An Introduction to using JAGS for Bayesian Regression Analysis

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1 Preface

This paper is an introduction to constructing Bayesian regression models using the R programming language and the R package rjags. Familiarity with the R language and basic statistical background (means, standard deviations, etc) are necessary to understand the material.

The intent of this paper is to show how easy it is to fit complex regression models to experimental data with rjags. The techniques applied in this paper are surprisingly powerful, given their simplicity.

2 Background

2.1 Bayes’ Theorem

First, some notation: for an event \( A \), the probability of the event occurring is given by \( P(A) \). For instance, the probabilities of an unbiased coin flip can be written as \( P(\text{heads}) = 0.5 \) and \( P(\text{tails}) = 0.5 \).

In many cases, we wish to know the conditional probability of an event. \( P(A|B) \) represents the probability of event \( A \) occurring, given that event \( B \) occurs. To give an example of the difference between this and standard probability, if today is Wednesday (event \( A \)), the probability of tomorrow being Thursday (event \( B \)) is \( P(B|A) = 1 \), while without the condition, the probability is random: \( P(B) = 1/7 \).

The whole subject of Bayesian Inference rests on a mathematical rule called Bayes’ theorem:

\[
P(H|E) = \frac{P(E|H)P(H)}{P(E)}
\]
Here, $H$ stands for a hypothesis to be tested and $E$ stands for the evidence (data). The right side contains three terms. $P(E|H)$ is the likelihood of measuring the evidence, assuming that the hypothesis is true. The two probabilities $P(H)$ and $P(E)$ are called priors or prior distributions and represent relevant knowledge beyond the dataset itself. They are called “priors” because we know these probabilities before doing the analysis.

The left side of Bayes’ theorem reads “The probability of $H$ given the evidence”, which represents exactly what we are interested in – how likely is this hypothesis, according to the data that we collected? This probability is known as the posterior or the posterior distribution. In this paper, we’ll focus on fitting model parameters to datasets, and so what we are interested in are real numbers: slopes, intercepts, standard deviations, etc. These of course lie on the real axis and are continuous, and so the posterior for some model will be probability distributions for each parameter.

In general, each of these terms can be arbitrarily complex, and so actually using Bayes’ theorem for analytic calculation is often impractical. To get around this, we use a numerical technique called Markov Chain Monte Carlo.

2.2 MCMC

Monte Carlo methods are algorithms that use randomly generated numbers to estimate numbers that are too hard to calculate analytically. A common use case for Monte Carlo techniques is evaluating complex multidimensional integrals. We won’t cover the theory of Markov Chain Monte Carlo here, as many resources are available for this. Suffice to say, we will generate Markov Chains from which the posterior distributions can be calculated.

3 Bayesian Regression

3.1 Basic Linear Model

The overall idea with using rjags is to define a model structure, give this, our datasets, and prior distributions to the MCMC engine, and get back posterior distributions of specified parameters.

First, the package needs to be loaded, and we may as well set a seed for the random number generator so that our results are reproducible:

```r
library(rjags)
set.seed(1)
```

Now let’s make a basic model to test rjags. The simplest realistic example is a linear relationship with some y-scatter. Let’s make an artificial dataset for testing:

```r
## Create an artificial dataset:
true_slope = 1
dtrue_intercept = -5
dtrue_sigma = 2
N = 50
dx = runif(N,0,10)
dy = rnorm(N, true_slope * x + true_intercept, true_sigma)
```

At least for now, we should take a look at our data before analyzing it, just to make sure it is how we expect it to be:

```r
plot(x, y)
```
Now let’s talk about the model we will use. We are modeling the data as linear with gaussian scatter:

\[ y_i \sim \mathcal{N}(ax_i + b, \sigma^2) \]

To actually implement this model, we will need to express it in the JAGS language. The JAGS language is a little different from normal programming languages like R. It is a declarative language, meaning that the code you write is not followed as a sequence of steps, but rather as a description of logic. For instance, the line \( y.hat[i] = a * x[i] + b \) does not evaluate the right side and set the left side equal to it, as R would. Instead, this code only specifies the model structure that JAGS should use.

For now, the model code will be separated into two sections. The first is for specifying priors on our parameters of interest. Here, we are interested in the slope \( a \), intercept \( b \), and standard deviation \( \sigma \) of our dataset. The second section is for describing how our different variables are related to each other. Then, the whole chunk of JAGS code is wrapped in `model {...}` and passed into the JAGS engine.

For this dataset, the priors might be as follows. The slope \( a \) we expect to be non-negative and no greater than 5, so we could use a uniform density between 0 and 5. The intercept \( b \) could be anywhere between \( \pm 10 \), and the scatter’s standard deviation \( \sigma \) is expected to be between 0 and 3. Note that the choice of priors is domain specific and not the emphasis here, but we have chosen priors that include the “true” values.

Let’s write the JAGS code for this model and capture it into a string:

```r
model_string = "
model {
  ## priors:
a ~ dunif(0,5)
}
```

Density functions in JAGS always start with “d”: `dunif` for uniform density, `dnorm` for gaussian density, `dlnorm` for lognormal density, etc. The tildes are read as “is distributed as”. For instance, \( a \sim \text{dunif}(0,5) \) is read as “the variable \( a \) is distributed uniformly between 0 and 5”.

In the structure block, we have a traditional for loop. This allows us to relate each \( y \) value to each \( x \) value such that each \( y \) value is normally distributed around the line \( a \times x + b \) with standard deviation \( \sigma \). For historical reasons, JAGS distribution functions use a “precision” that is defined as one over the variance. Usually it is more convenient to speak in terms of standard deviation and variance, so most models will have a small conversion between standard deviation and precision included.

Note that the order of lines is somewhat unimportant – the priors could have been included after the structure and it would make no difference.

Now that we have a model structure and some data, we can give this to JAGS and see what comes back. Normally the JAGS engine wants the model structure in a separate file, but to keep it easy we’ll use a `textConnection` instead. This allows us to create a fake file whose contents are the model string we created above, and we’ll give this to JAGS instead.

Now, we want to give our model structure and data to JAGS and get back the output of the MCMC process to analyze.

```r
model = jags.model(file = textConnection(model_string),
                    data = list('x' = x,
                                'y' = y,
                                'N' = N),
                    n.chains = 1,
                    n.adapt = 1000,
                    inits = list('.RNG.name' = 'base::Mersenne-Twister',
                                 '.RNG.seed' = 1))
```

This has created a model, and printed some information that is not particularly interesting. We can then actually generate a Markov chain with

```r
output = coda.samples(model = model,
                       variable.names = c("a", "b", "sigma"),
                       n.iter=1000,
                       thin=1)
```
We get back an object `output` that contains the Markov chain. First, as always in R, have a look at the summary of it:

```r
print(summary(output))
```

```
##
## Iterations = 1001:2000
## Thinning interval = 1
## Number of chains = 1
## Sample size per chain = 1000
##
## 1. Empirical mean and standard deviation for each variable, plus standard error of the mean:
##
##     Mean   SD Naive SE Time-series SE
##  a  1.015 0.0986 0.003117    0.0109
##  b -4.905 0.5791 0.018312    0.0635
## sigma 1.891 0.1939 0.006131    0.0079
##
## 2. Quantiles for each variable:
##
##     2.5%   25%   50%   75%  97.5%
##  a  0.8372 0.9484 1.013 1.078 1.220
##  b -6.0694 -5.2835 -4.876 -4.513 -3.857
## sigma 1.5659 1.7509 1.876 2.016 2.306
```

This gives us information about the distributions of the parameters we asked JAGS to calculate (\(a\), \(b\), and \(\sigma\)). Notice that the means for each parameter are quite close to the true values. We can also see this visually:

```r
plot(output)
```
We see mixing diagrams on the left, and posterior distributions on the right. The mixing diagrams appear qualitatively acceptable, and the posterior distributions are centered on or quite near the true values of 1, -5, and 2, respectively. The model has successfully recovered the values we used to create the data. The total, self-contained code for this is as follows:

```r
library(rjags)
set.seed(1)

true_slope = 1
true_intercept = -5
true_sigma = 2
N = 50
x = runif(N,0,10)
y = rnorm(N,true_slope * x + true_intercept, true_sigma)
plot(x,y)

model_string = "
model {

  
}
```

## priors:
a \sim \text{dunif}(0,5)
b \sim \text{dunif}(-10,10)
sigma \sim \text{dunif}(0,3)

## structure:
for (i in 1:N) {
y[i] \sim \text{dnorm}(a \times x[i] + b, \text{pow}(\sigma, -2))
}

```
model = jags.model(file = textConnection(model_string),
                   data = list('x' = x, 'y' = y, 'N' = N),
                   n.chains = 1, n.adapt = 1000, inits = list('.RNG.name' = 'base::Mersenne-Twister',
                                       '.RNG.seed' = 1))

output = coda.samples(model = model,
                       variable.names = c("a", "b", "sigma"),
                       n.iter=1000, thin=1)

print(summary(output))

plot(output)
```

The rest of the examples in this paper will follow more or less the same format: create or load in some data, define the model, pass it to JAGS, and have a look at the output.

### 3.2 Linear Model with Error Bars

The basic model we assumed last time is rarely the most applicable to real-life data analysis. In general, there will be some measurement error (that is not necessarily constant across measurements) associated with the dataset in addition to scatter from other variables. Let’s generate some data that reflect this:

```r
N = 25
true_x = runif(N,0,10)
true_slope = 1
true_intercept = 0
scatter = 1
true_y = rnorm(N, true_slope * true_x + true_intercept, scatter)
```

```r
## known measurement uncertainties
x_sigma = rlnorm(N, -2, 0.5)
y_sigma = rlnorm(N, -2, 0.5)
obs_x = rnorm(N, true_x, x_sigma)
ox_y = rnorm(N, true_y, y_sigma)
```

```r
plot(obs_x, obs_y)
segments(obs_x, obs_y - 2*y_sigma, obs_x, obs_y + 2*y_sigma)
```
segments(obs_x - 2*x_sigma, obs_y, obs_x + 2*x_sigma, obs_y)

Clearly, the group scatter is larger than the individual measurement error bars allow, implying that one or more unmeasured variables are influencing the y values. The model we’ll use is a linear relationship between y and x, with (uniform) measurement error on both y and x and additional scatter in y. The JAGS code is as follows:

```jags
model_string = "
model {
  ## priors:
  a ~ dunif(0,5)
  b ~ dunif(-10,10)
  scatter ~ dunif(0,3)

  ## structure:
  for (i in 1:N) {
    ## the true x:
    x[i] ~ dunif(0,10)
    ## the observed x:
    obs_x[i] ~ dnorm(x[i], pow(x_sigma[i],-2))

    ## y, as it would be if it only depended on the true x:
    y[i] = a*x[i] + b
    ## y, with the effect of the unmeasured confounding variable
```

```
y_scatter[i] ~ dnorm(y[i], pow(scatter,-2))
## y, with the confounding variable, with observational error:
obs_y[i] ~ dnorm(y_scatter[i], pow(y_sigma[i],-2))

Now we proceed as before: feed the data and model structure into JAGS and look at the output:

```r
model = jags.model(file = textConnection(model_string),
                  data = list('obs_x' = obs_x,
                              'x_sigma' = x_sigma,
                              'obs_y' = obs_y,
                              'y_sigma' = y_sigma,
                              'N' = N),
                  n.chains = 1,
                  n.adapt = 1000,
                  inits = list('.RNG.name' = 'base::Mersenne-Twister',
                              '.RNG.seed' = 1))

output = coda.samples(model = model,
                       variable.names = c("a", "b", "scatter"),
                       n.iter=1000,
                       thin=1)

plot(output)
```
Again, the model has reproduced the parameters used to generate the data. What would happen if we ran the code again, but increased the measurement uncertainty?

```r
## these values are the same as in the previous model:
#N = 25
#true_x = runif(N,0,10)
#true_slope = 1
#true_intercept = 0
#scatter = 0.25
#true_y = rnorm(N, true_slope * true_x + true_intercept, scatter)
## known measurement uncertainties (much larger than before)
x_sigma = rlnorm(N, 1, 0.5)
y_sigma = rlnorm(N, 1, 0.5)
obs_x = rnorm(N, true_x, x_sigma)
obs_y = rnorm(N, true_y, y_sigma)

plot(obs_x, obs_y)
segments(obs_x, obs_y - 2*y_sigma, obs_x, obs_y + 2*y_sigma)
segments(obs_x - 2*x_sigma, obs_y, obs_x + 2*x_sigma, obs_y)
```
This time, the uncertainty bars are much larger, and you would think that very little information could be extracted from these data. Using the same model as before, let’s see what the output looks like:
Here, the number of MCMC iterations has been increased to 10,000. With the 1,000 iterations used before, the mixing diagrams did not appear robust. The slope and intercept posterior distributions are not as smooth and are wider than before, and the scatter posterior is maximized far from the true value. As expected, using uninformative data results in uninformative posteriors.

### 3.3 Linear Model with Multiple Datasets and Systematic Error

Systematic error is something that is typically difficult to deal with in statistical analysis, but is easy here. First, let’s examine the case when the systematic error is proportional to $x$. Imagine we have two data sets with qualitatively different slopes:

```r
## generate some data
slope = 2
intercept = 5
N1 = 20
shift1 = 0.7;
obs_x1 = runif(N1,0,10)
err_y1 = runif(N1, 0.1, 0.2)
obs_y1 = shift1 * rnorm(N1, slope * obs_x1 + intercept, err_y1)
N2 = 30
shift2 = 1.3;
obs_x2 = runif(N2,0,10)
```
```r
err_y2 = runif(N2, 0.1, 0.2)
obs_y2 = shift2 * rnorm(N2, slope * obs_x2 + intercept, err_y2)

plot(obs_x1, obs_y1, xlim = c(0,10), ylim = c(4,35), xlab = "x", ylab = "y")
points(obs_x2, obs_y2, pch=19)
segments(obs_x1, obs_y1 - 2*err_y1, obs_x1, obs_y1 + 2*err_y1)
segments(obs_x2, obs_y2 - 2*err_y2, obs_x2, obs_y2 + 2*err_y2)
```

This could be caused by, say, the result of a lab instrument that became miscalibrated between the data collections. Some researchers would take a weighted average of some kind to combine the two datasets, but that method is statistically dubious at best. Let's construct and run a model that includes a multiplicative factor for the two datasets:

```r
model_string = "
model {
  ## priors:
a ~ dunif(0,5)
b ~ dunif(-10,10)
  ## shifts must be > 0. Choose centered near 1 (0% shift), with ~0.1 = 10% spread
multiplier1 ~ dlnorm(log(1.0), pow(log(1.1),-2))
multiplier2 ~ dlnorm(log(1.0), pow(log(1.1),-2))

  ## structure:
  for (i in 1:length(obs_x1)) {
```

---
\[ y_{1[i]} = \text{multiplier1} \times (a \times \text{obs}_{x1[i]} + b) \]
\[ \text{obs}_{y1[i]} \sim \text{dnorm}(y_{1[i]}, \text{pow}(\text{err}_{y1[i]}, -2)) \]

for (i in 1:length(\text{obs}_x2)) {
  \[ y_{2[i]} = \text{multiplier2} \times (a \times \text{obs}_{x2[i]} + b) \]
  \[ \text{obs}_{y2[i]} \sim \text{dnorm}(y_{2[i]}, \text{pow}(\text{err}_{y2[i]}, -2)) \]
}
}

```
model = jags.model(file = textConnection(model_string),
data = list('obs_x1' = obs_x1,
    'obs_x2' = obs_x2,
    'obs_y1' = obs_y1,
    'obs_y2' = obs_y2,
    'err_y1' = err_y1,
    'err_y2' = err_y2),
n.chains = 1,
    n.adapt = 1000,
inits = list('.RNG.name' = 'base::Mersenne-Twister',
    '.RNG.seed' = 1))
output = coda.samples(model = model,
    variable.names = c("a", "b", "multiplier1", "multiplier2"),
n.iter=500000,
    #n.iter =10000,
thin=1)
```

Note that the number of iterations has been increased to 500,000 from the standard 10,000. This model's added complexity required more iterations for the Markov chains to converge. The posterior distributions are amazingly accurate:

```
plot(output)
```
The slope, intercept, and both systematic error multipliers are all centered exactly on their true values. Now, let’s look at an additive systematic error. Imagine we have two datasets, each with a positive systematic error (implying that taking a weighted average would not help very much).

```r
## generate some data
slope = 2
intercept = 5

N1 = 20
shift1 = 1.5;
obs_x1 = runif(N1,0,10)
err_y1 = runif(N1, 0.1, 0.2)
obs_y1 = shift1 + rnorm(N1, slope * obs_x1 + intercept, err_y1)

N2 = 30
```
shift2 = 3;
obs_x2 = runif(N2, 0, 10)
err_y2 = runif(N2, 0.1, 0.2)
obs_y2 = shift2 + rnorm(N2, slope * obs_x2 + intercept, err_y2)

plot(obs_x1, obs_y1, xlim = c(0,10), ylim = c(5,25), xlab = "x", ylab = "y")
points(obs_x2, obs_y2, pch=19)
segments(obs_x1, obs_y1 - 2*err_y1, obs_x1, obs_y1 + 2*err_y1)
segments(obs_x2, obs_y2 - 2*err_y2, obs_x2, obs_y2 + 2*err_y2)

The model will be similar to before:

```r
model_string = "
model {
  ## priors:
a ~ dunif(0,5)
b ~ dunif(-10,10)
shift1 ~ dnorm(0, 1)
shift2 ~ dnorm(0, 1)

  ## structure:
  for (i in 1:length(obs_x1)) {
    y1[i] = shift1 + (a*obs_x1[i] + b)
    obs_y1[i] ~ dnorm(y1[i], pow(err_y1[i],-2))

  }
}
```

for (i in 1:length(obs_x2)) {
    y2[i] = shift2 + (a*obs_x2[i] + b)
    obs_y2[i] ~ dnorm(y2[i], pow(err_y2[i],-2))
}

model = jags.model(file = textConnection(model_string),
                     data = list('obs_x1' = obs_x1,
                                 'obs_x2' = obs_x2,
                                 'obs_y1' = obs_y1,
                                 'obs_y2' = obs_y2,
                                 'err_y1' = err_y1,
                                 'err_y2' = err_y2),
                     n.chains = 1,
                     n.adapt = 1000,
                     inits = list('.RNG.name' = 'base::Mersenne-Twister',
                                 '.RNG.seed' = 1))

output = coda.samples(model = model,
                        variable.names = c("a", "b", "shift1", "shift2"),
                        n.iter = 500000,
                        thin=1)

Again the number of iterations has been increased to 500,000.

plot(output)
This time, the results are rather disappointing. The systematic error posteriors are not centered near the true values at all. The intercept posterior has been shifted as well. This is not too unexpected— we didn’t give it much to work with, and really no additive shift would be unreasonable to report here.

### 3.4 Nonlinear models

In general, relationships between variables may not be linear. One of the conveniences of using JAGS is the ability to analyze data without transforming columns of your data back and forth.

#### 3.4.1 Malus’s Law

For instance, say that you collected data on light intensity after traveling through a polarizer. Then you would expect Malus’s Law to hold:

\[ I = I_0 \cos^2 \theta \]
If you measured $I$ as a function of $\theta$, perhaps the goal is to calculate the value of $I_0$, or to verify that it indeed varies with $\cos^2 \theta$ rather than $\cos^2 a\theta$ for $a \neq 1$.

```r
## theta in degrees, I in lux. data taken from
## http://www.physicslabs.umb.edu/Physics/sum13/182_Exp1_Sum13.pdf

data.table = read.table(header = TRUE, text =
"theta I
0 24.45
10 23.71
20 21.59
30 18.34
40 14.35
50 10.10
60 6.11
70 2.86
80 0.74
90 0.00"
)

# convert to radians
data.table$theta = data.table$theta * pi/180

Now, let’s write the model to test the two parameters $I_0$ and $a$, and get an idea of what the scatter around Malus’s Law is:

```r
model_string = "
model {
    ## priors:
a ~ dunif(0,10)
I0 ~ dunif(0,50)
sigma ~ dunif(0,100)

    for (i in 1:length(theta)) {
        I[i] ~ dnorm(I0 * (cos(a*theta[i]))^2, pow(sigma,-2))
    }
}
"

model = jags.model(file = textConnection(model_string),
data = list('theta' = data.table$theta,
'I' = data.table$I),
n.chains = 1,
n.adapt = 1000,
inits = list('.RNG.name' = 'base::Mersenne-Twister',
'.RNG.seed' = 1))

output = coda.samples(model = model,
variable.names = c("a", "I0", "sigma"),
n.iter =10000,
thin=1)

plot(output)
```
Note the x-scales on the probability densities— all of them are very tight, and it would appear that \( a \) is certainly indistinguishable from 1, and our measurements hardly deviate at all from Malus’s Law predictions.

### 3.4.2 Growing Signal

To give another example, one with more parameters, let’s analyze a simulated time-varying voltage signal. First, let’s generate some data:

```r
N = 100
A = 5
w = 2
d = 1.5
sigma = 1
t = seq(from = 0,
to = 10,
length.out = N)
y = rnorm(N,
    A*t*cos(w*t + d),
sigma)
plot(t,y)

Note that now we have four parameters: an amplitude, a frequency, a phase shift, and the noise. The model is simple:

```r
model_string = "
model {
    A ~ dunif(0,10)
    w ~ dunif(0,10)
    d ~ dunif(-3.14, 3.14)
    sigma ~ dunif(0,10)

    for (i in 1:length(t)) {
        y[i] ~ dnorm(A*t[i]*cos(w*t[i] + d), pow(sigma, -2))
    }
}
"

model = jags.model(file = textConnection(model_string),
    data = list('t' = t,

'y' = y),

`n.chains = 1,`  
`n.adapt = 1000)`

\[ \text{output} = \text{coda.samples(model = model,} \]
\[ \text{variable.names = c("A", "w", "sigma", "d"),} \]
\[ \text{n.iter = 10000,} \]
\[ \text{thin=1)} \]

And the output is surprisingly good:

```r
plot(output)
```
3.4.3 The Slow Fourier Transform

Just for fun, let’s see if we can emulate the Fourier Transform with JAGS. First, let’s make a plausible signal to transform. Choose some random lattice points, then spline between them and sample the interpolation:

```r
set.seed(2)
anchor.x = 1:10
anchor.y = rnorm(10,0,0.5)
x = seq(from=0,to=10,by=0.1)
spline_values = spline(x = anchor.x, y = anchor.y, xout = x, method = "fmm")
y = spline_values$y
plot(anchor.x, anchor.y)
lines(x,y)
```

Looks like a reasonable signal to analyze. Now, let’s assume that we can fit a model of the form

\[ y(x) \approx \sum_{n=1}^{5} \left[ a_n \sin(nx) + b_n \cos(nx) \right] \]

This is going to be a pretty rough approximation, since we are only using 5 terms and not including the \( n = 0 \) contribution. No matter. Let’s now define the model. The values for \( a_n \) and \( b_n \) probably won’t be too large, since the signal’s amplitude is relatively small. Hopefully, the difference between our approximated signal and the real thing will be relatively small as well.
This model is a bit of a mouthful, but should be understandable after some thought. Now, let’s calculate some values for the $a_n$ and $b_n$ and recreate the signal from each frequency component:

```r
N_terms = 5

model_string = 
  model {
    ## priors:
    for(i in 1:N){
      a[i] ~ dunif(-100,100)
      b[i] ~ dunif(-100,100)
    }
    for(i in 1:length(x)) {
      err[i] ~ dunif(0,100)
    }
    
    # loop over x
    for (i in 1:length(x)) {
      # loop over frequencies
      for (j in 1:N){
        y.hat[i,j] = a[j]*sin(j*x[i]) + b[j]*cos(j*x[i])
      }
      y[i] ~ dnorm(sum(y.hat[i,]), pow(err[i],-2))
    }
  }

model = jags.model(file = textConnection(model_string),
data = list('x' = x,
              'y' = y,
              'N' = N_terms),
n.chains = 1,
n.adapt = 1000,
inits = list('.RNG.name' = 'base::Mersenne-Twister',
              '.RNG.seed' = 1))

output = coda.samples(model = model,
                      variable.names = c("a", "b", "err"),
n.iter = 10000,
                      thin=1)

This model is a bit of a mouthful, but should be understandable after some thought. Now, let’s calculate some values for the $a_n$ and $b_n$ and recreate the signal from each frequency component:

```}

```r

a = rep(0,N_terms)
b = rep(0,N_terms)
for(i in 1:N_terms){
a[i] = median(output[[1]][,i])
b[i] = median(output[[1]][,N_terms+i])
}

y2 = rep(0,length(x))
for(i in 1:length(x)){
y2[i] = sum(a * sin((1:N_terms)*x[i]) + b * cos((1:N_terms)*x[i]))
}
```
It's not that bad! It is thoroughly impressive to me that such a sequence of bad approximations turned out to be so close to the original – even if it takes a minute or three to crunch the numbers (thus, the “Slow Fourier Transform”). This is by no means an appropriate use of JAGS, but it shows the flexibility of the package.

4 Choosing a Prior

The choice of prior to use for parameters can be somewhat tricky. If the parameters in question are well-studied, there may be reasonably precise bounds around the parameter value. However, previous information doesn’t exist about all parameters, so sometimes “vague priors” and “uninformative priors” are used to let the model have more freedom in determining parameter values. We’ll focus first on this kind of prior.

4.1 Uninformative Priors

A common choice of uninformative prior is the “flat” or uniform prior. In rjags code, a flat prior between two numbers \(a\) and \(b\) is represented by \(\text{dunif}(a, b)\). This is easy to understand and weights each value in the interval \([a, b]\) with equal value. However, the “fairness” of the uniform prior does need some careful consideration. Consider the case when the parameter of interest is the slope of a line. Using a uniform prior on \([0, 100]\) means that lines with slope greater than unity are 99% more likely than lines with slope less than unity. This is easy to see graphically: if we plot lines with slope 0, 1, 2, 3, ..., we get
Clearly, more steep lines exist than shallow lines, so this prior is probably less “fair” than you might have thought. A more fair alternative might be a uniform prior on $\phi$, the angle between the line and the x-axis. Then the slope corresponding to each $\phi$ is $b = \tan \phi$ (because slope is $\Delta y/\Delta x = \sin \phi/\cos \phi$). To see this graphically:

```r
plot(0,0)
phi_array = seq(from = 0, to = pi/2, by = 0.1)
for(phi in phi_array){
  abline(0,tan(phi),col='red');
}
```
So, if a uniformly-weighted prior is desired, sometimes it takes a bit of thought to achieve. It is a good idea to think about whether you would rather be totally ignorant of the scale of the parameter rather than the value of the parameter – if you are ignorant of the parameter’s order of magnitude, then it is as likely to be in [1, 10] as it is to be in [100, 1000]. This corresponds to a logarithmic decaying prior, which could be created as a uniform prior on the power of ten and then taking the logarithm for the parameter value.

In the past, people have put a lot of effort into find the “best” non-informative prior to use. The current consensus is that there is not one single uninformative prior that is the best to use for all models, though some fields do have standard default priors.

Vague priors are usually very broad in the sense that they cover a large amount of the parameter’s possible values. Examples of this include a wide uniform distribution and a Gaussian with large variance. A vague prior may still have some information; for instance, using a wide lognormal distribution will require the posterior to be non-negative.

### 4.2 Informative Priors

If some information about the parameters is already known before the data analysis, this can (and should) be encoded in the prior. For example, if previous experiments have estimated the value of the parameter of interest, you might use a prior of a Gaussian centered on the existing estimate. Strictly non-negative parameters can be described with a lognormal distribution, and in general the more flexible distributions (e.g., gamma) can be used with carefully chosen shape parameters to get a wide range of shapes.

### 5 Notes

There are a few tricks to help get good results with JAGS. For example, the time-varying signal had a phase shift included, and the prior was chosen to be \( \text{dunif}(-3.14, 3.14) \) rather than \( \text{dunif}(0, 6.28) \). Sometimes, the Markov Chain can “get stuck” and fail to sample accurately, and the choice of prior can affect this.

Another way to avoid this problem is by specifying reasonable initial values for each parameter with the \textit{inits} variable. If you do not specify the initial value for a parameter, JAGS will try to pick an appropriate
starting value. It usually works well, but can fail for some models.

6 Modifying JAGS

6.1 Overview

JAGS has the standard functions built into its model description language – log, sin, etc. However, more complex models may require custom domain-specific functions. Unfortunately, JAGS doesn’t provide a way to include custom functions if the function can’t be implemented in the model itself as a combination of the builtins. For instance, a nuclear physics model might require calculation of Coulomb wavefunctions with some given parameters. Existing fortran codes exist for this, and they are a thousand lines or more long, meaning that implementing them in the model directly is not feasible.

This document shows the process of creating new JAGS functions that can be used in a model description. They can use existing executables or be self-contained. This involves recompiling JAGS with the new function added in, and so the process of installing dependencies, compilers, etc will also be covered.

This document was written for JAGS version 4.2.0, R version 3.0.2, and R packages rjags 4-6 and coda 0.18-1, running on Ubuntu 14.04. It may be helpful for more recent versions of these packages, but things tend to change over time.

6.2 Installing Dependencies

This was originally done on a remote VPS, but a standard personal computer will also suffice. These instructions assume a Debian-based GNU/Linux OS, as I have no experience with writing code on Mac OSX or Windows computers.

First, if your computer does not have much ram, you may want to enable a swapfile. This will allow your computer to start using hard drive space as a (much slower) replacement for ram if it runs out. Running JAGS models is not very memory-intensive, but compiling the JAGS source code can take a decent amount. This may not be necessary for you, but if you run into “memory full” issues later, this is one solution. The following commands at a bash terminal will create a 2GB swapfile that will persist until the computer next shuts down:

```
fallocate -l 2G /swapfile
chmod 600 /swapfile
mkswap /swapfile
swapon /swapfile
```

To make the swapfile persist across reboots, use

```
echo '/swapfile none swap sw 0 0' >> /etc/fstab
```

Now, onto the actual dependencies. I started with a clean Ubuntu 14.04 installation. After installing R with

```
sudo apt-get install r-base-core
```

I installed the following packages to compile the JAGS source code:

```
sudo apt-get install gcc g++ gfortran liblapack-dev r-base-core
sudo apt-get install autoconf automake libtool libltdl-dev libcppunit-dev
```

At the time of writing, JAGS is hosted on SourceForge. The source code can be downloaded with a browser, and then unpacked with a file manager, or in the terminal:

```
wget 'https://sourceforge.net/projects/mcmc-jags/files/JAGS/4.x/Source/JAGS-4.2.0.tar.gz/download'
tar -xvf download
rm download
```
Now, to compile and install JAGS without any modifications:

cd JAGS-4.2.0
./configure
make
sudo make install

If make throws errors, it might be that the linking path is wrong. If running the command
/sbin/ldconfig -p | grep jags
doesn’t print anything, then open /etc/ld.so.conf with your favorite text editor and insert the line
include /usr/local/lib

at the bottom. Save the file, and run /sbin/ldconfig to load the new configuration file. Then try make again.

Finally, to install the R-language bindings to JAGS,
Rscript -e "install.packages('rjags');"

6.3 JAGS functions

The JAGS source code defines several types of functions. By looking in /JAGS-4.2.0/src/include/function,
you can see several class definition files – ArrayFunction.h, VectorFunction.h, ScalarVectorFunction.h, etc. These describe the types of the function parameters and return variables – ScalarVectorFunction takes vector arguments and returns a scalar, for instance. In our case, we wanted a function that accepts three scalar values and returns a 2-D array, so we chose to implement an ArrayFunction. Other function types will have different methods that need defining.

6.4 ArrayFunction

ArrayFunction defines several virtual methods that our code must implement. They describe the inputs and outputs of the function in addition to what the function actually does.

6.4.1 the constructor

If you look at ArrayFunction.h, you can see that the constructor takes two parameters, a string name and an unsigned int npar. These correspond to the name that you want to be able to use in JAGS model descriptions and the number of parameters that the function will take. In our case, we want to call the function sfactor and it takes three parameters.

6.4.2 evaluate

The first method is evaluate, which defines the actual function definition. It has the parameters of a double pointer value, a vector of double pointers args, and a vector of vectors of unsigned ints dims. The argument value is a pointer to a region of memory for the return value – because ArrayFunction is supposed to be a very generic template, the specific details of how to use that memory is up to you. Note: JAGS arrays are stored in column-major order (like Fortran), not row-major order like C++ in general! The size of this memory region is defined by the return value of the dim function.

The args parameter contains the arguments that the model description gave to the function. It is a vector of double pointers, and so each element of the vector can represent an array. The dimensions of these arrays must be accepted by checkParameterDim. In our case, we want it to be three scalars, so each element of the args vector should point to only one double value.

The dims parameter provides the dimensions of the arrays in args. In our case, they should be all ones because our parameters are scalars, but in general they define the shape of the memory regions pointed to in args.
6.4.3 checkParameterDim

The method checkParameterDim checks whether the function parameters are correct. It has one argument, a vector of vectors of unsigned ints dims. The outer vector has npar (the parameter of the constructor) elements, and each subvector contains the dimensions of the corresponding argument to your function. Our function accepts only scalars, so we use this function to check that all our arguments are scalars.

6.4.4 checkParameterValue

The method checkParameterValue is used to check whether the parameter values lie in the function’s domain. Our function did not require any constraints on the parameter values, so it always returned true.

6.4.5 dim

The method dim is used to tell JAGS how much memory to allocate for given input values. In our case, we are outsourcing the calculations to a fortran code that returns a table with 99 rows and 2 columns, so we return a 2-element vector containing the values 99 and 2.

6.5 C++ Implementation

Now, onto the specifics of implementing a new function in C++. All existing functions are located in

JAGS-4.2.0/src/modules/bugs/functions

and we will put our code there as well. A JAGS function has two files: a main .cc file that defines the bodies of the functions mentioned above, and a header file .h that is more or less just boilerplate. To begin, it is easiest to copy the .cc and .h files of a function that already exists and is the same type as yours. We want an ArrayFunction, and so we could copy, for instance, Transpose.cc and Transpose.h, because Transpose inherits from ArrayFunction. Note: when in JAGS-4.2.0/src/modules/bugs/functions/, you can use grep ArrayFunction * to find all functions that contain the phrase “ArrayFunction”.

After copying an existing function, we can modify the new files to fit our needs. In SFactor.cc and SFactor.h, the first thing to do is change all the Transposes to SFactors, so that #include "Transpose.h" turns into #include "SFactor.h", Transpose::evaluate becomes SFactor::evaluate, and so on. The method parameters and return types should all stay the same.

6.5.1 SFactor.cc

Now let’s talk about method bodies. The methods are more or less independent, and so we’ll discuss their implementation individually.

6.5.1.1 the constructor

Our JAGS function will be named sfactor and will take three parameters, so we define our constructor as

SFactor::SFactor ()
    : ArrayFunction ("sfactor", 3)
    {
    
   
6.5.1.2 evaluate

evaluate is the big function. Our objective is to provide a bridge between JAGS and an existing pre-compiled Fortran77 executable binary. The executable has an input file that contains all the parameter values used in the calculation and creates an output file with the 99x2 table of calculated values. The idea of this method is to create the input file with the three parameter values given to it by JAGS, execute the binary, and parse the table from the output file to return to JAGS.

Because we’ll be reading and writing files, we’ll need a few libraries. At the top of SFactor.cc, we have the following lines:
#include <iostream>
#include <fstream>
#include <string>
#include <stdlib.h>

First, we have to get the three parameter values. Recall that args is a vector of double pointers. In our case, these pointers are pointing to single values (or equivalently, 1x1 arrays), so to access them, we simply use

double resonance_energy = args[0][0];
double proton_width = args[1][0];
double gamma_width = args[2][0];

Now, we write them to the binary’s input file, called “extrappg.in”. The file also contains values for many other parameters, but those are treated as constants in this analysis, so we will hardcode them. The input file is assumed to be in a certain order, which must be preserved by this code:

// open the fortran input file for writing
std::ofstream paramfile;
paramfile.open ("extrappg.in");
paramfile << "17O+p ! title
";
paramfile << "17 1.0078 ! mass target, projectile MT,MP\n";
paramfile << "8 1 ! charge target, projectile ZT,ZP\n";
paramfile << "1.25 ! radius parameter r0 (fm) R0\n";
paramfile << resonance_energy << " ! resonance energy (MeV) ER ***\n";
paramfile << "2.5 0.5 2.0 ! spins target, projectile, resonance JT,JP,JR\n";
paramfile << "5.6065 ! reaction Q-value (MeV) Q\n";
paramfile << "1 ! orbital angular momentum of resonance LP\n";
paramfile << proton_width << " ! proton width at ER (MeV) GAMP ***\n";
paramfile << gamma_width << " ! gamma widths at ER (MeV) GAMG ***\n";
paramfile << "0.00 ! proton spectroscopic factor C2S\n";
paramfile << "0.00 ! dim. single-particle reduced width at ER (formal) THSP\n";
paramfile << "1.887 ! excitation energy of final state (MeV) EXF\n";
paramfile << "1.00 ! gamma-ray branching ratio BG\n";
paramfile << "1 ! gamma-ray multipolarity LG\n";
paramfile << "0.02 1.0 0.01 ! start energy, final energy, step size (MEV) ES,EF,SS\n";
paramfile << "1 ! (1) exact calculation; (else) Thomas approximation;\n";
paramfile.close();

Now that the input file is written, we can run the external executable, which we assume is called s_factor. It is assumed to be in the same working directory as your R session. If this is not the case, you’ll have to provide a full filepath to it.

// now that the parameter file is written, run the fortran executable
int retcode = system("./s_factor");

The return value retcode signals whether the process completed successfully or exited with an error. In true bad-practice style, we’ll ignore it here. Note that calling outside executables in this way will have our code wait until the external process finishes and returns. In this case, this is exactly what we want.

Now, we must read the table of values from the Fortran’s output file, called extrappg.out. The output file contains 14 lines of diagnostic info before getting to the table, at which point it has 99 lines of data, each line containing two numbers separated by a space.

//read the fortran executable's output file:
std::string line;
std::ifstream ifile ("extrappg.out");
if (ifile.is_open()) {
    // skip the first 14 lines
    for(int i = 0; i < 14; i++){
        getline(ifile, line);
    }
    // read 99 lines. Each line contains two numbers separated by a space.
    // `value` is a 1-D array, so we need to do some tricky indexing.
    // IMPORTANT: JAGS stores arrays in column-major order, so entire columns
    // are stored in contiguous memory. Unlike C/C++, which is row-major.
    // You will tear your hair out if you don't know this.
    for(int i = 0; i < 99; i++){
        ifile >> value[i] >> value[i+99];
    }
    ifile.close();
} else {
    // it's bad if this happens
    // TODO: figure out how to throw an error
    std::cout << "Unable to open file";
}

This deserves some explanation. Because the block of memory represented by `value` is given to us as a pointer, rather than a 2-D array, we have to do manual memory indexing to make sure all values go where they are supposed to go. Because JAGS arrays are stored in column-major format, each column of a 2-D array is stored in contiguous memory. Therefore, if we want to return a 99-row, 2-column array, it must be represented as a chunk of 99 values for the first column, followed by a chunk of 99 values for the second column. Note that we are guaranteed to have sufficient memory for this indexing because of what the dim method returns.

6.5.1.3 checkParameterDim The method checkParameterDim must ensure that our parameters are scalar values. JAGS has a few handy libraries around to check these sorts of things. We will use a function called isScalar from dim.h, in JAGS-4.2.0/src/include/util/dim.h

This requires adding a line `#include <util/dim.h>` at the top of SFactor.cc. Implementing this method now becomes very easy:

```cpp
bool SFactor::checkParameterDim(std::vector<std::vector<unsigned int>> const &dims) const
{
    // the three arguments should be scalars
    return isScalar(dims[0]) && isScalar(dims[1]) && isScalar(dims[2]);
}
```

Note that many other useful functions can be found in JAGS-4.2.0/src/include; have a look around in there before reinventing a wheel yourself.

6.5.1.4 checkParameterValue Our function has no restrictions on parameter values (strictly positive, nonnegative, etc), so this function always returns true. In general, you would have some logical expression involving the parameter values that evaluates to a boolean.

```cpp
bool SFactor::checkParameterValue(std::vector<double const *> const &args,
                                   std::vector<std::vector<unsigned int>> const &dims) const
```
6.5.1.5 dim
dim tells JAGS what the dimensions of the output of evaluate should be. In our case, we know that we will be returning a 2-D, 99x2 array of doubles. dim returns a vector of unsigned ints, with each element corresponding to a dimension of an array. By convention, it seems that JAGS code assumes dimension vectors to contain first the number of rows, and then the number of columns, and so our dim will look like

```cpp
std::vector<unsigned int> SFactor::dim(std::vector<std::vector<unsigned int>> const &dims,
                   std::vector<double const *> const &values) const
{
  // the size of the table that the fortran code calculates is 99 row by 2 col
  vector<unsigned int> ans(2);
  ans[0] = 99;
  ans[1] = 2;
  return ans;
}
```

6.5.2 SFactor.h

The header file is much easier to implement. More or less just changing everything to fit your function’s name is all that’s necessary. Also, be sure that the #ifndef line has a unique identifier that won’t match any other function’s.

6.6 Recompiling JAGS

Now that you’ve defined a function that JAGS can talk to, we have to tell JAGS about it. At the time of writing, there are two configuration files that must be edited. The first is found in

JAGS-4.2.0/src/modules/bugs/functions/Makefile.am

This file is a template used to generate a real makefile during the compilation process. Any functions you create that you want to be available in a JAGS model description must be listed here. There are two long lists in this file, one for .cc files and one for .h files. Just append your two new files to the ends of these lists.

The second file that requires editing is

JAGS-4.2.0/src/modules/bugs/bugs.cc

This file is a long list of #include statements. Scrolling down the file, there will be a list of all the functions we saw before, with lines like #include <functions/Transpose.h>. Add a similar line for your .h file in this list (eg, #include <functions/SFactor.h>).

Then, farther down the file, there will be a long list of lines like insert(new Transpose);. Add a new line for your function (eg, insert(new SFactor);).

After editing these two files, go back to the top level of the JAGS directory (JAGS-4.2.0 here), and run autoreconf --force --install to regenerate new configuration files from the templates you just edited. Then run the configure program in this directory with ./configure. After this, we are done configuring, and can proceed with make and sudo make install as before.

Note that the autoreconf --force --install and ./configure only need to be done after you edit the configuration templates Makefile.am and bugs.cc. After doing this once, you can skip those steps if you edit your new function’s .cc and .h files and go straight to the make and sudo make install. After this, using the rjags library in R will point to the new custom version of JAGS.

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6.7 Appendix

6.7.1 Timings

As a test, we used the extrappg Fortran binary to generate an output table for known parameters. Some noise was then added to the data and used in JAGS to try to recreate the original parameter values. The code and results are shown below:

```
library(rjags)

# parameters used to generate the data:
# MT,MP,ZT,ZP = 17. 1. 9. 1.
# RO (fm) = 1.25
# LP, LG = 0 1
# GAMP, GAMG (MeV) = .180E-01 .250E-07
# ER, Q, EXF (MeV) = .600 3.924 1.887
# JT, JP, JR = 2.5 .53.0
# THSP, C2S = .000 .000
# BG = 1.0000

# so the analysis should return
# ER = 0.600
# GAMP = 0.180e-01
# GAMG = 0.250e-07

df1 = read.table(header = TRUE, text =
"E  S
0.020 4.883E-06
0.030 5.110E-06
0.040 5.351E-06
0.050 5.607E-06
0.060 5.878E-06
0.070 6.166E-06
0.080 6.473E-06
0.090 6.799E-06
0.100 7.147E-06
0.110 7.518E-06
0.120 7.914E-06
0.130 8.338E-06
0.140 8.792E-06
0.150 9.279E-06
0.160 9.802E-06
0.170 1.036E-05
0.180 1.097E-05
0.190 1.162E-05
0.200 1.233E-05
0.210 1.310E-05
0.220 1.393E-05
0.230 1.483E-05
0.240 1.581E-05
0.250 1.688E-05
0.260 1.806E-05
0.270 1.935E-05
0.280 2.076E-05
0.290 2.233E-05
0.300 2.406E-05"
)
```
<table>
<thead>
<tr>
<th>0.310</th>
<th>2.597E-05</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.320</td>
<td>2.811E-05</td>
</tr>
<tr>
<td>0.330</td>
<td>3.050E-05</td>
</tr>
<tr>
<td>0.340</td>
<td>3.318E-05</td>
</tr>
<tr>
<td>0.350</td>
<td>3.620E-05</td>
</tr>
<tr>
<td>0.360</td>
<td>3.962E-05</td>
</tr>
<tr>
<td>0.370</td>
<td>4.352E-05</td>
</tr>
<tr>
<td>0.380</td>
<td>4.797E-05</td>
</tr>
<tr>
<td>0.390</td>
<td>5.310E-05</td>
</tr>
<tr>
<td>0.400</td>
<td>5.903E-05</td>
</tr>
<tr>
<td>0.410</td>
<td>6.596E-05</td>
</tr>
<tr>
<td>0.420</td>
<td>7.410E-05</td>
</tr>
<tr>
<td>0.430</td>
<td>8.376E-05</td>
</tr>
<tr>
<td>0.440</td>
<td>9.533E-05</td>
</tr>
<tr>
<td>0.450</td>
<td>1.093E-04</td>
</tr>
<tr>
<td>0.460</td>
<td>1.265E-04</td>
</tr>
<tr>
<td>0.470</td>
<td>1.479E-04</td>
</tr>
<tr>
<td>0.480</td>
<td>1.750E-04</td>
</tr>
<tr>
<td>0.490</td>
<td>2.098E-04</td>
</tr>
<tr>
<td>0.500</td>
<td>2.558E-04</td>
</tr>
<tr>
<td>0.510</td>
<td>3.180E-04</td>
</tr>
<tr>
<td>0.520</td>
<td>4.052E-04</td>
</tr>
<tr>
<td>0.530</td>
<td>5.324E-04</td>
</tr>
<tr>
<td>0.540</td>
<td>7.281E-04</td>
</tr>
<tr>
<td>0.550</td>
<td>1.050E-03</td>
</tr>
<tr>
<td>0.560</td>
<td>1.635E-03</td>
</tr>
<tr>
<td>0.570</td>
<td>2.849E-03</td>
</tr>
<tr>
<td>0.580</td>
<td>5.948E-03</td>
</tr>
<tr>
<td>0.590</td>
<td>1.628E-02</td>
</tr>
<tr>
<td>0.600</td>
<td>3.410E-02</td>
</tr>
<tr>
<td>0.610</td>
<td>1.423E-02</td>
</tr>
<tr>
<td>0.620</td>
<td>5.471E-03</td>
</tr>
<tr>
<td>0.630</td>
<td>2.737E-03</td>
</tr>
<tr>
<td>0.640</td>
<td>1.622E-03</td>
</tr>
<tr>
<td>0.650</td>
<td>1.069E-03</td>
</tr>
<tr>
<td>0.660</td>
<td>7.575E-04</td>
</tr>
<tr>
<td>0.670</td>
<td>5.651E-04</td>
</tr>
<tr>
<td>0.680</td>
<td>4.381E-04</td>
</tr>
<tr>
<td>0.690</td>
<td>3.499E-04</td>
</tr>
<tr>
<td>0.700</td>
<td>2.861E-04</td>
</tr>
<tr>
<td>0.710</td>
<td>2.385E-04</td>
</tr>
<tr>
<td>0.720</td>
<td>2.021E-04</td>
</tr>
<tr>
<td>0.730</td>
<td>1.735E-04</td>
</tr>
<tr>
<td>0.740</td>
<td>1.507E-04</td>
</tr>
<tr>
<td>0.750</td>
<td>1.323E-04</td>
</tr>
<tr>
<td>0.760</td>
<td>1.170E-04</td>
</tr>
<tr>
<td>0.770</td>
<td>1.044E-04</td>
</tr>
<tr>
<td>0.780</td>
<td>9.370E-05</td>
</tr>
<tr>
<td>0.790</td>
<td>8.463E-05</td>
</tr>
<tr>
<td>0.800</td>
<td>7.686E-05</td>
</tr>
<tr>
<td>0.810</td>
<td>7.013E-05</td>
</tr>
<tr>
<td>0.820</td>
<td>6.428E-05</td>
</tr>
<tr>
<td>0.830</td>
<td>5.916E-05</td>
</tr>
<tr>
<td>0.840</td>
<td>5.465E-05</td>
</tr>
</tbody>
</table>
sigma = 0.001
x = df1$E
y = rnorm(length(x), df1$S, sigma)

# so the analysis should return
# ER = 0.600
# GAMP = 0.180e-01
# GAMG = 0.250e-07

model_string = "
model {
  ER ~ dunif(0.5,0.7)
  GAMP ~ dunif(0.1e-01, 0.2e-01)
  GAMG ~ dunif(0.1e-07, 0.3e-07)
  # sigma is zero if it gets the other parameters right
  sigma ~ dunif(0,10)

  # a 99x2 table of E and S(E)
  table = sfactor(ER, GAMP, GAMG)

  for (i in 1:length(E)) {
    S.hat[i] = interp.lin(E[i], table[1:99,1], table[1:99,2])
    S[i] ~ dnorm(S.hat[i], pow(sigma,-2))
  }
}
"

model = jags.model(file = textConnection(model_string),
data = list('E' = x,
            'S' = y),
n.chains = 1,
n.adapt = 1000)

output = coda.samples(model = model,
                 variable.names = c("ER", "GAMP", "GAMG", "sigma"),
n.iter=3000,
The quantiles of the parameter values are shown below. Note that they nicely include the original true parameter values of ER = 0.600, GAMG = 0.250e-07, GAMP = 0.180e-01, and sigma = 1e-3.

<table>
<thead>
<tr>
<th></th>
<th>2.5%</th>
<th>25%</th>
<th>50%</th>
<th>75%</th>
<th>97.5%</th>
</tr>
</thead>
<tbody>
<tr>
<td>ER</td>
<td>5.995e-01</td>
<td>6.001e-01</td>
<td>6.004e-01</td>
<td>6.007e-01</td>
<td>6.012e-01</td>
</tr>
<tr>
<td>GAMG</td>
<td>2.308e-08</td>
<td>2.422e-08</td>
<td>2.489e-08</td>
<td>2.556e-08</td>
<td>2.675e-08</td>
</tr>
<tr>
<td>GAMP</td>
<td>1.600e-02</td>
<td>1.693e-02</td>
<td>1.748e-02</td>
<td>1.802e-02</td>
<td>1.900e-02</td>
</tr>
<tr>
<td>sigma</td>
<td>9.454e-04</td>
<td>1.034e-03</td>
<td>1.084e-03</td>
<td>1.137e-03</td>
<td>1.262e-03</td>
</tr>
</tbody>
</table>

I ran this code on a single-core, 1GB ram computer with a solid-state harddrive. The model consumed a pretty small amount of ram, and as we discussed, it consumed about 20-25% CPU, indicating that 75-80% of its time is spent on filesystem operations rather than direct cpu calculations. I used 3000 iterations, and the timings were

- real 4m42.614s
- user 1m8.469s
- sys 3m29.102s

### 6.7.2 Code

For reference, the complete `SFactor.cc` and `SFactor.h` files are included here:

**SFactor.cc:**

```cpp
#include "SFactor.h"
#include <config.h>
#include <cmath>

namespace jags {
namespace bugs {

/**
 * @short Matrix- or array-valued function
 *
 * Array-valued functions are the most general class of function. The
 * arguments of an array-valued function, and the value may be a
 * scalar, vector, or array.
 *
 * We use ArrayFunction here because there is no more specific class
 * that accepts scalars and returns vectors
 */

SFactor::SFactor ()

```
ArrayFunction ("sfactor", 3)
{
}

/**
 * Evaluates the function.
 *
 * @param value array of doubles which contains the result of
 * the evaluation on exit
 * @param args Vector of arguments.
 * @param dims Respective dimensions of each element of args.
 */
void SFactor::evaluate(double *value,
    std::vector<double const *> const &args,
    std::vector<std::vector<unsigned int> > const &dims) const
{
    // parameters to be written to the fortran input file
    double resonance_energy = args[0][0];
    double proton_width = args[1][0];
    double gamma_width = args[2][0];

    // open the fortran input file
    std::ofstream paramfile;
    paramfile.open ("extrappg.in");

    paramfile << "17O+p ! title
    paramfile << "17 1.0078 ! mass target, projectile MT,MP\n"
    paramfile << "8 1 ! charge target, projectile ZT,ZP\n"
    paramfile << "1.25 ! radius parameter r0 (fm) R0\n"
    paramfile << resonance_energy << " ! resonance energy (MeV) ER ***\n"
    paramfile << "2.5 0.5 2.0 ! spins target, projectile, resonance JT,JP,JR\n"
    paramfile << "5.6065 ! reaction Q-value (MeV) Q\n"
    paramfile << "1 ! orbital angular momentum of resonance LP\n"
    paramfile << proton_width << " ! proton width at ER (MeV) GAMP ***\n"
    paramfile << gamma_width << " ! gamma widths at ER (MeV) GAMG ***\n"
    paramfile << "0.00 ! proton spectroscopic factor C2S\n"
    paramfile << "0.00 ! dim. single-particle reduced width at ER (formal) THSP\n"
    paramfile << "1.887 ! excitation energy of final state (MeV) EXF\n"
    paramfile << "1.00 ! gamma-ray branching ratio BG\n"
    paramfile << "1 ! gamma-ray multipolarity LG\n"
    paramfile << "0.02 1.0 0.01 ! start energy, final energy, step size (MEV) ES,EF,SS\n"
    paramfile << "0 ! (1) exact calculation; (else) Thomas approximation;\n"

    paramfile.close();

    // now that the parameter file is written, run the fortran executable
    int retcode = system("./s_factor");

    //read the fortran executable's output file:
    std::string line;
    std::ifstream ifile ("extrappg.out");
    if (ifile.is_open()) {

// skip the first 14 lines
for(int i = 0; i < 14; i++){
    getline(ifile, line);
}
// read 99 lines. Each line contains two numbers separated by a space.
// `value` is a 1-D array, so we need to do some tricky indexing.
// IMPORTANT: JAGS stores arrays in column-major order, so entire columns
// are stored in contiguous memory. Unlike C, which is row-major.
// You will tear your hair out if you don’t know this.
for(int i = 0; i < 99; i++){  
    ifile >> value[i] >> value[i+99];
}
ifile.close();
else {
    // it’s really bad if this happens
    // TODO: figure out how to throw an error
    std::cout << "Unable to open file";
}

/**
 * Checks whether dimensions of the function parameters are correct.
 * @param dims Vector of length npar denoting the dimensions of
 * the parameters, with any redundant dimensions dropped.
 */
bool SFactor::checkParameterDim(std::vector<std::vector<unsigned int> > const &dims) const
{
    // the three arguments should be scalars
    return isScalar(dims[0]) && isScalar(dims[1]) && isScalar(dims[2]);
}

/**
 * Checks whether the parameter values lie in the domain of the
 * function. The default implementation returns true.
 */
bool SFactor::checkParameterValue(std::vector<double const *> const &args,
std::vector<std::vector<unsigned int> > const &dims) const
{
    // TODO: should any parameters be eg strictly positive?
    return true;
}

/**
 * Calculates what the dimension of the return value should be,
 * based on the arguments.
 *
@param dims Vector of Indices denoting the dimensions of the parameters. This vector must return true when passed to checkParameterDim.

@param values Vector of pointers to parameter values.

*std::vector<unsigned int>
SFactor::dim(std::vector <std::vector<unsigned int> > const &dims,
            std::vector <double const *> const &values) const
{
    // the size of the table that the fortran code calculates is 99 row by 2 col
    vector<unsigned int> ans(2);
    ans[0] = 99;
    ans[1] = 2;
    return ans;
}

SFactor.h:

#ifndef S_FACTOR_H_
#define S_FACTOR_H_

#include <function/ArrayFunction.h>

namespace jags {
namespace bugs {

/**
 * @short Astronomical S Factors
 * SFactor returns the astronomical S-factor as a function of energy. It
 * returns a 99x2 table where column 1 is energy and column 2 is the S-factor.
 * It requires a fortran executable to perform the calculations.
 * <pre>
 * table = sfactor(ER, GAMP, GAMG)
 * </pre>
 */
class SFactor : public ArrayFunction
{
public:
    SFactor ();
    void evaluate(double *x, std::vector<double const *> const &args,
                  std::vector<std::vector<unsigned int> > const &dims)
    const;
    bool checkParameterDim(std::vector<std::vector<unsigned int> > const &dims) const;
    std::vector<unsigned int>
dim(std::vector<std::vector<unsigned int> > const &dims,
       std::vector<double const *> const &values) const;
    bool checkParameterValue(std::vector<double const *> const &args,
                               std::vector<std::vector<unsigned int> > const &dims) const;
};

}}