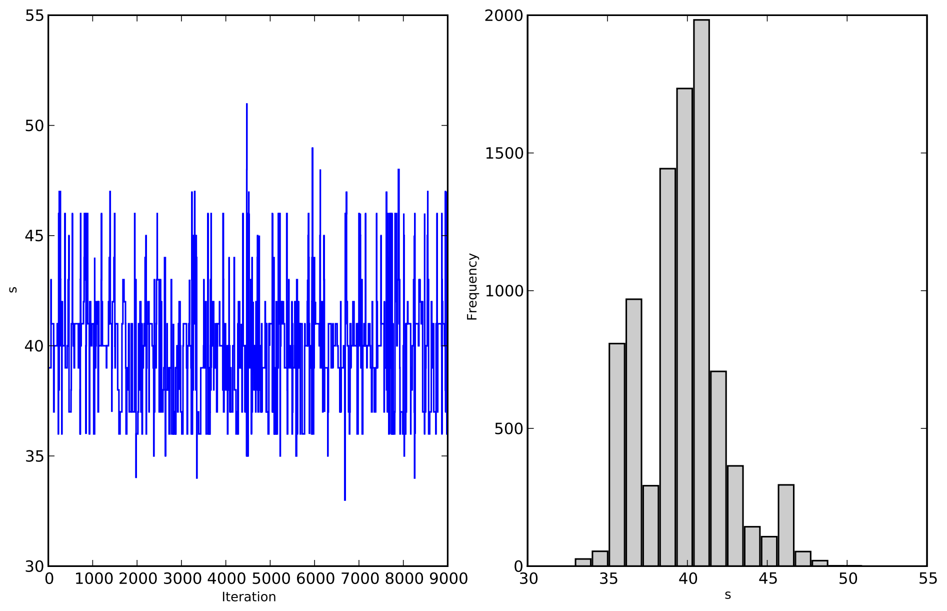
[1]Note that the unknown variables s, e, l and r will all accrue samples, but D will not because its value has been observed and is not updated. Hence D has no trace and calling `M.trace('D')[:]` will raise an error.



PyMC has its own plotting functionality, via the optional `matplotlib` module as noted in the installation notes. The `Matplot` module includes a `plot` function that takes the model (or a single parameter) as an argument:

```
>>> from pymc.Matplot import plot
>>> plot(M)
```

For each variable in the model, `plot` generates a composite figure, such as this one for the switchpoint in the disasters model:



The left-hand pane of this figure shows the temporal series of the samples from s, while the right-hand pane shows a histogram of the trace. The trace is useful for evaluating and diagnosing the algorithm's performance (see Gelman, Carlin, Stern, and Rubin [2004]), while the histogram is useful for visualizing the posterior.

For a non-graphical summary of the posterior, simply call `M.stats()`.

Imputation of Missing Data

As with most "textbook examples", the models we have examined so far assume that the associated data are complete. That is, there are no missing values corresponding to any observations in the dataset. However, many real-world datasets contain one or more missing values, usually due to some logistical problem during the data collection process. The easiest way of dealing with observations that contain missing values is simply to exclude them from the analysis. However, this results in loss of information if an excluded observation contains valid values for other quantities. An alternative is to impute the missing values, based on information in the rest of the model.

For example, consider a survey dataset for some wildlife species:

Count	Site	Observer	Temperature
15	1	1	15
10	1	2	NA
6	1	1	11

Each row contains the number of individuals seen during the survey, along with three covariates: the site on which the survey was conducted, the observer that collected the data, and the temperature during the survey. If we are interested in modelling, say, population size as a function of the count and the associated covariates, it is difficult to accommodate the second observation because the temperature is missing (perhaps the thermometer was broken that day). Ignoring this observation will allow us to fit the model, but it wastes information that is contained in the other covariates.

In a Bayesian modelling framework, missing data are accommodated simply by treating them as unknown model parameters. Values for the missing data $\tilde{y}$ are estimated naturally, using the posterior predictive distribution:

$$p(\tilde{y}|y) = \int p(\tilde{y}|\theta) f(\theta|y) d\theta \tag{3.2}$$

This describes additional data $\tilde{y}$, which may either be considered unobserved data or potential future observations. We can use the posterior predictive distribution to model the likely values of missing data.

Consider the coal mining disasters data introduced previously. Assume that two years of data are missing from the time series; we indicate this in the data array by the use of an arbitrary placeholder value, -999.

```
x = numpy.array([ 4, 5, 4, 0, 1, 4, 3, 4, 0, 6, 3, 3, 4, 0, 2, 6,
3, 3, 5, 4, 5, 3, 1, 4, 4, 1, 5, 5, 3, 4, 2, 5,
2, 2, 3, 4, 2, 1, 3, -999, 2, 1, 1, 1, 1, 3, 0, 0,
1, 0, 1, 1, 0, 0, 3, 1, 0, 3, 2, 2, 0, 1, 1, 1,
0, 1, 0, 1, 0, 0, 0, 2, 1, 0, 0, 0, 1, 1, 0, 2,
3, 3, 1, -999, 2, 1, 1, 1, 1, 2, 4, 2, 0, 0, 1, 4,
0, 0, 0, 1, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0, 1])
```

To estimate these values in PyMC, we generate a masked array. These are specialised NumPy arrays that contain a matching True or False value for each element to indicate if that value should be excluded from any computation. Masked arrays can be generated using NumPy's `ma.masked_equal` function:

```
>>> masked_data = numpy.ma.masked_equal(x, value=-999)
>>> masked_data
masked_array(data = [4 5 4 0 1 4 3 4 0 6 3 3 4 0 2 6 3 3 5 4 5 3 1 4 4 1 5 5 3
 4 2 5 2 2 3 4 2 1 3 -- 2 1 1 1 1 3 0 0 1 0 1 1 0 0 3 1 0 3 2 2 0 1 1 1 0 1 0
 1 0 0 0 2 1 0 0 0 1 1 0 2 3 3 1 -- 2 1 1 1 1 2 4 2 0 0 1 4 0 0 0 1 0 0 0 0 0 1
 0 0 1 0 1],
 mask = [False False False False False False False False False False False False
 False False False False False False False False False False False False
 False False False False False False False False False False False False
 False False False  True False False False False False False False False
 False False False False False False False False False False False False
 False False False False False False False False False False False False
 False False False False False False False False False False False  True
 False False False False False False False False False False False False
 False False False False False False False False False False False False
 False False False],
      fill_value=999999)
```

This masked array, in turn, can then be passed to PyMC's own `ImputeMissing` function, which replaces the missing values with Stochastic variables of the desired type. For the coal mining disasters problem, recall that disaster events were modelled as Poisson variates:

```
>>> D = ImputeMissing('D', Poisson, masked_data, mu=r)
>>> D
[<pymc.distributions.Poisson 'D[0]' at 0x4ba42d0>,
 <pymc.distributions.Poisson 'D[1]' at 0x4ba4330>,
 <pymc.distributions.Poisson 'D[2]' at 0x4ba44d0>,
 <pymc.distributions.Poisson 'D[3]' at 0x4ba45f0>,
...
 <pymc.distributions.Poisson 'D[110]' at 0x4ba46d0>]
```

Here r is an array of means for each year of data, allocated according to the location of the switchpoint. Each element in D is a Poisson Stochastic, irrespective of whether the observation was missing or not. The difference is that actual observations are data Stochastics (`observed=True`), while the missing values are non-data Stochastics. The latter are considered unknown, rather than fixed, and therefore estimated by the MCMC algorithm, just as unknown model parameters.

The entire model looks very similar to the original model:

```
# Switchpoint
s = DiscreteUniform('s', lower=0, upper=110)
# Early mean
e = Exponential('e', beta=1)
# Late mean
l = Exponential('l', beta=1)

@deterministic(plot=False)
def r(s=s, e=e, l=l):
    """Allocate appropriate mean to time series"""
    out = np.empty(len(disasters_array))
    # Early mean prior to switchpoint
    out[:s] = e
    # Late mean following switchpoint
    out[s:] = l
    return out

# Where the mask is true, the value is taken as missing.
masked_data = np.ma.masked_array(disasters_array, disasters_mask)
D = ImputeMissing('D', Poisson, masked_data, mu=r)
```

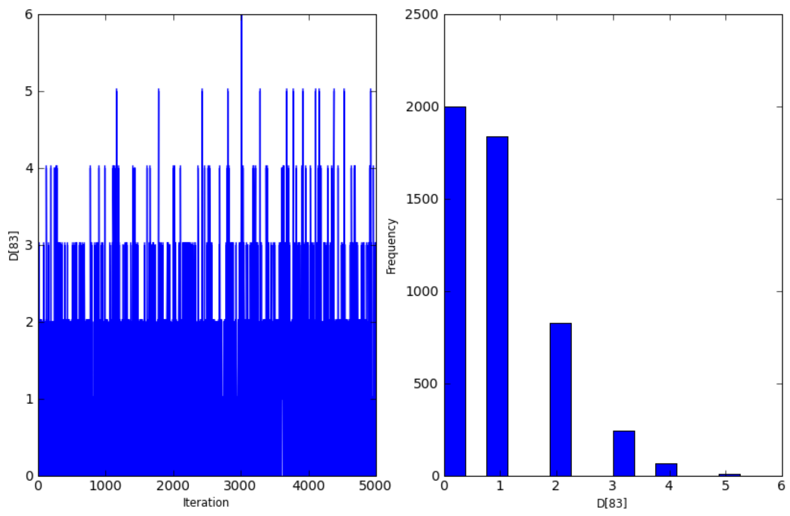


Figure 3.1: Trace and posterior distribution of the second missing data point in the example.

The main limitation of this approach for imputation is performance. Because each element in the data array is modelled by an individual Stochastic, rather than a single Stochastic for the entire array, the number of nodes in the overall model increases from 4 to 113. This significantly slows the rate of sampling, since the model iterates over each node at every iteration.

3.6 Fine-tuning the MCMC algorithm

MCMC objects handle individual variables via *step methods*, which determine how parameters are updated at each step of the MCMC algorithm. By default, step methods are automatically assigned to variables by PyMC. To see which step methods M is using, look at its `step_method_dict` attribute with respect to each parameter:

```
>>> M.step_method_dict[s]
>>> [<pymc.StepMethods.DiscreteMetropolis object at 0x3e8cb50>]

>>> M.step_method_dict[e]
>>> [<pymc.StepMethods.Metropolis object at 0x3e8cbb0>]

>>> M.step_method_dict[l]
>>> [<pymc.StepMethods.Metropolis object at 0x3e8ccb0>]
```

The value of `step_method_dict` corresponding to a particular variable is a list of the step methods M is using to handle that variable.

You can force M to use a particular step method by calling `M.use_step_method` before telling it to sample. The following call will cause M to handle l with a standard `Metropolis` step method, but with proposal standard deviation equal to 2:

```
M.use_step_method(Metropolis, l, proposal_sd=2.)
```

Another step method class, `AdaptiveMetropolis`, is better at handling highly-correlated variables. If your model mixes poorly, using `AdaptiveMetropolis` is a sensible first thing to try.

3.7 Beyond the basics

That was a brief introduction to basic PyMC usage. Many more topics are covered in the subsequent sections, including:

- Class `Potential`, another building block for probability models in addition to `Stochastic` and `Deterministic`
- Normal approximations
- Using custom probability distributions
- Object architecture
- Saving traces to the disk, or streaming them to the disk during sampling
- Writing your own step methods and fitting algorithms.

Also, be sure to check out the documentation for the Gaussian process extension, which is available on the webpage.

CHAPTER
FOUR

Building models

Bayesian inference begins with specification of a probability model relating unknown variables to data. PyMC provides three basic building blocks for Bayesian probability models: `Stochastic`, `Deterministic` and `Potential`.

A `Stochastic` object represents a variable whose value is not completely determined by its parents, and a `Deterministic` object represents a variable that is entirely determined by its parents. In object-oriented programming parlance, `Stochastic` and `Deterministic` are subclasses of the `Variable` class, which only serves as a template and is never actually implemented in models.

The third basic class, `Potential`, represents 'factor potentials' (Lauritzen et al. [1990], Jordan [2004]), which are *not* variables but simply terms and/or constraints that are multiplied into joint distributions to modify them. `Potential` and `Variable` are subclasses of `Node`.

PyMC probability models are simply linked groups of `Stochastic`, `Deterministic` and `Potential` objects. These objects have very limited awareness of the models in which they are embedded and do not themselves possess methods for updating their values in fitting algorithms. Objects responsible for fitting probability models are described in chapter 5.

4.1 The `Stochastic` class

A stochastic variable has the following primary attributes:

`value`: The variable's current value.

`logp`: The log-probability of the variable's current value given the values of its parents.

A stochastic variable can optionally be endowed with a method called `random`, which draws a value for the variable given the values of its parents[1]. Stochastic objects have the following additional attributes that are generally specified automatically, or only specified under particular circumstances:

`parents`: A dictionary containing the variable's parents. The keys of the dictionary correspond to the names assigned to the variable's parents by the variable, and the values correspond to the actual parents. For example, the keys of s's parents dictionary in model (3.1) would be `'t_l'` and `'t_h'`. Thanks to Python's dynamic typing, the actual parents (*i.e.* the values of the dictionary) may be of any class or type.

`children`: A set containing the variable's children.

[1]Note that the `random` method does not provide a Gibbs sample unless the variable has no children.

`extended_parents`: A set containing all the stochastic variables on which the variable depends either directly or via a sequence of deterministic variables. If the value of any of these variables changes, the variable will need to recompute its log-probability.

`extended_children`: A set containing all the stochastic variables and potentials that depend on the variable either directly or via a sequence of deterministic variables. If the variable's value changes, all of these variables will need to recompute their log-probabilities.

`observed`: A flag (boolean) indicating whether the variable's value has been observed (is fixed).

`dtype`: A NumPy dtype object (such as `numpy.int`) that specifies the type of the variable's value to fitting methods. If this is `None` (default) then no type is enforced.

Creation of stochastic variables

There are three main ways to create stochastic variables, called the **automatic**, **decorator**, and **direct** interfaces.

Automatic Stochastic variables with standard distributions provided by PyMC (see chapter 9) can be created in a single line using special subclasses of `Stochastic`. For example, the uniformly-distributed discrete variable s in (3.1) could be created using the automatic interface as follows:

```
s = DiscreteUniform('s', 1851, 1962, value=1900)
```

In addition to the classes in chapter 9, `scipy.stats.distributions`' random variable classes are wrapped as `Stochastic` subclasses if SciPy is installed. These distributions are in the submodule `pymc.SciPyDistributions`.

Users can call the class factory `stochastic_from_dist` to produce `Stochastic` subclasses of their own from probability distributions not included with PyMC.

Decorator Uniformly-distributed discrete stochastic variable s in (3.1) could alternatively be created from a function that computes its log-probability as follows:

```
@stochastic(dtype=int)
def s(value=1900, t_l=1851, t_h=1962):
    """The switchpoint for the rate of disaster occurrence."""
    if value > t_h or value < t_l:
        # Invalid values
        return -numpy.inf
    else:
        # Uniform log-likelihood
        return -numpy.log(t_h - t_l + 1)
```

Note that this is a simple Python function preceded by a Python expression called a **decorator**, here called `@stochastic`. Generally, decorators enhance functions with additional properties or functionality. The `Stochastic` object produced by the `@stochastic` decorator will evaluate its log-probability using the function s. The `value` argument, which is required, provides an initial value for the variable. The remaining arguments will be assigned as parents of s (*i.e.* they will populate the `parents` dictionary).

To emphasize, the Python function decorated by `@stochastic` should compute the *log*-density or *log*-probability of the variable. That is why the return value in the example above is $-\log(t_h - t_l + 1)$ rather than $1/(t_h - t_l + 1)$.

The value and parents of stochastic variables may be any objects, provided the log-probability function return a real number (float). PyMC and SciPy both provide implementations of several standard probability distributions that may be helpful for creating custom stochastic variables. Based on informal comparison, the distributions in PyMC tend to be approximately an order of magnitude faster than their counterparts in SciPy.

The decorator stochastic can take several arguments:

- A flag called trace, which signals to MCMC instances whether an MCMC trace should be kept for this variable. @stochastic(trace = False) would turn tracing off. Defaults to True.
- A flag called plot, which signals to MCMC instances whether summary plots should be produced for this variable. Defaults to True.
- An integer-valued argument called verbose that controls the amount of output the variable prints to the screen. The default is 0, no output; the maximum value is 3.
- A Numpy datatype called dtype. Decorating a log-probability function with @stochastic(dtype=int) would produce a discrete random variable. Such a variable will cast its value to either an integer or an array of integers. The default dtype is float.

The decorator interface has a slightly more complex implementation which allows you to specify a random method for sampling the stochastic variable's value conditional on its parents.

```
@stochastic(dtype=int)
def s(value=1900, t_l=1851, t_h=1962):
    """The switchpoint for the rate of disaster occurrence."""

    def logp(value, t_l, t_h):
        if value > t_h or value < t_l:
            return -Inf
        else:
            return -log(t_h - t_l + 1)

    def random(t_l, t_h):
        return round( (t_l - t_h) * random() ) + t_l
```

The stochastic variable again gets its name, docstring and parents from function *s*, but in this case it will evaluate its log-probability using the logp function. The random function will be used when s.random() is called. Note that random doesn't take a value argument, as it generates values itself. The optional rseed variable provides a seed for the random number generator. The stochastic's value argument is optional when a random method is provided; if no initial value is provided, it will be drawn automatically using the random method.

Direct It's possible to instantiate Stochastic directly:

```
def s_logp(value, t_l, t_h):
    if value > t_h or value < t_l:
        return -Inf
    else:
        return -log(t_h - t_l + 1)

def s_rand(t_l, t_h):
    return round( (t_l - t_h) * random() ) + t_l

s = Stochastic( logp = s_logp,
                doc = 'The switchpoint for the rate of disaster occurrence.',
                name = 's',
                parents = {'t_l': 1851, 't_h': 1962},
                random = s_rand,
                trace = True,
                value = 1900,
                dtype=int,
                rseed = 1.,
                observed = False,
                cache_depth = 2,
                plot=True,
                verbose = 0)
```

Notice that the log-probability and random variate functions are specified externally and passed to `Stochastic` as arguments. This is a rather awkward way to instantiate a stochastic variable; consequently, such implementations should be rare.

Don't update stochastic variables' values in-place

`Stochastic` objects' values should not be updated in-place. This confuses PyMC's caching scheme and corrupts the process used for accepting or rejecting proposed values in the MCMC algorithm. The only way a stochastic variable's value should be updated is using statements of the following form:

```
A.value = new_value
```

The following are in-place updates and should *never* be used:

- `A.value += 3`
- `A.value[2,1] = 5`
- `A.value.attribute = new_attribute_value`.

This restriction becomes onerous if a step method proposes values for the elements of an array-valued variable separately. In this case, it may be preferable to partition the variable into several scalar-valued variables stored in an array or list.

4.2 Data

Although the data are modelled with statistical distributions, their values should be treated as immutable (since they have been observed). Data are represented by `Stochastic` objects whose `observed` attribute is set to `True`. If a stochastic variable's `observed` flag is `True`, its value cannot be changed, and it won't be sampled by the fitting method..

Declaring stochastic variables to be data

In the short and long interfaces, a `Stochastic` object's `observed` flag can be set to true by stacking an `@observed` decorator on top of the `@stochastic` decorator:

```
@observed
@stochastic(dtype=int)
def D(value = count_array, switchpoint = s, early_rate = e, late_rate = l):
    """The observed annual disaster counts."""
    logp = sum(-value[:switchpoint]) + early_rate * log(value[:switchpoint]) \
            - gammaln(early_rate))
    logp += sum(-value[switchpoint:] + late_rate * log(value[switchpoint:]) \
            - gammaln(late_rate))
    return logp
```

In the automatic and direct interfaces, the `observed` argument can be simply set to `True`.

4.3 The `Deterministic` class

The `Deterministic` class represents variables whose values are completely determined by the values of their parents. For example, in model (3.1), r is a `deterministic` variable. Recall it was defined by

$$r_t = \begin{cases} e & t \leq s \\ l & t > s \end{cases},$$

so r's value can be computed exactly from the values of its parents e, l and s.

A `deterministic` variable's most important attribute is `value`, which gives the current value of the variable given the values of its parents. Like `Stochastic`'s `logp` attribute, this attribute is computed on-demand and cached for efficiency.

A Deterministic variable has the following additional attributes:

`parents`: A dictionary containing the variable's parents. The keys of the dictionary correspond to the names assigned to the variable's parents by the variable, and the values correspond to the actual parents. Thanks to Python's dynamic typing, parents may be of any class or type.

`children`: A set containing the variable's children, which must be nodes.

Deterministic variables have no methods.

Creation of deterministic variables

Deterministic variables are less complicated than stochastic variables, and have similar **automatic**, **decorator**, and **direct** interfaces:

Automatic A handful of common functions have been wrapped in Deterministic objects. These are brief enough to list:

`LinearCombination`: Has two parents x and y, both of which must be iterable (*i.e.* vector-valued). This function returns:

$$\sum_i x_i^T y_i.$$

`Index`: Has three parents x, y and `index`. x and y must be iterables, `index` must be valued as an integer. Index returns the dot product of x and y for the elements specified by `index`:

$$x[\mathtt{index}]^T y[\mathtt{index}].$$

`Index` is useful for implementing dynamic models, in which the parent-child connections change.

`Lambda`: Converts an anonymous function (in Python, called **lambda functions**) to a `Deterministic` instance on a single line.

`CompletedDirichlet`: PyMC represents Dirichlet variables of length k by the first $k-1$ elements; since they must sum to 1, the k^{th} element is determined by the others. `CompletedDirichlet` appends the k^{th} element to the value of its parent D.

`Logit`, `InvLogit`, `StukelLogit`, `StukelInvLogit`: Various common link functions for generalized linear models.

It's a good idea to use these classes when feasible, because certain fitting methods (Gibbs step methods in particular) implicitly know how to take them into account.

Decorator A deterministic variable can be created via a decorator in a way very similar to `Stochastic`'s decorator interface:

```
@deterministic
def r(switchpoint = s, early_rate = e, late_rate = l):
    """The rate of disaster occurrence."""
    value = zeros(N)
    value[:switchpoint] = early_rate
    value[switchpoint:] = late_rate
    return value
```

Notice that rather than returning the log-probability, as is the case for `Stochastic` objects, the function returns the value of the deterministic object, given its parents. This return value may be of any type, as is suitable for the problem at hand. Arguments' keys and values are converted into a parent dictionary as with `Stochastic`'s short interface. The `deterministic` decorator can take `trace`, `verbose` and `plot` arguments, like the `stochastic` decorator[2].

Of course, since deterministic nodes are not expected to generate random variates, the longer implementation of the decorator interface available to `Stochastic` objects is not relevant here.

[2]Note that deterministic variables have no `observed` flag. If a deterministic variable's value were known, its parents would be restricted to the inverse image of that value under the deterministic variable's evaluation function. This usage would be extremely difficult to support in general, but it can be implemented for particular applications at the `StepMethod` level.

Direct Deterministic objects can also be instantiated directly, by passing the evaluation function to the `Deterministic` class as an argument:

```
def r_eval(switchpoint = s, early_rate = e, late_rate = l):
    value = zeros(N)
    value[:switchpoint] = early_rate
    value[switchpoint:] = late_rate
    return value

r = Deterministic(  eval = r_eval,
                    name = 'r',
                    parents = {'switchpoint': s, 'early_rate': e, 'late_rate': l}),
                    doc = 'The rate of disaster occurrence.',
                    trace = True,
                    verbose = 0,
                    dtype=float,
                    plot=False,
                    cache_depth = 2)
```

4.4 Containers

In some situations it would be inconvenient to assign a unique label to each parent of some variable. Consider y in the following model:

$$\begin{aligned} x_0 &\sim \mathrm{N}(0, \tau_x) \\ x_{i+1}|x_i &\sim \mathrm{N}(x_i, \tau_x) \qquad\qquad i = 0, \ldots, N-2 \\ y|x &\sim \mathrm{N}\left(\sum_{i=0}^{N-1} x_i^2, \tau_y\right) \end{aligned}$$

Here, y depends on every element of the Markov chain x, but we wouldn't want to manually enter N parent labels `‘x_0’`, `‘x_1’`, etc.

This situation can be handled naturally in PyMC:

```
x_0 = Normal('x_0', mu=0, tau=1)

# Initialize array of stochastics
x = [x_0]

# Loop over number of elements in N
for i in range(1,N):

   # Instantiate Normal stochastic, based on value of previous element in x
   xi = Normal('x_%i' % i, mu=x[-1], tau=1)

   # Append to x
   x.append(xi)

@observed
@stochastic
def y(value = 1, mu = x, tau = 100):

    # Initialize sum of mu's
    mu_sum = 0

    for i in range(N):
        # Append squared mu
        mu_sum += mu[i] ** 2

    # Calculate and return log-likelihood
    return normal_like(value, mu_sum, tau)
```

PyMC automatically wraps list x in an appropriate `Container` class. The expression `'x_%i' %i` labels each `Normal` object in the container with the appropriate index i.

Containers, like variables, have an attribute called `value`. This attribute returns a copy of the (possibly nested) iterable that was passed into the container function, but with each variable inside replaced with its corresponding value.

Containers can currently be constructed from lists, tuples, dictionaries, Numpy arrays, modules, sets or any object with a `__dict__` attribute. Variables and non-variables can be freely mixed in these containers, and different types of containers can be nested[3]. Containers attempt to behave like the objects they wrap. All containers are subclasses of `ContainerBase`.

Containers have the following useful attributes in addition to `value`:

- `variables`
- `stochastics`
- `potentials`
- `deterministics`
- `data_stochastics`
- `step_methods`.

[3]Nodes whose parents are containers make private shallow copies of those containers. This is done for technical reasons rather than to protect users from accidental misuse.

Each of these attributes is a set containing all the objects of each type in a container, and within any containers in the container.

4.5 The `Potential` class

The joint density corresponding to model (3.1) can be written as follows:

$$p(D,s,l,e) = p(D|s,l,e)p(s)p(l)p(e).$$

Each factor in the joint distribution is a proper, normalized probability distribution for one of the variables conditional on its parents. Such factors are contributed by `Stochastic` objects.

In some cases, it's nice to be able to modify the joint density by incorporating terms that don't correspond to probabilities of variables conditional on parents, for example:

$$p(x_0, x_2, \ldots x_{N-1}) \propto \prod_{i=0}^{N-2} \psi_i(x_i, x_{i+1}).$$

In other cases we may want to add probability terms to existing models. For example, suppose we want to constrain the difference between e and l in (3.1) to be less than 1, so that the joint density becomes

$$p(D,s,l,e) \propto p(D|s,l,e)p(s)p(l)p(e)1_{|e-l|<1}.$$

It's possible to express this constraint by adding variables to the model, or by grouping e and l to form a vector-valued variable, but it's uncomfortable to do so.

Arbitrary factors such as ψ and $1_{|e-l|<1}$ are contributed by objects of class `Potential` (Lauritzen et al. [1990] and Jordan [2004] call these terms 'factor potentials'). Bayesian hierarchical notation (cf model (3.1)) doesn't accomodate these potentials. They are often used in cases where there is no natural dependence hierarchy, such as the first example above (which is known as a Markov random field). They are also useful for expressing 'soft data' [Christakos, 2002] as in the second example above.

Potentials have one important attribute, `logp`, the log of their current probability or probability density value given the values of their parents. The only other additional attribute of interest is `parents`, a dictionary containing the potential's parents. Potentials have no methods. They have no `trace` attribute, because they are not variables. They cannot serve as parents of variables (for the same reason), so they have no `children` attribute.

A more extended example

The role of potentials can be confusing, so we will provide another example: we have a dataset t consisting of the days on which several marked animals were recaptured. We believe that the probability S that an animal is not recaptured on any given day can be explained by a covariate vector x. We model this situation as follows:

$$\begin{aligned} t_i|S_i &\sim \text{Geometric}(S_i), \quad i = 1 \ldots N \\ S_i &= \text{logit}^{-1}(\beta x_i), \quad i = 1 \ldots N \\ \beta &\sim \text{N}(\mu_\beta, V_\beta). \end{aligned}$$

So far, so good. Now suppose we have some knowledge of other related experiments and we have a good idea of what S will be independent of the value of β. It's not obvious how to work this 'soft data', because as we've written the model S is completely determined by β. There are three options within the strict Bayesian hierarchical framework:

- Work the soft data into the prior on β.
- Incorporate the data from the previous experiments explicitly into the model.
- Refactor the model so that S is at the bottom of the hierarchy, and assign the prior directly.

Factor potentials provide a convenient way to incorporate the soft data without the need for such major modifications. We can simply modify the joint distribution from

$$p(t|S(x,\beta))p(\beta)$$

to

$$\gamma(S)p(t|S(x,\beta))p(\beta),$$

where the value of γ is large if S's value is plausible (based on our external information) and small otherwise. We do not know the normalizing constant for the new distribution, but we don't need it to use most popular fitting algorithms. It's a good idea to check the induced priors on S and β for sanity. This can be done in PyMC by fitting the model with the data t removed.

It's important to understand that γ is not a variable, so it does not have a value. That means, among other things, there will be no γ column in MCMC traces. γ is simply an extra term that we are incorporating in the joint distribution.

Creation of `Potentials`

There are two ways to create potentials:

Decorator A potential can be created via a decorator in a way very similar to `Deterministic`'s decorator interface:

```
@potential
def psi_i(x_lo = x[i], x_hi = x[i+1]):
    """A pair potential"""
    return -(xlo - xhi)**2
```

The function supplied should return the potential's current *log*-probability or *log*-density as a Numpy `float`. The `potential` decorator can take `verbose` and `cache_depth` arguments like the `stochastic` decorator.

Direct The same potential could be created directly as follows:

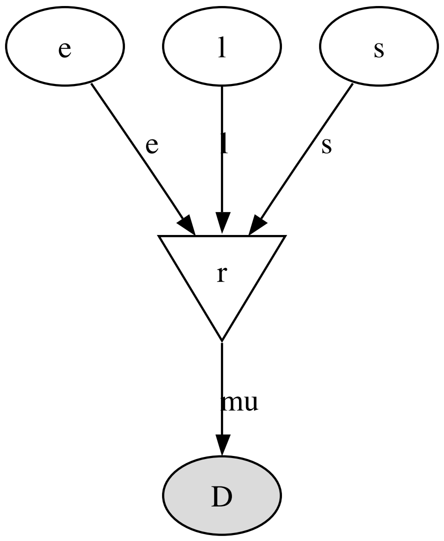
```
def psi_i_logp(x_lo = x[i], x_hi = x[i+1]):
    return -(xlo - xhi)**2

psi_i = Potential(  logp = psi_i_logp,
                    name = 'psi_i',
                    parents = {'xlo': x[i], 'xhi': x[i+1]},
                    doc = 'A pair potential',
                    verbose = 0,
                    cache_depth = 2)
```

4.6 Graphing models

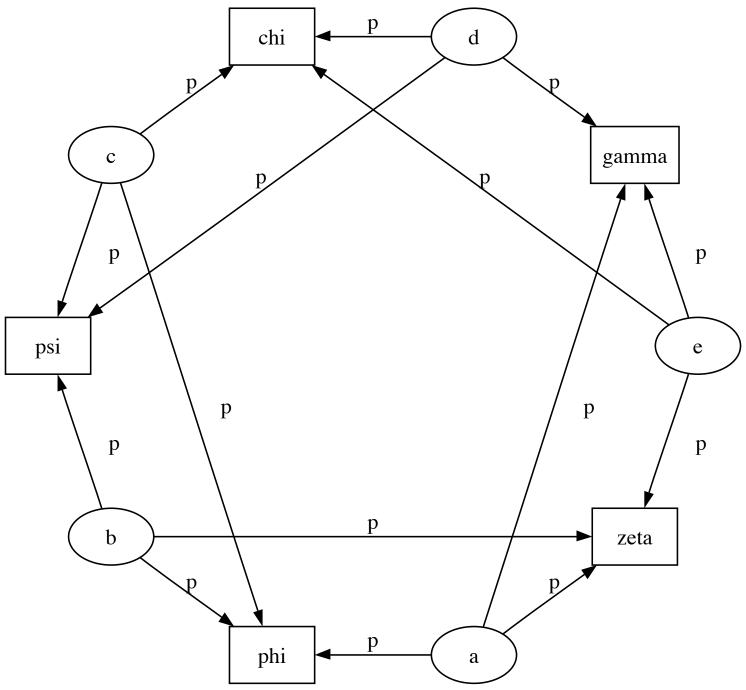
The function `pymc.graph.graph` draws graphical representations of `Model` (Chapter 5) instances using GraphViz via the Python package PyDot (if they are installed). See Lauritzen et al. [1990] and Jordan [2004] for more discussion of useful information that can be read off of graphical models. Note that these authors do not consider deterministic variables.

The symbol for stochastic variables is an ellipse. Parent-child relationships are indicated by arrows. These arrows point from parent to child and are labeled with the names assigned to the parents by the children. PyMC's symbol for deterministic variables is a downward-pointing triangle. A graphical representation of model 3.1 follows:

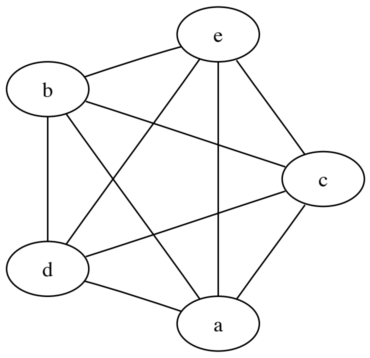


D is shaded because it is flagged as data.

The symbol for factor potentials is a rectangle, as in the following model.



Factor potentials are usually associated with *undirected* grahical models. In undirected representations, each parent of a potential is connected to every other parent by an undirected edge. The undirected representation of the model pictured above is much more compact:



Directed or mixed graphical models can be represented in an undirected form by 'moralizing', which is done by the function `pymc.graph.moral_graph`.

4.7 Class `LazyFunction` and caching

This section gives an overview of PyMC's computational innards. You don't need this information to use PyMC.

The `logp` attributes of stochastic variables and potentials and the `value` attributes of deterministic variables are wrappers for instances of class `LazyFunction`. Lazy functions are wrappers for ordinary Python functions. A lazy function `L` could be created from a function `fun` as follows:

```
L = LazyFunction(fun, arguments)
```

The argument `arguments` is a dictionary container; `fun` must accept keyword arguments only. When L's `get()` method is called, the return value is the same as the call

```
fun(**arguments.value)
```

Note that no arguments need to be passed to `L.get`; lazy functions memorize their arguments.

Before calling `fun`, `L` will check the values of `arguments.variables` against an internal cache. This comparison is done *by reference*, not by value, and this is part of the reason why stochastic variables' values cannot be updated in-place. If `arguments.variables`' values match a frame of the cache, the corresponding output value is returned and `fun` is not called. If a call to `fun` is needed, `arguments.variables`' values and the return value replace the oldest frame in the cache. The depth of the cache can be set using the optional init argument `cache_depth`, which defaults to 2.

Caching is helpful in MCMC, because variables' log-probabilities and values tend to be queried multiple times for the same parental value configuration. The default cache depth of 2 turns out to be most useful in Metropolis-Hastings-type algorithms involving proposed values that may be rejected.

Lazy functions are implemented in C using Pyrex, a language for writing Python extensions.

CHAPTER

FIVE

Fitting models

PyMC probability models are linked collections of nodes. These nodes are only informed by the values of their parents. `Deterministic` instances can compute their values given their parents' values, `Stochastic` instances can compute their log-probabilities or draw new values, and `Potential` instances can compute their log-probabilities. Fitting probability models requires larger-scale coordination and communication.

PyMC provides three objects that fit models:

- `MCMC`, which coordinates Markov chain Monte Carlo algorithms. The actual work of updating stochastic variables conditional on the rest of the model is done by `StepMethod` objects, which are described in this chapter.
- `MAP`, which computes maximum *a posteriori* estimates.
- `NormApprox`, which computes the 'normal approximation' [Gelman et al., 2004]: the joint distribution of all stochastic variables in a model is approximated as normal using local information at the maximum *a posteriori* estimate.

All three objects are subclasses of `Model`, which is PyMC's base class for fitting methods. `MCMC` and `NormApprox`, both of which can produce samples from the posterior, are subclasses of `Sampler`, which is PyMC's base class for Monte Carlo fitting methods. `Sampler` provides a generic sampling loop method and database support for storing large sets of joint samples. These base classes implement some basic methods that are inherited by the three implemented fitting methods, so they are documented at the end of this chapter.

5.1 Creating models

The first argument to any fitting method's `init` method, including that of `MCMC`, is called `input`. The `input` argument can be just about anything; once you have defined the nodes that make up your model, you shouldn't even have to think about how to wrap them in a `Model` instance. Some examples of model instantiation using nodes `a`, `b` and `c` follow:

- `M = Model(set([a,b,c]))`
- `M = Model({'a': a, 'd': [b,c]})` In this case, M will expose a and d as attributes: `M.a` will be a, and `M.d` will be `[b,c]`.
- `M = Model([[a,b],c])`
- If file `MyModule` contains the definitions of `a`, `b` and `c`:

```
        import MyModule
        M = Model(MyModule)
```

In this case, M will expose a, b and c as attributes.

- Using a 'model factory' function:

```
        def make_model(x):
            a = Exponential('a',.5,beta=x)

            @deterministic
            def b(a=a):
                return 100-a

            @stochastic
            def c(value=.5, a=a, b=b);
                return (value-a)**2/b

            return locals()

        M = Model(make_model(3))
```

In this case, M will also expose a, b and c as attributes.

5.2 Maximum *a posteriori* estimates

The `MAP` class sets all stochastic variables to their maximum *a posteriori* values using functions in SciPy's `optimize` package. SciPy must be installed to use it. `MAP` can only handle variables whose dtype is `float`, so it will not work on model 3.1. To fit the model in 'examples/gelman_bioassay.py' using `MAP`, do the following

```
    >>> import gelman_bioassay
    >>> M = MAP(gelman_bioassay)
    >>> M.fit()
```

This call will cause M to fit the model using Nelder-Mead optimization, which does not require derivatives. The variables in `DisasterModel` have now been set to their maximum *a posteriori* values:

```
    >>> M.alpha.value
    array(0.8465892309923545)
    >>> M.beta.value
    array(7.7488499785334168)
```

In addition, the AIC and BIC of the model are now available:

```
>>> M.AIC
7.9648372671389458
>>> M.BIC
6.7374259893787265
```

`MAP` has two useful methods:

`fit(method ='fmin', iterlim=1000, tol=.0001)`: The optimization method may be `fmin`, `fmin_l_bfgs_b`, `fmin_ncg`, `fmin_cg`, or `fmin_powell`. See the documentation of SciPy's `optimize` package for the details of these methods. The `tol` and `iterlim` parameters are passed to the optimization function under the appropriate names.

`revert_to_max()`: If the values of the constituent stochastic variables change after fitting, this function will reset them to their maximum *a posteriori* values.

If you're going to use an optimization method that requires derivatives, `MAP`'s `init` method can take additional parameters `eps` and `diff_order`. `diff_order`, which must be an integer, specifies the order of the numerical approximation (see the SciPy function `derivative`). The step size for numerical derivatives is controlled by `eps`, which may be either a single value or a dictionary of values whose keys are variables (actual objects, not names).

The useful attributes of `MAP` are:

`logp`: The joint log-probability of the model.

`logp_at_max`: The maximum joint log-probability of the model.

`AIC`: Akaike's information criterion for this model [Akaike, 1973, Burnham and Anderson, 2002].

`BIC`: The Bayesian information criterion for this model [Schwarz, 1978].

One use of the `MAP` class is finding reasonable initial states for MCMC chains. Note that multiple `Model` subclasses can handle the same collection of nodes.

5.3 Normal approximations

The `NormApprox` class extends the `MAP` class by approximating the posterior covariance of the model using the Fisher information matrix, or the Hessian of the joint log probability at the maximum. To fit the model in 'examples/gelman_bioassay.py' using `NormApprox`, do:

```
>>> N = NormApprox(gelman_bioassay)
>>> N.fit()
```

The approximate joint posterior mean and covariance of the variables are available via the attributes `mu` and `C`:

```
>>> N.mu[N.alpha]
array([ 0.84658923])
>>> N.mu[N.alpha, N.beta]
array([ 0.84658923,  7.74884998])
>>> N.C[N.alpha]
matrix([[ 1.03854093]])
>>> N.C[N.alpha, N.beta]
matrix([[  1.03854093,   3.54601911],
        [  3.54601911,  23.74406919]])
```

As with MAP, the variables have been set to their maximum *a posteriori* values (which are also in the mu attribute) and the AIC and BIC of the model are available.

In addition, it's now possible to generate samples from the posterior as with MCMC:

```
>>> N.sample(100)
>>> N.trace('alpha')[::10]
array([-0.85001278,  1.58982854,  1.0388088 ,  0.07626688,  1.15359581,
       -0.25211939,  1.39264616,  0.22551586,  2.69729987,  1.21722872])
>>> N.trace('beta')[::10]
array([  2.50203663,  14.73815047,  11.32166303,   0.43115426,
        10.1182532 ,   7.4063525 ,  11.58584317,   8.99331152,
        11.04720439,   9.5084239 ])
```

Any of the database backends can be used (chapter 6).

In addition to the methods and attributes of MAP, NormApprox provides the following methods:

sample(iter): Samples from the approximate posterior distribution are drawn and stored.

isample(iter): An 'interactive' version of sample(): sampling can be paused, returning control to the user.

draw: Sets all variables to random values drawn from the approximate posterior.

It provides the following additional attributes:

mu: A special dictionary-like object that can be keyed with multiple variables. N.mu[p1, p2, p3] would return the approximate posterior mean values of stochastic variables p1, p2 and p3, ravelled and concatenated to form a vector.

C: Another special dictionary-like object. N.C[p1, p2, p3] would return the approximate posterior covariance matrix of stochastic variables p1, p2 and p3. As with mu, these variables' values are ravelled and concatenated before their covariance matrix is constructed.

5.4 Markov chain Monte Carlo: the MCMC class

The MCMC class implements PyMC's core business: producing 'traces' for a model's variables which, with careful thinning, can be considered independent joint samples from the posterior. See chapter 3 for an example of basic usage.

MCMC's primary job is to create and coordinate a collection of 'step methods', each of which is responsible for updating one or more variables. The available step methods are described below. Instructions on how to create your own step method are available in chapter 8.

MCMC provides the following useful methods:

`sample(iter, burn=0, thin=1, tune_interval=1000, verbose=0)`: Runs the MCMC algorithm and produces the traces. The `iter` argument controls the total number of MCMC iterations. No tallying will be done during the first `burn` iterations; these samples will be forgotten. After this burn-in period, tallying will be done each `thin` iterations. Tuning will be done each `tune_interval` iterations.

`isample(iter, burn=0, thin=1, tune_interval=1000, verbose=0)`: An interactive version of `sample`. The sampling loop may be paused at any time, returning control to the user.

`use_step_method(method, *args, **kwargs)`: Creates an instance of step method class `method` to handle some stochastic variables. The extra arguments are passed to the `init` method of `method`. Assigning a step method to a variable manually will prevent the MCMC instance from automatically assigning one. However, you may handle a variable with multiple step methods.

`goodness()`: Calculates goodness-of-fit (GOF) statistics according to Brooks et al. [2000].

`save_state()`: Saves the current state of the sampler, including all stochastics, to the database. This allows the sampler to be reconstituted at a later time to resume sampling. This is not supported yet for the RDBMS backends, sqlite and mysql.

`restore_state()`: Restores the sampler to the state stored in the database.

`stats()`: Generate summary statistics for all nodes in the model.

`remember(trace_index)`: Set all variables' values from frame `trace_index` in the database.

MCMC samplers' step methods can be accessed via the `step_method_dict` attribute. `M.step_method_dict[x]` returns a list of the step methods `M` will use to handle the stochastic variable `x`.

5.5 Step methods

Step method objects handle individual stochastic variables, or sometimes groups of them. They are responsible for making the variables they handle take single MCMC steps conditional on the rest of the model. Each subclass of `StepMethod` implements a method called `step()`, which is called by MCMC. Step methods with adaptive tuning parameters can optionally implement a method called `tune()`, which causes them to assess performance so far and adjust.

The major subclasses of `StepMethod` are `Metropolis` and `Gibbs`. PyMC provides several flavors of the basic Metropolis steps, but the Gibbs steps are not ready for use as of the current release.

Metropolis step methods

`Metropolis` and subclasses implement Metropolis-Hastings steps. To tell an MCMC object M to handle a variable x with a Metropolis step method, you might do the following:

```
M.use_step_method(Metropolis, x, proposal_sd=1., proposal_distribution='Normal')
```

Metropolis itself handles float-valued variables, and subclasses DiscreteMetropolis and BinaryMetropolis handle integer- and boolean-valued variables, respectively. Subclasses of Metropolis must implement the following methods:

propose(): Sets the values of the variables handled by the Metropolis step method to proposed values.

reject(): If the Metropolis-Hastings acceptance test fails, this method is called to reset the values of the variables to their values before propose() was called.

Note that there is no accept() method; if a proposal is accepted, the variables' values are simply left alone. Subclasses that use proposal distributions other than symmetric random-walk may specify the 'Hastings factor' by changing the hastings_factor method. See chapter 8 for an example.

Metropolis' init method takes the following arguments:

stochastic: The variable to handle.

proposal_sd: A float or array of floats. This sets the proposal standard deviation if the proposal distribution is normal.

scale: A float, defaulting to 1. If the scale argument is provided but not proposal_sd, proposal_sd is computed as follows:

```
if all(self.stochastic.value != 0.):
    self.proposal_sd = ones(shape(self.stochastic.value)) * \
                        abs(self.stochastic.value) * scale
else:
    self.proposal_sd = ones(shape(self.stochastic.value)) * scale
```

proposal_distribution: A string indicating which distribution should be used for proposals. Current options are 'Normal' and 'Prior'. If proposal_distribution=None, the proposal distribution is chosen automatically. It is set to 'Prior' if the variable has no children and has a random method, and to 'Normal' otherwise.

verbose: An integer.

Metropolis step methods adjust their initial proposal standard deviations using an attribute called adaptive_scale_factor. When tune() is called, the acceptance ratio of the step method is examined and this scale factor is updated accordingly. If the proposal distribution is normal, proposals will have standard deviation self.proposal_sd * self.adaptive_scale_factor. It is usually OK to keep tuning throughout the MCMC loop even though the resulting chain is not actually Markov [Levine et al., 2005].

If a Metropolis step method handles an array-valued variable, it proposes all elements independently but simultaneously. That is, it decides whether to accept or reject all elements together but it does not attempt to take the posterior correlation between elements into account. The AdaptiveMetropolis class (see below), on the other hand, does make correlated proposals.

The DiscreteMetropolis class

This class is just like Metropolis, but specialized to handle Stochastic instances with dtype int. The jump proposal distribution can either be 'Normal', 'Prior' or 'Poisson'. In the normal case, the proposed value is drawn from a normal distribution centered at the current value and then rounded to the nearest integer.

The `BinaryMetropolis` class

This class is specialized to handle `Stochastic` instances with dtype `bool`.

For array-valued variables, `BinaryMetropolis` can be set to propose from the prior by passing in `dist="Prior"`. Otherwise, the argument `p_jump` of the init method specifies how probable a change is. Like `Metropolis`' attribute `proposal_sd`, `p_jump` is tuned throughout the sampling loop via `adaptive_scale_-factor`.

For scalar-valued variables, `BinaryMetropolis` behaves like a Gibbs sampler, since this requires no additional expense. The `p_jump` and `adaptive_scale_factor` parameters are not used in this case.

The `AdaptiveMetropolis` class

The `AdaptatativeMetropolis` (AM) step method works like a regular Metropolis step method, with the exception that its variables are block-updated using a multivariate jump distribution whose covariance is tuned during sampling. Although the chain is non-Markovian, it has correct ergodic properties (see Haario et al. [2001]).

To tell an `MCMC` object M to handle variables x, y and z with an `AdaptiveMetropolis` instance, you might do the following:

```
M.use_step_method(AdaptiveMetropolis, [x,y,z], \
                  scales={'x':1, 'y':2, 'z':.5}, delay=10000)
```

`AdaptatativeMetropolis`' init method takes the following arguments:

`stochastics`: The stochastic variables to handle. These will be updated jointly.

`cov` **(optional):** An initial covariance matrix. Defaults to the identity matrix, adjusted according to the `scales` argument.

`delay` **(optional):** The number of iterations to delay before computing the empirical covariance matrix.

`scales` **(optional):** The initial covariance matrix will be diagonal, and its diagonal elements will be set to `scales` times the stochastics' values, squared.

`interval` **(optional):** The number of iterations between updates of the covariance matrix. Defaults to 1000.

`greedy` **(optional):** If `True`, only accepted jumps will be counted toward the delay before the covariance is first computed. Defaults to `True`.

`verbose`: An integer from 0 to 3 controlling the verbosity of the step method's printed output.

In this algorithm, jumps are proposed from a multivariate normal distribution with covariance matrix Σ. The algorithm first iterates until `delay` samples have been drawn (if `greedy` is true, until `delay` jumps have been accepted). At this point, Σ is given the value of the empirical covariance of the trace so far and sampling resumes. The covariance is then updated each `interval` iterations throughout the entire sampling run[1]. It is this constant adaptation of the proposal distribution that makes the chain non-Markovian.

[1]The covariance is estimated recursively from the previous value and the last `interval` samples, instead of computing it each time from the entire trace.

Granularity of step methods: one-at-a-time vs. block updating

There is currently no way for a stochastic variable to compute individual terms of its log-probability; it is computed all together. This means that updating the elements of a array-valued variable individually would be inefficient, so all existing step methods update array-valued variables together, in a block update.

To update an array-valued variable's elements individually, simply break it up into an array of scalar-valued variables. Instead of this:

```
A = Normal('A', value=zeros(100), mu=0., tau=1.)
```

do this:

```
A = [Normal('A_%i'%i, value=0., mu=0., tau=1.) for i in xrange(100)]
```

An individual step method will be assigned to each element of `A` in the latter case, and the elements will be updated individually. Note that `A` can be broken up into larger blocks if desired.

Automatic assignment of step methods

Every step method subclass (including user-defined ones) that does not require any `init` arguments other than the stochastic variable to be handled adds itself to a list called `StepMethodRegistry` in the PyMC namespace. If a stochastic variable in an `MCMC` object has not been explicitly assigned a step method, each class in `StepMethodRegistry` is allowed to examine the variable.

To do so, each step method implements a class method called `competence(stochastic)`, whose only argument is a single stochastic variable. These methods return values from 0 to 3; 0 meaning the step method cannot safely handle the variable and 3 meaning it will most likely perform well for variables like this. The `MCMC` object assigns the step method that returns the highest competence value to each of its stochastic variables.

5.6 The `Model` class

This class serves as a container for probability models and as a base class for the classes responsible for model fitting, such as `MCMC`. Like any Python class, its properties are inherited by subclasses.

`Model`'s init method takes the following arguments:

`input`: Some collection of PyMC nodes defining a probability model. These may be stored in a list, set, tuple, dictionary, array, module, or any object with a `__dict__` attribute.

`verbose` **(optional):** An integer controlling the verbosity of the model's output.

Models' useful methods are:

`draw_from_prior()`: Sets all stochastic variables' values to new random values, which would be a sample from the joint distribution if all data and `Potential` instances' log-probability functions returned zero. If any stochastic variables lack a`random()` method, PyMC will raise an exception.

`seed()`: Same as `draw_from_prior`, but only `stochastics` whose `rseed` attribute is not `None` are changed.

`find_generations()`: Sets the `generations` attribute. This attribute is a list whose elements are sets of stochastic variables. The zeroth set has no extended parents in the model, the first set only has extended parents in the zeroth set, and so on.

The helper function `graph` produces graphical representations of models [Jordan, 2004, see].

Models have the following important attributes:

- `variables`
- `stochastics`
- `potentials`
- `deterministics`
- `data_stochastics`
- `step_methods`
- `value`

In addition, models expose each node they contain as an attribute. For instance, if model `M` were produced from model (3.1) `M.s` would return the switchpoint variable. It's a good idea to give each variable a unique name if you want to access them this way.

5.7 The Sampler class

Samplers fit models with Monte Carlo fitting methods, which characterize the posterior distribution by approximate samples from it. They are initialized as follows: `Sampler(input=None, db='ram', name='Sampler', reinit_model=True, calc_deviance=False)`. The `input` argument is a module, list, tuple, dictionary, set, or object that contains all elements of the model, the `db` argument indicates which database backend should be used to store the samples (see chapter 6), `reinit_model` is a boolean flag that indicates whether the model should be re-initialised before running, and `calc_deviance` is a boolean flag indicating whether deviance should be calculated for the model at each iteration. Samplers have the following important methods:

`sample(iter, length=None, verbose=0)`: Samples from the joint distribution. The `iter` argument controls how many times the sampling loop will be run, and the `length` argument controls the initial size of the database that will be used to store the samples.

`isample(iter, length=None, verbose=0)`: The same as `sample`, but the sampling is done interactively: you can pause sampling at any point and be returned to the Python prompt to inspect progress and adjust fitting parameters. While sampling is paused, the following methods are useful:

`icontinue()`: Continue interactive sampling.

`halt()`: Truncate the database and clean up.

`tally()`: Write all variables' current values to the database. The actual write operation depends on the specified database backend.

`save_state()`: Saves the current state of the sampler, including all stochastics, to the database. This allows the sampler to be reconstituted at a later time to resume sampling. This is not supported yet for the RDBMS backends, sqlite and mysql.

`restore_state()`: Restores the sampler to the state stored in the database.

`stats()`: Generate summary statistics for all nodes in the model.

`remember(trace_index)`: Set all variables' values from frame `trace_index` in the database. Note that the `trace_index` is different from the current iteration, since not all samples are necessarily saved due to burning and thinning.

In addition, the sampler attribute `deviance` is a deterministic variable valued as the model's deviance at its current state.

CHAPTER
SIX

Saving and managing sampling results

In the examples seen so far, traces are simply held in memory and discarded once the Python session ends. PyMC provides the means to store these traces on disk, load them back and add additional samples. Internally, this is implemented in what we call *database backends*. Each one of these backends is simply made of two classes: `Database` and `Trace` which all present a similar interface to users. At the moment, PyMC counts seven such backends: `ram`, `no_trace`, `pickle`, `txt`, `sqlite`, `mysql` and `hdf5`. In the following, we present the common interface to those backends and a description of each individual backend.

6.1 Accessing Sampled Data

To recommended way to access data from an MCMC run, irrespective of the database backend, is to use the `trace(name, chain=-1)` method:

```
>>> M = MCMC(DisasterModel)
>>> M.sample(10)
>>> M.trace('e')[:]
array([ 2.28320992,  2.28320992,  2.28320992,  2.28320992,  2.28320992,
        2.36982455,  2.36982455,  3.1669422 ,  3.1669422 ,  3.14499489])
```

`M.trace('e')` returns the `Trace` instance associated with the tallyable object *e*:

```
>>> M.trace('e')
<pymc.database.ram.Trace object at 0x7fa4877a8b50>
```

This `Trace` object from the `ram` backend has a `__getitem__` method that is used to access the trace, just as with any other NumPy array. By default, `trace` returns the samples from the last chain (chain=-1), which in this case is equivalent to `chain=0`. To return the samples from all the chains, use `chain=None`:

```
>>> M.sample(5)
>>> M.trace('e', chain=None)[:]
array([ 2.28320992,  2.28320992,  2.28320992,  2.28320992,  2.28320992,
        2.36982455,  2.36982455,  3.1669422 ,  3.1669422 ,  3.14499489,
        3.14499489,  3.14499489,  3.14499489,  2.94672454,  3.10767686])
```

6.2 Saving Data to Disk

By default, the database backend selected by the `MCMC` sampler is the `ram` backend, which simply holds the data in RAM memory. Now, we will create a sampler that, instead, will write data to a pickle file:

```
>>> M = MCMC(DisasterModel, db='pickle', dbname='Disaster.pickle')
>>> M.db
<pymc.database.pickle.Database object at 0x7fa486623d90>

>>> M.sample(10)
>>> M.db.commit()
```

Note that in this particular case, no data is written to disk before the call to `db.commit`. The `commit` call creates a file named *Disaster.pickle* that contains the trace of each tallyable object as well as the final state of the sampler. This means that a user that forgets to call the `commit` method runs the risk of losing his data. Some backends write the data to disk continuously, so that not calling `commit` is less of an issue.

In general, however, it is recommended to always call the `db.close` method before closing the session. The `close` method first calls `commit`, and goes further in making sure that the database is in a safe state. Once `close` has been called, further call to `sample` will likely fail, at least for some backends.

Warning

Always call the `close` method before closing the session to avoid running the risk of losing your data.

6.3 Loading Back a Database

To load a file created in a previous session, use the `load` function from the backend that created the database:

```
>>> db = pymc.database.pickle.load('Disaster.pickle')
>>> len(db.trace('e')[:])
10
```

The `db` object also has a `trace` method identical to that of `Sampler`. You can hence inspect the results of a model, even when you don't have the model around.

To add samples to this file, we need to create an MCMC instance. This time, instead of setting `db='pickle'`, we will pass the existing `Database` instance:

```
>>> M = MCMC(DisasterModel, db=db)
>>> M.sample(5)
>>> len(M.trace('e', chain=None)[:])
15
>>> M.db.close()
```

6.4 Backends Description

ram

Used by default, this backend simply holds a copy in memory, with no output written to disk. This is useful for short runs or testing. For long runs generating large amount of data, using this backend may fill the available memory, forcing the OS to store data in the cache, slowing down all running applications on your computer.

no_trace

This backend simply does not store the trace. This may be useful for testing purposes.

txt

With the `txt` backend, the data is written to disk in ASCII files. More precisely, the `dbname` argument is used to create a top directory into which chain directories, called `Chain_<#>`, are going to be created each time `sample` is called:

```
dbname/
  Chain_0/
    <object0 name>.txt
    <object1 name>.txt
    ...
  Chain_1/
    <object0 name>.txt
    <object1 name>.txt
    ...
  ...
```

In each one of these chain directories, files named `<variable name>.txt` are created, storing the values of the variable as rows of text:

```
# Variable: e
# Sample shape: (5,)
# Date: 2008-11-18 17:19:13.554188
3.033672373807017486e+00
3.033672373807017486e+00
...
```

Although this backend makes it easy to load the data using another application, for large datasets files tend to be embarassingly large and slow to load into memory.

pickle

The `pickle` database relies on the `cPickle` module to save the traces. Use of this backend is appropriate for small scale, short-lived projects. For longer term or larger projects, the `pickle` backend should be avoided since generated files might be unreadable across different Python versions. The *pickled* file is a simple dump of a dictionary containing the NumPy arrays storing the traces, as well as the state of the `Sampler`'s step methods.

sqlite

The `sqlite` backend is based on the python module sqlite3 (a Python 2.5 built-in) . It opens an SQL database named `dbname`, and creates one table per tallyable objects. The rows of this table store a key, the chain index and the values of the objects as:

```
key (INT), trace (INT),  v1 (FLOAT), v2 (FLOAT), v3 (FLOAT) ...
```

The key is autoincremented each time a new row is added to the table.

Warning

Note that the state of the sampler is not saved by the `sqlite` backend.

mysql

The `mysql` backend depends on the MySQL library and its python wrapper MySQLdb. Like the `sqlite` backend, it creates an SQL database containing one table per tallyable object. The main difference of `mysql` compared to `sqlite` is that it can connect to a remote database, provided the url and port of the host server is given, along with a valid user name and password. These parameters are passed when the `Sampler` is instantiated:

- `dbname` (*string*) The name of the database file.
- `dbuser` (*string*) The database user name.
- `dbpass` (*string*) The user password for this database.
- `dbhost` (*string*) The location of the database host.
- `dbport` (*int*) The port number to use to reach the database host.
- `dbmode` {`a`, `w`} File mode. Use `a` to append values, and `w` to overwrite an existing database.

Warning

Note that the state of the sampler is not saved by the `mysql` backend.

hdf5

The `hdf5` backend uses pyTables to save data in binary HDF5 format. The `hdf5` database is fast and can store huge traces, far larger than the available RAM. This data can be compressed and decompressed on the fly to reduce the memory footprint. Another feature of this backends is that it can store arbitrary objects. Whereas the other backends are limited to numerical values, `hdf5` can tally any object that can be pickled, opening the door for powerful and exotic applications (see `pymc.gp`).

The internal structure of an HDF5 file storing both numerical values and arbitrary objects is as follows:

```
/ (root)
  /chain0/ (Group) 'Chain #0'
    /chain0/PyMCSamples (Table(N,)) 'PyMC Samples'
    /chain0/group0 (Group) 'Group storing objects.'
      /chain0/group0/<object0 name> (VLArray(N,)) '<object0 name> samples.'
      /chain0/group0/<object1 name> (VLArray(N,)) '<object1 name> samples.'
      ...
  /chain1/ (Group) 'Chain #1'
    ...
```

All standard numerical values are stored in a `Table`, while `objects` are stored in individual `VLArrays`.

The `hdf5` Database takes the following parameters:

- `dbname` (*string*) Name of the hdf5 file.
- `dbmode` {`a`, `w`, `r`} File mode: `a`: append, `w`: overwrite, `r`: read-only.
- `dbcomplevel` : (*int* (0-9)) Compression level, 0: no compression.
- `dbcomplib` (*string*) Compression library (`zlib`, `bzip2`, `lzo`)

According the the pyTables manual, *zlib* has a fast decompression, relatively slow compression, and a good compression ratio. *LZO* has a fast compression, but a low compression ratio. *bzip2* has an excellent compression ratio but requires more CPU. Note that some of these compression algorithms require additional software to work (see the pyTables manual).

6.5 Writing a New Backend

It is relatively easy to write a new backend for `PyMC`. The first step is to look at the `database.base` module, which defines barebone `Database` and `Trace` classes. This module contains documentation on the methods that should be defined to get a working backend.

Testing your new backend should be trivial, since the `test_database` module contains a generic test class that can easily be subclassed to check that the basic features required of all backends are implemented and working properly.

CHAPTER
SEVEN

Model checking and diagnostics

7.1 Convergence Diagnostics

Valid inferences from sequences of MCMC samples are based on the assumption that the samples are derived from the true posterior distribution of interest. Theory guarantees this condition as the number of iterations approaches infinity. It is important, therefore, to determine the minimum number of samples required to ensure a reasonable approximation to the target posterior density. Unfortunately, no universal threshold exists across all problems, so convergence must be assessed independently each time MCMC estimation is performed. The procedures for verifying convergence are collectively known as convergence diagnostics.

One approach to analyzing convergence is analytical, whereby the variance of the sample at different sections of the chain are compared to that of the limiting distribution. These methods use distance metrics to analyze convergence, or place theoretical bounds on the sample variance, and though they are promising, they are generally difficult to use and are not prominent in the MCMC literature. More common is a statistical approach to assessing convergence. With this approach, rather than considering the properties of the theoretical target distribution, only the statistical properties of the observed chain are analyzed. Reliance on the sample alone restricts such convergence criteria to heuristics; that is, convergence cannot be guaranteed. Although evidence for lack of convergence using statistical convergence diagnostics will correctly imply lack of convergence in the chain, the absence of such evidence will not *guarantee* convergence in the chain. Nevertheless, negative results for one or more criteria will provide some measure of assurance to most users that their sample will provide valid inferences.

For most simple models, convergence will occur quickly, sometimes within a the first several hundred iterations, after which all remaining samples of the chain may be used to calculate posterior quantities. For many more complex models, convergence requires a significantly longer burn-in period; sometimes orders of magnitude more samples are needed. Frequently, lack of convergence will be caused by poor mixing (Figure 7.1). Recall that *mixing* refers to the degree to which the Markov chain explores the support of the posterior distribution. Poor mixing may stem from inappropriate proposals (if one is using the Metropolis-Hastings sampler) or from attempting to estimate models with highly correlated variables.

Informal Methods

The most straightforward approach for assessing convergence is based on simply plotting and inspecting traces and histograms of the observed MCMC sample. If the trace of values for each of the stochastics exhibits asymptotic behaviour[1] over the last m iterations, this may be satisfactory evidence for convergence. A similar approach involves plotting a histogram for every set of k iterations (perhaps 50-100) beyond some burn in threshold n; if the histograms are not visibly different among the sample intervals, this is reasonable evidence for convergence. Note that such diagnostics should be carried out for each stochastic estimated by the MCMC algorithm, because

[1]Asymptotic behaviour implies that the variance and the mean value of the sample stays relatively constant over some arbitrary period.

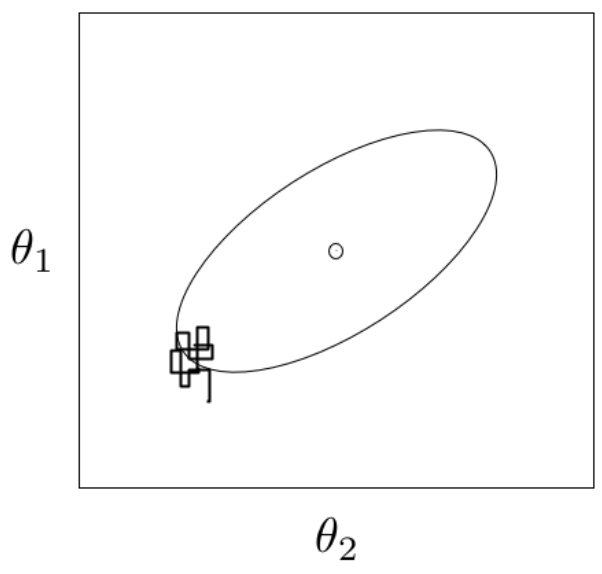


Figure 7.1: An example of a poorly-mixing sample in two dimensions. Notice that the chain is trapped in a region of low probability relative to the mean (dot) and variance (oval) of the true posterior quantity.

convergent behaviour by one variable does not imply evidence for convergence for other variables in the analysis. An extension of this approach can be taken when multiple parallel chains are run, rather than just a single, long chain. In this case, the final values of c chains run for n iterations are plotted in a histogram; just as above, this is repeated every k iterations thereafter, and the histograms of the endpoints are plotted again and compared to the previous histogram. This is repeated until consecutive histograms are indistinguishable.

Another *ad hoc* method for detecting convergence is to examine the traces of several MCMC chains initialized with different starting values. Overlaying these traces on the same set of axes should (if convergence has occurred) show each chain tending toward the same equilibrium value, with approximately the same variance. Recall that the tendency for some Markov chains to converge to the true (unknown) value from diverse initial values is called *ergodicity*. This property is guaranteed by the reversible chains constructed using MCMC, and should be observable using this technique. Again, however, this approach is only a heuristic method, and cannot always detect lack of convergence, even though chains may appear ergodic.

A principal reason that evidence from informal techniques cannot guarantee convergence is a phenomenon called metastability. Chains may appear to have converged to the true equilibrium value, displaying excellent qualities by any of the methods described above. However, after some period of stability around this value, the chain may suddenly move to another region of the parameter space (Figure 7.2). This period of metastability can sometimes be very long, and therefore escape detection by these convergence diagnostics. Unfortunately, there is no statistical technique available for detecting metastability.

Formal Methods

Along with the *ad hoc* techniques described above, a number of more formal methods exist which are prevalent in the literature. These are considered more formal because they are based on existing statistical methods, such as time series analysis.

PyMC currently includes two formal convergence diagnostic methods. The first, proposed by Geweke [1992], is

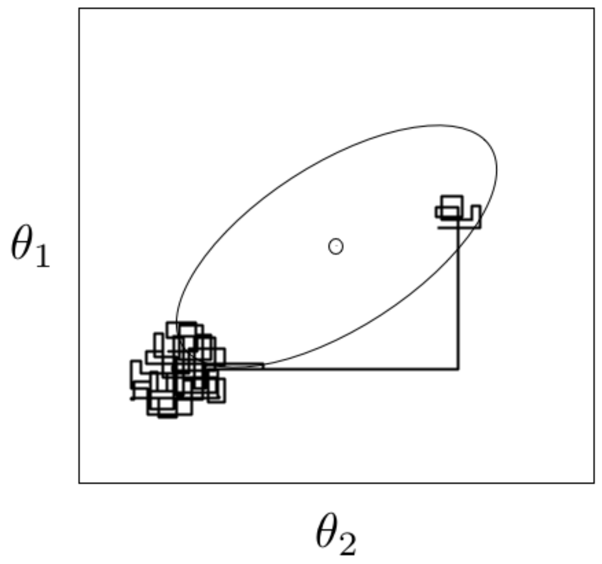


Figure 7.2: An example of metastability in a two-dimensional parameter space. The chain appears to be stable in one region of the parameter space for an extended period, then unpredictably jumps to another region of the space.

a time-series approach that compares the mean and variance of segments from the beginning and end of a single chain.

$$z = \frac{\bar{\theta}_a - \bar{\theta}_b}{\sqrt{Var(\theta_a) + Var(\theta_b)}} \tag{7.1}$$

where a is the early interval and b the late interval. If the z-scores (theoretically distributed as standard normal variates) of these two segments are similar, it can provide evidence for convergence. PyMC calculates z-scores of the difference between various initial segments along the chain, and the last 50% of the remaining chain. If the chain has converged, the majority of points should fall within 2 standard deviations of zero.

Diagnostic z-scores can be obtained by calling the `geweke` function. It accepts either (1) a single trace, (2) a dictionary of traces, (3) a Node object, or (4) an entire Model object.

Method Usage

```
geweke(x, first=0.1, last=0.5, intervals=20)
```

- `x`: The object that is or contains the output trace(s).
- `first` (optional): First portion of chain to be used in Geweke diagnostic. Defaults to 0.1 (i.e. first 10% of chain).
- `last` (optional): Last portion of chain to be used in Geweke diagnostic. Defaults to 0.5 (i.e. last 50% of chain).
- `intervals` (optional): Number of sub-chains to analyze. Defaults to 20.

The resulting scores are best interpreted graphically, using the `geweke_plot` function. This displays the scores in series, in relation to the 2 standard deviation boundaries around zero. Hence, it is easy to see departures from the standard normal assumption.

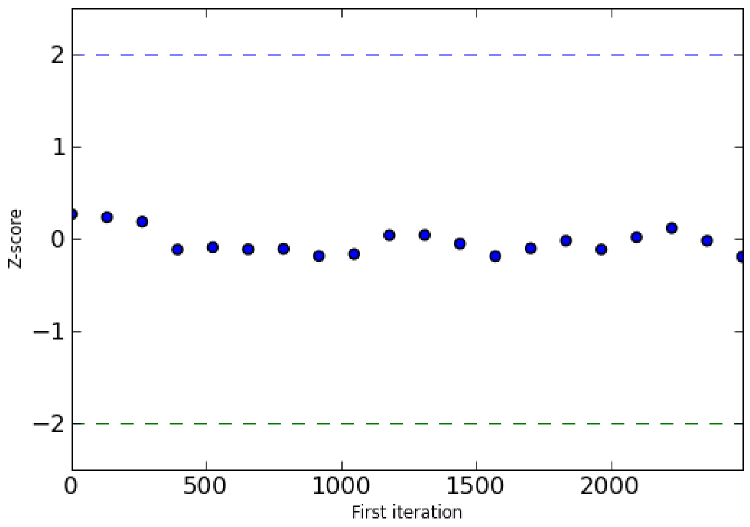


Figure 7.3: Sample plot of Geweke z-scores for a variable using **geweke_plot**. The occurrence of the scores well within 2 standard deviations of zero gives not indication of lack of convergence.

`geweke_plot` takes either a single set of scores, or a dictionary of scores (output by `geweke` when an entire Sampler is passed) as its argument:

Method Usage

```
def geweke_plot(data, name='geweke', format='png', suffix='-diagnostic', \
                path='./', fontmap = {1:10, 2:8, 3:6, 4:5, 5:4}, verbose=1)
```

- `data`: The object that contains the Geweke scores. Can be a list (one set) or a dictionary (multiple sets).
- `name` (optional): Name used for output files. For multiple scores, the dictionary keys are used as names.
- `format` (optional): Graphic output file format (defaults to *png*).
- `suffix` (optional): Suffix to filename (defaults to *-diagnostic*)
- `path` (optional): The path for output graphics (defaults to working directory).
- `fontmap` (optional): Dictionary containing the font map for the labels of the graphic.
- `verbose` (optional): Verbosity level for output (defaults to 1).

To illustrate, consider a model `my_model` that is used to instantiate a MCMC sampler. The sampler is then run for a given number of iterations:

```
>>> S = pymc.MCMC(my_model)
>>> S.sample(10000, burn=5000)
```

It is easiest simply to pass the entire sampler S the `geweke` function:

```
>>> scores = pymc.geweke(S, intervals=20)
>>> pymc.geweke_plot(scores)
```

Alternatively, individual stochastics within S can be analyzed for convergence:

```
>>> trace = S.alpha.trace()
>>> alpha_scores = pymc.geweke(trace, 'alpha', intervals=20)
>>> pymc.geweke_plot(alpha_scores)
```

The second diagnostic provided by PyMC is the Raftery and Lewis [1995] procedure. This approach estimates the number of iterations required to reach convergence, along with the number of burn-in samples to be discarded and the appropriate thinning interval. A separate estimate of both quantities can be obtained for each variable in a given model.

As the criterion for determining convergence, the Raftery and Lewis approach uses the accuracy of estimation of a user-specified quantile. For example, we may want to estimate the quantile $q = 0.975$ to within $r = 0.005$ with probability $s = 0.95$. In other words,

$$Pr(|\hat{q} - q| \leq r) = s \tag{7.2}$$

From any sample of θ, one can construct a binary chain:

$$Z^{(j)} = I(\theta^{(j)} \leq u_q) \tag{7.3}$$

where u_q is the quantile value and I is the indicator function. While $\{\theta^{(j)}\}$ is a Markov chain, $\{Z^{(j)}\}$ is not necessarily so. In any case, the serial dependency among $Z^{(j)}$ decreases as the thinning interval k increases. A value of k is chosen to be the smallest value such that the first order Markov chain is preferable to the second order Markov chain.

This thinned sample is used to determine number of burn-in samples. This is done by comparing the remaining samples from burn-in intervals of increasing length to the limiting distribution of the chain. An appropriate value is one for which the truncated sample's distribution is within ϵ (arbitrarily small) of the limiting distribution. See Raftery and Lewis [1995] or Gamerman [1997] for computational details. Estimates for sample size tend to be conservative.

This diagnostic is best used on a short pilot run of a particular model, and the results used to parameterize a subsequent sample that is to be used for inference.

Method Usage

```
raftery_lewis(x, q, r, s=.95, epsilon=.001, verbose=1)
```

- `x`: The object that contains the Geweke scores. Can be a list (one set) or a dictionary (multiple sets).
- `q`: Desired quantile to be estimated.
- `r`: Desired accuracy for quantile.
- `s`(optional): Probability of attaining the requested accuracy (defaults to 0.95).
- `epsilon` (optional) : Half width of the tolerance interval required for the q-quantile (defaults to 0.001).
- `verbose` (optional) : Verbosity level for output (defaults to 1).

The code for `raftery_lewis` is based on the FORTRAN program *gibbsit*, which was written by Steven Lewis.

Additional convergence diagnostics are available in the R statistical package, via the CODA module. PyMC includes a method `coda` for exporting model traces in a format that may be directly read by CODA.

Method Usage

```
pymc.utils.coda(pymc_object)
```

- `pymc_object`: The PyMC sampler for which output is desired.

Calling `coda` yields a file containing raw trace values (suffix `.out`) and a file containing indices to the trace values (suffix `.ind`).

7.2 Autocorrelation Plots

Samples from MCMC algorithms are ususally autocorrelated, due partly to the inherent Markovian dependence structure. The degree of autocorrelation can be quantified using the autocorrelation function:

$$\begin{aligned}\rho_k &= \frac{\text{Cov}(X_t, X_{t+k})}{\sqrt{\text{Var}(X_t)\text{Var}(X_{t+k})}} \\ &= \frac{E[(X_t-\theta)(X_{t+k}-\theta)]}{\sqrt{E[(X_t-\theta)^2]E[(X_{t+k}-\theta)^2]}}\end{aligned}$$

PyMC includes a function for plotting the autocorrelation function for each stochastics in the sampler (Figure 7.4). This allows users to examine the relationship among successive samples within sampled chains. Significant autocorrelation suggests that chains require thinning prior to use of the posterior statistics for inference.

```
autocorrelation(data, name, maxlag=100, format='png', suffix='-acf',
path='./', fontmap = {1:10, 2:8, 3:6, 4:5, 5:4}, verbose=1)
```

- `data`: The object that is or contains the output trace(s).
- `name`: Name used for output files.

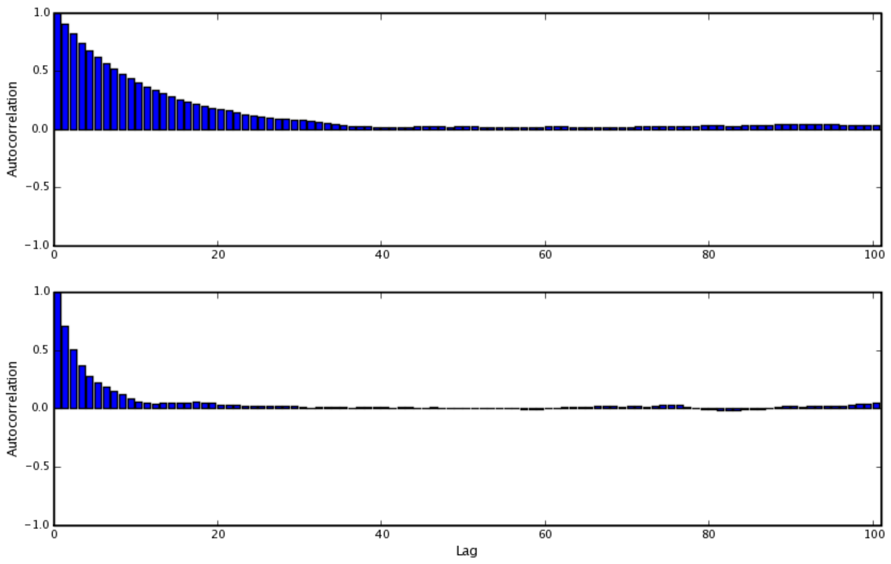


Figure 7.4: Sample autocorrelation plots for two Poisson variables from coal mining disasters example model.

- `maxlag`: The highest lag interval for which autocorrelation is calculated.
- `format` (optional): Graphic output file format (defaults to *png*).
- `suffix` (optional): Suffix to filename (defaults to *-diagnostic*)
- `path` (optional): The path for output graphics (defaults to working directory).
- `fontmap` (optional): Dictionary containing the font map for the labels of the graphic.
- `verbose` (optional): Verbosity level for output (defaults to 1).

7.3 Goodness of Fit

Checking for model convergence is only the first step in the evaluation of MCMC model outputs. It is possible for an entirely unsuitable model to converge, so additional steps are needed to ensure that the estimated model adequately fits the data. One intuitive way for evaluating model fit is to compare model predictions with actual observations. In other words, the fitted model can be used to simulate data, and the distribution of the simulated data should resemble the distribution of the actual data.

Fortunately, simulating data from the model is a natural component of the Bayesian modelling framework. Recall, from the discussion on imputation of missing data, the posterior predictive distribution:

$$p(\tilde{y}|y) = \int p(\tilde{y}|\theta) f(\theta|y) d\theta \tag{7.4}$$

Here, $\tilde{y}$ represents some hypothetical new data that would be expected, taking into account the posterior uncertainty in the model parameters. Sampling from the posterior predictive distribution is easy in PyMC. The code looks identical to the corresponding data stochastic, with two modifications: (1) the node should be specified as deterministic and (2) the statistical likelihoods should be replaced by random number generators. As an example, consider the Poisson data likelihood of the coal mining disasters example:

```
@pm.stochastic(observed=True, dtype=int)
def disasters(  value = disasters_array,
                early_mean = early_mean,
                late_mean = late_mean,
                switchpoint = switchpoint):
    """Annual occurences of coal mining disasters."""
    return pm.poisson_like(value[:switchpoint],early_mean) +
 pm.poisson_like(value[switchpoint:],late_mean)
```

This is a mixture of Poisson processes, one with a higher early mean and another with a lower late mean. Here is the corresponding sample from the posterior predictive distribution:

```
@pm.deterministic
def disasters_sim(early_mean = early_mean,
                late_mean = late_mean,
                switchpoint = switchpoint):
    """Coal mining disasters sampled from the posterior predictive distribution"""
    return concatenate( (pm.rpoisson(early_mean, size=switchpoint),
 pm.rpoisson(late_mean, size=n-switchpoint)))
```

Notice that `@pm.stochastic` has been replaced with `@pm.deterministic` and `pm.poisson_like` with `pm.rpoisson`. The simulated values from each of the Poisson processes are concatenated together before returning them.

The degree to which simulated data correspond to observations can be evaluated in at least two ways. First, these quantities can simply be compared visually. This allows for a qualitative comparison of model-based replicates and observations. If there is poor fit, the true value of the data may appear in the tails of the histogram of replicated data, while a good fit will tend to show the true data in high-probability regions of the posterior predictive distribution (Figure 7.5).

The Matplot package in PyMC provides an easy way of producing such plots, via the `gof_plot` function. To illustrate, consider a single data point `x` and an array of values `x_sim` sampled from the posterior predictive distribution. The histogram is generated by calling:

```
pm.Matplot.gof_plot(x_sim, x, name='x')
```

A second approach for evaluating goodness of fit using samples from the posterior predictive distribution involves the use of a statistical criterion. For example, the Bayesian p-value [Gelman et al., 1996] uses a discrepancy measure that quantifies the difference between data (observed or simulated) and the expected value, conditional on some model. One such discrepancy measure is the Freeman-Tukey statistic [Brooks et al., 2000]:

$$D(x|\theta) = \sum_j (\sqrt{x_j} - \sqrt{e_j})^2 \tag{7.5}$$

Model fit is assessed by comparing the discrepancies from observed data to those from simulated data. On

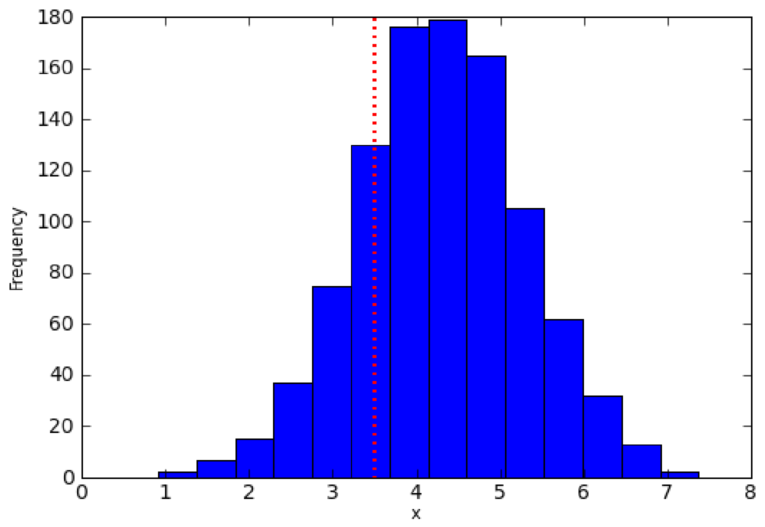


Figure 7.5: Data sampled from the posterior predictive distribution of a model for some observation **x**. The true value of **x** is shown by the dotted red line.

average, we expect the difference between them to be zero; hence, the Bayesian p-value is simply the proportion of simulated discrepancies that are larger than their corresponding observed discrepancies:

$$p = Pr[D(\text{sim}) > D(\text{obs})] \tag{7.6}$$

If p is very large (e.g. > 0.975) or very small (e.g. < 0.025) this implies that the model is not consistent with the data, and thus is evidence of lack of fit. Graphically, data and simulated discrepancies plotted together should be clustered along a 45 degree line passing through the origin, as shown in Figure 7.6.

The `discrepancy` function in the `utils` package can be used to generate discrepancy statistics from arrays of data, simulated values, and expected values:

```
D = pm.utils.discrepancy(observed, simulated, expected)
```

A call to this function returns two arrays of discrepancy values, which can be passed to the `discrepancy_plot` function in the Matplot module to generate a scatter plot, and if desired, a p-value:

```
pm.Matplot.discrepancy_plot(D, name='D', report_p=True)
```

Additional optional arguments for `discrepancy_plot` are identical to other PyMC plotting functions.

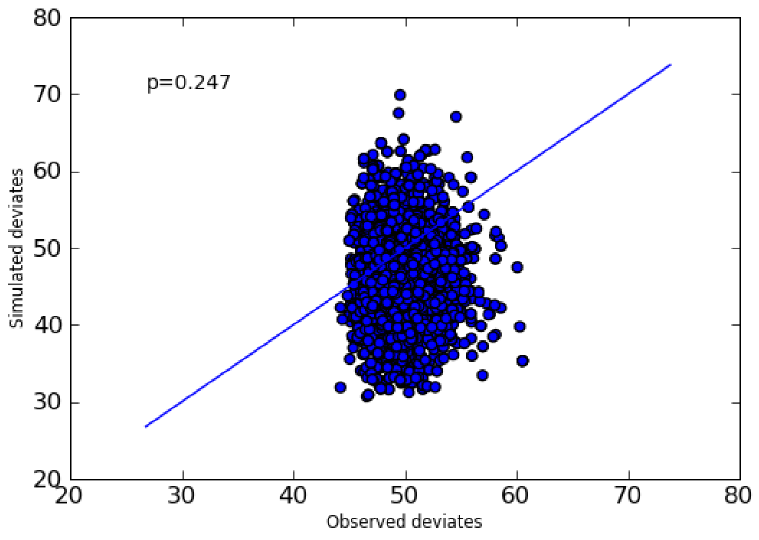


Figure 7.6: Plot of deviates of observed and simulated data from expected values. The cluster of points symmetrically about the 45 degree line (and the reported p-value) suggests acceptable fit for the modeled parameter.

CHAPTER
EIGHT

Extending PyMC

qPyMC tries to make standard things easy, but keep unusual things possible. Its openness, combined with Python's flexibility, invite extensions from using new step methods to exotic stochastic processes (see the Gaussian process module). This chapter briefly reviews the ways PyMC is designed to be extended.

8.1 Nonstandard Stochastics

The simplest way to create a `Stochastic` object with a nonstandard distribution is to use the medium or long decorator syntax. See chapter 4. If you want to create many stochastics with the same nonstandard distribution, the decorator syntax can become cumbersome. An actual subclass of `Stochastic` can be created using the class factory `stochastic_from_dist`. This function takes the following arguments:

- The name of the new class,
- A `logp` function,
- A `random` function,
- The NumPy datatype of the new class (for continuous distributions, this should be `float`; for discrete distributions, `int`; for variables valued as non-numerical objects, `object`),
- A flag indicating whether the resulting class represents a vector-valued variable.

The necessary parent labels are read from the `logp` function, and a docstring for the new class is automatically generated. Instances of the new class can be created in one line.

Full subclasses of `Stochastic` may be necessary to provide nonstandard behaviors (see `gp.GP`).

8.2 User-defined step methods

The `StepMethod` class is meant to be subclassed. There are an enormous number of MCMC step methods in the literature, whereas PyMC provides only about half a dozen. Most user-defined step methods will be either Metropolis-Hastings or Gibbs step methods, and these should subclass `Metropolis` or `Gibbs` respectively. More unusual step methods should subclass `StepMethod` directly.

Example: an asymmetric Metropolis step

Consider the probability model in 'examples/custom_step.py':

```
mu = pm.Normal('mu',0,.01, value=0)
tau = pm.Exponential('tau',.01, value=1)
cutoff = pm.Exponential('cutoff',1, value=1.3)
D = pm.Truncnorm('D',mu,tau,-np.inf,cutoff,value=data,observed=True)
```

The stochastic variable `cutoff` cannot be smaller than the largest element of D, otherwise D's density would be zero. The standard `Metropolis` step method can handle this case without problems; it will propose illegal values occasionally, but these will be rejected.

Suppose we want to handle `cutoff` with a smarter step method that doesn't propose illegal values. Specifically, we want to use the nonsymmetric proposal distribution

$$x_p|x \sim \text{Truncnorm}(x, \sigma, \max(D), \infty).$$

We can implement this Metropolis-Hastings algorithm with the following step method class:

```
class TruncatedMetropolis(pm.Metropolis):
    def __init__(self, stochastic, low_bound, up_bound, *args, **kwargs):
        self.low_bound = low_bound
        self.up_bound = up_bound
        pm.Metropolis.__init__(self, stochastic, *args, **kwargs)

    # Propose method written by hacking Metropolis.propose()
    def propose(self):
        tau = 1./(self.adaptive_scale_factor * self.proposal_sd)**2
        self.stochastic.value = \
        pm.rtruncnorm(self.stochastic.value, tau, self.low_bound, self.up_bound)

    # Hastings factor method accounts for asymmetric proposal distribution
    def hastings_factor(self):
        tau = 1./(self.adaptive_scale_factor * self.proposal_sd)**2
        cur_val = self.stochastic.value
        last_val = self.stochastic.last_value

        lp_for = pm.truncnorm_like(cur_val, last_val, tau, self.low_bound, self.up_bound)
        lp_bak = pm.truncnorm_like(last_val, cur_val, tau, self.low_bound, self.up_bound)

        if self.verbose > 1:
            print self._id + ': Hastings factor %f'%(lp_bak - lp_for)
        return lp_bak - lp_for
```

The `propose` method sets the step method's stochastic's value to a new value, drawn from a truncated normal distribution. The precision of this distribution is computed from two factors: `self.proposal_sd`, which can be set with an input argument to Metropolis, and `self.adaptive_scale_factor`. Metropolis step methods' default tuning behavior is to reduce `adaptive_scale_factor` if the acceptance rate is too low, and to increase `adaptive_scale_factor` if it is too high. By incorporating `adaptive_scale_factor` into the proposal standard deviation, we avoid having to write our own tuning infrastructure. If we don't want the proposal to tune, we don't have to use `adaptive_scale_factor`.

The `hastings_factor` method adjusts for the asymmetric proposal distribution Gelman et al. [2004]. It computes the log of the quotient of the 'backward' density and the 'forward' density. For symmetric proposal distributions, this quotient is 1, so its log is zero. We have added some code to print the Hastings factor if the step method's verbosity level is set high.

Having created our custom step method, we need to tell MCMC instances to use it to handle the variable `cutoff`. This is done in 'custom_step.py' with the following line:

```
M.use_step_method(TruncatedMetropolis, cutoff, D.value.max(), np.inf)
```

This call causes M to pass the arguments `cutoff, D.value.max(), np.inf` to a `TruncatedMetropolis` object's `init` method, and use the object to handle `cutoff`.

It's often convenient to get a handle to a custom step method instance directly for debugging purposes. `M.step_method_dict[cutoff]` returns a list of all the step methods M will use to handle `cutoff`:

```
>>> M.step_method_dict[cutoff]
[<custom_step.TruncatedMetropolis object at 0x3c91130>]
```

There may be more than one, and conversely step methods may handle more than one stochastic variable. To see which variables step method S is handling, try

```
>>> S.stochastics
set([<pymc.distributions.Exponential 'cutoff' at 0x3cd6b90>])
```

General step methods

All step methods must implement the following methods:

`step()`: Updates the values of `self.stochastics`.

`tune()`: Tunes the jumping strategy based on performance so far. A default method is available that increases `self.adaptive_scale_factor` (see below) when acceptance rate is high, and decreases it when acceptance rate is low. This method should return `True` if additional tuning will be required later, and `False` otherwise.

`competence(s)`: A class method that examines stochastic variable s and returns a value from 0 to 3 expressing the step method's ability to handle the variable. This method is used by `MCMC` instances when automatically assigning step methods. Conventions are:

0 I cannot safely handle this variable.

1 I can handle the variable about as well as the standard `Metropolis` step method.

2 I can do better than `Metropolis`.

3 I am the best step method you are likely to find for this variable in most cases.

For example, if you write a step method that can handle `MyStochasticSubclass` well, the competence method might look like this:

```
class MyStepMethod(pm.StepMethod):
   def __init__(self, stochastic, *args, **kwargs):
      ...

   @classmethod
   def competence(self, stochastic):
      if isinstance(stochastic, MyStochasticSubclass):
         return 3
      else:
         return 0
```

Note that PyMC will not even attempt to assign a step method automatically if its `init` method cannot be called with a single stochastic instance, that is `MyStepMethod(x)` is a legal call. The list of step methods that PyMC will consider assigning automatically is called `pymc.StepMethodRegistry`.

`current_state()`: This method is easiest to explain by showing the code:

```
state = {}
for s in self._state:
    state[s] = getattr(self, s)
return state
```

`self._state` should be a list containing the names of the attributes needed to reproduce the current jumping strategy. If an `MCMC` object writes its state out to a database, these attributes will be preserved. If an `MCMC` object restores its state from the database later, the corresponding step method will have these attributes set to their saved values.

Step methods should also maintain the following attributes:

`_id`: A string that can identify each step method uniquely (usually something like `<class_name>_<stochastic_name>`).

`adaptive_scale_factor`: An 'adaptive scale factor'. This attribute is only needed if the default `tune()` method is used.

All step methods have a property called `loglike`, which returns the sum of the log-probabilities of the union of the extended children of `self.stochastics`. This quantity is one term in the log of the Metropolis-Hastings acceptance ratio.

Metropolis-Hastings step methods

A Metropolis-Hastings step method only needs to implement the following methods, which are called by `Metropolis.step()`:

`reject()`: Usually just

```
def reject(self):
    self.rejected += 1
    [s.value = s.last_value for s in self.stochastics]
```

`propose()`: Sets the values of all `self.stochastics` to new, proposed values. This method may use the `adaptive_scale_factor` attribute to take advantage of the standard tuning scheme.

Metropolis-Hastings step methods may also override the `tune` and `competence` methods.

Metropolis-Hastings step methods with asymmetric jumping distributions may implement a method called `hastings_factor()`, which returns the log of the ratio of the 'reverse' and 'forward' proposal probabilities. Note that no `accept()` method is needed or used.

By convention, Metropolis-Hastings step methods use attributes called `accepted` and `rejected` to log their performance.

Gibbs step methods

Gibbs step methods handle conjugate submodels. These models usually have two components: the 'parent' and the 'children'. For example, a gamma-distributed variable serving as the precision of several normally-distributed variables is a conjugate submodel; the gamma variable is the parent and the normal variables are the children.

This section describes PyMC's current scheme for Gibbs step methods, several of which are in a semi-working state in the sandbox. It is meant to be as generic as possible to minimize code duplication, but it is admittedly complicated. Feel free to subclass StepMethod directly when writing Gibbs step methods if you prefer.

Gibbs step methods that subclass PyMC's `Gibbs` should define the following class attributes:

`child_class`: The class of the children in the submodels the step method can handle.

`parent_class`: The class of the parent.

`parent_label`: The label the children would apply to the parent in a conjugate submodel. In the gamma-normal example, this would be `tau`.

`linear_OK`: A flag indicating whether the children can use linear combinations involving the parent as their actual parent without destroying the conjugacy.

A subclass of `Gibbs` that defines these attributes only needs to implement a `propose()` method, which will be called by `Gibbs.step()`. The resulting step method will be able to handle both conjugate and 'non-conjugate' cases. The conjugate case corresponds to an actual conjugate submodel. In the nonconjugate case all the children are of the required class, but the parent is not. In this case the parent's value is proposed from the likelihood and accepted based on its prior. The acceptance rate in the nonconjugate case will be less than one.

The inherited class method `Gibbs.competence` will determine the new step method's ability to handle a variable x by checking whether:

- all x's children are of class `child_class`, and either apply `parent_label` to x directly or (if `linear_OK=True`) to a `LinearCombination` object (chapter 4), one of whose parents contains x.
- x is of class `parent_class`

If both conditions are met, `pymc.conjugate_Gibbs_competence` will be returned. If only the first is met, `pymc.nonconjugate_Gibbs_competence` will be returned.

8.3 New fitting algorithms

PyMC provides a convenient platform for non-MCMC fitting algorithms in addition to MCMC. All fitting algorithms should be implemented by subclasses of `Model`. There are virtually no restrictions on fitting algorithms, but many of `Model`'s behaviors may be useful. See chapter 5.

Monte Carlo fitting algorithms

Unless there is a good reason to do otherwise, Monte Carlo fitting algorithms should be implemented by subclasses of `Sampler` to take advantage of the interactive sampling feature and database backends. Subclasses using the standard `sample()` and `isample()` methods must define one of two methods:

`draw()`: If it is possible to generate an independent sample from the posterior at every iteration, the `draw` method should do so. The default `_loop` method can be used in this case.

`_loop()`: If it is not possible to implement a `draw()` method, but you want to take advantage of the interactive sampling option, you should override `_loop()`. This method is responsible for generating the posterior samples and calling `tally()` when it is appropriate to save the model's state. In addition, `_loop` should monitor the sampler's `status` attribute at every iteration and respond appropriately. The possible values of `status` are:

- `'ready'`: Ready to sample.
- `'running'`: Sampling should continue as normal.
- `'halt'`: Sampling should halt as soon as possible. `_loop` should call the `halt()` method and return control. `_loop` can set the status to `'halt'` itself if appropriate (eg the database is full or a `KeyboardInterrupt` has been caught).
- `'paused'`: Sampling should pause as soon as possible. `_loop` should return, but should be able to pick up where it left off next time it's called.

Samplers may alternatively want to override the default `sample()` method. In that case, they should call the `tally()` method whenever it is appropriate to save the current model state. Like custom `_loop()` methods, custom `sample()` methods should handle `KeyboardInterrupts` and call the `halt()` method when sampling terminates to finalize the traces.

8.4 Don't update stochastic variables' values in-place

If you're going to implement a new step method, fitting algorithm or unusual (non-numeric-valued) `Stochastic` subclass, you should understand the issues related to in-place updates of `Stochastic` objects' values. Fitting methods should never update variables' values in-place for two reasons:

- In algorithms that involve accepting and rejecting proposals, the 'pre-proposal' value needs to be preserved uncorrupted. It would be possible to make a copy of the pre-proposal value and then allow in-place updates, but in PyMC we have chosen to store the pre-proposal value as `Stochastic.last_value` and require proposed values to be new objects. In-place updates would corrupt `Stochastic.last_value`, and this would cause problems.
- `LazyFunction`'s caching scheme checks variables' current values against its internal cache by reference. That means if you update a variable's value in-place, it or its child may miss the update and incorrectly skip recomputing its value or log-probability.

However, a `Stochastic` object's value can make in-place updates to itself if the updates don't change its identity. For example, the `Stochastic` subclass `gp.GP` is valued as a `gp.Realization` object. GP realizations represent random functions, which are infinite-dimensional stochastic processes, as literally as possible. The strategy they employ is to 'self-discover' on demand: when they are evaluated, they generate the required value conditional on previous evaluations and then make an internal note of it. This is an in-place update, but it is done to provide the same behavior as a single random function whose value everywhere has been determined since it was created.

CHAPTER
NINE

Probability distributions

PyMC provides 35 built-in probability distributions. For each distribution, it provides:

- A function that evaluates its log-probability or log-density: `normal_like()`.
- A function that draws random variables: `rnormal()`.
- A function that computes the expectation associated with the distribution: `normal_expval()`.
- A `Stochastic` subclass generated from the distribution: `Normal`.

This section describes the likelihood functions of these distributions.

9.1 Discrete distributions

`binomial_like`(*x, n, p*)

Binomial log-likelihood. The discrete probability distribution of the number of successes in a sequence of n independent yes/no experiments, each of which yields success with probability p.

$$f(x \mid n,p) = \frac{n!}{x!(n-x)!}p^x(1-p)^{n-x}$$

Parameters

x : integer
    Number of successes, > 0.

n : integer
    Number of Bernoulli trials, $>$ x.

p : float
    Probability of success in each trial, $p \in [0,1]$.

Notes

- $E(X) = np$
- $Var(X) = np(1-p)$

`geometric_like`(*x, p*)

Geometric log-likelihood. The probability that the first success in a sequence of Bernoulli trials occurs on the x'th trial.

$$f(x \mid p) = p(1-p)^{x-1}$$

Parameters

x : integer
    Number of trials before first success, > 0.

p : float
    Probability of success on an individual trial, $p \in [0,1]$

Notes

- $E(X) = 1/p$
- $Var(X) = \frac{1-p}{p^2}$

`hypergeometric_like`(*x, n, m, N*)

Hypergeometric log-likelihood. Discrete probability distribution that describes the number of successes in a sequence of draws from a finite population without replacement.

$$f(x \mid n, m, N) = \frac{\binom{m}{x}\binom{N-m}{n-x}}{\binom{N}{n}}$$

Parameters

x : integer
    Number of successes in a sample drawn from a population. $\max(0, draws - failures) \leq x \leq \min(draws, success)$

n : integer
    Size of sample drawn from the population.

m : integer
    Number of successes in the population.

N : integer
    Total number of units in the population.

Notes

- $E(X) = \frac{nm}{N}$

`poisson_like`(*x, mu*)

Poisson log-likelihood. The Poisson is a discrete probability distribution. It is often used to model the number of events occurring in a fixed period of time when the times at which events occur are independent. The Poisson distribution can be derived as a limiting case of the binomial distribution.

$$f(x \mid \mu) = \frac{e^{-\mu}\mu^x}{x!}$$

Parameters

x : integer
$x \in 0, 1, 2, \ldots$

mu : float
Expected number of occurrences that occur during the given interval, $\mu \geq 0$.

Notes

- $E(x) = \mu$
- $Var(x) = \mu$

`negative_binomial_like`(*x, mu, alpha*)

Negative binomial log-likelihood. The negative binomial distribution describes a Poisson random variable whose rate parameter is gamma distributed. PyMC's chosen parameterization makes this mixture interpretation more convenient to work with.

$$f(x \mid \mu, \alpha) = \frac{\Gamma(x+\alpha)}{x!\Gamma(\alpha)}(\alpha/(\mu+\alpha))^\alpha(\mu/(\mu+\alpha))^x$$

Parameters

x : integer
$x > 0$

mu : float
Expected number of occurrences, > 0.

alpha : float
Shape parameter of the gamma distribution of the Poisson rate, > 0.

Notes

- $E(x) = \mu$
- In Wikipedia's parameterization, $r = \alpha$, $p = \alpha/(\mu+\alpha)$ and $\mu = r(1-p)/p$.

`categorical_like`(*x, p*)

Categorical log-likelihood. The most general discrete distribution.

$$f(x = i \mid p) = p_i$$

$$i \in 0 \ldots k-1$$

Parameters

x : integer

$x \in 0 \ldots k-1$

p : (k) float

$p > 0, \sum p = 1$

`discrete_uniform_like` (*x, lower, upper*)

Discrete uniform log-likelihood.

$$f(x \mid lower, upper) = \frac{1}{upper - lower}$$

Parameters

x : integer

$lower \leq x \leq upper$

lower : float

Lower limit.

upper : float

Upper limit.

`bernoulli_like` (*x, p*)

Bernoulli log-likelihood. The Bernoulli distribution describes the probability of successes (x=1) and failures (x=0).

$$f(x \mid p) = p^x (1-p)^{1-x}$$

Parameters

x : sequence of Booleans

Series of successes (1) and failures (0). $x = 0, 1$

p : float

Probability of success. $0 < p < 1$.

Notes

- $E(x) = p$
- $Var(x) = p(1-p)$

9.2 Continuous distributions

`beta_like` (*x, alpha, beta*)

Beta log-likelihood. The conjugate prior for the parameter p of the binomial distribution.

$$f(x \mid \alpha, \beta) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} x^{\alpha-1} (1-x)^{\beta-1}$$

Parameters

x : float

$0 < x < 1$

alpha : float

$\alpha > 0$

beta : float

$\beta > 0$

Notes

- $E(X) = \frac{\alpha}{\alpha+\beta}$
- $Var(X) = \frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}$

`cauchy_like` (*x, alpha, beta*)

Cauchy log-likelihood. The Cauchy distribution is also known as the Lorentz or the Breit-Wigner distribution.

$$f(x \mid \alpha, \beta) = \frac{1}{\pi\beta[1+(\frac{x-\alpha}{\beta})^2]}$$

Parameters

alpha : float

Location parameter.

beta : float

Scale parameter > 0.

Notes

- Mode and median are at alpha.

`chi2_like` (*x, nu*)

Chi-squared (χ^2) log-likelihood.

$$f(x \mid \nu) = \frac{x^{(\nu-2)/2}e^{-x/2}}{2^{\nu/2}\Gamma(\nu/2)}$$

Parameters

x : float

$x \geq 0$

nu : integer

Degrees of freedom ($nu > 0$)

Notes

- $E(X) = \nu$
- $Var(X) = 2\nu$

degenerate_like(*x, k*)

Degenerate log-likelihood, also known as point mass.

$$f(x \mid k) = \begin{cases} 1 \text{ if } x = k \\ 0 \text{ if } x \neq k \end{cases}$$

Parameters

x : float
  $x = k$

k : float
  degenerate value or location of point mass.

exponential_like(*x, beta*)

Exponential log-likelihood. The exponential distribution is a special case of the gamma distribution with alpha=1. It often describes the time until the first occurrence of an event.

$$f(x \mid \beta) = \frac{1}{\beta} e^{-x/\beta}$$

Parameters

x : float
  $x \geq 0$

beta : float
  Survival parameter $\beta > 0$

Notes

- $E(X) = \beta$
- $Var(X) = \beta^2$

exponweib_like(*x, alpha, k, loc=0, scale=1*)

Exponentiated Weibull log-likelihood. The exponentiated Weibull distribution is a generalization of the Weibull family. Its value lies in being able to model monotone and non-monotone failure rates.

$$f(x \mid \alpha, k, loc, scale) = \frac{\alpha k}{scale}(1 - e^{-z^k})^{\alpha-1} e^{-z^k} z^{k-1}$$
$$z = \frac{x - loc}{scale}$$

Parameters

x : float
: $x > 0$

alpha : float
: Shape parameter

k : float
: $k > 0$

loc : float
: Location parameter

scale : float
: Scale parameter > 0.

`gamma_like`(*x, alpha, beta*)

Gamma log-likelihood. A useful two-parameter distribution for positive variables. It can serve as a conjugate prior for the precision parameter of a normal distribution. When alpha is an integer, it can represent the sum of alpha exponentially distributed random variables, each of which has mean beta.

$$f(x \mid \alpha, \beta) = \frac{\beta^{\alpha} x^{\alpha-1} e^{-\beta x}}{\Gamma(\alpha)}$$

Parameters

x : float
: $x \geq 0$

alpha : float
: Shape parameter $\alpha > 0$.

beta : float
: Scale parameter $\beta > 0$.

Notes

- $E(X) = \frac{\alpha}{\beta}$
- $Var(X) = \frac{\alpha}{\beta^2}$

`half_normal_like`(*x, tau*)

Half-normal log-likelihood, a normal distribution with mean 0 and limited to the domain $x \in [0, \infty)$.

$$f(x \mid \tau) = \sqrt{\frac{2\tau}{\pi}} \exp\left\{\frac{-x^2 \tau}{2}\right\}$$

Parameters

x : float
: $x \geq 0$

tau : float
: $\tau > 0$

`inverse_gamma_like`(*x, alpha, beta*)

Inverse gamma log-likelihood. If X is gamma distributed, $1/X$ is inverse gamma distributed. The inverse gamma is the conjugate prior for the variance of a normal random variable.

$$f(x \mid \alpha, \beta) = \frac{\beta^{\alpha}}{\Gamma(\alpha)} x^{-\alpha-1} \exp\left(\frac{-\beta}{x}\right)$$

Parameters

x : float
    x > 0

alpha : float
    Shape parameter, $\alpha > 0$.

beta : float
    Scale parameter, $\beta > 0$.

Notes

- $E(X) = \frac{1}{\beta(\alpha-1)}$ for $\alpha > 1$.

`laplace_like`(*x, mu, tau*)

Laplace (double exponential) log-likelihood. The Laplace (or double exponential) distribution describes the difference between two independent, identically distributed exponential events. It is often used as a heavier-tailed alternative to the normal.

$$f(x \mid \mu, \tau) = \frac{\tau}{2} e^{-\tau|x-\mu|}$$

Parameters

x : float
    $-\infty < x < \infty$

mu : float
    Location parameter $-\infty < \mu < \infty$

tau : float
    Scale parameter $\tau > 0$

Notes

- $E(X) = \mu$
- $Var(X) = \frac{2}{\tau^2}$

`logistic_like`(*x, mu, tau*)

Logistic log-likelihood. The logistic distribution is often used as a growth model for populations or markets. It resembles a heavy-tailed normal distribution.

$$f(x \mid \mu, \tau) = \frac{\tau \exp(-\tau[x-\mu])}{[1+\exp(-\tau[x-\mu])]^2}$$

Parameters

x : float

$-\infty < x < \infty$

mu : float

Location parameter $-\infty < \mu < \infty$

tau : float

Scale parameter $\tau > 0$

Notes

- $E(X) = \mu$
- $Var(X) = \frac{\pi^2}{3\tau^2}$

`lognormal_like`(*x, mu, tau*)

Log-normal log-likelihood. Distribution of any random variable whose logarithm is normally distributed. A variable might be modeled as log-normal if it can be thought of as the multiplicative product of many small independent factors.

$$f(x \mid \mu, \tau) = \sqrt{\frac{\tau}{2\pi}} \frac{\exp\left\{-\frac{\tau}{2}(\ln(x)-\mu)^2\right\}}{x}$$

Parameters

x : float

x > 0

mu : float

Location parameter.

tau : float

Scale parameter, > 0.

Notes $E(X) = e^{\mu+\frac{1}{2\tau}}$

`normal_like`(*x, mu, tau*)

Normal log-likelihood. The sum of many independent random terms, suitably scaled, is approximately normally distributed.

$$f(x \mid \mu, \tau) = \sqrt{\frac{\tau}{2\pi}} \exp\left\{-\frac{\tau}{2}(x-\mu)^2\right\}$$

Parameters

x : float

Input data.

mu : float

Mean of the distribution.

tau : float

Precision of the distribution, $\tau > 0$ (corresponds to $1/\sigma^2$).

Notes

- $E(X) = \mu$
- $Var(X) = 1/\tau$

`t_like` (*x, nu*)

Student's T log-likelihood. Describes a zero-mean normal variable whose precision is gamma distributed. Alternatively, describes the mean of several zero-mean normal random variables divided by their sample standard deviation.

$$f(x \mid \nu) = \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})\sqrt{\nu\pi}} \left(1 + \frac{x^2}{\nu}\right)^{-\frac{\nu+1}{2}}$$

Parameters

x : float
  Input data.

nu : float
  Degrees of freedom.

`uniform_like` (*x, lower, upper*)

Uniform log-likelihood.

$$f(x \mid lower, upper) = \frac{1}{upper - lower}$$

Parameters

x : float
  $lower \leq x \leq upper$

lower : float
  Lower limit.

upper : float
  Upper limit.

`weibull_like` (*x, alpha, beta*)

Weibull log-likelihood.

$$f(x \mid \alpha, \beta) = \frac{\alpha x^{\alpha-1} \exp(-(\frac{x}{\beta})^{\alpha})}{\beta^{\alpha}}$$

Parameters

x : float
  $x \geq 0$

alpha : float
  $\alpha > 0$

beta : float
  $\beta > 0$

Notes

- $E(x) = \beta\Gamma(1 + \frac{1}{\alpha})$
- $Var(x) = \beta^2\Gamma(1 + \frac{2}{\alpha} - \mu^2)$

`skew_normal_like` (*x, mu, tau, alpha*)

Azzalini's skew-normal log-likelihood,

$$f(x \mid \mu, \tau, \alpha) = 2\Phi((x-\mu)\sqrt{\tau}\alpha)\phi(x,\mu,\tau)$$

where Φ is the normal CDF and ϕ is the normal PDF.

Parameters

x : float
  Input data.
mu : float
  Mean of the distribution.
tau : float
  Precision of the distribution, > 0.
alpha : float
  Shape parameter of the distribution.

Notes

- See http://azzalini.stat.unipd.it/SN/

`truncnorm_like` (*x, mu, tau, a, b*)

Truncated normal log-likelihood. Describes a normal variable conditioned to be inside an interval.

$$f(x \mid \mu, \tau, a, b) = \frac{\phi(\frac{x-\mu}{\sigma})}{\Phi(\frac{b-\mu}{\sigma}) - \Phi(\frac{a-\mu}{\sigma})},$$

where $\sigma^2 = 1/\tau$.

Parameters

x : float
  Input data.
mu : float
  Mean of the distribution.
tau : float
  Precision of the distribution, $\tau > 0$ (corresponds to $1/\sigma^2$).
a : float
  Left bound of the distribution.
b : float
  Right bound of the distribution.

9.3 Multivariate discrete distributions

multivariate_hypergeometric_like(*x, m*)

The multivariate hypergeometric describes the probability of drawing x[i] elements of the ith category, when the number of items in each category is given by m.

$$\frac{\prod_i \binom{m_i}{x_i}}{\binom{N}{n}}$$

where $N = \sum_i m_i$ and $n = \sum_i x_i$.

Parameters

x : integer sequence

Number of draws from each category, $< m$

m : integer sequence

Number of items in each category.

multinomial_like(*x, n, p*)

Multinomial log-likelihood. Generalization of the binomial distribution, but instead of each trial resulting in "success" or "failure", each one results in exactly one of some fixed finite number k of possible outcomes over n independent trials. 'x[i]' indicates the number of times outcome number i was observed over the n trials.

$$f(x \mid n, p) = \frac{n!}{\prod_{i=1}^k x_i!} \prod_{i=1}^k p_i^{x_i}$$

Parameters

x : (ns, k) integer

Random variable indicating the number of time outcome i is observed, $\sum_{i=1}^k x_i = n$, $x_i \geq 0$.

n : integer

Number of trials.

p : (k,) float

Probability of each one of the different outcomes, $\sum_{i=1}^k p_i = 1$, $p_i \geq 0$.

Notes

- A Multinomial's parent p may be Dirichlet, even though its value is length $k - 1$.
- $E(X_i) = np_i$
- $var(X_i) = np_i(1 - p_i)$
- $cov(X_i, X_j) = -np_i p_j$

9.4 Multivariate continuous distributions

`dirichlet_like`(*x, theta*)

Dirichlet log-likelihood. A convenient distribution for variables that take values on the simplex, it is the conjugate prior for the multinomial distribution's p parameter.

$$f(\mathbf{x}) = \frac{\Gamma(\sum_{i=1}^k \theta_i)}{\prod \Gamma(\theta_i)} \prod_{i=1}^k x_i^{\theta_i - 1}$$

Parameters

x : (n,k-1) array

Where n is the number of samples and k the dimension. $0 < x_i < 1$, $\sum_{i=1}^{k-1} x_i < 1$

theta : (n,k) or (1,k) float

$\theta > 0$

`inverse_wishart_like`(*X, n, Tau*)

Inverse Wishart log-likelihood. The inverse Wishart distribution is the conjugate prior for the covariance matrix of a multivariate normal distribution.

$$f(X \mid n, T) = \frac{\mid T \mid^{n/2} \mid X \mid^{(n-k-1)/2} \exp\left\{-\frac{1}{2} Tr(TX^{-1})\right\}}{2^{nk/2}\Gamma_p(n/2)}$$

where k is the rank of X.

Parameters

X : matrix

Symmetric, positive definite.

n : integer

Degrees of freedom, > 0.

Tau : matrix

Symmetric and positive definite

`mv_normal_like`(*x, mu, tau*)

Multivariate normal log-likelihood parameterized by precision.

$$f(x \mid \pi, T) = \frac{T^{n/2}}{(2\pi)^{1/2}} \exp\left\{-\frac{1}{2}(x-\mu)'T(x-\mu)\right\}$$

Parameters

x : (n,k) float
mu : (k,) float
tau : (k,k) float, positive definite

See Also:

`mv_normal_chol_like`, `mv_normal_cov_like`

`mv_normal_cov_like`(*x, mu, C*)

Multivariate normal log-likelihood parameterized by covariance.

$$f(x \mid \pi, C) = \frac{T^{n/2}}{(2\pi)^{1/2}} \exp\left\{-\frac{1}{2}(x-\mu)'C^{-1}(x-\mu)\right\}$$

Parameters

x : (n,k) float
mu : (k,) float
C : (k,k) float, positive definite

See Also:

`mv_normal_like`, `mv_normal_chol_like`

`mv_normal_chol_like`(*x, mu, tau*)

Multivariate normal log-likelihood parameterized by the Cholesky factor of the covariance.

$$f(x \mid \pi, \sigma) = \frac{T^{n/2}}{(2\pi)^{1/2}} \exp\left\{-\frac{1}{2}(x-\mu)'(\sigma\sigma')^{-1}(x-\mu)\right\}$$

Parameters

x : (n,k) float
mu : (k,) float
sigma : (k,k) float, lower triangular

See Also:

`mv_normal_like`, `mv_normal_cov_like`

`wishart_like`(*X, n, Tau*)

Wishart log-likelihood. The conjugate prior for the precision parameter of a multivariate normal distribution. For an alternative parameterization based on $C = T^{-1}$, see `wishart_cov_like`.

$$f(X \mid n, T) = \mid T \mid^{n/2} \mid X \mid^{(n-k-1)/2} \exp\left\{-\frac{1}{2}Tr(TX)\right\}$$

where k is the rank of X.

Parameters

X : matrix
    Symmetric, positive definite.
n : integer
    Degrees of freedom, > 0.
Tau : matrix
    Symmetric and positive definite

wishart_cov_like(*X, n, C*)

Wishart log-likelihood. The conjugate prior for the precision parameter of a multivariate normal distribution. For an alternative parameterization based on $T = C^{-1}$, see `wishart_like`.

$$f(X \mid n, C) = \mid C^{-1} \mid^{n/2} \mid X \mid^{(n-k-1)/2} \exp\left\{-\frac{1}{2} Tr(C^{-1}X)\right\}$$

where k is the rank of X.

Parameters

X : matrix

Symmetric, positive definite.

n : integer

Degrees of freedom, > 0.

C : matrix

Symmetric and positive definite

CHAPTER TEN

Conclusion

MCMC is a surprisingly difficult and bug-prone algorithm to implement by hand. We find PyMC makes it much easier and less stressful. PyMC also makes our work more dynamic; getting hand-coded MCMC's working used to be so much work that we were reluctant to change anything, but with PyMC changing models is a breeze. We hope it does the same for you!

10.1 What's next?

A partial list of the features we would like to include in future releases follows. Three stars means that only debugging and checking is needed, so the feature is likely to be available in release 2.1; two stars means that there are no conceptual hurdles to be overcome but there's a lot of work left to do; and one star means only experimental development has been done.

- (***) Gibbs step methods to handle conjugate and nearly-conjugate submodels,
- (***) Handling all-normal submodels with sparse linear algebra [Wilkinson and Yeung, 2004]. This will help PyMC handle Markov random fields and time-series models based on the 'dynamic linear model' [West and Harrison, 1997] (among others) more efficiently, in some cases fitting them in closed form,
- (**) Generic Monte Carlo EM and SEM algorithms,
- (**) Parallelizing single chains with a thread pool,
- (**) Terse syntax inspired by Kerman and Gelman [2004] for creating variables: `C=A*B` should return a deterministic object if A and/or B is a PyMC variable,
- (**) Distributing multiple chains across multiple processes,
- (*) Parsers for model-definition syntax from R and WinBugs,
- (*) Dirichlet processes and other stick-breaking processes [Ishwaran and James, 2001].

These features will make their way into future releases as (and if) we are able to finish them and make them reliable.

10.2 How to get involved

We welcome new contributors at all levels. If you would like to contribute to any of the features above, or to improve PyMC itself in some other way, please introduce yourself on our mailing list. If you would like to share code written in PyMC, for example a tutorial or a specialized step method, please feel free to edit our wiki page.

APPENDIX
A

Appendix: Markov chain Monte Carlo

A.1 Monte Carlo Methods in Bayesian Analysis

Bayesian analysis often requires integration over multiple dimensions that is intractable both via analytic methods or standard methods of numerical integration. However, it is often possible to compute these integrals by simulating (drawing samples) from posterior distributions. For example, consider the expected value of a random variable $\mathbf{x}$:

$$E[\mathbf{x}] = \int \mathbf{x} f(\mathbf{x}) d\mathbf{x}, \qquad \mathbf{x} = \{x_1, ..., x_k\}$$

where k (the dimension of vector x) is perhaps very large. If we can produce a reasonable number of random vectors $\{\mathbf{x_i}\}$, we can use these values to approximate the unknown integral. This process is known as *Monte Carlo integration*. In general, MC integration allows integrals against probability density functions:

$$I = \int h(\mathbf{x}) f(\mathbf{x}) \mathbf{dx}$$

to be estimated by finite sums:

$$\hat{I} = \frac{1}{n} \sum_{i=1}^{n} h(\mathbf{x}_i),$$

where $\mathbf{x}_i$ is a sample from f. This estimate is valid and useful because:

- By the strong law of large numbers:
$$\hat{I} \to I \text{ with probability } 1$$
- Simulation error can be measured and controlled:
$$Var(\hat{I}) = \frac{1}{n(n-1)} \sum_{i=1}^{n} (h(\mathbf{x}_i) - \hat{I})^2$$

Why is this relevant to Bayesian analysis? If we replace $f(\mathbf{x})$ with a posterior, $f(\theta|d)$ and make $h(\theta)$ an interesting function of the unknown parameter, the resulting expectation is that of the posterior of $h(\theta)$:

$$E[h(\theta)|d] = \int f(\theta|d) h(\theta) d\theta \approx \frac{1}{n} \sum_{i=1}^{n} h(\theta)$$

Rejection Sampling

Though Monte Carlo integration allows us to estimate integrals that are unassailable by analysis and standard numerical methods, it relies on the ability to draw samples from the posterior distribution. For known parametric forms, this is not a problem; probability integral transforms or bivariate techniques (e.g Box-Muller method) may be used to obtain samples from uniform pseudo-random variates generated from a computer. Often, however, we cannot readily generate random values from non-standard posteriors. In such instances, we can use rejection sampling to generate samples.

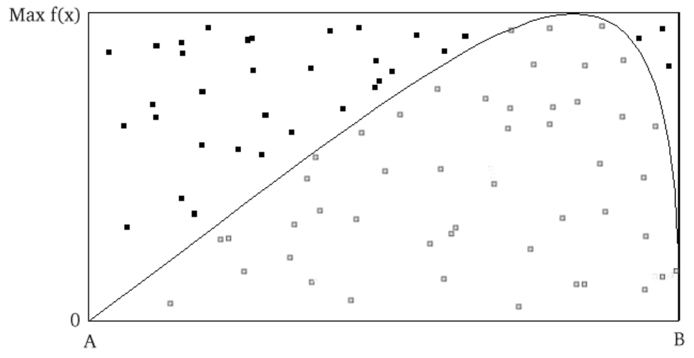


Figure A.1: Rejection sampling of a bounded form. Area is estimated by the ratio of accepted (open squares) to total points, multiplied by the rectangle area.

Posit a function, $f(x)$ which can be evaluated for any value on the support of $x : S_x = [A, B]$, but may not be integrable or easily sampled from. If we can calculate the maximum value of $f(x)$, we can then define a rectangle that is guaranteed to contain all possible values $(x, f(x))$. It is then trivial to generate points over the box and enumerate the values that fall under the curve (Figure A.1).

$$\frac{\text{Points under curve}}{\text{Points generated}} \times \text{box area} = \lim_{n\to\infty} \int_A^B f(x)dx$$

This approach is useful, for example, in estimating the normalizing constant for posterior distributions.

If $f(x)$ has unbounded support (i.e. infinite tails), such as a Gaussian distribution, a bounding box is no longer appropriate. We must specify a majorizing (or, enveloping) function, $g(x)$, which implies:

$$g(x) \geq f(x) \qquad \forall x \in (-\infty, \infty)$$

Having done this, we can now sample x_i from $g(x)$ and accept or reject each of these values based upon $f(x_i)$. Specifically, for each draw x_i, we also draw a uniform random variate u_i and accept x_i if $u_i < f(x_i)/cg(x_i)$, where c is a constant (Figure A.2). This approach is made more efficient by choosing an enveloping distribution that is "close" to the target distribution, thus maximizing the number of accepted points. Further improvement is gained by using optimized algorithms such as importance sampling which, as the name implies, samples more frequently from important areas of the distribution.

Rejection sampling is usually subject to declining performance as the dimension of the parameter space increases, so it is used less frequently than MCMC for evaluation of posterior distributions [Gamerman, 1997].

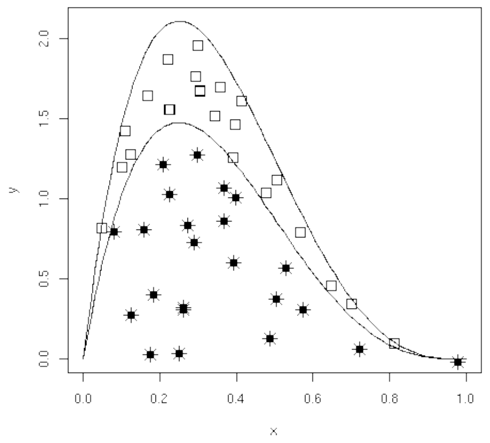


Figure A.2: Rejection sampling of an unbounded form using an enveloping distribution.

A.2 Markov Chains

A Markov chain is a special type of *stochastic process*. The standard definition of a stochastic process is an ordered collection of random variables:

$$\{X_t : t \in T\}$$

where t is frequently (but not necessarily) a time index. If we think of X_t as a state X at time t, and invoke the following dependence condition on each state:

$$Pr(X_{t+1} = x_{t+1} | X_t = x_t, X_{t-1} = x_{t-1}, \dots, X_0 = x_0) = Pr(X_{t+1} = x_{t+1} | X_t = x_t)$$

then the stochastic process is known as a Markov chain. This conditioning specifies that the future depends on the current state, but not past states. Thus, the Markov chain wanders about the state space, remembering only where it has just been in the last time step. The collection of transition probabilities is sometimes called a *transition matrix* when dealing with discrete states, or more generally, a *transition kernel*.

In the context of Markov chain Monte Carlo, it is useful to think of the Markovian property as "mild non-independence". MCMC allows us to indirectly generate independent samples from a particular posterior distribution.

Jargon-busting

Before we move on, it is important to define some general properties of Markov chains. They are frequently encountered in the MCMC literature, and some will help us decide whether MCMC is producing a useful sample from the posterior.

- *Homogeneity*: A Markov chain is homogeneous at step t if the transition probabilities are independent of time t.

- *Irreducibility*: A Markov chain is irreducible if every state is accessible in one or more steps from any other state. That is, the chain contains no absorbing states. This implies that there is a non-zero probability of eventually reaching state k from any other state in the chain.
- *Recurrence*: States which are visited repeatedly are *recurrent*. If the expected time to return to a particular state is bounded, this is known as *positive recurrence*, otherwise the recurrent state is *null recurrent*. Further, a chain is *Harris recurrent* when it visits all states $X \in S$ infinitely often in the limit as $t \to \infty$; this is an important characteristic when dealing with unbounded, continuous state spaces. Whenever a chain ends up in a closed, irreducible set of Harris recurrent states, it stays there forever and visits every state with probability one.
- *Stationarity*: A stationary Markov chain produces the same marginal distribution when multiplied by the transition kernel. Thus, if P is some $n \times n$ transition matrix:

  $$\pi \mathbf{P} = \pi$$

  for Markov chain π. Thus, π is no longer subscripted, and is referred to as the *limiting distribution* of the chain. In MCMC, the chain explores the state space according to its limiting marginal distribution.
- *Ergodicity*: Ergodicity is an emergent property of Markov chains which are irreducible, positive Harris recurrent and aperiodic. Ergodicity is defined as:

  $$\lim_{n\to\infty} Pr^{(n)}(\theta_i \to \theta_j) = \pi(\theta) \quad \forall \theta_i, \theta_j \in \Theta$$

  or in words, after many steps the marginal distribution of the chain is the same at one step as at all other steps. This implies that our Markov chain, which we recall is dependent, can generate samples that are independent if we wait long enough between samples. If it means anything to you, ergodicity is the analogue of the strong law of large numbers for Markov chains. For example, take values $\theta_{i+1}, \ldots, \theta_{i+n}$ from a chain that has reached an ergodic state. A statistic of interest can then be estimated by:

  $$\frac{1}{n} \sum_{j=i+1}^{i+n} h(\theta_j) \approx \int f(\theta) h(\theta) d\theta$$

A.3 Why MCMC Works: Reversible Markov Chains

Markov chain Monte Carlo simulates a Markov chain for which some function of interest (*e.g.* the joint distribution of the parameters of some model) is the unique, invariant limiting distribution. An invariant distribution with respect to some Markov chain with transition kernel $Pr(y \mid x)$ implies that:

$$\int_x Pr(y \mid x) \pi(x) dx = \pi(y).$$

Invariance is guaranteed for any **reversible** Markov chain. Consider a Markov chain in reverse sequence: $\{\theta^{(n)}, \theta^{(n-1)}, ..., \theta^{(0)}\}$. This sequence is still Markovian, because:

$$Pr(\theta^{(k)} = y \mid \theta^{(k+1)} = x, \theta^{(k+2)} = x_1, \ldots) = Pr(\theta^{(k)} = y \mid \theta^{(k+1)} = x)$$

Forward and reverse transition probabilities may be related through Bayes theorem:

$$\begin{aligned} Pr(\theta^{(k)} = y \mid \theta^{(k+1)} = x) &= \frac{Pr(\theta^{(k+1)} = x \mid \theta^{(k)} = y)Pr(\theta^{(k)} = y)}{Pr(\theta^{(k+1)} = x)} \\ &= \frac{Pr(\theta^{(k+1)} = x \mid \theta^{(k)} = y)\pi^{(k)}(y)}{\pi^{(k+1)}(x)} \end{aligned}$$

$$\frac{Pr(\theta^{(k+1)} = x \mid \theta^{(k)} = y)\pi^{(k)}(y)}{\pi^{(k+1)}(x)}$$

Though not homogeneous in general, π becomes homogeneous if **Do you ever call the stationary distribution itself homogeneous?**:

- $n \to \infty$
- $\pi^{(0)} = \pi$ for some $i < k$ **Is it meant to be $\pi^(i)$, and**

If this chain is homogeneous it is called reversible, because it satisfies the **detailed balance equation**:

$$\pi(x)Pr(y \mid x) = \pi(y)Pr(x \mid y)$$

Reversibility is important because it has the effect of balancing movement through the entire state space. When a Markov chain is reversible, π is the unique, invariant, stationary distribution of that chain. Hence, if π is of interest, we need only find the reversible Markov chain for which π is the limiting distribution. This is what MCMC does!

A.4 Gibbs Sampling

The Gibbs sampler is the simplest and most prevalent MCMC algorithm. If a posterior has k parameters to be estimated, we may condition each parameter on current values of the other $k-1$ parameters, and sample from the resultant distributional form (usually easier), and repeat this operation on the other parameters in turn. This procedure generates samples from the posterior distribution. Note that we have now combined Markov chains (conditional independence) and Monte Carlo techniques (estimation by simulation) to yield Markov chain Monte Carlo.

Here is a stereotypical Gibbs sampling algorithm:

1 Choose starting values for states (parameters): $\theta = [\theta_1^{(0)}, \theta_2^{(0)}, \ldots, \theta_k^{(0)}]$

2 Initialize counter $j = 1$

3 Draw the following values from each of the k conditional distributions:

$$\begin{aligned} \theta_1^{(j)} &\sim \pi(\theta_1|\theta_2^{(j-1)}, \theta_3^{(j-1)}, \ldots, \theta_{k-1}^{(j-1)}, \theta_k^{(j-1)}) \\ \theta_2^{(j)} &\sim \pi(\theta_2|\theta_1^{(j)}, \theta_3^{(j-1)}, \ldots, \theta_{k-1}^{(j-1)}, \theta_k^{(j-1)}) \\ \theta_3^{(j)} &\sim \pi(\theta_3|\theta_1^{(j)}, \theta_2^{(j)}, \ldots, \theta_{k-1}^{(j-1)}, \theta_k^{(j-1)}) \\ &\vdots \\ \theta_{k-1}^{(j)} &\sim \pi(\theta_{k-1}|\theta_1^{(j)}, \theta_2^{(j)}, \ldots, \theta_{k-2}^{(j)}, \theta_k^{(j-1)}) \\ \theta_k^{(j)} &\sim \pi(\theta_k|\theta_1^{(j)}, \theta_2^{(j)}, \theta_4^{(j)}, \ldots, \theta_{k-2}^{(j)}, \theta_{k-1}^{(j)}) \end{aligned}$$

4 Increment j and repeat until convergence occurs.

As we can see from the algorithm, each distribution is conditioned on the last iteration of its chain values, constituting a Markov chain as advertised. The Gibbs sampler has all of the important properties outlined in the previous section: it is aperiodic, homogeneous and ergodic. Once the sampler converges, all subsequent samples are from the target distribution. This convergence occurs at a geometric rate.

A.5 The Metropolis-Hastings Algorithm

The key to success in applying the Gibbs sampler to the estimation of Bayesian posteriors is being able to specify the form of the complete conditionals of θ. In fact, the algorithm cannot be implemented without them. Of course, the posterior conditionals cannot always be neatly specified. In contrast to the Gibbs algorithm, the Metropolis-Hastings algorithm generates candidate state transitions from an alternate distribution, and accepts or rejects each candidate probabilistically.

Let us first consider a simple Metropolis-Hastings algorithm for a single parameter, θ. We will use a standard sampling distribution, referred to as the *proposal distribution*, to produce candidate variables $q_t(\theta'|\theta)$. That is, the generated value, θ', is a *possible* next value for θ at step $t+1$. We also need to be able to calculate the probability of moving back to the original value from the candidate, or $q_t(\theta|\theta')$. These probabilistic ingredients are used to define an *acceptance ratio*:

$$a(\theta', \theta) = \frac{q_t(\theta'|\theta)\pi(\theta')}{q_t(\theta|\theta')\pi(\theta)}$$

The value of $\theta^{(t+1)}$ is then determined by:

$$\theta^{(t+1)} = \begin{cases} \theta' & \text{with prob.} \quad \min(a(\theta', \theta), 1) \\ \theta^{(t)} & \text{with prob.} \quad 1 - \min(a(\theta', \theta), 1) \end{cases}$$

This transition kernel implies that movement is not guaranteed at every step. It only occurs if the suggested transition is likely based on the acceptance ratio.

A single iteration of the Metropolis-Hastings algorithm proceeds as follows:

1 Sample θ' from $q(\theta'|\theta^{(t)})$.

2 Generate a Uniform[0,1] random variate u.

3 If $a(\theta', \theta) > u$ then $\theta^{(t+1)} = \theta'$, otherwise $\theta^{(t+1)} = \theta^{(t)}$.

The original form of the algorithm specified by Metropolis required that $q_t(\theta'|\theta) = q_t(\theta|\theta')$, which reduces $a(\theta', \theta)$ to $\pi(\theta')/\pi(\theta)$, but this is not necessary. In either case, the state moves to high-density points in the distribution with high probability, and to low-density points with low probability. After convergence, the Metropolis-Hastings algorithm describes the full target posterior density, so all points are recurrent.

Random-walk Metropolis-Hastings

A practical implementation of the Metropolis-Hastings algorithm makes use of a random-walk proposal. Recall that a random walk is a Markov chain that evolves according to:

$$\begin{aligned} \theta^{(t+1)} &= \theta^{(t)} + \epsilon_t \\ \epsilon_t &\sim f(\phi) \end{aligned}$$

As applied to the MCMC sampling, the random walk is used as a proposal distribution, whereby dependent proposals are generated according to:

$$q(\theta'|\theta^{(t)}) = f(\theta' - \theta^{(t)}) = \theta^{(t)} + \epsilon_t$$

Generally, the density generating ϵ_t is symmetric about zero, resulting in a symmetric chain. Chain symmetry implies that $q(\theta'|\theta^{(t)}) = q(\theta^{(t)}|\theta')$, which reduces the Metropolis-Hastings acceptance ratio to:

$$a(\theta', \theta) = \frac{\pi(\theta')}{\pi(\theta)}$$

The choice of the random walk distribution for ϵ_t is frequently a normal or Student's t density, but it may be any distribution that generates an irreducible proposal chain.

An important consideration is the specification of the scale parameter for the random walk error distribution. Large values produce random walk steps that are highly exploratory, but tend to produce proposal values in the tails of the target distribution, potentially resulting in very small acceptance rates. Conversely, small values tend to be accepted more frequently, since they tend to produce proposals close to the current parameter value, but may result in chains that mix very slowly. Some simulation studies suggest optimal acceptance rates in the range of 20-50%. It is often worthwhile to optimize the proposal variance by iteratively adjusting its value, according to observed acceptance rates early in the MCMC simulation [Gamerman, 1997].

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