

Bayesian modelling - high strain, one component (1C), GSI

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1. Libraries and Data

The following libraries are essential for the modelling and visualisation

- JAGS <https://sourceforge.net/projects/mcmc-jags/>
- R2jags <https://cran.r-project.org/web/packages/R2jags/index.html>
- lattice <https://cran.r-project.org/web/packages/lattice/index.html>
- ggplot2 <https://cran.r-project.org/web/packages/ggplot2/index.html>
- gridExtra <https://cran.r-project.org/web/packages/gridExtra/index.html>

```
# Import Libraries

library(R2jags)
library(lattice)
library(ggplot2)
library(gridExtra)

# Import data
file_path <- "D:\\Bayesian_modelling\\Input_data\\Supplement_S4_input_high_strain.csv"

data <- read.csv(file_path)

# Assignment of each column to a variable
Source <- data$Source
GS_ini_mean <- data$GS_ini_mean
GS_ini_upper <- data$GS_ini_upper
GS_ini_lower <- data$GS_ini_lower
rate_c <- data$rate_c
strain_c <- data$strain_c
stress_c <- data$stress_c
T_mean <- data$T_mean
T_upper <- data$T_upper
T_lower <- data$T_lower
exp_type <- data$exp_type
```

2. Bayesian Modelling

2.1 Set Bayesian modelling parameters and output dir

```
## Bayesian model parameters
# Iterations
n_iter <- 4000000
n_iter_str <- format (n_iter, scientific=FALSE)

# Burn-in
n_burnin <- 10000
n_burnin_str <- format (n_burnin, scientific=FALSE)

# Thinning
n_thin <- 20
n_thin_str <- format (n_thin, scientific=FALSE)

model <- "high_strain_single_component_GSI"
extension <- ".jags"
model_file <- paste0(model, extension)

## Output dir

strain_condition_input = "High-strain"

law <- "GSI"

# Get the current date
date_time_str <- format(Sys.time(), "%Y-%m-%d-%H-%M-%S")

# Create the folder name by concatenating the date and variable name
sub_folder_name <- paste(date_time_str, strain_condition_input, law, n_iter_str, n_burnin_str, n_thin_str)

# Create the folder under the master directory
new_dir <- file.path("D:\\Bayesian_modelling\\Results", sub_folder_name)

dir.create(new_dir)
```

2.2 Modelling

```
R <- 8.314*1e-3 #kJmol-1K-1

# number of observations
N <- length(stress_c)

rate_exp = log10(rate_c)

# model 0
data1 <- list("N"=N,
             "rate_exp" = rate_exp,
             "Stress"=stress_c,
```

```

        "R" = R,
        "T_mean"=T_mean,
        "T_upper"=T_upper,
        "T_lower"=T_lower)

vinits <- function(){
  list("n" = 4)
}

params <- c("n", "Q", "A_log")

# Start modelling
s1 <- Sys.time()
m0 = jags(data=data1, inits = vinits, parameters.to.save=params, n.chains = 3,
          n.iter = n_iter, n.burnin=n_burnin, n.thin=n_thin,
          model.file=model_file)

## module glm loaded

## Compiling model graph
##   Resolving undeclared variables
##   Allocating nodes
## Graph information:
##   Observed stochastic nodes: 160
##   Unobserved stochastic nodes: 163
##   Total graph size: 2034
##
## Initializing model

s2 <- Sys.time()
s2-s1

## Time difference of 1.612104 hours

m0

## Inference for Bugs model at "high_strain_single_component_GSI.jags", fit using jags,
## 3 chains, each with 4e+06 iterations (first 10000 discarded), n.thin = 20
## n.sims = 598500 iterations saved
##      mu.vect sd.vect   2.5%   25%   50%   75%  97.5%  Rhat n.eff
## A_log   11.901   0.902  10.153  11.288  11.897  12.509  13.677 1.002  2000
## Q       90.179   4.552  81.355  87.090  90.158  93.245  99.142 1.002  1900
## n        3.527   0.068   3.394   3.481   3.527   3.573   3.661 1.001  6900
## deviance 172.970   4.032 166.422 170.123 172.488 175.298 182.200 1.001  5300
##
## For each parameter, n.eff is a crude measure of effective sample size,
## and Rhat is the potential scale reduction factor (at convergence, Rhat=1).
##
## DIC info (using the rule, pD = var(deviance)/2)
## pD = 8.1 and DIC = 181.1
## DIC is an estimate of expected predictive error (lower deviance is better).

```

```
m0.mcmc <- as.mcmc(m0)
```

```
# Document the summary of output
```

```
jags_output_path <- file.path(new_dir, "jags_output.txt")
```

```
sink(file = jags_output_path)
```

```
print(m0)
```

```
## Inference for Bugs model at "high_strain_single_component_GSI.jags", fit using jags,  
## 3 chains, each with 4e+06 iterations (first 10000 discarded), n.thin = 20
```

```
## n.sims = 598500 iterations saved
```

	mu.vect	sd.vect	2.5%	25%	50%	75%	97.5%	Rhat	n.eff
## A_log	11.901	0.902	10.153	11.288	11.897	12.509	13.677	1.002	2000
## Q	90.179	4.552	81.355	87.090	90.158	93.245	99.142	1.002	1900
## n	3.527	0.068	3.394	3.481	3.527	3.573	3.661	1.001	6900
## deviance	172.970	4.032	166.422	170.123	172.488	175.298	182.200	1.001	5300

```
##
```

```
## For each parameter, n.eff is a crude measure of effective sample size,  
## and Rhat is the potential scale reduction factor (at convergence, Rhat=1).  
##
```

```
## DIC info (using the rule,  $pD = \text{var}(\text{deviance})/2$ )
```

```
##  $pD = 8.1$  and  $DIC = 181.1$ 
```

```
## DIC is an estimate of expected predictive error (lower deviance is better).
```

```
summary(m0.mcmc)
```

```
##
```

```
## Iterations = 10001:3999981
```

```
## Thinning interval = 20
```

```
## Number of chains = 3
```

```
## Sample size per chain = 199500
```

```
##
```

```
## 1. Empirical mean and standard deviation for each variable,  
## plus standard error of the mean:
```

```
##
```

	Mean	SD	Naive SE	Time-series SE
## A_log	11.901	0.90219	1.166e-03	0.0169693
## deviance	172.970	4.03216	5.212e-03	0.0514519
## n	3.527	0.06814	8.808e-05	0.0006257
## Q	90.179	4.55249	5.885e-03	0.0854609

```
##
```

```
## 2. Quantiles for each variable:
```

```
##
```

	2.5%	25%	50%	75%	97.5%
## A_log	10.153	11.288	11.897	12.509	13.677
## deviance	166.422	170.123	172.488	175.298	182.200
## n	3.394	3.481	3.527	3.573	3.661
## Q	81.355	87.090	90.158	93.245	99.142

```
gelman.diag(m0.mcmc)
```

```
## Potential scale reduction factors:
```

```
##
##           Point est. Upper C.I.
## A_log      1      1.01
## deviance    1      1.00
## n           1      1.00
## Q           1      1.01
##
## Multivariate psrf
##
## 1
```

```
sink(file = NULL)

# Save raw outputs
all_samples <- as.matrix (m0.mcmc[,])
all_samples_path <- file.path(new_dir, "all_samples.RDS")
save (all_samples, file=all_samples_path)

m0_file_path <- file.path(new_dir, "m0.RDS")
m0mc_file_path <- file.path(new_dir, "m0mc.RDS")

save(m0,file=m0_file_path)
save(m0.mcmc,file=m0mc_file_path)
```