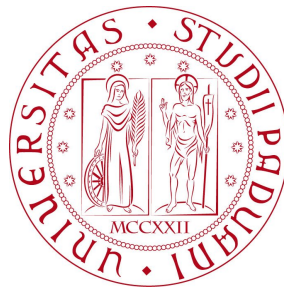


Gibbs sampling and JAGS

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AA 2020/2021 - Stat Lect. 12



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

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

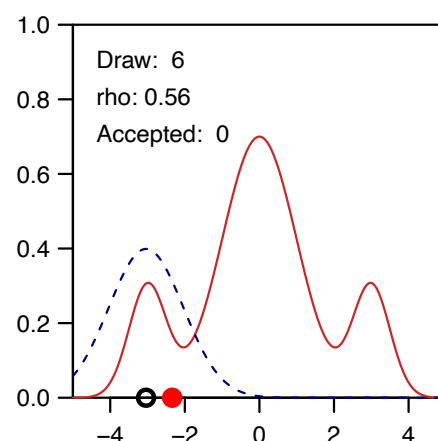
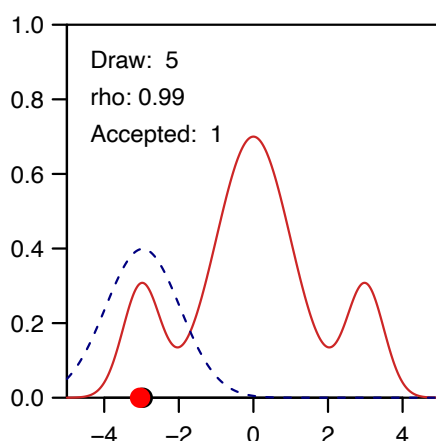
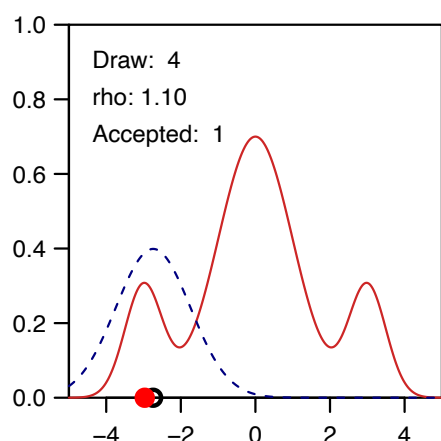
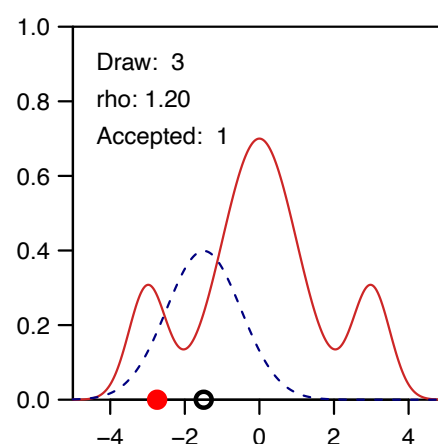
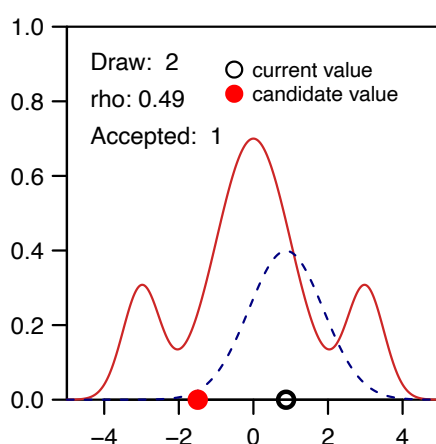
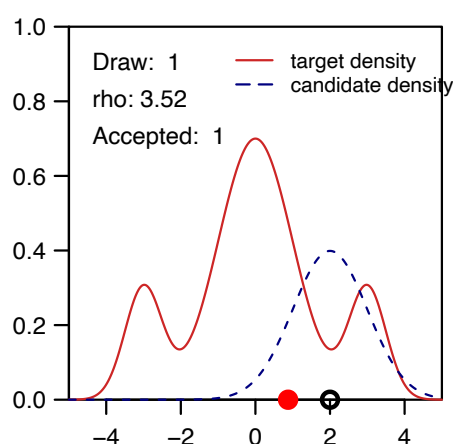
Problem

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

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

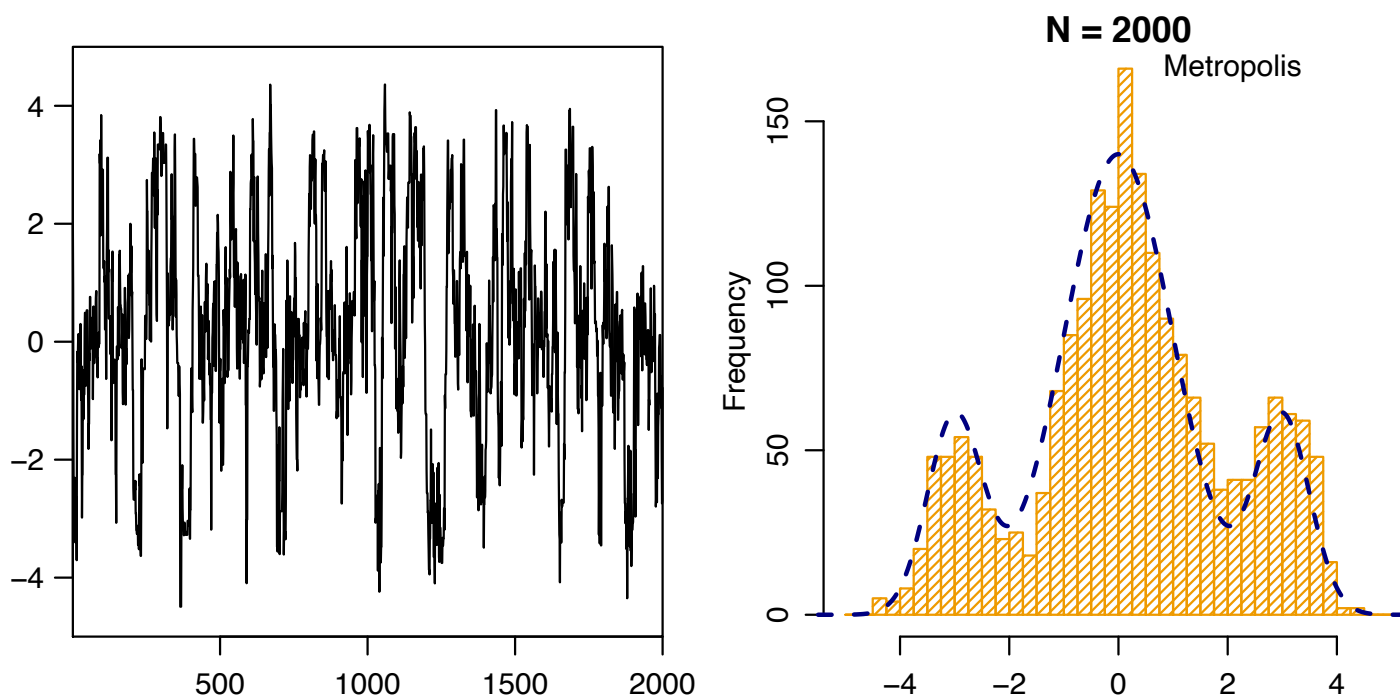
- with $a_1 = 0.7$, $a_2 = 0.15$ and $a_3 = 0.15$

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



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4

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

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

- Q_2 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

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

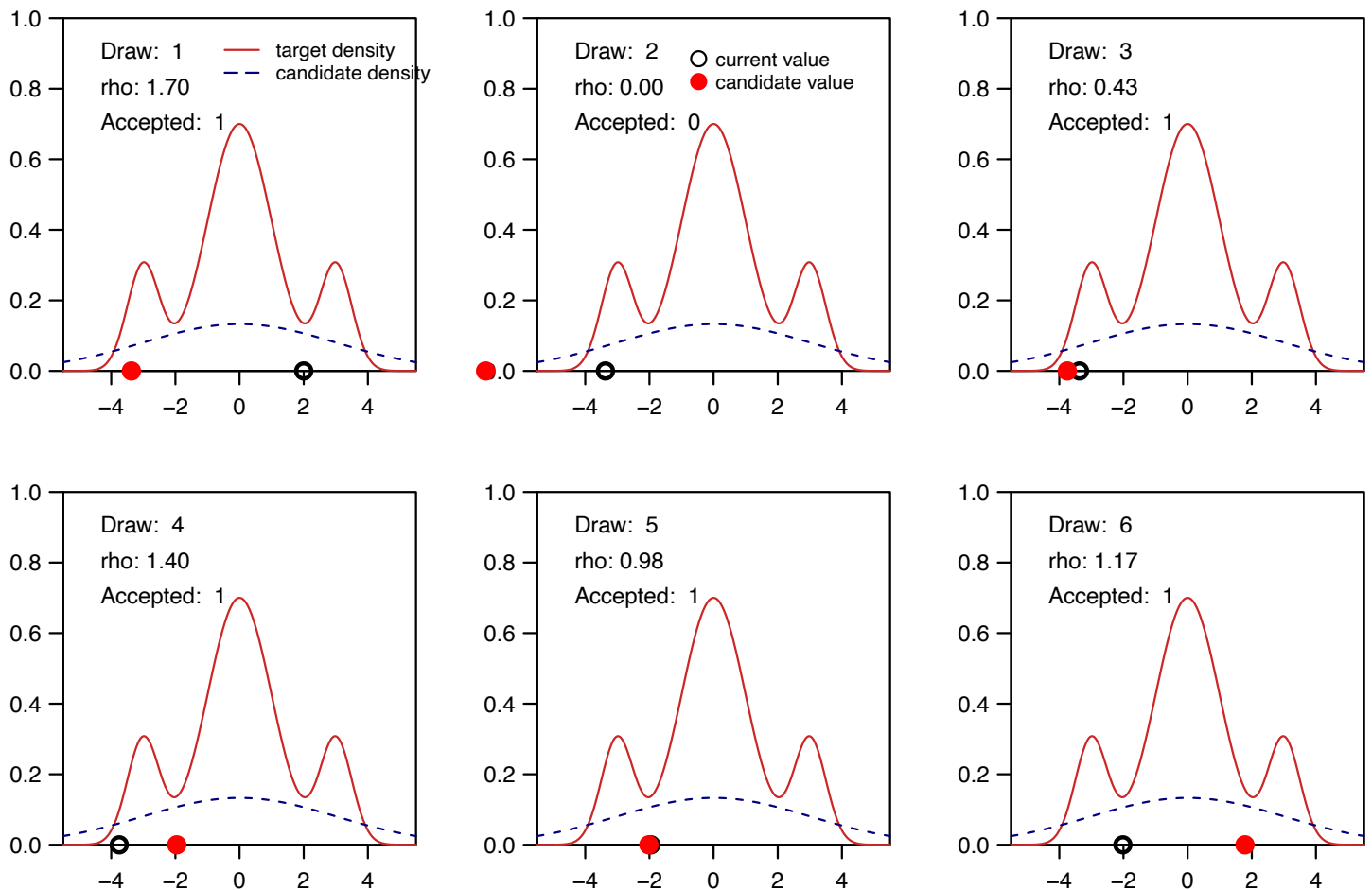
- with $a_1 = 0.7$, $a_2 = 0.15$ and $a_3 = 0.15$
- assuming that the candidate density is a $\text{Norm}(0, 3^2)$ distribution function

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5

Metropolis-Hastings : indep. cand. chain



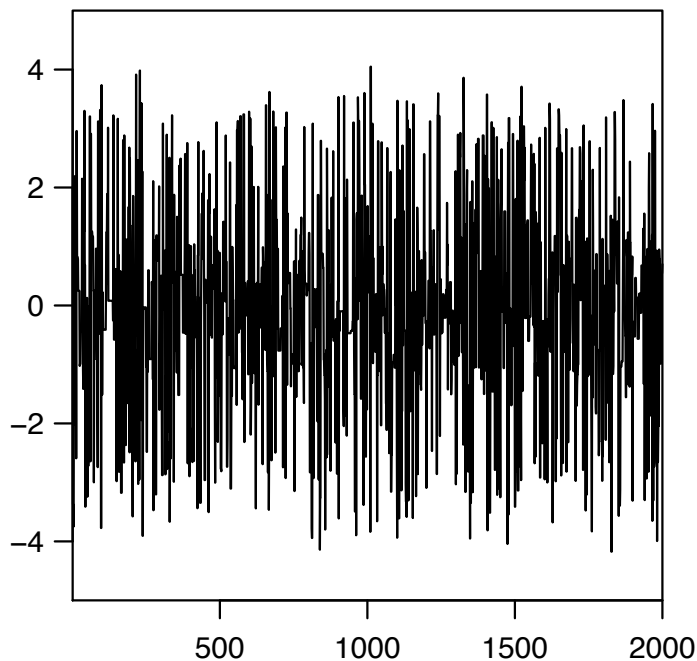
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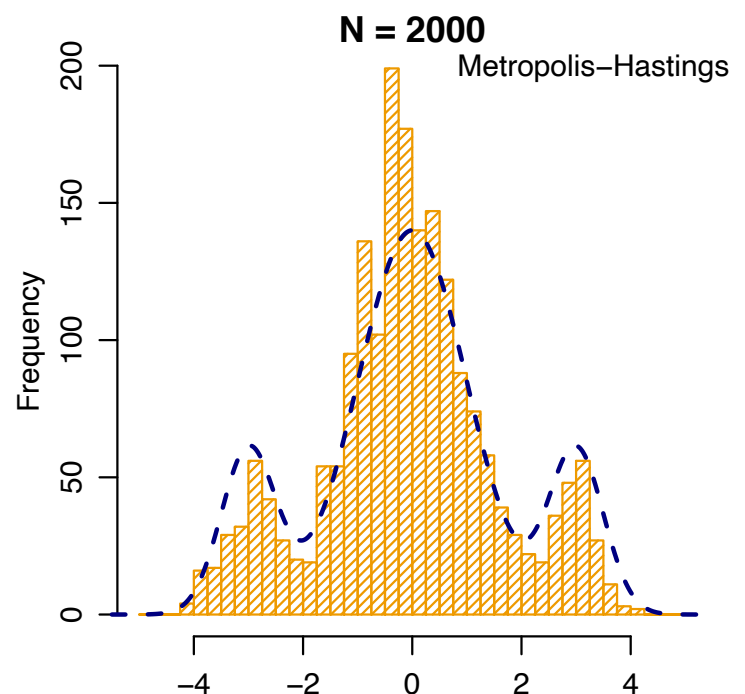
6

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



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7

- 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

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

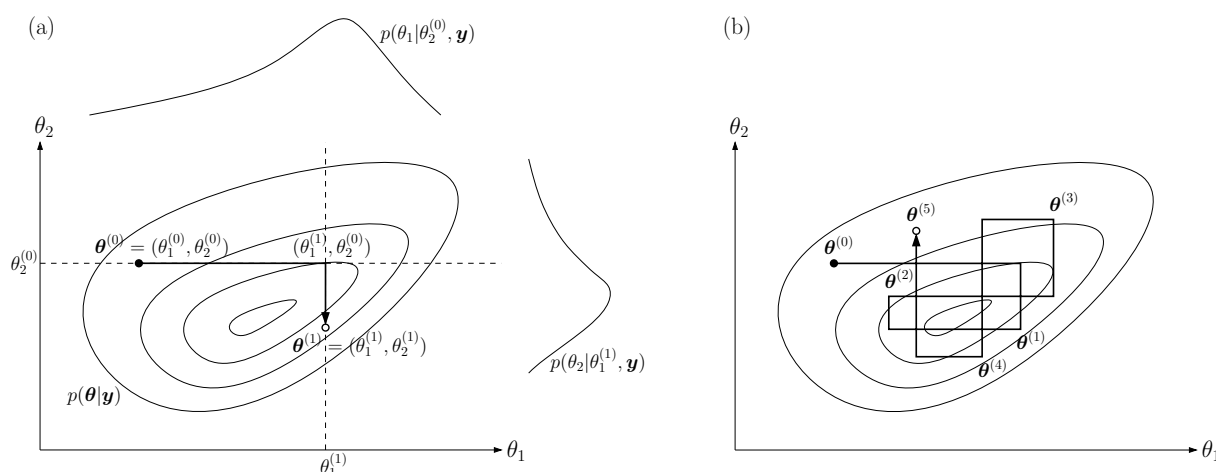
- sample a new $\theta_2^{(1)}$, for the second component, from its full conditional distribution

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

- 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

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 $\theta_1^{(1)}$ 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 4.3.0 (July 18, 2017)
- **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 (v4.6) and osx-64 (v4.6)
 - `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 (v0.5.7)
 - `conda install -c glaxosmithkline r-r2jags`

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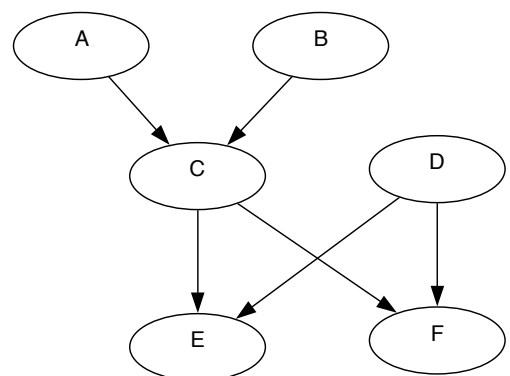
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11

- 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

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



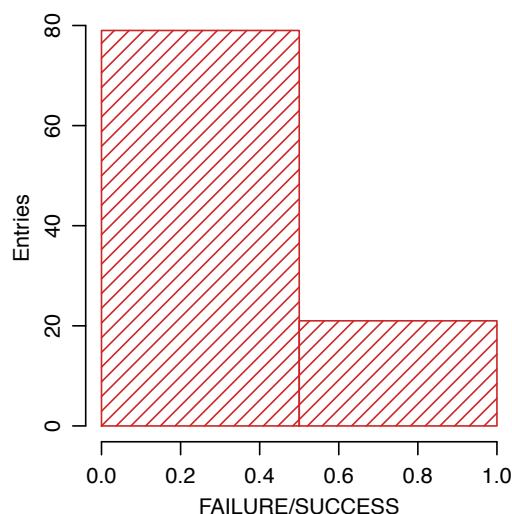
$$P(A, B, C, D, E, F) = P(A)P(B)P(C|A, B)P(D)P(E|C, D)P(F|C, D)$$

Ex 1: Bernoulli process

The Problem

- given a set of observation, coming from a **Bernoulli process**, we want to **infer 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:

```
X <- c(0, 0, 0, 0, 0, 0, 0, 1, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 1, 0, 1, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 1, 0, 0, 0, 0, 0, 1,
       0, 1, 0, 0, 0, 0, 0, 1, 0, 0,
       0, 0, 0, 0, 1, 0, 0, 0, 1, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 1, 1,
       0, 1, 0, 0, 1, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 1, 0, 0, 1, 0, 1)
```



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

Ex 1: BUGS model and parameters

- file: `s13_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
```

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

```
jlm <- jags.model(model, data)
```


Ex 1: running jags

```
# Update the Markov chain (Burn-in)
update(jm, 1000)
chain <- coda.samples(jm, c("p", "y"), n.iter=10000)
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%
| ***** | 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:
      Mean      SD Naive SE Time-series SE
p 0.1474 0.03495 0.0003495 0.0003547
y 1.4872 1.17489 0.0117489 0.0117489

2. Quantiles for each variable:
      2.5%    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
```

Ex 1: producing control plots

```
plot(chain, col="navy")

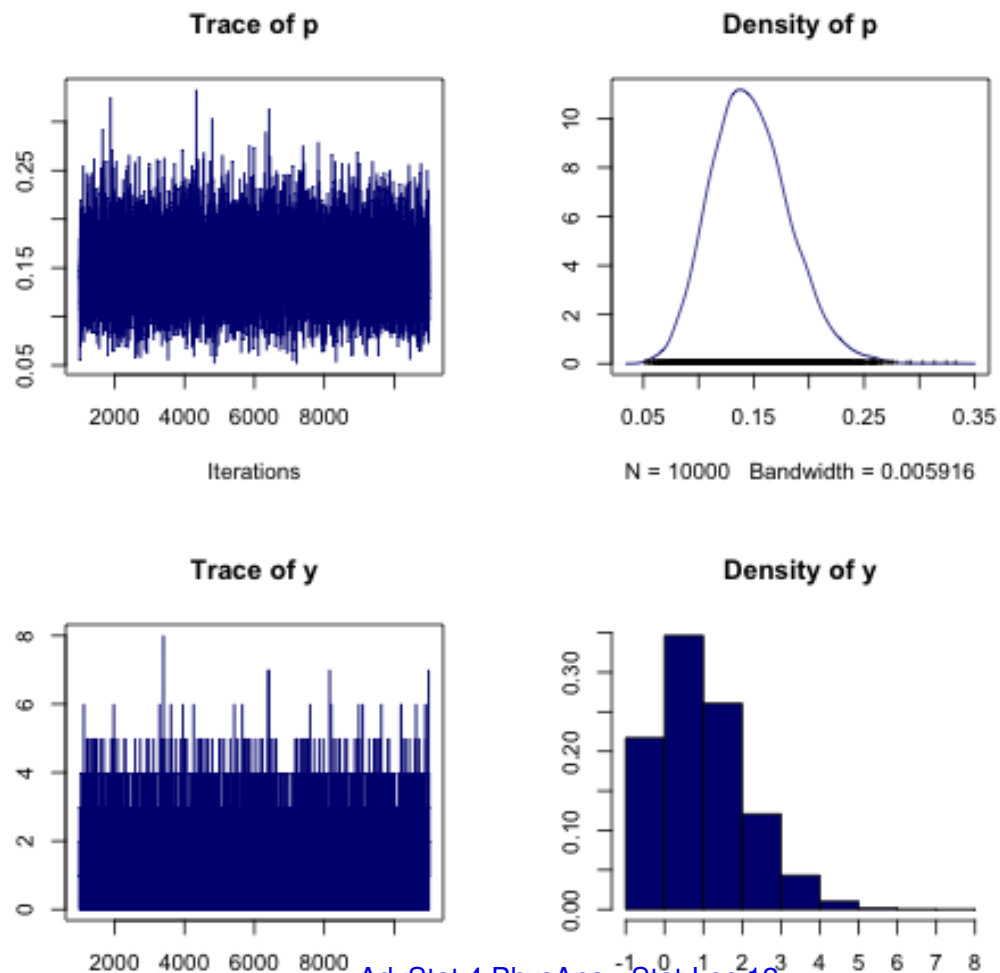
# Let's format our chain
chain.df <- as.data.frame( as.mcmc(chain) )
cat(sprintf("\nCorrelation matrix:\n"))
print(cor(chain.df))

#
# 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$y)
barplot(ty/sum(ty), col='firebrick2', xlab='y', ylab='f(y)',
        ylim=c(0,0.40),
        main=sprintf('Number of successes in %d future trials', data$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))
```

Ex 1: jags chains



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18

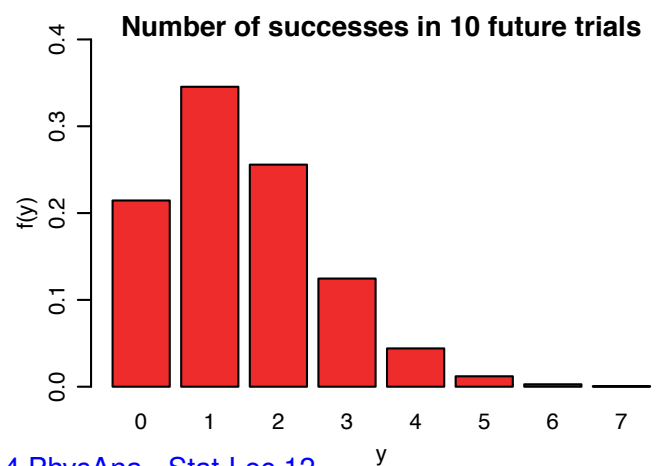
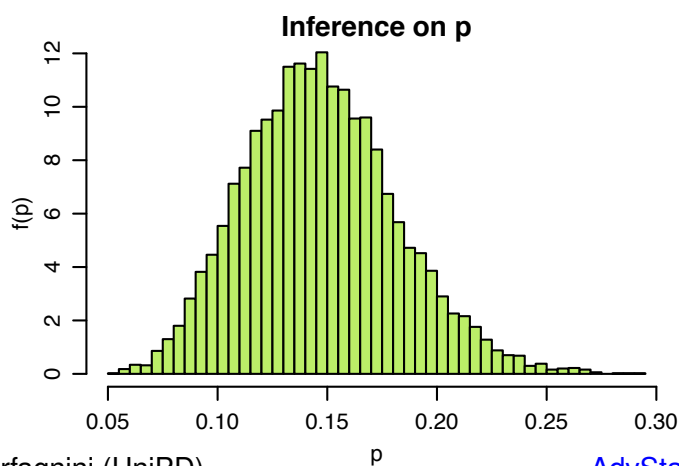
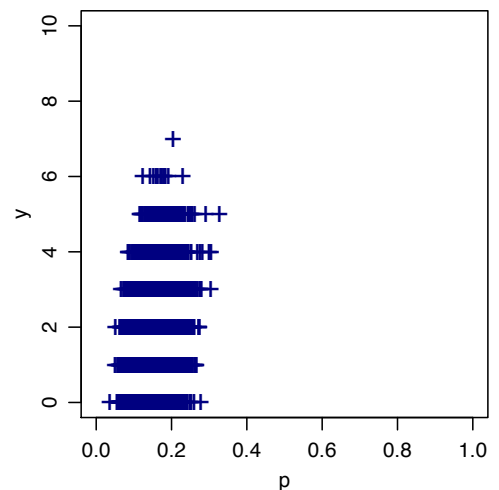
Ex 1: jags results

	Mean	SD	Naive SE	Time-series SE
p	0.1474	0.03495	0.0003495	0.0003547
y	1.4872	1.17489	0.0117489	0.0117489

	2.5%	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

Correlation matrix:

	p	y
p	1.0000000	0.3031662
y	0.3031662	1.0000000



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19

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: s13_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
```

- we create the jags model:

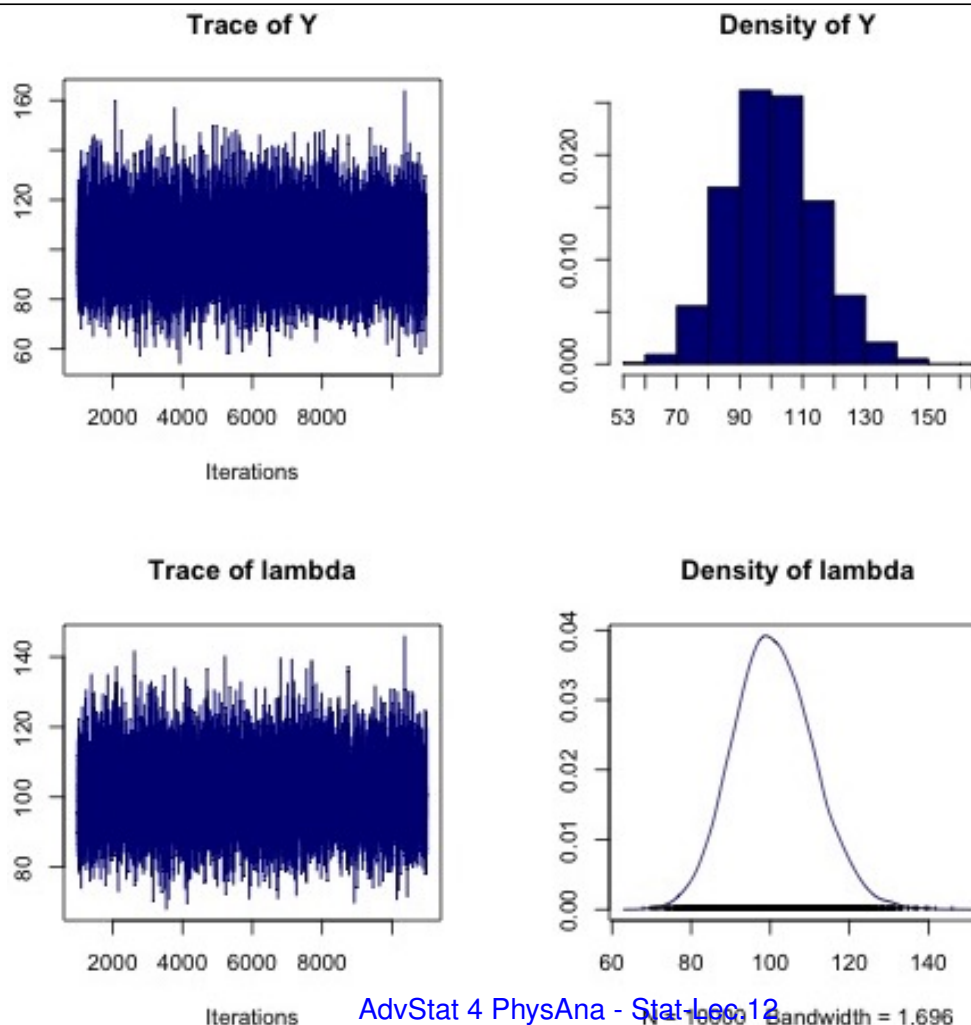
```
library(rjags)  
model <- "s13_inf_lambda_pred.bug"  
jm <- jags.model(model, data)
```

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)  
  
plot(chain, col="navy")  
  
# Let's format our chain  
chain.df <- as.data.frame( as.mcmc(chain) )  
  
#  
# 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)  
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))
```

Ex 2: jags chains



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22

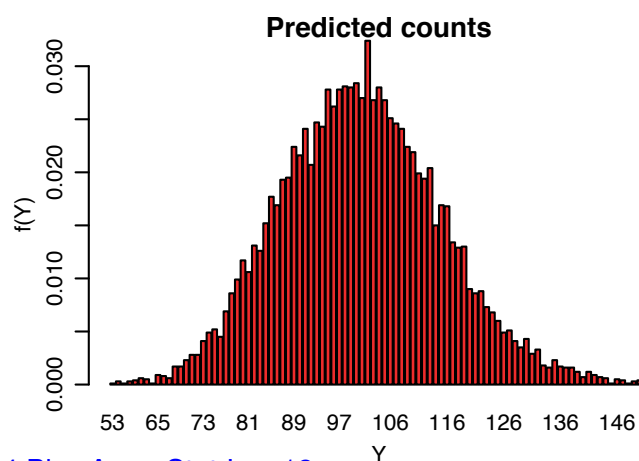
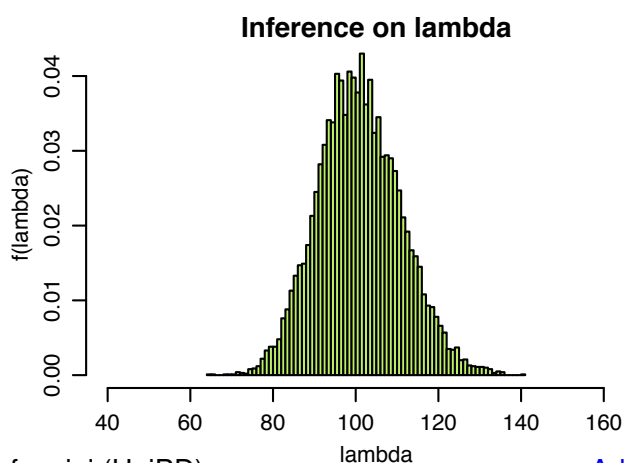
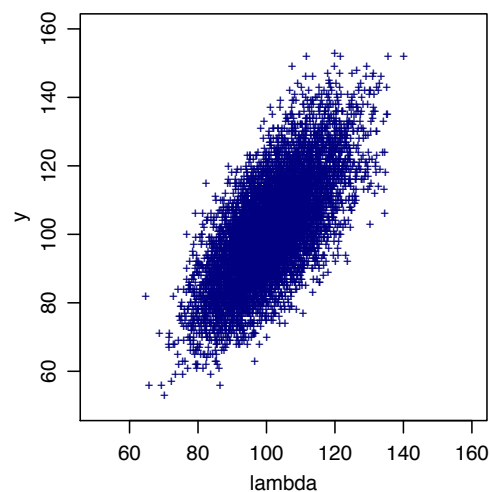
Ex 2: jags Poisson results

1. 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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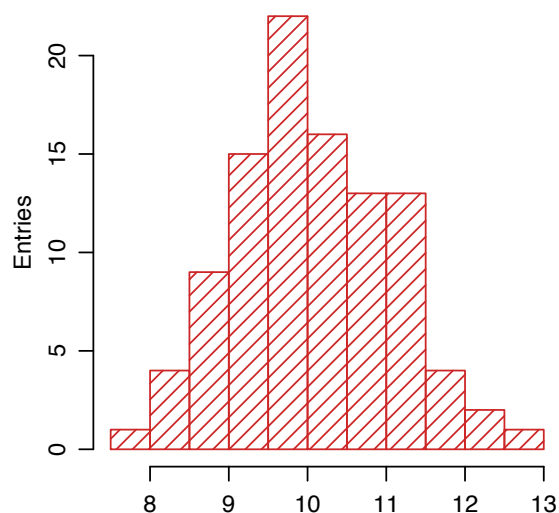
23

Ex 3: Normal inference

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: s13_norm_pred.bug) is the following:

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



Ex 3: Normal inference

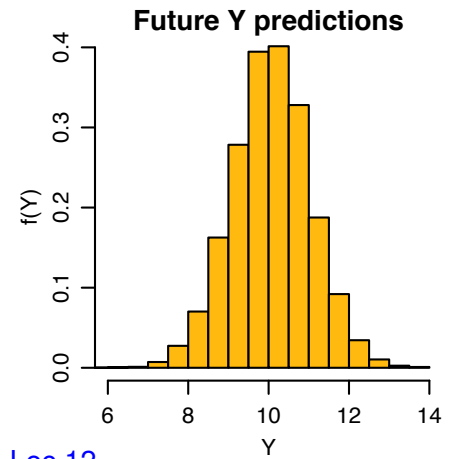
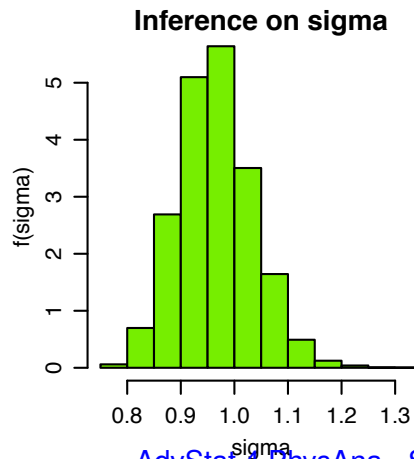
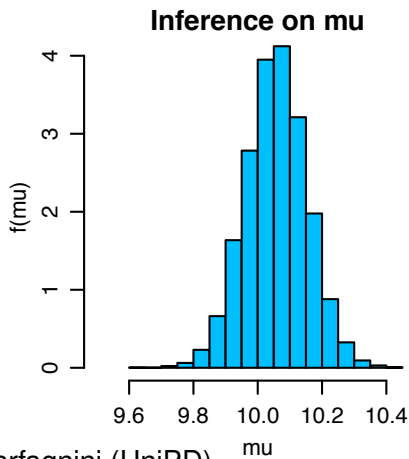
```
library(rjags)  
  
set.seed(20190522)  
  
#  
# Generate the observed data  
data_size <- 100  
data_mu <- 10  
data_sigma <- 1  
data_obs <- rnorm(data_size, data_mu, data_sigma)  
  
# - Specify the Generative Model with BUGS  
model <- "s13_norm_pred.bug"  
  
# Our data for the model  
data <- NULL  
data$X <- data_obs # Set of observations  
  
# Create the model and pass the parameters  
jm <- jags.model(model, data)  
  
# Update the Markov chain (Burn-in)  
update(jm, 1000)  
  
chain <- coda.samples(jm, c("mu", "sigma", "Y"), n.iter=10000)  
print(summary(chain))
```

Ex 3: jags Normal results

	Mean	SD	Naive SE	Time-series SE
Y	10.0655	0.97382	0.0097382	0.0097382
mu	10.0577	0.09610	0.0009610	0.0009610
sigma	0.9656	0.06926	0.0006926	0.0006926

	2.5%	25%	50%	75%	97.5%
Y	8.1399	9.4278	10.067	10.711	11.983
mu	9.8668	9.9945	10.058	10.122	10.247
sigma	0.8398	0.9176	0.962	1.009	1.111

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



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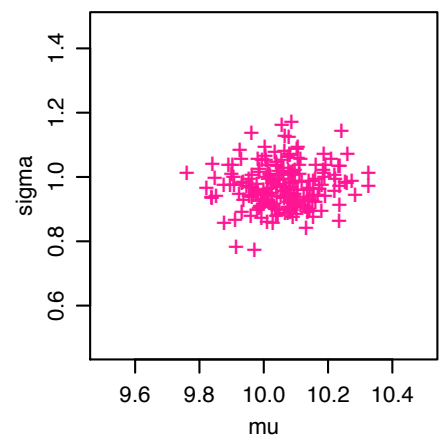
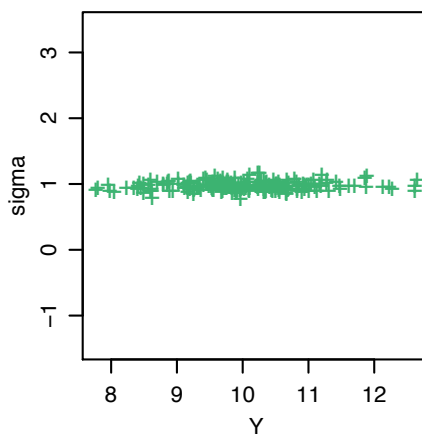
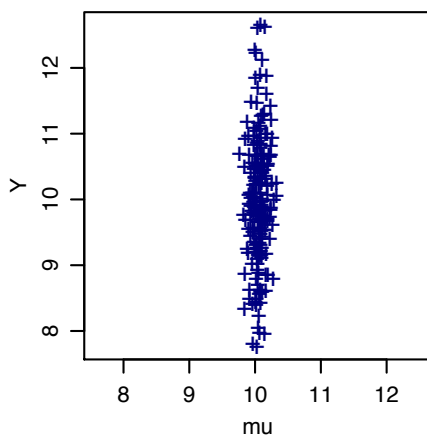
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26

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



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27

Ex 4: Hook's law inference

The Problem

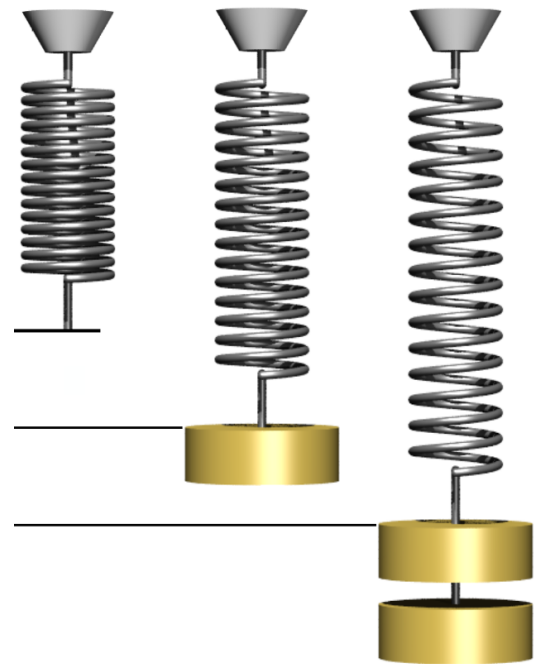
- a spring with elastic constant k and mass m_{spring} is held vertically, at rest, under the influence of the Earth's gravitational field
- the lower end of the spring is loaded with equal mass discs and both spring elongation and oscillation periods are measured
- we want to infer, from the data, the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

$$l = l_o + \frac{g}{k}(m_{spring} + n \cdot m_{disc})$$

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

- if one end of the spring is perturbed from the equilibrium position, it oscillates with period

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



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

Ex 4: the collected data

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

n	M	I series		II series		III series	
	(g)	l (mm)	$T \times 10$ (s)	l (mm)	$T \times 10$ (s)	l (mm)	$T \times 10$ (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: l_o , the unloaded spring rest length has been subtracted from data. Since the oscillation period is below 1 s, the measurements have been taken for 10 periods

Ex 4: the BUGS model

```
model {
  # l Vs m
  for (i in 1:length(l)) {
    mu.l[i] <- c.l + m.l * (m_spring + (Nmin-1 + i) * m_disc);
    l[i] ~ dnorm(mu.l[i], tau.l);
  }
  c.l ~ 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);

  # 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);
    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);

  # k e g
  k <- 4*pi2 / (m.t*m.t)
  g <- m.l * k
}
```

Ex 4: data, init values, and model running

```
# Experimental data - Series I
data <- NULL
data$m_spring <- 0.063
data$m_disc <- 0.0789
data$l <- c(0.014, 0.032, 0.049, 0.066, 0.085, 0.103, 0.119, 0.137)
data$t <- c(0.501, 0.557, 0.624, 0.678, 0.728, 0.779, 0.813, 0.863)
data$Nmin <- 3
data$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
inits$m.t <- 1

# Create the model and pass the parameters
jm <- jags.model("s13_spring.bug", data, inits)

# Update the Markov chain (Burn-in)
update(jm, 1000)

chain <- coda.samples(jm, c("c.l", "m.l", "sigma.l", "c.t",
                           "m.t", "sigma.t", "k", "g"),
                      n.iter = 50000, thin = 50)
```


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

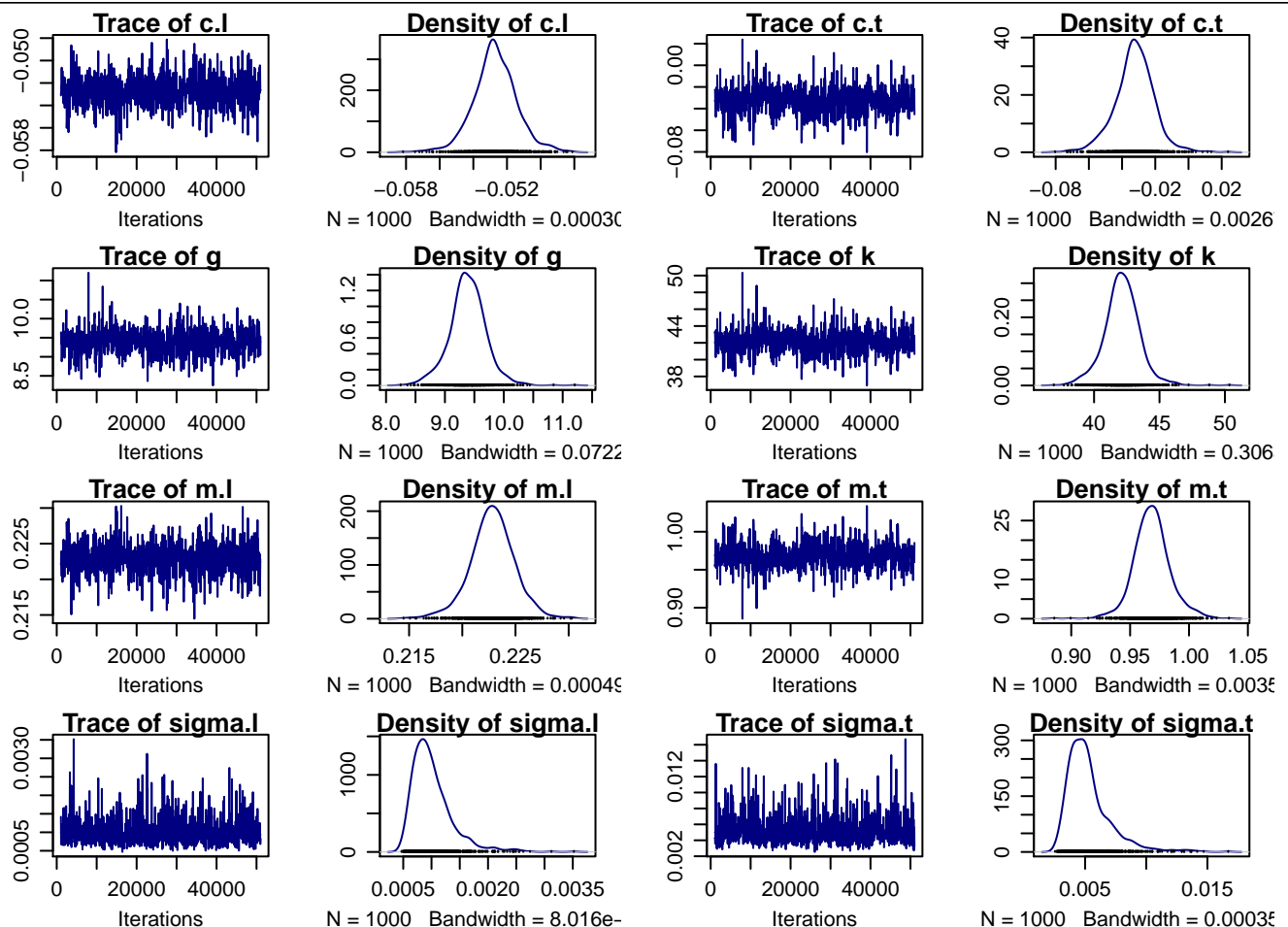
- Empirical mean and standard deviation for each variable,
plus standard error of the mean:

	Mean	SD	Naive SE	Time-series SE
c.l	-0.0527146	0.0012529	3.962e-05	3.962e-05
c.t	-0.0313581	0.0141587	4.477e-04	5.596e-04
g	9.4168338	0.3718726	1.176e-02	1.502e-02
k	42.2535756	1.6111324	5.095e-02	6.667e-02
m.l	0.2228622	0.0020382	6.445e-05	6.445e-05
m.t	0.9671275	0.0184045	5.820e-04	7.612e-04
sigma.l	0.0009943	0.0003414	1.080e-05	1.080e-05
sigma.t	0.0056743	0.0022657	7.165e-05	9.858e-05

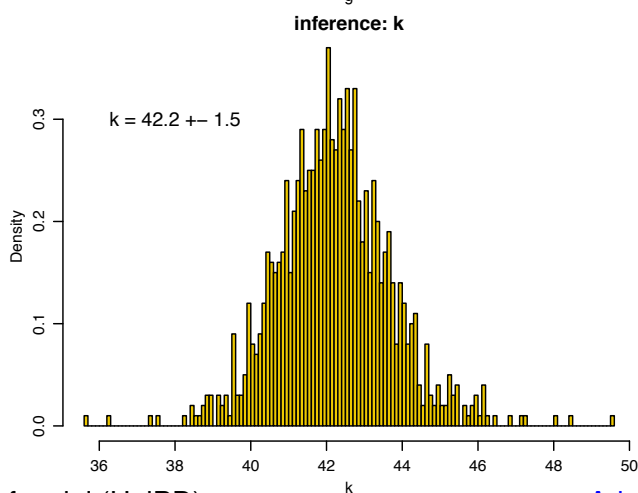
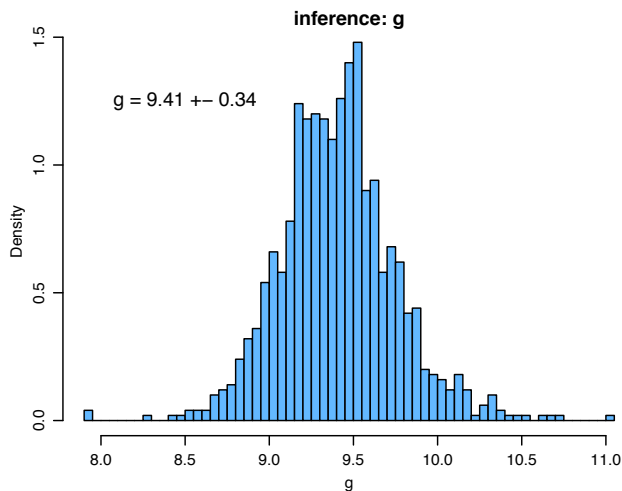
- Quantiles for each variable:

	2.5%	25%	50%	75%	97.5%
c.l	-0.0551276	-0.0534807	-0.0527385	-0.051996	-0.050116
c.t	-0.0622894	-0.0386805	-0.0312846	-0.023451	-0.003571
g	8.6816215	9.2058887	9.4212113	9.621637	10.127262
k	38.9954677	41.3512168	42.2117668	43.125521	45.426046
m.l	0.2188010	0.2216423	0.2229252	0.224129	0.226905
m.t	0.9322393	0.9567813	0.9670816	0.977093	1.006173
sigma.l	0.0005608	0.0007633	0.0009172	0.001125	0.001863
sigma.t	0.0030946	0.0042109	0.0050638	0.006621	0.011691

Ex 4: Markov chains plots



Ex 4: Inference, g and k results



```
sch <- summary(chain)
names(sch)
[1] "statistics" "quantiles"
"start"      "end"        "thin"
[6] "nchain"

> sch$statistics[,1:2]
              Mean
SD
c.l      -0.052742040 0.0013533757
c.t      -0.031768656 0.0131463627
g
9.407672249 0.3556819257
k
42.203673989 1.5186476007
m.l
0.222907961 0.0022597906
m.t
0.967640043 0.0173119299
sigma.l
0.001029015 0.0003875593
sigma.t
0.005411466 0.0018208406

sprintf("g_=%%.2f_+-%%.2f",
        sch$statistics["g","Mean"],
        sch$statistics["g","SD"])
[1] "g_=%9.41_+-%0.36"
```

References

Exercises

- <http://www.roma1.infn.it/~dagosa/prob+stat.html>

Reference Books

- C.P. Robert and G.Casella, *Introducing 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>