

Measurements, uncertainties and probabilistic inference/forecasting

Giulio D'Agostini

Università di Roma La Sapienza e INFN
Roma, Italy

A simple random walk on a plane

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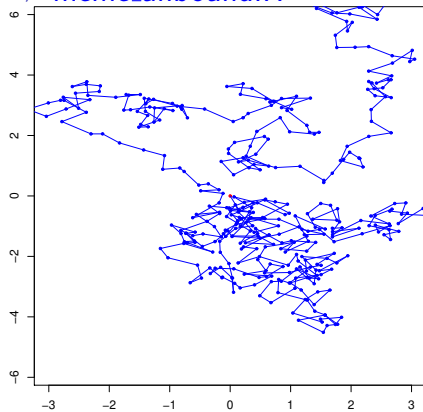
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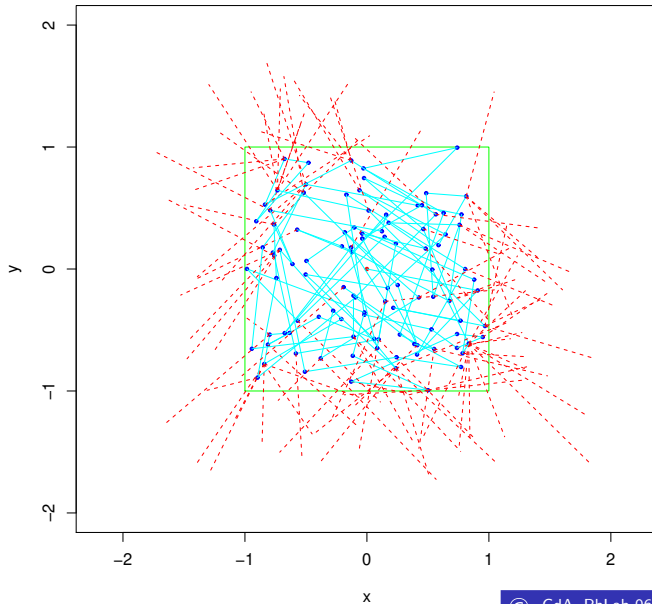
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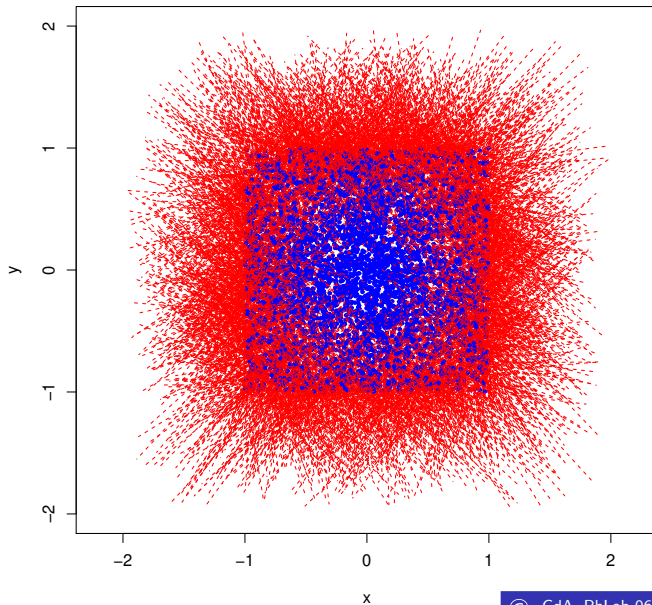
Visiting uniformly the points inside a square

200 attempts



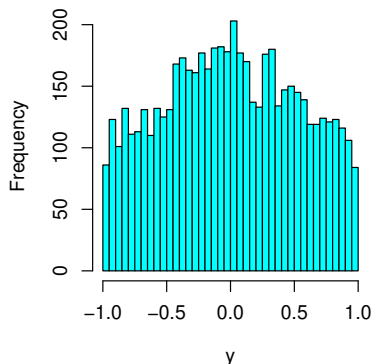
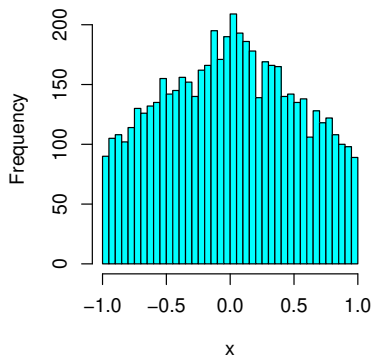
Visiting uniformly the points inside a square

10000 attempts (intermediate cyan 'lines' omitted)



Visiting uniformly the points inside a square

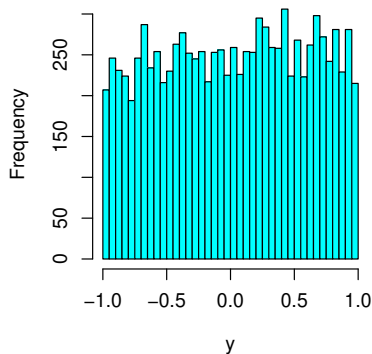
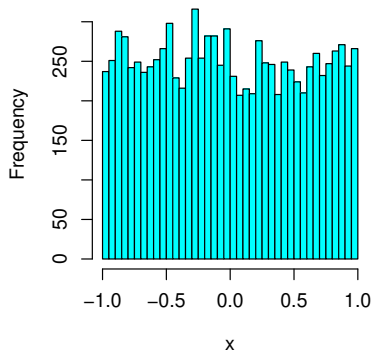
Method 1: count points only once



Not what we wanted!

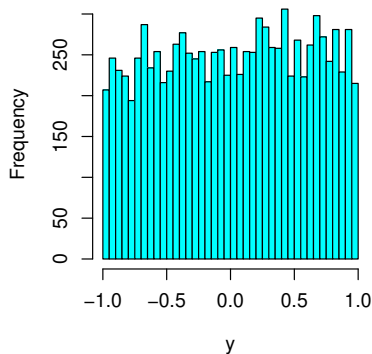
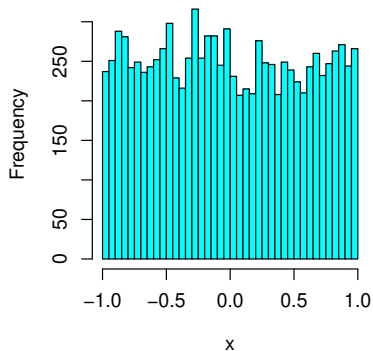
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Method 2: count points several times



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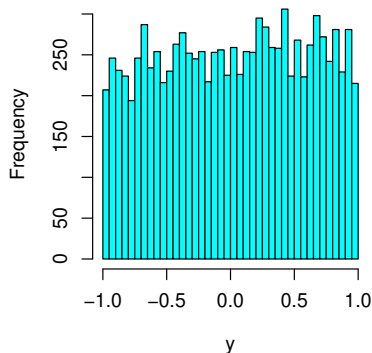
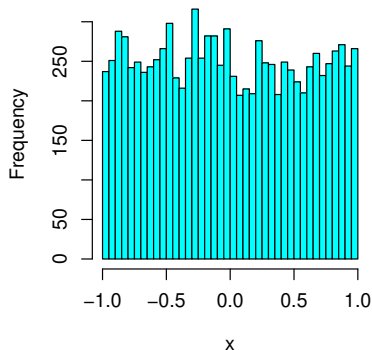
Method 2: count points several times



Why?

Visiting uniformly the points inside a square

Method 2: count points several times



Why?

MCMC theory left to self study

Inferring μ and σ from n 'independent' measurements

$$f(\mu, \sigma \mid \underline{x}, f_0(\mu, \sigma) = k) \propto \prod_i \frac{1}{\sigma} \exp \left[-\frac{(x_i - \mu)^2}{2\sigma^2} \right]$$

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Try to do it with Metropolis!

Back to $f(\mu, \sigma)$ from a sample

In practice

$$f(\mu, \sigma | \bar{x}, s, \dots) \propto \sigma^{-n} \exp \left[-\frac{s^2 + (\mu - \bar{x})^2}{2\sigma^2/n} \right] \cdot f_0(\mu, \sigma)$$

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Some remarks are in order:

- ▶ $f(\mu | \bar{x}, s)$ is in general not Gaussian (**not even starting from a flat prior!**) due to the uncertainty on σ

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→ See **appendix** with details on small numbers

Including uncertainties due to systematics

Exact solution in a special (important) case

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(But remember that many ' h 's are Physics:

for example you will not be able to get meaningful results on the primordial Universe if you do not first understand the Physics of Cosmic Dust)

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(see ISO GUM).

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(*) Usually this is not the case, but in some field of reaserch it is not impossible that e.g. the physical properties of the instrument depend on the physical properties (of materials) you are studying.

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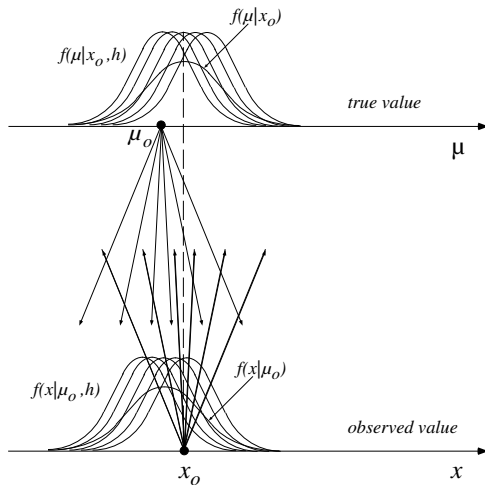
$$x \Rightarrow f(\mu | x, h).$$

Each conditional result is reweighed with the distribution of beliefs of h , using the well-known law of probability:

$$f(\mu | x) = \int f(\mu | x, h) f(h) dh.$$

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Conditional inference



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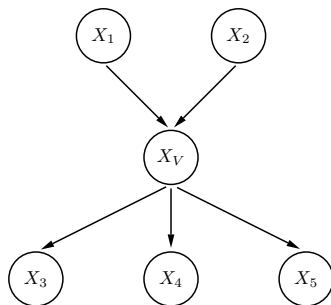
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Graphical model

In terms of the generic variables X_i ([arXiv:1504.02065](#))



$$X_1 \longleftrightarrow \mu$$

$$X_2 \longleftrightarrow Z$$

$$X_V \longleftrightarrow \mu + Z$$

$$X_{3-\dots} \longleftrightarrow X_i \text{ (observations)}$$

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Integrating we get

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Technical remark

It may help to know that

$$\int_{-\infty}^{+\infty} \exp \left[b x - \frac{x^2}{a^2} \right] dx = \sqrt{a^2 \pi} \exp \left[\frac{a^2 b^2}{4} \right]$$

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- ▶ This result (a theorem under well stated conditions!) is often used as a ‘**prescription**’, although there are still some “old-fashioned” recipes which require different combinations of the contributions to be performed.

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Systematics due to uncertain offset

Measuring two quantities with the same instrument

$$f(\mu_1, \mu_2 | x_1, x_2) = \frac{\int f(x_1, x_2 | \mu_1, \mu_2, z) f_o(\mu_1, \mu_2, z) dz}{\int \dots d\mu_1 d\mu_2 dz}$$

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where

$$\rho = \frac{\sigma_Z^2}{\sqrt{\sigma_1^2 + \sigma_Z^2} \sqrt{\sigma_2^2 + \sigma_Z^2}}.$$

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⇒ bivariate normal distribution!

Systematics due to uncertain offset

Summary:

$$\mu_1 \sim \mathcal{N}\left(x_1, \sqrt{\sigma_1^2 + \sigma_Z^2}\right)$$

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As more or less intuitively expected from an offset!

A simple example with JAGS

```
model {  
  for (i in 1:length(x)) {  
    x[i] ~ dnorm(mu.s, tau)  
  }  
  mu.s <- mu + z;  
  mu ~ dnorm(0.0, 1.0E-6)  
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=> norm_sist_z.R

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- ▶ include also derived quantities, like sum and difference;
- ▶ modify the model in order to describe a systematics affecting the scale: $f = 1 \pm \sigma_f$;
- ▶ then, add other derived quantities, like product and ratio.

Fits – introduction

- ▶ In a probabilistic framework the issue of the fits is nothing but **parametric inference**.
- ▶ set up the **model**,
e.g. $\mu_{y_i} = m \mu_{x_i} + c$

Fits – introduction

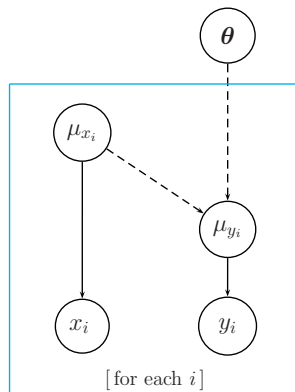
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- ▶ **perform the calculations**.

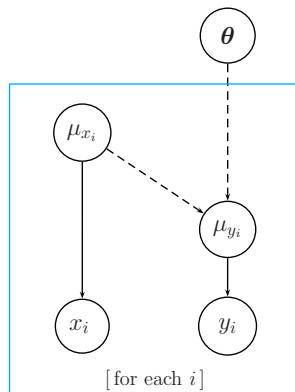


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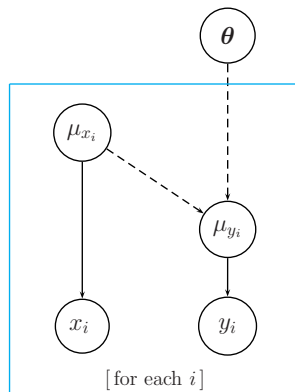
$$\rightarrow f(\theta \mid x, y, l)$$



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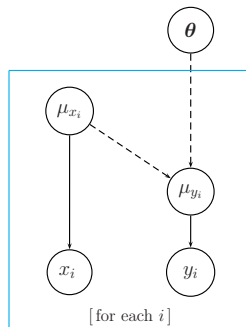
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→ $f(\theta | x, y, l)$

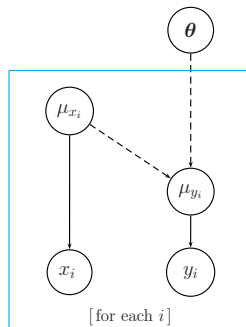
→ $f(m, c | x, y, \sigma)$, in the case of case of **linear fit**
with “ σ ’s known a priori” (!)

Linear fit – introduction



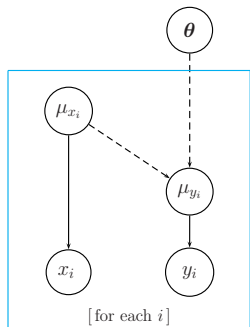
- Deterministic links between μ_x 's and μ_y 's.

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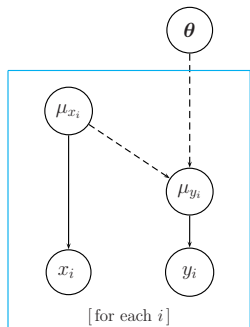
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- ▶ \Rightarrow aim of fit (σ 's known): $\{\mathbf{x}, \mathbf{y}\} \rightarrow \boldsymbol{\theta} = (m, c)$
- ▶ If σ_x 's and σ_y 's are unknown and assumed all equal
 $\{\mathbf{x}, \mathbf{y}\} \rightarrow \boldsymbol{\theta} = (m, c, \sigma_x, \sigma_y)$
- ▶ etc. . .

Linear fit – simplest case

$$f(m, c \mid \mathbf{x}, \mathbf{y}, l) \propto f(\mathbf{x}, \mathbf{y} \mid m, c, l) \cdot f_0(m, c)$$

Simplifying hypotheses:

- ▶ No error on $\mu_x \Rightarrow \mu_{x_i} = x_i$:
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$$\begin{aligned} f(m, c | \mathbf{x}, \mathbf{y}, \sigma) &\propto \exp \left[- \sum_i \frac{(y_i - \mu_{y_i})^2}{2 \sigma_i^2} \right] \cdot f_0(m, c) \\ &\propto \exp \left[- \frac{1}{2} \sum_i \frac{(y_i - m x_i - c)^2}{\sigma_i^2} \right] \cdot f_0(m, c) \end{aligned}$$

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\Rightarrow flat priors: inference only depends on $\exp \left[- \frac{1}{2} \sum_i \frac{(y_i - m x_i - c)^2}{\sigma_i^2} \right]$.

Least squares and 'Gaussian tricks' on linear fits

$$f(m, c \mid \mathbf{x}, \mathbf{y}, \boldsymbol{\sigma}) \propto \exp \left[-\frac{\sum_i (y_i - m x_i - c)^2}{2 \sigma_i^2} \right] \cdot f_0(m, c)$$

- If the prior is irrelevant and the σ 's are all equal, then the maximum of the posterior is obtained when the sum of the squares is minimized:
⇒ Least Square 'Principle'.

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 - ▶ As an approximation, one can obtain best fit parameters and covariance matrix by the 'Gaussian trick'
 $\Rightarrow \varphi(m, c) \propto \chi^2$.
- \Rightarrow same result of the detailed one is achieved, simply because the problem is linear!
- (No guarantee in general!)

Uncertain standard deviation

In the probabilistic approach it is rather simple: just add σ in θ to infer.

- For example, if we have good reasons to believe that the σ 's are all equal, then

$$f(m, c, \sigma | \mathbf{x}, \mathbf{y}) \propto \sigma^{-n} \exp \left[-\frac{\sum_i (y_i - m x_i - c)^2}{2 \sigma^2} \right] \cdot f_0(m, c, \sigma)$$

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Even if the prior is flat in all parameters

- methods “based only on the properties of the argument of the exponent” fail, because they miss the contribution from σ^{-n} !

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- ▶ methods “based only on the properties of the argument of the exponent” fail, because they miss the contribution from σ^{-n} !
- ▶ The Gaussian trick applied to the full posterior performs better.

Uncertain standard deviation

In the probabilistic approach it is rather simple: just add σ in θ to infer.

- ▶ For example, if we have good reasons to believe that the σ 's are all equal, then

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Residuals? Ok if there are many points, otherwise we do not take into account the uncertainty on σ and its effect on the probability function of m and c .

Note: as long as σ is constant (although unknown) and the prior flat in m and c the best estimates of m and c do not depend in σ .

Linear fits with uncertain σ in JAGS

Model

```
var mu.y[N];  
model{  
  for (i in 1:N) {  
    y[i] ~ dnorm(mu.y[i], tau);  
    mu.y[i] <- x[i]*m + c;  
  }  
  c ~ dnorm(0, 1.0E-6);  
  m ~ dnorm(0, 1.0E-6);  
  tau ~ dgamma(1.0, 1.0E-6);  
  sigma <- 1.0/sqrt(tau);  
}
```


Linear fits with uncertain σ in JAGS

Model

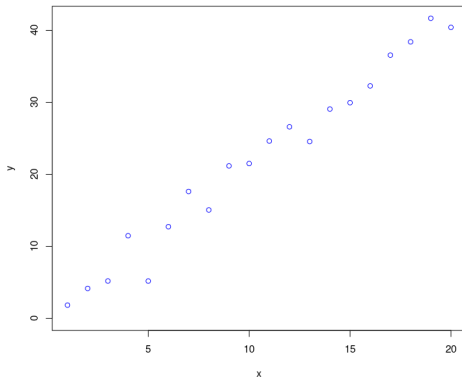
```
var mu.y[N];  
model{  
  for (i in 1:N) {  
    y[i] ~ dnorm(mu.y[i], tau);  
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  m ~ dnorm(0, 1.0E-6);  
  tau ~ dgamma(1.0, 1.0E-6);  
  sigma <- 1.0/sqrt(tau);  
}
```

Simulated data

```
m.true = 2; c.true = 1; sigma.true=2  
x = 1:20  
y = m.true * x + c.true + rnorm(length(x), 0, sigma.true)  
  
plot(x,y, col='blue',ylim=c(0,max(y)) )
```

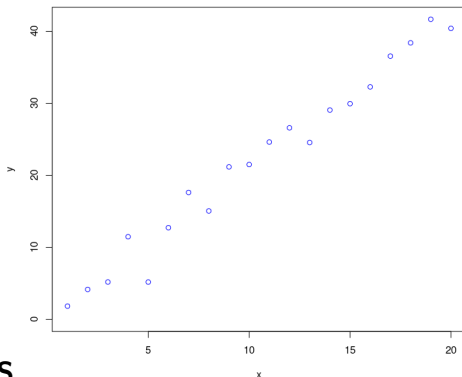
Linear fits with uncertain σ in JAGS

Plot of simulated data



Linear fits with uncertain σ in JAGS

Plot of simulated data



Calling JAGS

```
ns=10000
```

```
jm <- jags.model(model, data, inits)
```

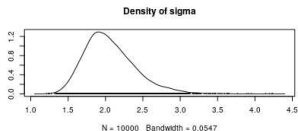
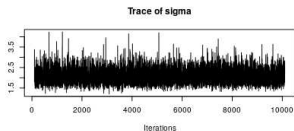
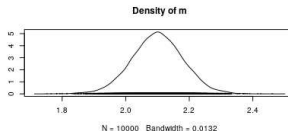
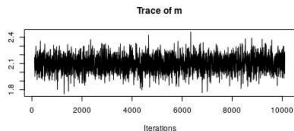
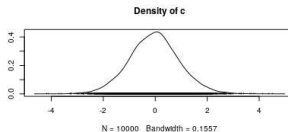
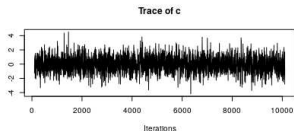
```
update(jm, 100)
```

```
chain <- coda.samples(jm, c("c","m","sigma"), n.iter=ns)
```

Linear fits with uncertain σ in JAGS

⇒ `linear_fit.R`

JAGS summary



$$c = -0.04 \pm 0.96; m = 2.10 \pm 0.08; \sigma = 2.06 \pm 0.34$$

Linear fits with uncertain σ in JAGS

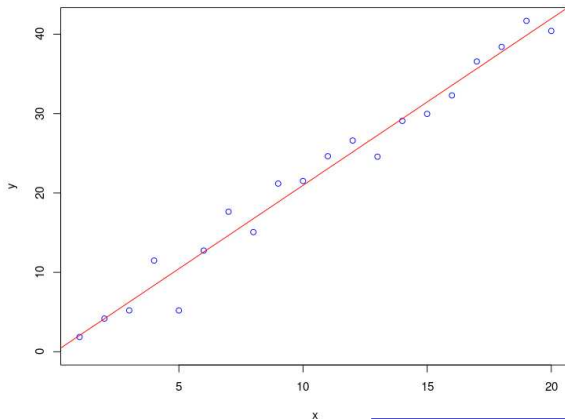
'Check' the result

```
c      <- as.vector(chain[[1]][,1])  
m      <- as.vector(chain[[1]][,2])  
sigma <- as.vector(chain[[1]][,3])  
plot(x,y, col='blue',ylim=c(0,max(y)) )  
abline(mean(c), mean(m), col='red')
```

Linear fits with uncertain σ in JAGS

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c      <- as.vector(chain[[1]][,1])  
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Linear fits with uncertain σ in JAGS

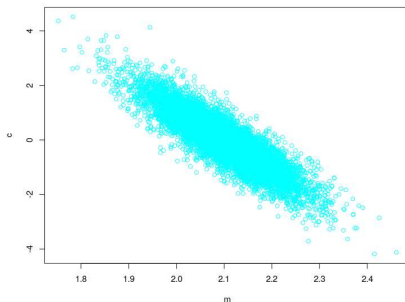
Correlation between m and c

```
plot(m,c,col='cyan')  
cat(sprintf("rho(m,x) = %.3f\n", cor(m,c) ))
```

Linear fits with uncertain σ in JAGS

Correlation between m and c

```
plot(m,c,col='cyan')  
cat(sprintf("rho(m,x) = %.3f\n", cor(m,c) ))
```



$$\rho(m, c) = -0.88$$

Linear fits with uncertain σ in JAGS

Check with R `lm()` (least square)

```
plot(x,y, col='blue',ylim=c(0,max(y)) )
```

```
abline(mean(c), mean(m), col='red') # JAGS
```

```
abline(lm(y~x), col='black')      # least squares
```

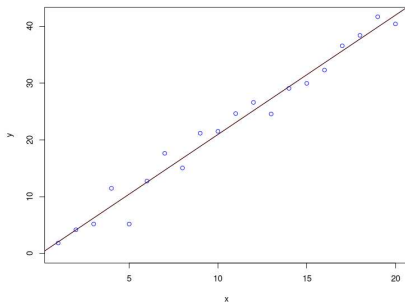
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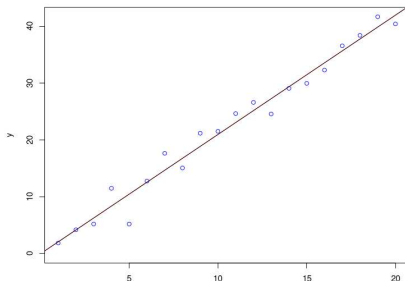
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Linear fits with uncertain σ in JAGS

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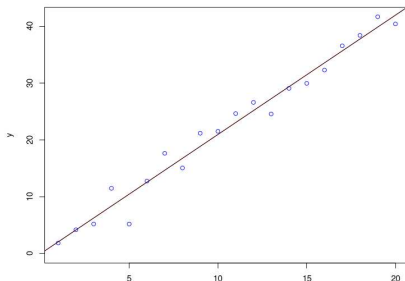


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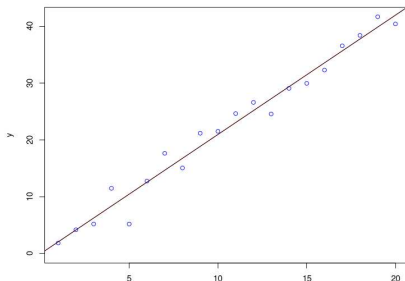


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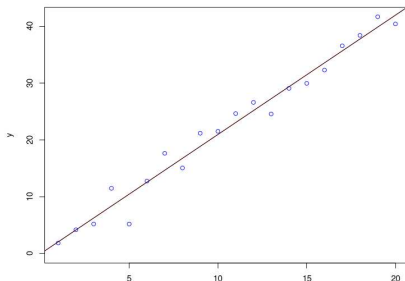


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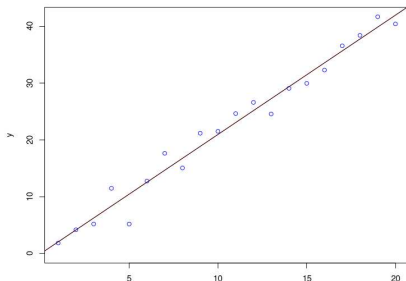
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Linear fits with uncertain σ in JAGS

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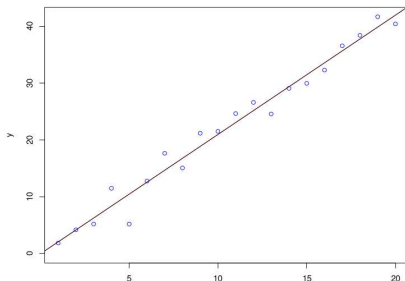
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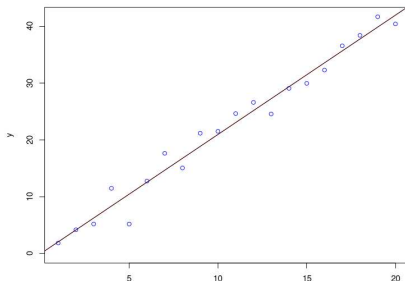
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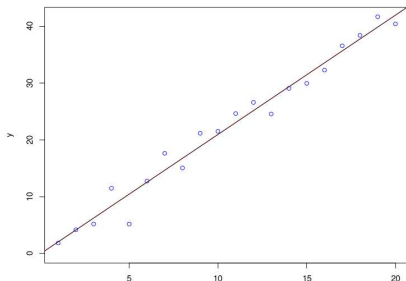
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Otherwise: $\Rightarrow f(c, m, \sigma \mid \text{data points})$

Forecasting new μ_y and new y

Imagine we are interested at “ y at $x_f = 30$ ” (referring to our ‘data’).

Forecasting new μ_y and new y

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- First at all it is important to distinguish

$$\mu_y(x_f) \rightarrow \mu_y(\mu_{x_f}) \quad (\text{no error on } x)$$

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Our problem

$$f(\mu_{y_f} \mid \text{data}, x_f) = \int f(\mu_{y_f} \mid m, c, x_f) \cdot f(m, c \mid \text{data}) dc dm$$

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Our problem

$$\begin{aligned}f(\mu_{y_f} \mid \text{data}, x_f) &= \int f(\mu_{y_f} \mid m, c, x_f) \cdot f(m, c \mid \text{data}) \, dc \, dm \\ f(y_f \mid \text{data}, x_f) &= \int f(y_f \mid \mu_{y_f}) \cdot f(\mu_{y_f} \mid \text{data}, x_f) \, d\mu_{y_f}\end{aligned}$$

Forecasting new μ_y and new y

Including prediction in the JAGS model

```
var mu.y[N];
model{
  for (i in 1:N) {
    y[i] ~ dnorm(mu.y[i], tau);
    mu.y[i] <- x[i] * m + c;
  }
  mu.yf <- xf * m + c;      # future 'true value' for x=xf
  yf ~ dnorm(mu.yf, tau);  # future 'observation for x=xf'
  c ~ dnorm(0, 1.0E-6);
  m ~ dnorm(0, 1.0E-6);
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}
```

Or we can do the '[integral](#)' by sampling, using the MCMC histories of the quantities of interest
(see previous model, without prediction)

Forecasting new μ_y and new y

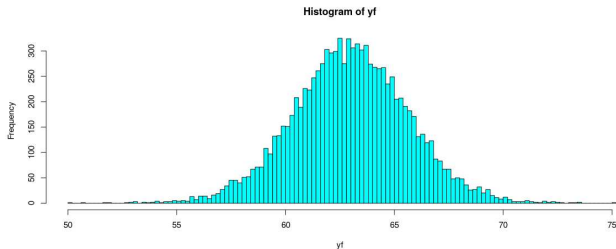
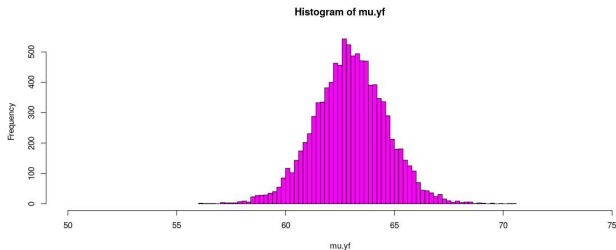
Including prediction in the JAGS model

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}
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Or we can do the '[integral](#)' by sampling, using the MCMC histories of the quantities of interest
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⇒ Left as exercise

Forecasting new μ_y and new y with JAGS



$$\mu_y(x = 30) = 63.0 \pm 1.7; \quad y(x = 30) = 63.0 \pm 2.7$$

Try with Root ;-) ['data' on the web site]

The End

Appendix on small samples

Inferring μ and σ from a sample

(Gaussian, independent observations)

$$f(\mu, \sigma | \underline{x}) \propto \sigma^{-n} \exp \left[-\frac{\overline{x^2} - 2\mu \bar{x} + \mu^2}{2\sigma^2/n} \right] \cdot f_0(\mu, \sigma)$$

Inferring μ and σ from a sample

(Gaussian, independent observations)

$$\begin{aligned} f(\mu, \sigma | \underline{x}) &\propto \sigma^{-n} \exp \left[-\frac{\overline{x^2} - 2\mu \bar{x} + \mu^2}{2\sigma^2/n} \right] \cdot f_0(\mu, \sigma) \\ &\propto \sigma^{-n} \exp \left[-\frac{\overline{x^2} - \bar{x}^2 + \bar{x}^2 - 2\mu \bar{x} + \mu^2}{2\sigma^2/n} \right] \cdot f_0(\mu, \sigma) \end{aligned}$$

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with $s^2 = \overline{x^2} - \bar{x}^2$, variance of the sample.

Inferring μ and σ from a sample

(Gaussian, independent observations)

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with $s^2 = \overline{x^2} - \bar{x}^2$, variance of the sample.

- the inference on μ and σ depends only on s^2 and \bar{x} (and on the priors, as it has to be!).

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- ▶ the inference on μ and σ depends only on s^2 and \bar{x} (and on the priors, as it has to be!).
- ▶ Evaluate $f(\mu, \sigma | \bar{x}, s)$ and then

$$f(\mu | \bar{x}, s) = \int_0^\infty f(\mu, \sigma | \bar{x}, s) d\sigma$$

Inferring μ and σ from a sample

(Gaussian, independent observations)

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$$f(\sigma | \bar{x}, s) = \int_{-\infty}^{+\infty} f(\mu, \sigma | \bar{x}, s) d\mu$$

Inferring μ and σ from a sample

(Gaussian, independent observations – prior uniform on σ)

$$f(\mu, \sigma | \underline{x}) \propto \sigma^{-n} \exp \left[-\frac{s^2 + (\mu - \bar{x})^2}{2\sigma^2/n} \right]$$

Marginalizing¹

$$f(\mu | \underline{x}) = \int_0^\infty f(\mu, \sigma | \underline{x}) d\sigma$$

¹The integral of interest is

$$\int_0^\infty z^{-n} \exp \left[-\frac{c}{2z^2} \right] dz = 2^{(n-3)/2} \Gamma \left[\frac{1}{2}(n-1) \right] c^{-(n-1)/2}.$$

Inferring μ and σ from a sample

(Gaussian, independent observations – prior uniform on σ)

$$f(\mu, \sigma | \underline{x}) \propto \sigma^{-n} \exp \left[-\frac{s^2 + (\mu - \bar{x})^2}{2\sigma^2/n} \right]$$

Marginalizing¹

$$\begin{aligned} f(\mu | \underline{x}) &= \int_0^\infty f(\mu, \sigma | \underline{x}) d\sigma \\ &\propto ((\bar{x} - \mu)^2 + s^2)^{-(n-1)/2} \end{aligned}$$

¹The integral of interest is

$$\int_0^\infty z^{-n} \exp \left[-\frac{c}{2z^2} \right] dz = 2^{(n-3)/2} \Gamma \left[\frac{1}{2}(n-1) \right] c^{-(n-1)/2}.$$

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with

$$\begin{aligned}\nu &= n - 2 \\t &= \frac{\mu - \bar{x}}{s/\sqrt{n-2}},\end{aligned}$$

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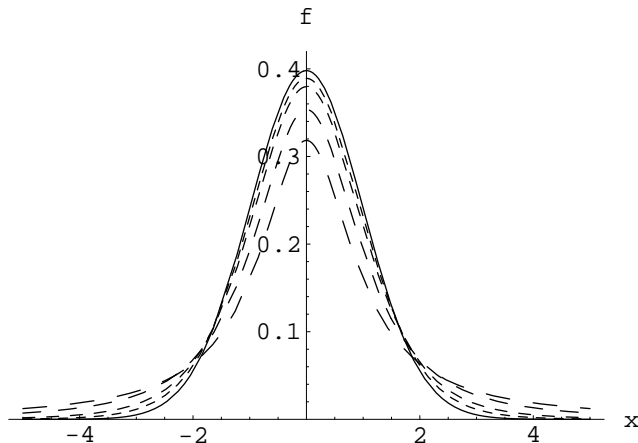
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that is

$$\mu = \bar{x} + \frac{s}{\sqrt{n-2}} t,$$

where t is a “Student t ” with $\nu = n - 2$

Student t



Examples of Student t for ν equal to 1 , 2, 5, 10 and 100 ($\approx \infty$).

Inferring μ and σ from a sample

(Gaussian, independent observations – prior uniform on μ and σ)

In summary,

$$\frac{\mu - \bar{x}}{s/\sqrt{n-2}} \sim \text{Student}(\nu = n - 2)$$

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- not only the standard uncertainty increases, but the distribution itself changes and, as ‘well know’ the t distribution has ‘higher’ tails.

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- not only the standard uncertainty increases, but the distribution itself changes and, as ‘well know’ the t distribution has ‘higher’ tails.

However, when n is very large the Gaussian distribution is recovered (the t-distribution tends to a gaussian), with $\sigma(\mu) = s/\sqrt{n}$.

Inferring μ and σ from a sample

Misunderstandings and 'myths' related to the Student t distribution

Expected value and variance only exist above certain values of n :

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So what?

It is just a reflex of the fact that we have used, for lazyness,² priors which are indeed absurd.

- ▶ In no measurement we believe that μ and/or σ could be 'infinite'.
- ▶ Just plug in some reasonable, although very vague, proper priors, and the problem disappears.

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Inferring μ and σ from a sample

(Gaussian, independent observations – prior uniform on μ and σ)

► Large n limit:

$$\begin{aligned} E(\mu) &\xrightarrow{n \rightarrow \infty} \bar{x} \\ \sigma(\mu) &\xrightarrow{n \rightarrow \infty} \frac{s}{\sqrt{n}} \\ \mu &\xrightarrow{n \rightarrow \infty} \sim \mathcal{N}(\bar{x}, \frac{s}{\sqrt{n}}). \end{aligned}$$

Inferring μ and σ from a sample

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Marginal $f(\sigma)$

$$f(\sigma | \bar{x}, s) = \int_{-\infty}^{+\infty} f(\mu, \sigma | \bar{x}, s) d\mu$$

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$$\begin{aligned} f(\sigma | \bar{x}, s) &= \int_{-\infty}^{+\infty} f(\mu, \sigma | \bar{x}, s) d\mu \\ &\propto \sigma^{-n} \exp \left[-\frac{n s^2}{2 \sigma^2} \right] \int_{-\infty}^{+\infty} \exp \left[-\frac{n (\bar{x} - \mu)^2}{2 \sigma^2} \right] d\mu \end{aligned}$$

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That is... (no special function)

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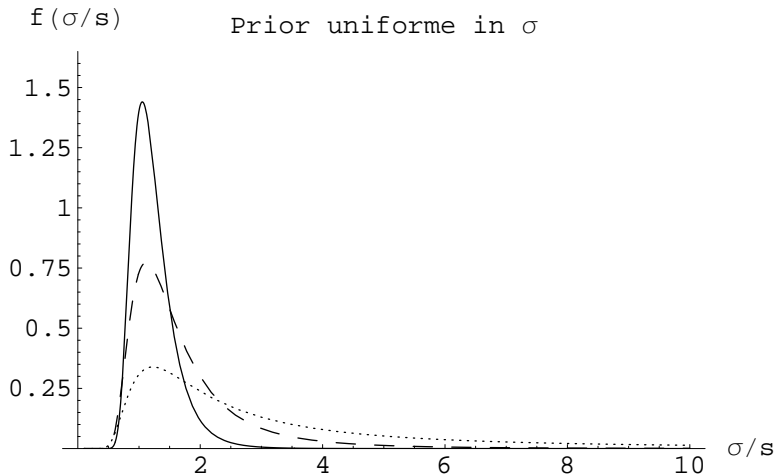
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[But if we would use $\tau = 1/\sigma^2$ we would recognize a Gamma...]

Inferring μ and σ from a sample

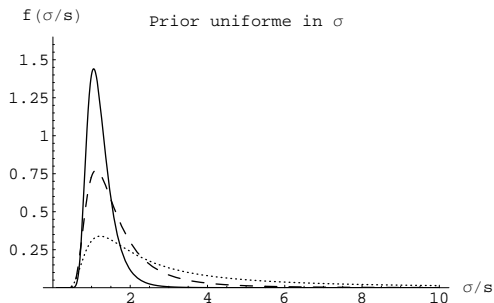
(Gaussian, independent observations – prior uniform on μ and σ)



$n = 3$ (dotted), $n = 5$ (dashed) e $n = 10$ (continuous).

Inferring μ and σ from a sample

(Gaussian, independent observations – prior uniform on μ and σ)



$$E(\sigma) \xrightarrow[n \rightarrow \infty]{} s$$

$$\text{std}(\sigma) \xrightarrow[n \rightarrow \infty]{} \frac{s}{\sqrt{2n}}$$

$$\sigma \xrightarrow[n \rightarrow \infty]{} \sim \mathcal{N}(s, \frac{s}{\sqrt{2n}}).$$

Inferring μ and σ from a sample

(Gaussian, independent observations – prior uniform on μ and σ)

Using the “Gaussian trick”

$$\varphi(\mu, \sigma) = n \ln \sigma + \frac{s^2 + (\mu - \bar{x})^2}{2\sigma/n}$$

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First derivatives:

$$\frac{\partial \varphi}{\partial \mu} = \frac{\mu - \bar{x}}{\sigma/n}$$

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From which it follows (equating the derivatives to zero)

$$\begin{aligned}E(\mu) &= \bar{x} \\ E(\sigma) &= s\end{aligned}$$

(They are indeed the modes!)

Inferring μ and σ from a sample

(Gaussian, independent observations – prior uniform on μ and σ)

Hessian calculated at $\mu = \bar{x}$ and $\sigma = s$ (hereafter ' m ')

$$\left. \frac{\partial^2 \varphi}{\partial \mu^2} \right|_m = \left. \frac{n}{\sigma^2} \right|_m = \frac{n}{s^2}$$

$$\left. \frac{\partial^2 \varphi}{\partial \sigma^2} \right|_m = \left(-\frac{n}{\sigma^2} + \frac{3(s^2 + (\mu - \bar{x})^2)}{\sigma^4/n} \right) \Big|_m = \frac{2n}{s^2}$$

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$$\text{std}(\mu) = \frac{s}{\sqrt{n}}$$

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reobtaining the large number limit.

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Q.: Are they independent?

Inferring μ and σ from a sample

(Gaussian, independent observations. Expression the Gaussian in terms of $\tau = 1/\sigma^2$)

$$f(\mu, \sigma | \underline{x}) \propto \sigma^{-n} \exp \left[-\frac{s^2 + (\mu - \bar{x})^2}{2 \sigma^2 / n} \right] \cdot f_0(\mu, \sigma)$$

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$$f(\tau | \underline{x}, \mu) \propto \tau^\alpha e^{-\beta\tau} \cdot f_0(\tau)$$

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\Rightarrow Gibbs sampling

Practical introduction to BUGS

- ▶ Introducing the *bug* language to build up the models.
- ▶ Running the model (including data and 'inits') in the OpenBUGS GUI.
- ▶ Analysing the resulting chain in R.