Gibbs sampling and JAGS

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AA 2023/2024 - Stat Lect 10





Computational Bayesian Statistics

• the posterior distribution itself is the essence of bayesian inference

$$P(\theta \mid y) = \frac{f(y \mid \theta) g(\theta)}{\int f(y \mid \theta) g(\theta) d \theta}$$

- but most of the time it is not known analytically, and it must be computed numerically with Monte Carlo methods
- Markov Chain Monte Carlo (MCMC) methods are commonly used for sampling from a posterior distribution: we let the Markov chain run long enough → a random draw from the chain can be considered a random draw from the posterior
- it's a radically different approach: instead of computing numerically the posterior distribution, we draw a sample from the posterior distribution.
- two main MCMC methods are commonly used:
- the Metropolis-Hastings algorithm
- the Gibbs sampling algorithm

Metropolis-Hastings: 1-dim example

- it samples from a target density by choosing values from a candidate density
- the acceptance of the new value (*proposal*) depends only on the previously accepted value (*current value*)
- using a symmetric transition probability, we generate a Markov Chain
- the acceptance probability, also called Metropolis ratio, is

$$\rho = \text{MIN}\left(1, \frac{f(s)}{f(\theta_t)} \frac{Q(\theta_t \mid s)}{Q(s \mid \theta_t)}\right)$$

Problem

• let's assume ve have a target density that is the sum of three Normal distributions

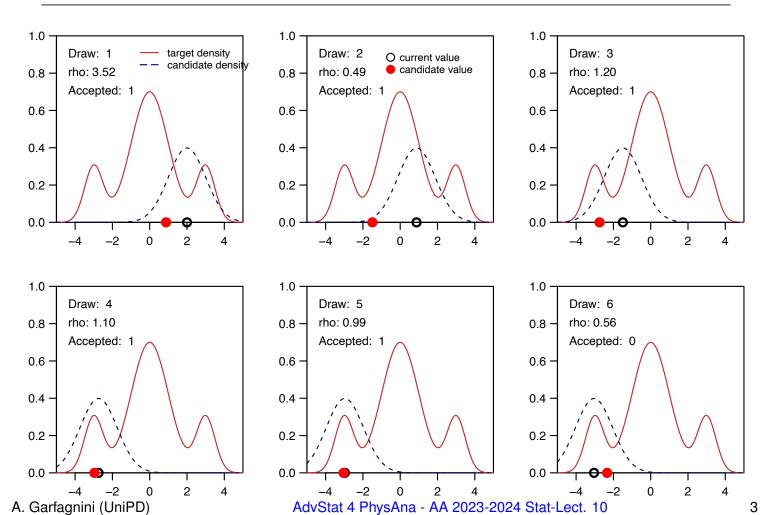
$$f(x) = a_1 \text{ Norm}(0, 1) + a_2 \text{ Norm}(3, 0.5^2) + a_3 \text{ Norm}(-3, 0.5^2)$$

• with $a_1 = 0.7$, $a_2 = 0.15$ and $a_3 = 0.15$

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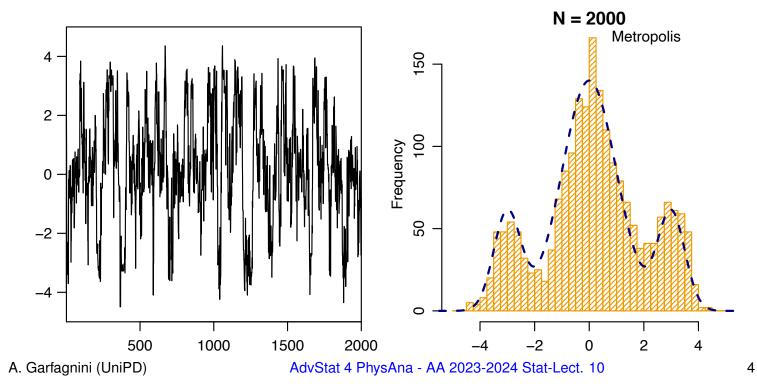
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Metropolis-Hastings: 1-dim example



Metropolis-Hastings: 1-dim example

- the sample is moving through the space quite satisfactory
- extreme values are selected, from time to time, but the chain tends to jump back to the central region (with higher probability) very quickly



Metropolis-Hastings: indep. cand. chain

- a variant to the Metropolis-hastings algorithm uses an independent candidate density
- Hastings (1970) introduced Markov Chains with candidate densities that did not depend on the current value in the chain

$$Q(s \mid \theta) = Q_2(s)$$

- Q₂ is some function that dominates the target density in the tails
- therefore the acceptance probability, the Metropolis ratio, simplifies to

$$\rho = \min\left(1, \frac{f(s)}{f(\theta_t)} \frac{Q(\theta_t \mid s)}{Q(s \mid \theta_t)}\right) = \min\left(1, \frac{f(s)}{f(\theta_t)} \frac{Q_2(\theta_t)}{Q_2(s)}\right)$$

Problem

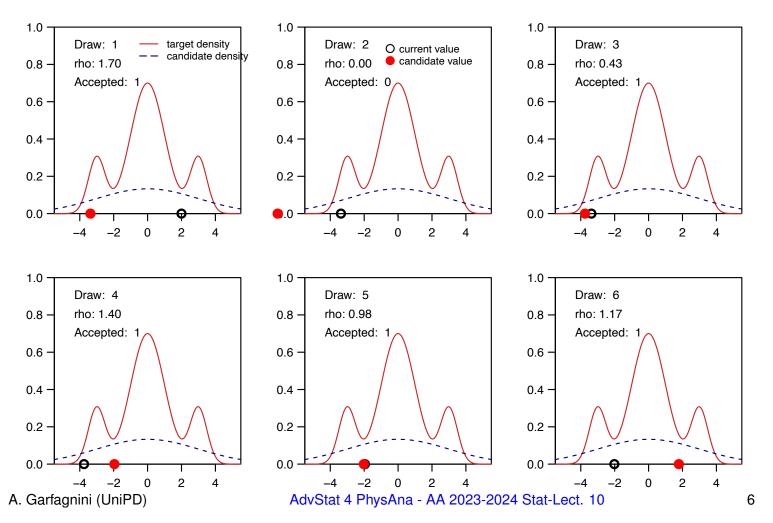
let's study the same problem

$$f(x) = a_1 \text{ Norm}(0, 1) + a_2 \text{ Norm}(3, 0.5^2) + a_3 \text{ Norm}(-3, 0.5^2)$$

- with $a_1 = 0.7$, $a_2 = 0.15$ and $a_3 = 0.15$
- assuming that the candidate density is a Norm $(0,3^2)$ distribution function

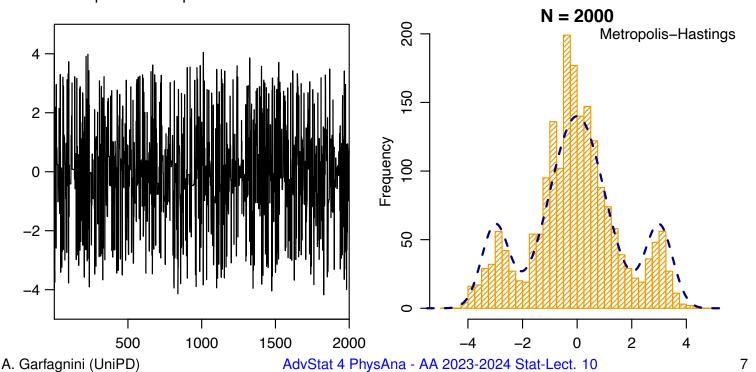
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Metropolis-Hastings: indep. cand. chain



Metropolis-Hastings: indep. cand. chain

- the sample is moving through the space quite satisfactory
- the independent candidate density allows for larger jumps, but it may accept fewer proposals than the random-walk chain
- nevertheless the acceptance is larger and the chain will potentially explore the parameter space faster



Gibbs sampling

- it is one of the most widely used algorithms for simulating Markov chains
- it is a special case of the Metropolis-Hastings algorithm and it is most relevant with multi-parameters problems
- in general, Metropolis-hasting can be improved by only updating a block of parameters at each iteration → blockwise Metropolis-Hastings algorithm
- the Gibbs sampling algorithm is a special case of the blockwise Metropolis-Hastings
- it generates a multi-dimensional Markov chain by splitting the vector of random variables θ into subvectors and sampling each subvector in turn, conditional on the most recent values of all other elements of θ
- the beauty of Gibbs sampling is that simulation from a complex, high-dimensional joint posterior distribution is reduced to a sequence of algorithms for sampling from one or low-dimensional distributions
- Gibbs sampling is most suited for hierarchical models, where the dependencies between model parameters is well-defined

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Gibbs sampling algorithm

- (1) choose arbitrary starting values $\theta_1^{(0)}, \theta_2^{(0)}, \dots, \theta_k^{(0)}$ (subscript = component, superscript = iteration step)
- (2) sample new values for each element with the following steps:
 - sample $\theta_1^{(1)}$ from the full-conditional distribution,

$$\theta_1^{(1)} \sim P(\theta_1 \mid \theta_2^{(0)}, \theta_3^{(0)}, \dots \theta_k^{(0)}, y)$$

where y indicates the data

- sample a new $\theta_2^{(1)}$, for the second component, from its full conditional distribution

$$\theta_2^{(1)} \sim P(\theta_2 \mid \theta_1^{(1)}, \theta_3^{(0)}, \dots \theta_k^{(0)}, y)$$

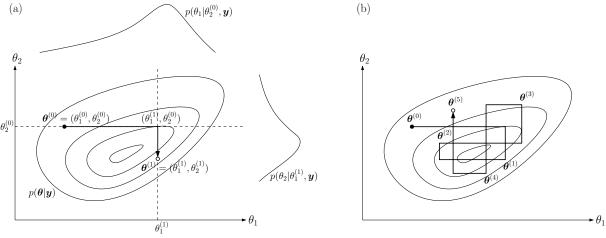
- complete the step for all the other components, obtaining a sequence of dependent realization of $\theta_1^{(1)}, \theta_2^{(1)}, \dots, \theta_k^{(1)}$
- (3) repeat step 2 many times conditioning on the most recent values of other parameters

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Gibbs sampling algorithm: 2-dim example

- picture (b) shows the first five iterations of the Gibbs sampler
- the sampler always moves parallel to the axes
- the starting point, $\theta^{(0)} = (\theta_1^{(0)}, \theta_2^{(0)})$ is shown
- $p(\theta_1 | \theta_2^{(0)}, y)$, shown on top, is the univariate density and is obtained by taking a horizontal "slice" through the 2 joint posterior distribution at the value $\theta_2 = \theta_2^{(0)}$ (horizontal dashed line)
- a new value for $\theta_1^{(0)}$ is generated from this full conditional, and then a "slice" parallel to the θ_2 axis is taken through the joint posterior (vertical dashed line)



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JAGS: Just Another Gibbs Sampler

- JAGS is a program mainly written by M. Plummer with the aim of providing a BUGS (Bayesian Inference Using Gibbs Sampling) engine for UNIX
- more infos are available at http://sourceforge.net/projects/mcmc-jags/
- the latest version is 4.3.2 (March 4, 2023)
- rjags is another R package that allows to run JAGS from within R https://cran.r-project.org/web/packages/rjags/ https://cran.r-project.org/web/packages/rjags/rjags.pdf
- available for Linux-64 (v4.15) and osx-64 (v4.15) conda install -c conda-forge r-rjags
- R2jags is an R package that allow to fit JAGS models from within R https://cran.r-project.org/web/packages/R2jags/ https://cran.r-project.org/web/packages/R2jags/R2jags.pdf
- available only for Linux-64/Windows and osx-64 (v0.8_5) conda install conda-forge::r-r2jags

- an analysis with rjags proceeds through the following steps:
- (1) define the model using the BUGS language in a separate file
- (2) read in the model file using the jags.model function. This creates an object of class jags
- (3) update the model using the update method for jags objects. This constitutes the *burn-in* part
- (4) extract samples from the model object using the coda.samples function. This creates an object of class mcmc.list which can be used to summarize the posterior distribution. The coda package also provides convergence diagnostics to check that the output is valid for analysis

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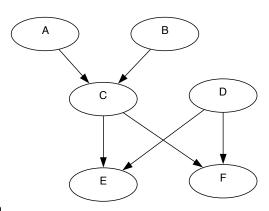
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The BUGS language

- BUGS (Bayesian inference Using Gibbs Sampling) is also a language that allows to specify Bayesian models for Bayesian computation
- it is based on graphical representation which is used to express the joint relationship between all known and unknown quantities in a model through a series of simple local relationships
- let's consider the graph in the figure:
- A, B and D have no parents and are therefore marginally independent
- A and B are parents of C which, in turn, is a parent (with D) of E and F
- if we observe E, this will induce a dependency between C and D and between A and B, since two nodes without common parents are only independent given no descendants have been observed
- from the graph we can see that the joint distribution of the set of quantities may be written

P(A, B, C, D, E, F) = P(A)P(B)P(C|A, B)P(D)P(E|C, D)P(F|C, D)



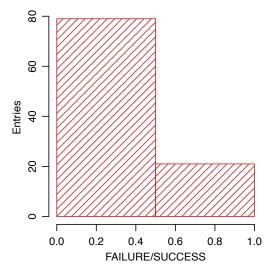
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Ex 1: Bernoulli process

The Problem

- given a set of observation, coming from a Bernoulli process, we want to infere the probability p of the process from the sequence of success/failure, and predict the number of successes in the future
- the observed sequence is the following:



we describe the model with BUGS and let jags solve our inference problem

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Ex 1: BUGS model and parameters

• file: s11_inf_p_pred.bug

```
model {
    # data likelihood
    for (i in 1:length(X)) {
        X[i] ~ dbern(p);
    }
    # a uniform prior for p
    p ~ dbeta(1, 1);

# Predicted data, given p
    y ~ dbin(p, n_next);
}
```

a list with the data for the model :

```
data <- NULL
data$X <- data_obs  # Set of observations
data$n <- length(X)  # those to be considered
data$n_next <- 10  # Predictions</pre>
```

 the model is created passing the BUGS data file and a list with all the data and model parameters

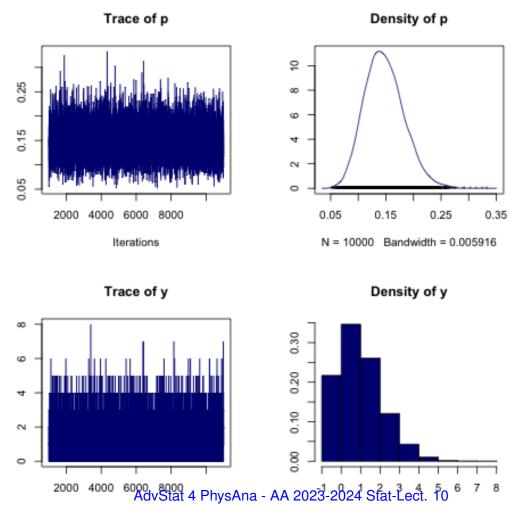
```
jm <- jags.model(model, data)</pre>
```

Ex 1: running jags

```
# Update the Markov chain (Burn-in)
          update(jm, 1000)
          chain <- coda.samples(jm, c("p", "y"), n.iter=10000)</pre>
          print(summary(chain))
       Output from R:
          Compiling model graph
            Resolving undeclared variables / Allocating nodes
          Graph information:
            Observed stochastic nodes: 100 / Unobserved stochastic nodes: 2
            Total graph size: 105
          Initializing model
           | *********** | 100%
            Iterations = 1001:11000
          Thinning interval = 1 / Number of chains = 1 | SampSize/chain = 10000
          1. Empirical mean and standard deviation for each variable,
            plus standard error of the mean:
                       SD Naive SE Time-series SE
             Mean
          p 0.1474 0.03495 0.0003495
                                    0.0003547
          y 1.4872 1.17489 0.0117489
                                      0.0117489
          2. Quantiles for each variable:
                      25%
                            50%
                                   75% 97.5%
          p 0.08681 0.1225 0.1448 0.1695 0.2224
         y 0.00000 1.0000 1.0000 2.0000 4.0000
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```

Ex 1: producting control plots

```
plot(chain, col="navy")
# Let's format our chain
chain.df <- as.data.frame( as.mcmc(chain) )</pre>
cat(sprintf("\n_Correlation_matrix:_\n"))
print(cor(chain.df))
# p inference result
hist(chain.df$p, nc=50, prob=TRUE, col='darkolivegreen2',
     xlab='p', ylab='f(p)', main='Inference_on_p')
# next data prediction probability
ty <- table(chain.df$y)</pre>
barplot(ty/sum(ty), col='firebrick2', xlab='y', ylab='f(y)',
        ylim=c(0,0.40),
        main=sprintf('Number_of_successes_in_%d_future_trials', data$n_next))
# Correlation between p and predicted variable
plot(chain.df$p, chain.df$y, xlab='p', ylab='y', main="",
     pch='+', col='navy', cex=1.5,
     xlim=c(0,1), ylim=c(0,10))
```



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Ex 1: jags results

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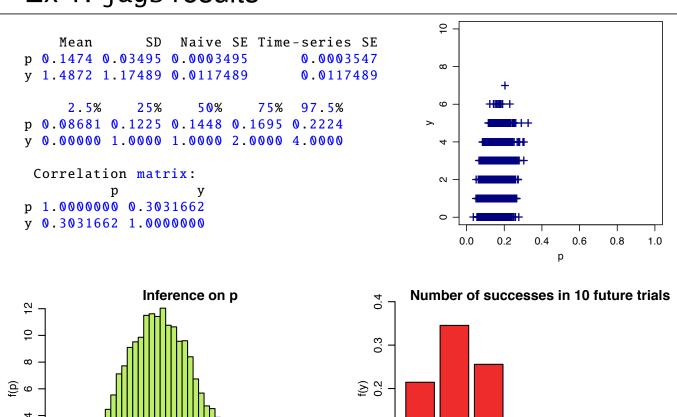
 α

0.05

0.10

0.15

0.20



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0.25

0.30

9

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Ex 2: Poisson inference

The Problem

- given the number of counts from a ionizing radiation detector, we want to infer the parameter λ of the underlying Poisson process
- the BUGS model (file: s11_inf_lambda_pred.bug) is the following:

```
model {
    # data likelihood
    X ~ dpois(lambda);

    # a uniform prior for lambda
    lambda ~ dexp(0.00001)

    # Predicted data, given lambda
    Y ~ dpois(lambda);
}
```

and our data:

```
data <- NULL
data$X <- 100 # number of counts</pre>
```

we create the jags model:

```
library(rjags)
model <- "s11_inf_lambda_pred.bug"
jm <- jags.model(model, data)</pre>
```

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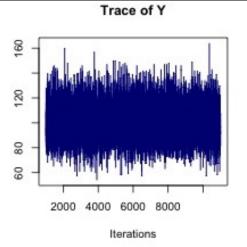
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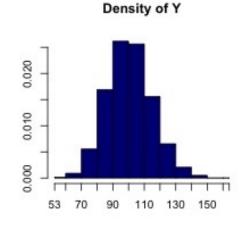
20

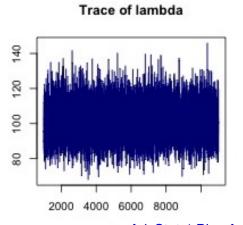
Ex 2: Poisson inference

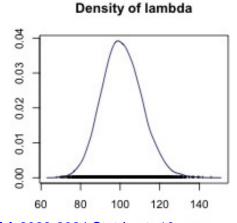
• the rest of the code is:

```
# Update the Markov chain (Burn-in)
update(jm, 1000)
chain <- coda.samples(jm, c("lambda", "Y"), n.iter=10000)</pre>
plot(chain, col="navy")
# Let's format our chain
chain.df <- as.data.frame( as.mcmc(chain) )</pre>
# Probability plots
par(mfrow=c(3,2), mgp=c(2.0,0.8,0), mar=c(3.5,3.5,1,1), oma=0.1*c(1,1,1,1))
hist(chain.df$lambda, nc=100, prob=TRUE, col='darkolivegreen2',
     xlim=c(40, 170),
     xlab='lambda', ylab='f(lambda)', main='Inference_on_lambda')
ty <- table(chain.df$Y)</pre>
barplot(ty/sum(ty), col='firebrick2', xlab='Y', ylab='f(Y)',
        # ylim=c(0,0.40),
        main=sprintf('Predicted_counts'))
# And present/ future prediction correlations
plot(chain.df$lambda, chain.df$Y, xlab='lambda', ylab='y', main="",
     pch='+', col='navy', cex=0.75, asp=1,
     xlim=c(50,160), ylim=c(50,160))
```









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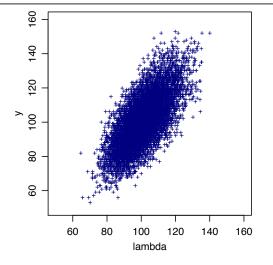
Ex 2: jags Poisson results

 Empirical mean and standard deviation for each variable, plus standard error of the mean:

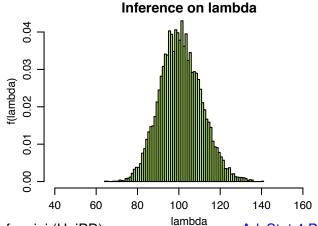
```
Mean SD Naive SE Time-series SE
Y 101.1 14.26 0.1426 0.1426
lambda 100.9 10.10 0.1010 0.1010
```

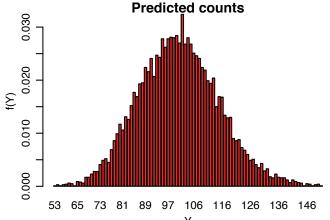
2. Quantiles for each variable:

```
2.5% 25% 50% 75% 97.5%
Y 75.00 91.00 101.0 110.0 131.0
lambda 82.24 93.99 100.5 107.6 121.7
```



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Problem

- given a set of 100 measurements, we want to infer the mean and sigma, assuming they are coming from a gaussian distribution with unknown mean and sigma
- the BUGS model (file: s11_norm_pred.bug) is the following:

```
# Gaussian model with unknown mean and sigma
model {
   for (i in 1:length(X)) {
                                            20
      X[i] ~ dnorm(mu, tau);
   mu ~ dnorm(0.0, 1.0E-6);
                                            15
   tau ~ dgamma(1.0, 1.0E-4);
   sigma <- 1.0/sqrt(tau);
                                            9
   # future observation
   Y ~ dnorm(mu, tau);
                                            2
}
                                                  8
                                                       9
                                                           10
                                                                11
                                                                     12
                                                                          13
```

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Ex 3: Normal inference

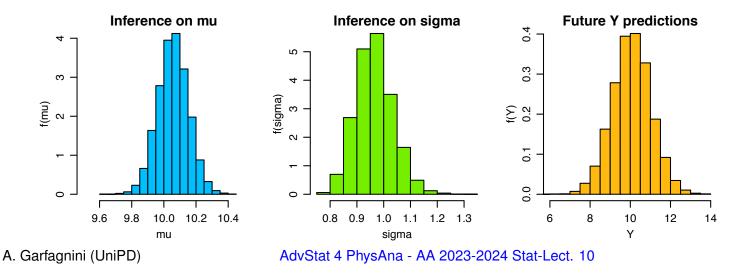
```
library(rjags)
set.seed(20190522)
# Generate the observed data
data_size <- 100
data_mu <- 10
data_sigma <- 1
data_obs <- rnorm(data_size, data_mu, data_sigma)</pre>
# - Specify the Generative Model with BUGS
model <- "s11_norm_pred.bug"</pre>
# Our data for the model
data <- NULL
data$X <- data_obs</pre>
                       # Set of observations
# Create the model and pass the parameters
jm <- jags.model(model, data)</pre>
# Update the Markov chain (Burn-in)
update(jm, 1000)
chain <- coda.samples(jm, c("mu", "sigma", "Y"), n.iter=10000)</pre>
print(summary(chain))
```

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Ex 3: jags Normal results

```
Naive SE Time-series SE
                    SD
Y
      10.0655 0.97382 0.0097382
                                       0.0097382
      10.0577 0.09610 0.0009610
                                       0.0009610
       0.9656 0.06926 0.0006926
                                       0.0006926
sigma
                               75%
        2.5%
                 25%
                        50%
                                     97.5%
Y
      8.1399 9.4278 10.067 10.711 11.983
      9.8668 9.9945 10.058 10.122 10.247
sigma 0.8398 0.9176
                      0.962
                             1.009
```

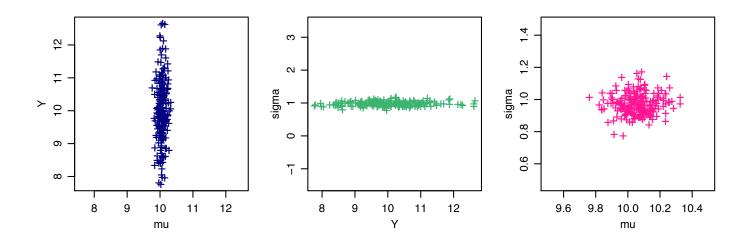
Note the different x-axis limits for μ and future Y predictions



Ex 3: jags Normal variables correlations

```
Correlation matrix:

Y mu sigma
Y 1.000000000 0.101044364 0.008388187
mu 0.101044364 1.000000000 0.002831711
sigma 0.008388187 0.002831711 1.000000000
```



Ex 4: Hook's law inference

The Problem

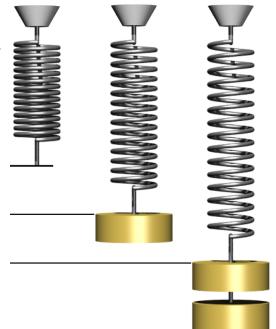
- a spring with elastic constant k and mass m_{spring} is held vertically, at rest, under the influence of the Earth's gravitational field
- the lower end of the spring is loaded with equal mass discs and both spring elongation and oscillation periods are measured
- we want to infer, from the data, the spring elastic constant, k and, eventualy, the Earth gravity constant, g
- calling *l*_o, the unloaded spring length, we get at equilibrum

$$I = I_{\circ} + rac{g}{k}(m_{spring} + n \cdot m_{disc})$$

where m_{disc} is a disc mass and n the number of discs connected to the spring

• if one end of the spring is perturbated from the equilibrium position, it oscillates with period

$$T = 2\pi \sqrt{M/k}$$
 where $M = m_{spring} + n \cdot m_{disc}$



measuring the oscillation period. as a function of the applied mass, it is possible to measure k, and from l, infer g

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Ex 4: the collected data

 the following data come from https://www.roma1.infn.it/~dagos/BMS/node22.html

		I series		II series		III series	
n	М	1	<i>T</i> × 10	1	<i>T</i> × 10	1	<i>T</i> × 10
	(g)	(mm)	(s)	(mm)	(s)	(mm)	(s)
0	63	0	-	0	-	0	-
1	142	0	-	0	-	0	-
2	221	0	-	0	-	0	-
3	300	14	5.01	16	5.09	16	5.19
4	379	32	5.57	33	5.66	33	5.68
5	458	49	6.24	51	6.27	51	6.34
6	536	66	6.78	68	6.82	69	6.94
7	615	85	7.28	86	7.33	87	7.28
8	694	103	7.79	103	7.81	103	7.86
9	773	119	8.13	121	8.31	121	8.24
10	852	137	8.63	139	8.77	139	8.70

 Notes: I_o, the unloaded spring rest length has been subtracted from data. Since the oscillation priod is below 1 s, the measurements have been taken for 10 periods

Ex 4: the BUGS model

```
model {
   # 1 Vs m
   for (i in 1:length(1)) {
      mu.l[i] <- c.l + m.l * (m_spring + (Nmin-1 + i) * m_disc);</pre>
      1[i] ~dnorm(mu.l[i], tau.l);
   c.1 ^{\sim} dnorm(0.0, 1.0E-4);
   m.l ~ dnorm(0.0, 1.0E-4);
   tau.l ~ dgamma(1.0E-3, 1.0E-6);
   sigma.l <- 1/sqrt(tau.l);</pre>
   # t vs sqrt(m)
   for (i in 1:length(t)) {
      mu.t[i] <- c.t + m.t * sqrt(m_spring + (Nmin-1 + i) * m_disc);</pre>
      t[i] ~dnorm(mu.t[i], tau.t);
   c.t ~ dnorm(0.0, 1.0E-4);
   m.t ~ dnorm(0.0, 1.0E-4);
   tau.t ~ dgamma(1.0E-3, 1.0E-5);
   sigma.t <- 1/sqrt(tau.t);</pre>
   #keg
   k \leftarrow 4*pi2 / (m.t*m.t)
   g \leftarrow m.1 * k
}
```

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Ex 4: data, init values, and model running

```
# Experimental data - Series I
data <- NULL
data$m_spring <- 0.063</pre>
data$m_disc <- 0.0789
              <- c(0.014, 0.032, 0.049, 0.066, 0.085, 0.103, 0.119, 0.137)</pre>
data$1
              <- c(0.501, 0.557, 0.624, 0.678, 0.728, 0.779, 0.813, 0.863)</pre>
data$t
              <- 3
data$Nmin
data$pi2
              <- pi^2
# Generative model initial values
inits <- NULL
inits$c.l
          <- 0
inits$m.l
          <- 0
inits$tau.l <- 1000
inits$tau.t <- 1000
           <- 1
inits$m.t
# Create the model and pass the parameters
jm <- jags.model("s13_spring.bug", data, inits)</pre>
# Update the Markov chain (Burn-in)
update(jm, 1000)
chain <- coda.samples(jm, c("c.1","m.1","sigma.1","c.t",</pre>
                             "m.t", "sigma.t", "k", "g"),
                       n.iter = 50000, thin = 50)
```

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Ex 4: jags run results

• the model produces the following output:

```
Iterations = 1050:51000 / Thinning interval = 50 / 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
c.1
        -0.0527146 0.0012529 3.962e-05
                                              3.962e - 05
                                              5.596e-04
c.t
        -0.0313581 0.0141587 4.477e-04
         9.4168338 0.3718726 1.176e-02
                                              1.502e-02
k
        42.2535756 1.6111324 5.095e-02
                                              6.667e-02
m.1
         0.2228622 0.0020382 6.445e-05
                                              6.445e-05
         0.9671275 0.0184045 5.820e-04
                                              7.612e-04
sigma.1
         0.0009943 0.0003414 1.080e-05
                                              1.080e-05
         0.0056743 0.0022657 7.165e-05
                                              9.858e-05
sigma.t
```

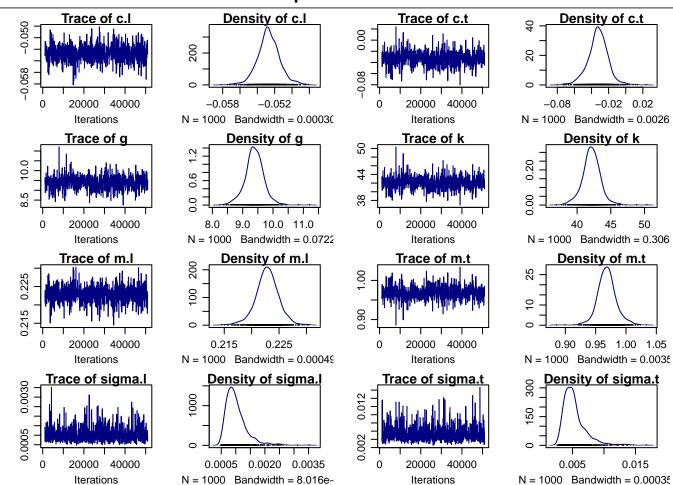
2. Quantiles for each variable:

```
2.5%
                            25%
                                        50%
                                                  75%
                                                           97.5%
        -0.0551276 -0.0534807 -0.0527385
                                           -0.051996 -0.050116
c.t
                   -0.0386805
                               -0.0312846
                                           -0.023451 -0.003571
        -0.0622894
         8.6816215
                     9.2058887
                                 9.4212113
                                             9.621637
a
k
        38.9954677 41.3512168 42.2117668 43.125521 45.426046
m.1
         0.2188010
                     0.2216423
                                 0.2229252
                                             0.224129
                                                       0.226905
         0.9322393
                     0.9567813
                                 0.9670816
                                             0.977093
                                                        1.006173
                                 0.0009172
sigma.l
         0.0005608
                     0.0007633
                                             0.001125
                                                        0.001863
         0.0030946
                     0.0042109
                                 0.0050638
                                             0.006621
                                                        0.011691
```

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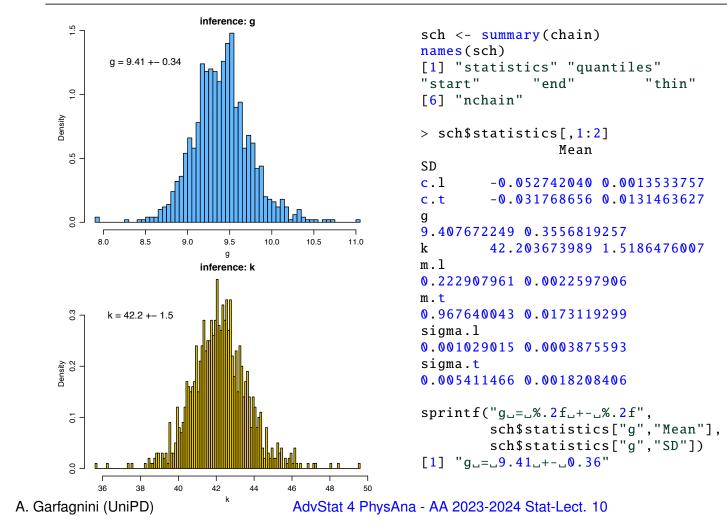
Ex 4: Markov chains plots



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Ex 4: Inference, g and k results



References

Exercises

• http://www.roma1.infn.it/~dagos/prob+stat.html

Reference Books

- C.P. Robert and G.Casella, *Introducting Monte Carlo Methods with R*, Springer, 2010
- C.P. Robert and G.Casella, Monte Carlo Statistical methods, Springer, 1999
- D. Lunn, et. al., The BUGS Book, a prctical introduction to Bayesian Analysis, CRC Press, 2012

Additional Material

- JAGS user manual: https://sourceforge.net/projects/mcmc-jags/files/Manuals/
- rjags user manual https://cran.r-project.org/web/packages/rjags/rjags.pdf
- BUGS reference manual https: //www.statslab.cam.ac.uk/Dept/People/djsteaching/bugsbook-syntax.pdf

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