

# Measurements, uncertainties and probabilistic inference/forecasting

Giulio D'Agostini

Università di Roma La Sapienza e INFN  
Roma, Italy

## An important clarification

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In this case  $P(W) < 1$ : probability of  $W$  before it was observed!



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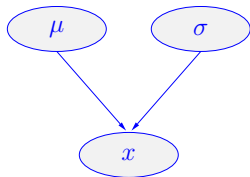
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Add this hypothesis in the model and apply probability theory!

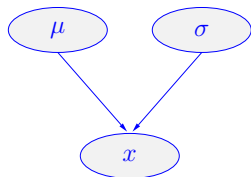
# Inferring $\mu$ of the normal distribution

Setting up the problem



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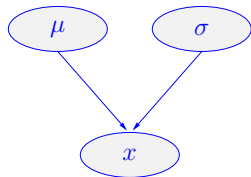
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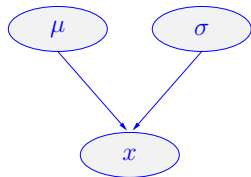
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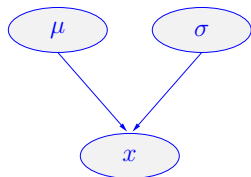
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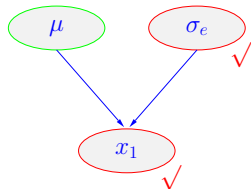


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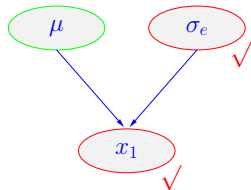
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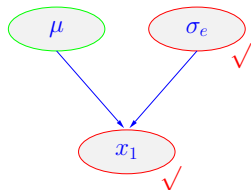
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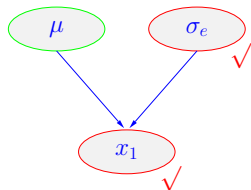
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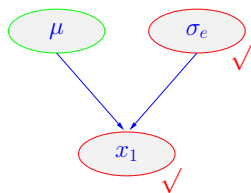


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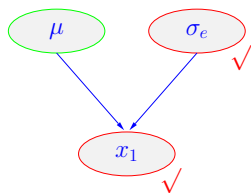
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'data' can be a set of observations

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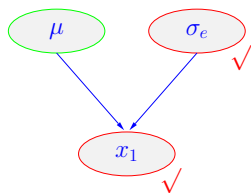
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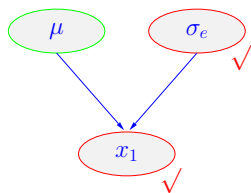
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Starting as usual from a flat prior

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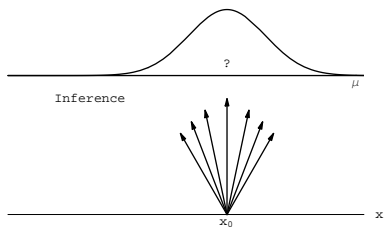
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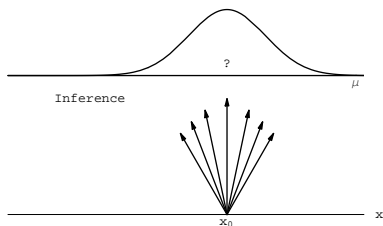
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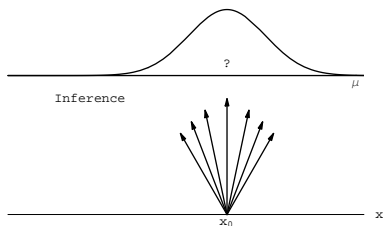


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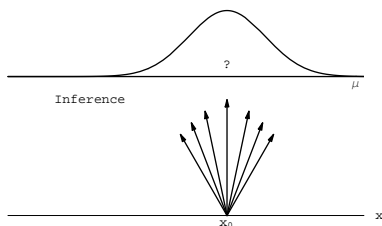
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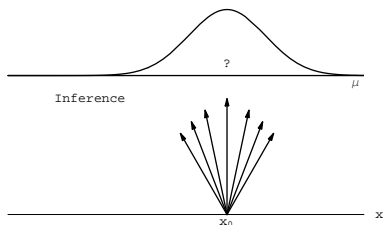
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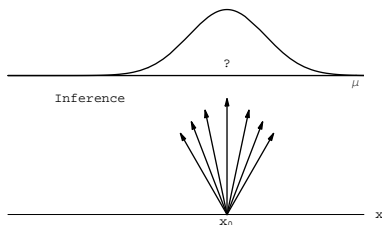
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(\*) The expressions "confidence interval" and "confidence limits" are jeopardized having often **little to do with 'confidence'** – sic!

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And Gauss was the first to realize that  
**the Gaussian is indeed 'wrong'!**

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## Use of a conjugate prior

As we have already, a 'trick' developed in order to simplify the calculations is the use of **conjugate priors**:

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with

$$\begin{aligned}\mu_A &= \frac{x_1/\sigma_e^2 + \mu_0/\sigma_0^2}{1/\sigma_e^2 + 1/\sigma_0^2} \\ \frac{1}{\sigma_A^2} &= \frac{1}{\sigma_e^2} + \frac{1}{\sigma_0^2}.\end{aligned}$$

## Other 'Gaussian tricks'

Here are the details of our to get the previous result

$$\begin{aligned} f(\mu) &\propto \exp \left[ -\frac{1}{2} \left( \frac{-2\mu x_1 \sigma_o^2 + \mu^2 \sigma_o^2 + -2\mu \mu_o \sigma_e^2 + \mu^2 \sigma_e^2}{\sigma_e^2 + \sigma_o^2} \right) \right] \\ &= \exp \left[ -\frac{1}{2} \left( \frac{\mu^2 - 2\mu \left( \frac{x_1 \sigma_o^2 + \mu_o \sigma_e^2}{\sigma_e^2 + \sigma_o^2} \right)}{(\sigma_e^2 \cdot \sigma_o^2) / (\sigma_e^2 + \sigma_o^2)} \right) \right] \\ &= \exp \left[ -\frac{1}{2} \left( \frac{\mu^2 - 2\mu \mu_A}{\sigma_A^2} \right) \right] \\ &\propto \exp \left[ -\frac{(\mu - \mu_A)^2}{2\sigma_A^2} \right] \end{aligned}$$

In particular, in the last step the trick of **complementing the exponential** has been used, since adding/removing constant terms in the exponential is equivalent to multiply/divide by factors. Once we recognize the structure, the normalization is automatic.

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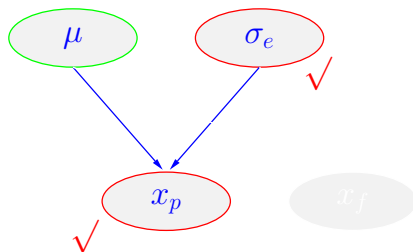
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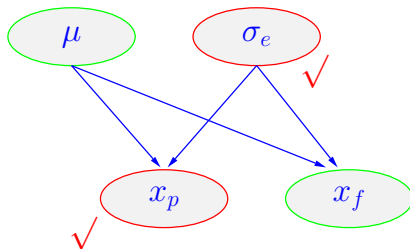
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- ▶ A **flat prior** is recovered for  $\sigma_0^2 \gg \sigma_e^2$  (and  $x_0$  'reasonable').

# Predictive distribution

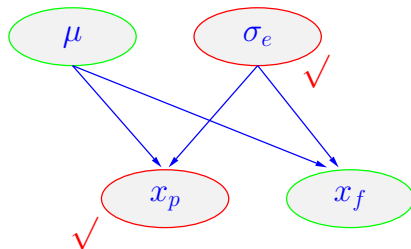


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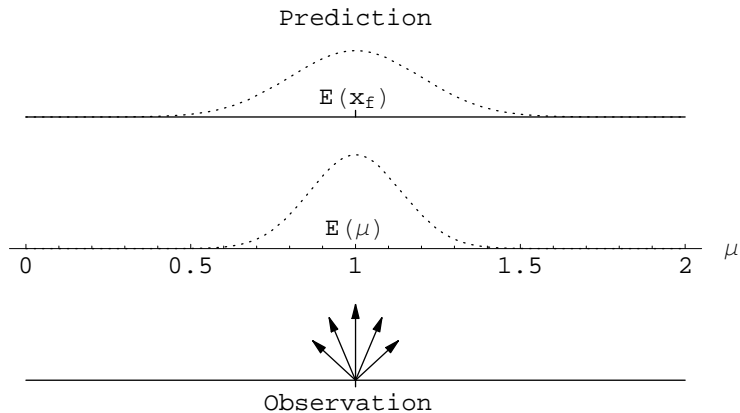
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What shall we observe in a **next measurement**  $x_f$  ('f' as 'future'), given our knowledge on  $\mu$  based on the **previous observation**  $x_p$ ? (Note the new evocative name for the observation, instead of  $x_1$ )

# Predictive distribution

$$x_p \rightarrow \mu \rightarrow x_f$$



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In particular, if  $\sigma_p = \sigma_f = \sigma$ , then

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*Classical confidence intervals (exact method)* **119**

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(Glen Cowan, *Statistical Data Analysis*)

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GdA, *Bayesian reasoning versus conventional statistics in High Energy Physics*,

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# Prescriptions?





## Objective prescriptions?

Mistrust those who promise you 'objective' methods to form up your confidence about the physical world!



# Principles?

Too many unnecessary 'principles' on the market.

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**Those are my  
principles, and  
if you don't like  
them ... well, I  
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**~ Groucho Marx**



# Introducing systematics

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From a probabilistic point of view, there is no distinction between  $\mu$  and  $h$ : they are all conditional hypotheses for the  $x$ , i.e. causes which produce the observed effects. The difference is simply that we are interested in  $\mu$  rather than in  $h$ .



# Introducing systematics

Several approaches (within probability theory – no adhoceries!)

Uncertainty due to systematic effects is also included in a natural way in this approach. Let us first define the notation ( $i$  is the generic index):

- ▶  $\mathbf{x} = \{x_1, x_2, \dots, x_{n_x}\}$  is the 'n-tuple' (vector) of observables  $X_i$ ;
- ▶  $\boldsymbol{\mu} = \{\mu_1, \mu_2, \dots, \mu_{n_\mu}\}$  is the n-tuple of true values  $\mu_i$ ;
- ▶  $\mathbf{h} = \{h_1, h_2, \dots, h_{n_h}\}$  is the n-tuple of *influence quantities*  $H_i$ . (see ISO GUM).

# Taking into account of uncertain $h$

Global inference on  $f(\boldsymbol{\mu}, \mathbf{h})$

- ▶ We can use Bayes' theorem to make an inference on  $\boldsymbol{\mu}$  and  $\mathbf{h}$ . A subsequent marginalization over  $\mathbf{h}$  yields the p.d.f. of interest:

$$\mathbf{x} \Rightarrow f(\boldsymbol{\mu}, \mathbf{h} | \mathbf{x}) \Rightarrow f(\boldsymbol{\mu} | \mathbf{x}).$$

This method, depending on the joint prior distribution  $f_{\circ}(\boldsymbol{\mu}, \mathbf{h})$ , can even model possible correlations between  $\boldsymbol{\mu}$  and  $\mathbf{h}$ .

# Taking into account of uncertain $h$

## Conditional inference

- ▶ Given the observed data, one has a joint distribution of  $\mu$  for all possible configurations of  $h$ :

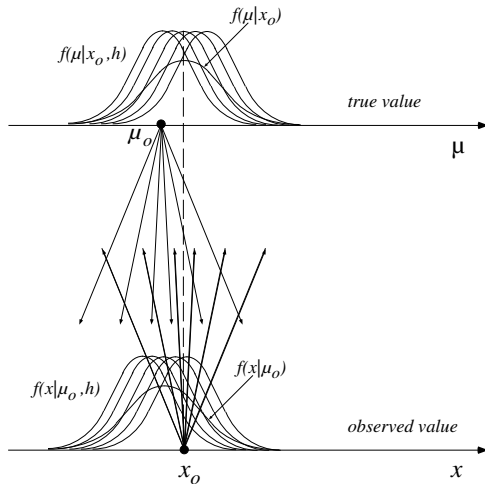
$$\mathbf{x} \Rightarrow f(\mu | \mathbf{x}, \mathbf{h}).$$

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

$$f(\mu | \mathbf{x}) = \int f(\mu | \mathbf{x}, \mathbf{h}) f(\mathbf{h}) d\mathbf{h}.$$

# Taking into account of uncertain $h$

## Conditional inference



# Taking into account of uncertain $h$

## Propagation of uncertainties

- ▶ Essentially, one applies the propagation of uncertainty, whose most general case has been illustrated in the previous section, making use of the following model: One considers a 'raw result' on raw values  $\mu_R$  for some nominal values of the influence quantities, i.e.

$$f(\mu_R | \mathbf{x}, \mathbf{h}_o);$$

then (corrected) true values are obtained as a function of the raw ones and of the possible values of the influence quantities, i.e.

$$\mu_i = \mu_i(\mu_{iR}, \mathbf{h}),$$

and  $f(\mu)$  is evaluated by probability rules.

The third form is particularly convenient to make linear expansions which lead to approximate solutions.

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$$f_{\circ}(\mu, z) = f_{\circ}(\mu) f_{\circ}(z) = k \frac{1}{\sqrt{2\pi}\sigma_Z} \exp\left[-\frac{z^2}{2\sigma_Z^2}\right].$$

- ▶  $X$  is no longer Gaussian distributed around  $\mu$ ,



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$$f_o(\mu, z) = f_o(\mu) f_o(z) = k \frac{1}{\sqrt{2\pi}\sigma_Z} \exp\left[-\frac{z^2}{2\sigma_Z^2}\right].$$

- ▶  $X$  is no longer Gaussian distributed around  $\mu$ , but around  $\mu + Z$ :

$$X \sim \mathcal{N}(\mu + Z, \sigma)$$

# Systematics due to uncertain offset

Application to the single (equivalent) measurement  $X_1$ , with std  $\sigma_1$

Likelihood:

$$f(x_1 | \mu, z) = \frac{1}{\sqrt{2\pi}\sigma_1} \exp\left[-\frac{(x_1 - \mu - z)^2}{2\sigma_1^2}\right].$$

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After joint inference and marginalization

$$f(\mu | x_1) = \frac{\int \frac{1}{\sqrt{2\pi}\sigma_1} \exp\left[-\frac{(x_1 - \mu - z)^2}{2\sigma_1^2}\right] \frac{1}{\sqrt{2\pi}\sigma_z} \exp\left[-\frac{z^2}{2\sigma_z^2}\right] dz}{\iint \frac{1}{\sqrt{2\pi}\sigma_1} \exp\left[-\frac{(x_1 - \mu - z)^2}{2\sigma_1^2}\right] \frac{1}{\sqrt{2\pi}\sigma_z} \exp\left[-\frac{z^2}{2\sigma_z^2}\right] d\mu dz}.$$

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Integrating we get

$$f(\mu) = f(\mu | x_1, \dots, f_o(z)) = \frac{1}{\sqrt{2\pi}\sqrt{\sigma_1^2 + \sigma_Z^2}} \exp\left[-\frac{(\mu - x_1)^2}{2(\sigma_1^2 + \sigma_Z^2)}\right].$$

# Systematics due to uncertain offset

Technical remark

It may help to know that

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

# Systematics due to uncertain offset

## Result

$$f(\mu) = f(\mu | x_1, \dots, f_o(z)) = \frac{1}{\sqrt{2\pi} \sqrt{\sigma_1^2 + \sigma_Z^2}} \exp \left[ -\frac{(\mu - x_1)^2}{2(\sigma_1^2 + \sigma_Z^2)} \right].$$

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- ▶ The global standard uncertainty is the quadratic combination of that due to the statistical fluctuation of the data sample and the uncertainty due to the imperfect knowledge of the *systematic effect*:

$$\sigma_{tot}^2 = \sigma_1^2 + \sigma_Z^2.$$



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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.

# Systematics due to uncertain offset

Measuring two quantities with the same instrument

Measuring  $\mu_1$  and  $\mu_2$ , resulting into  $x_1$  and  $x_2$ .

Setting up the model:

$$Z \sim \mathcal{N}(0, \sigma_Z)$$

$$X_1 \sim \mathcal{N}(\mu_1 + Z, \sigma_1)$$

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$$\begin{aligned} f(x_1, x_2 | \mu_1, \mu_2, z) &= \frac{1}{\sqrt{2\pi}\sigma_1} \exp\left[-\frac{(x_1 - \mu_1 - z)^2}{2\sigma_1^2}\right] \\ &\quad \times \frac{1}{\sqrt{2\pi}\sigma_2} \exp\left[-\frac{(x_2 - \mu_2 - z)^2}{2\sigma_2^2}\right] \\ &= \frac{1}{2\pi\sigma_1\sigma_2} \exp\left[-\frac{1}{2}\left(\frac{(x_1 - \mu_1 - z)^2}{\sigma_1^2} + \frac{(x_2 - \mu_2 - z)^2}{\sigma_2^2}\right)\right] \end{aligned}$$

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

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Measuring two quantities with the same instrument

$$\begin{aligned} f(\mu_1, \mu_2 | x_1, x_2) &= \frac{\int f(x_1, x_2 | \mu_1, \mu_2, z) f_0(\mu_1, \mu_2, z) dz}{\int \dots d\mu_1 d\mu_2 dz} \\ &= \frac{1}{2\pi \sqrt{\sigma_1^2 + \sigma_z^2} \sqrt{\sigma_2^2 + \sigma_z^2} \sqrt{1 - \rho^2}} \\ &\quad \times \exp \left\{ -\frac{1}{2(1 - \rho^2)} \left[ \frac{(\mu_1 - x_1)^2}{\sigma_1^2 + \sigma_z^2} \right. \right. \\ &\quad \left. \left. - 2\rho \frac{(\mu_1 - x_1)(\mu_2 - x_2)}{\sqrt{\sigma_1^2 + \sigma_z^2} \sqrt{\sigma_2^2 + \sigma_z^2}} + \frac{(\mu_2 - x_2)^2}{\sigma_2^2 + \sigma_z^2} \right] \right\} \end{aligned}$$

where

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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!

## An exercise

Two samples of data have been collected with the same instrument. These are the numbers, as they result from a printout (homogeneous quantities, therefore measurement unit omitted):

- ▶  $n_1 = 1000$ ,  $\bar{x}_1 = 10.4012$ ,  $s_1 = 5.7812$ ;
- ▶  $n_2 = 2000$ ,  $\bar{x}_2 = 10.2735$ ,  $s_2 = 5.9324$ .

We know that the instrument has an offset uncertainty of 0.15.

1. Report the results on  $\mu_1$ ,  $\mu_2$ ,  $\sigma_1$  and  $\sigma_2$ .
2. If you consider the  $\sigma$ 's of the two samples consistent you might combine the result.
3. Calculate the correlation coefficient between  $\mu_1$  and  $\mu_2$ .
4. Give also the result on  $s = \mu_1 + \mu_2$  and  $s = \mu_1 - \mu_2$ , including  $\rho(s, d)$ .
5. Give also the result on  $z_1 = \mu_1 \mu_2^2$  and  $z_2 = \mu_1/\mu_2$ , including  $\rho(z_1, z_2)$ .
6. Consider also a third data sample, recorded with the same instrument:  
 $n_3 = 4$ ,  $\bar{x}_3 = 13.8931$ ,  $s_3 = 4.5371$ .

# Inferring $\mu$ from a sample

(Gaussian, independent observations,  $\sigma$  **perfectly known**)

$$f(\mu | \underline{x}, \sigma) \propto f(\underline{x} | \mu, \sigma) \cdot f_0(\mu)$$

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**Trick:** complementing of exponential

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

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In the case of  $f_0(\mu)$  irrelevant (but we know how to act otherwise!)  
we recognize by eye a Gaussian



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$$f(\mu | \underline{x}, \sigma) = \frac{1}{\sqrt{2\pi} \sigma / \sqrt{n}} \exp \left[ -\frac{(\mu - \bar{x})^2}{2(\sigma / \sqrt{n})^2} \right]$$

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$\mu$  is Gaussian around arithmetic average, with standard deviation  
 $\sigma / \sqrt{n}$

$$\mu \sim \mathcal{N}(\bar{x}, \frac{\sigma}{\sqrt{n}})$$

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$\mu$  is Gaussian around arithmetic average, with standard deviation  $\sigma / \sqrt{n}$

$$\mu \sim \mathcal{N}(\bar{x}, \frac{\sigma}{\sqrt{n}})$$

►  $\bar{x}$  is a *sufficient statistic* (**very important concept!**)

# Inferring $\mu$ from a sample

(Gaussian, independent observations,  $\sigma$  perfectly known)

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

In the case of  $f_0(\mu)$  irrelevant (but we know how to act otherwise!) we recognize by eye a Gaussian

$$f(\mu | \underline{x}, \sigma) = \frac{1}{\sqrt{2\pi} \sigma / \sqrt{n}} \exp \left[ -\frac{(\mu - \bar{x})^2}{2(\sigma / \sqrt{n})^2} \right]$$

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$$\mu \sim \mathcal{N}(\bar{x}, \frac{\sigma}{\sqrt{n}})$$

- ▶  $\bar{x}$  is a *sufficient statistic* (**very important concept!**)  
⇒  $\bar{x}$  it provides the same information about  $\mu$   
contained in detailed knowledge of  $\underline{x}$

# Inferring $\mu$ from a sample

(Gaussian, independent observations,  $\sigma$  perfectly known)

## Exercise

- ▶ In the last steps we have used the technique of *complementing the exponential*.
- ▶ Restart, using a *flat prior*, from

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

and use the 'Gaussian tricks' (first and second derivatives of  $\varphi(\mu)$ ) to find  $E(\mu)$  and  $\text{Var}(\mu)$ .

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and use the 'Gaussian tricks' (first and second derivatives of  $\varphi(\mu)$ ) to find  $E(\mu)$  and  $\text{Var}(\mu)$ .

- ▶ In this case the result is **exact**, because  $f(\mu | \underline{x}, \sigma)$  is indeed Gaussian.  
(A hint is that  $\frac{d^2\varphi(\mu)}{d\mu^2}$  is constant  $\forall \mu$ )

## Joint inference of $\mu$ and $\sigma$ from a sample

$$f(\mu, \sigma | \underline{x}) \propto \prod_i \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x_i - \mu)^2}{2\sigma^2}} \cdot f_0(\mu, \sigma)$$

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$\Rightarrow \bar{x}$  and  $s$  are **sufficient statistics**

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In practice

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

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$$\Rightarrow n \rightarrow \infty$$

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Large sample behaviour starting from uniform priors<sup>(\*)</sup>

(with 'std' for **standard deviation** to avoid confusion with unknown  $\sigma$ )

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$\Rightarrow$  See references and links

# Joint inference of $\mu$ and $\sigma$ from a sample

Conditional distributions

**Joint** distribution:

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

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**Conditioning**  $\mu$  on a precise value of  $\sigma = \sigma_*$ :

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In the case of uniform  $f_0(\mu)$  it turns out that  $\mu$  is Gaussian around  $\bar{x}$  with standard deviation equal to  $\sigma_*/\sqrt{n}$ .

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In the case of uniform  $f_0(\mu)$  it turns out that  $\mu$  is Gaussian around  $\bar{x}$  with standard deviation equal to  $\sigma_*/\sqrt{n}$ .

“Obviously!”: this is equivalent to the choice  $f_0(\sigma) = \delta(\sigma - \sigma_*)$

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# Joint inference of $\mu$ and $\sigma$ from a sample

## Conditional distributions

**Joint** distribution:

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

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$\Rightarrow$  Gibbs sampler!

# Joint inference of $\mu$ and $\tau$ ( $\rightarrow \sigma$ ) from a sample

Sampling the posterior by **MCMC** using **Gibbs sampler**

0) Inizialization:

- ▶  $i = 0$
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Then **loop**  $n$  **times** :

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Try it!

You only need Gaussian and Gamma random number generators  
(e.g. in R)

## Joint inference of $\mu$ and $\tau$ ( $\rightarrow \sigma$ ) with JAGS/rjags

**Model** (to be written in the model file)

```
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-6);
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**Simulated data**

```
mu.true = 3; sigma.true = 2; sample.n = 20
x = rnorm(sample.n, mu.true, sigma.true)
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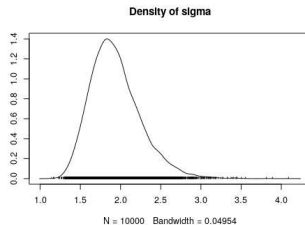
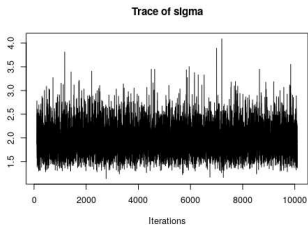
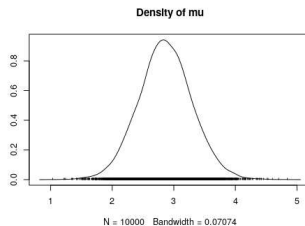
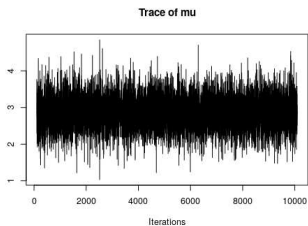
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## JAGS calls

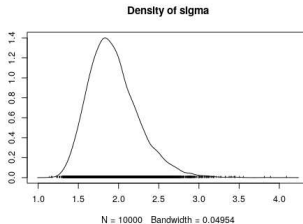
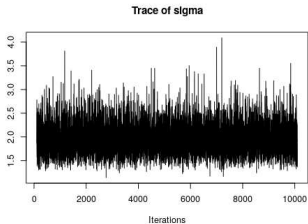
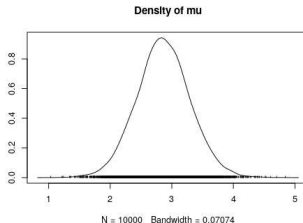
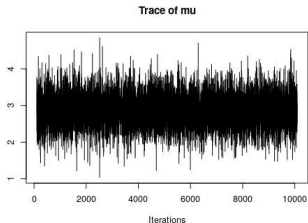
```
data = list(x=x)
inits = list(mu=mean(x), tau=1/var(x))
jm <- jags.model(model, data, inits)
update(jm, 100)
chain <- coda.samples(jm, c("mu", "sigma"), n.iter=10000)
```

# Joint inference of $\mu$ and $\tau$ ( $\rightarrow \sigma$ ) with JAGS/rjags

$\Rightarrow$  `inf_mu_sigma.R`



# Joint inference of $\mu$ and $\tau$ ( $\rightarrow \sigma$ ) with JAGS/rjags $\Rightarrow$ `inf_mu_sigma.R`



$\overline{\mu} = 2.87$ ,  $\text{std}(\mu) = 0.44$ ;

$\overline{\text{sigma}} = 1.94$ ,  $\text{std}(\text{sigma}) = 0.31$

## Fits – introduction

- ▶ In a probabilistic framework the issue of the fits is nothing but **parametric inference**.
  
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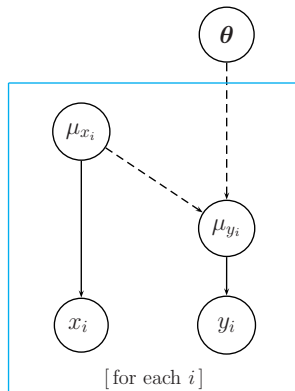


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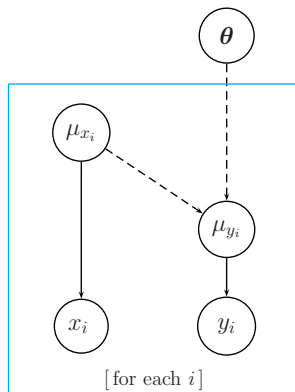
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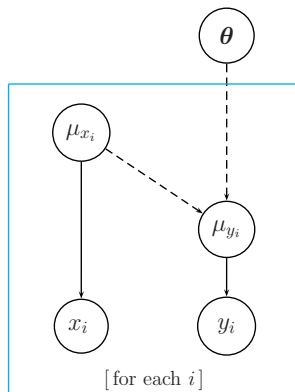
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$$\rightarrow f(\boldsymbol{\theta} | \mathbf{x}, \mathbf{y}, l)$$



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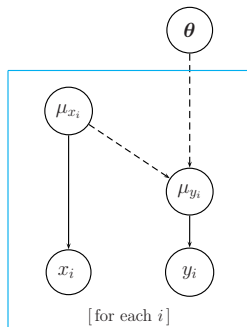
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→  $f(\boldsymbol{\theta} | \mathbf{x}, \mathbf{y}, I)$

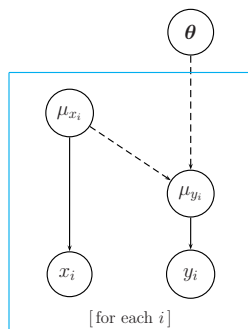
→  $f(m, c | \mathbf{x}, \mathbf{y}, \boldsymbol{\sigma})$ , in the case of case of **linear fit**  
with “ $\sigma$ ’s known a priori” (!)

## Linear fit – introduction



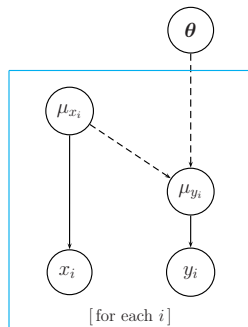
- ▶ Deterministic links between  $\mu_x$ 's and  $\mu_y$ 's.

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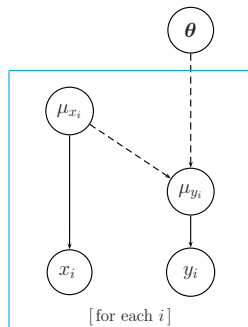
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- ▶ If  $\sigma_x$ 's and  $\sigma_y$ 's are unknown and assumed all equal  
 $\{\mathbf{x}, \mathbf{y}\} \rightarrow \boldsymbol{\theta} = (m, c, \sigma_x, \sigma_y)$
- ▶ etc. . .



## Linear fit – simplest case

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

Simplifying hypotheses:

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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

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

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⇒  $\chi^2$  minimization.
- ▶ As an approximation, one can obtain best fit parameters and covariance matrix by the 'Gaussian trick'  
⇒  $\varphi(m, c) \propto \chi^2$ .



## Least squares and 'Gaussian tricks' on linear fits

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

- ▶ If the prior is irrelevant and the  $\sigma$ 's are all equal, than the maximum of the posterior is obtained when the sum of the squares is minimized:  
⇒ Least Square 'Principle'.
  - ▶ You might recognize at the exponent:  $\chi^2/2$ :  
⇒  $\chi^2$  minimization.
  - ▶ As an approximation, one can obtain best fit parameters and covariance matrix by the 'Gaussian trick'  
⇒  $\varphi(m, c) \propto \chi^2$ .
- ⇒ 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  $\sigma$  in  $\theta$  to infer.

- ▶ For example, if we have good reasons to believe that the  $\sigma$ '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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**Residuals?** Ok if there are many points, otherwise we do not take into account the uncertainty on  $\sigma$  and its effect on the probability function of  $m$  and  $c$ .

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

# Linear fits with uncertain $\sigma$ 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);
}
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}
```

## Simulated data

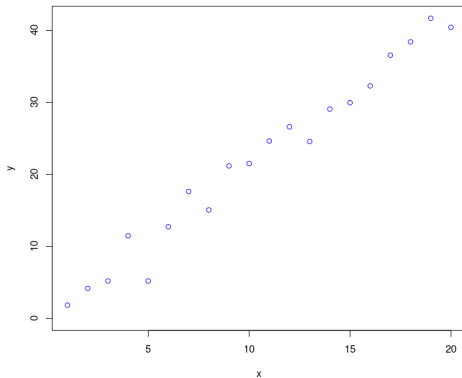
```
m.true = 2; c.true = 1; sigma.true=2
x = 1:20
y = m.true * x + c.true + rnorm(length(x), 0, sigma.true)

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



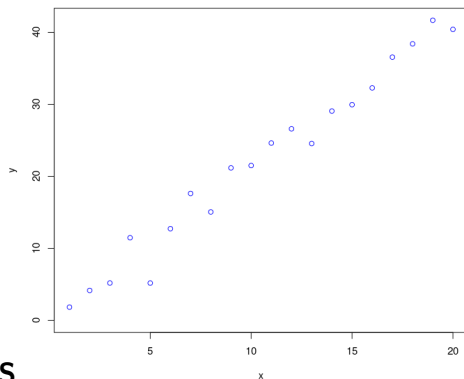
# Linear fits with uncertain $\sigma$ in JAGS

## Plot of simulated data



# Linear fits with uncertain $\sigma$ in JAGS

## Plot of simulated data



## Calling JAGS

```
ns=10000
```

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

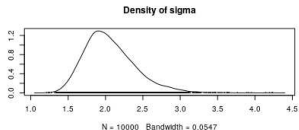
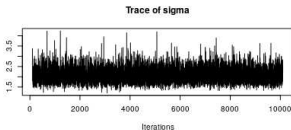
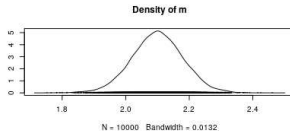
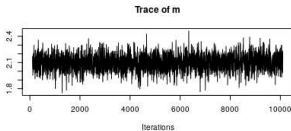
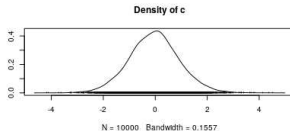
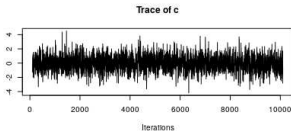
```
update(jm, 100)
```

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

# Linear fits with uncertain $\sigma$ 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 $\sigma$ in JAGS

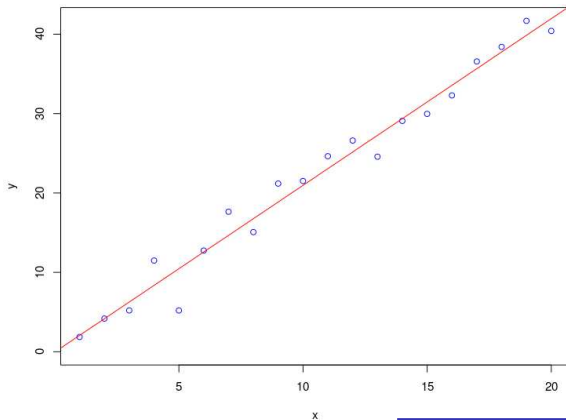
## 'Check' the result

```
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')
```

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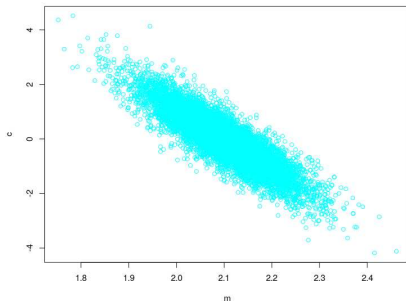
## Correlation between $m$ and $c$

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

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

## Linear fits with uncertain $\sigma$ in JAGS

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

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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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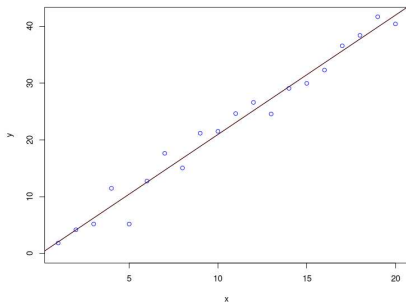
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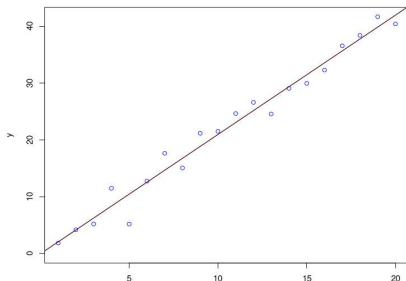
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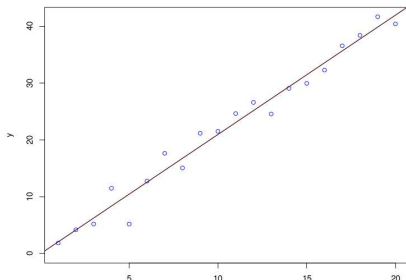


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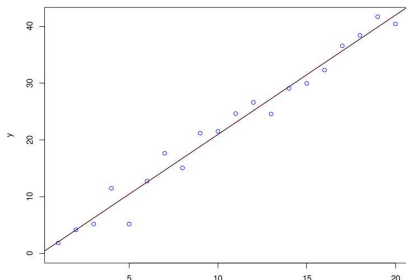


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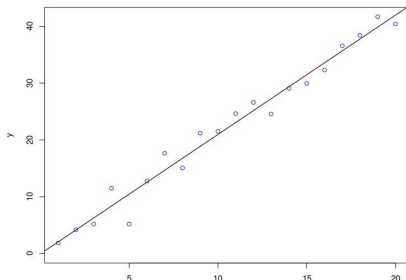


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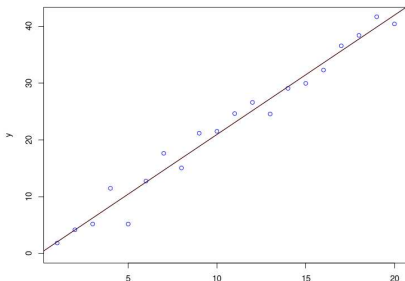
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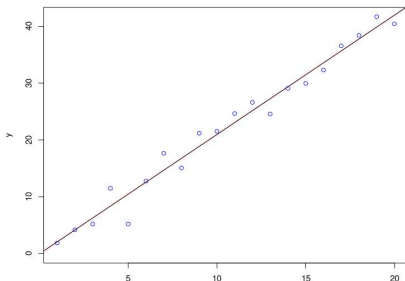
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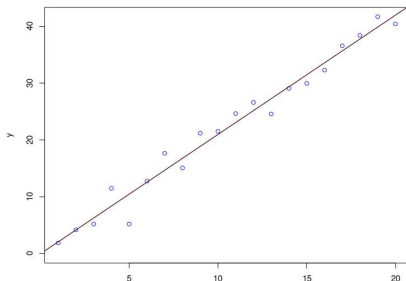
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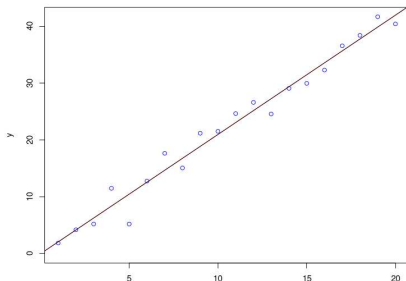
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**Otherwise:**  $\Rightarrow f(c, m, \sigma | \text{data points})$

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

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# Forecasting new $\mu_y$ and new $y$

## Including prediction in the JAGS model

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  mu.yf <- xf * m + c;      # future 'true value' for x=xf
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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)



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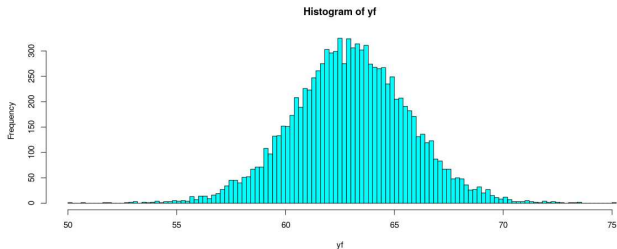
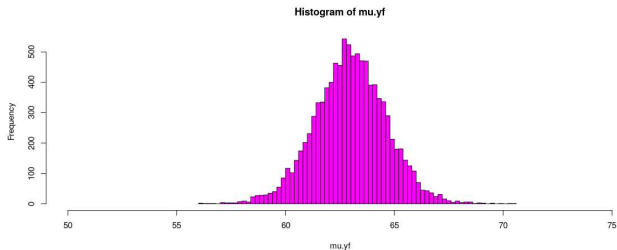
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⇒ Left as exercise

# Forecasting new $\mu_y$ 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 $\mu$ and $\sigma$ from a sample

(Gaussian, independent observations)

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

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

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



# Inferring $\mu$ and $\sigma$ from a sample

(Gaussian, independent observations)

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# Inferring $\mu$ and $\sigma$ from a sample

(Gaussian, independent observations – prior uniform on  $\sigma$ )

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

Marginalizing<sup>1</sup>

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

---

<sup>1</sup>The 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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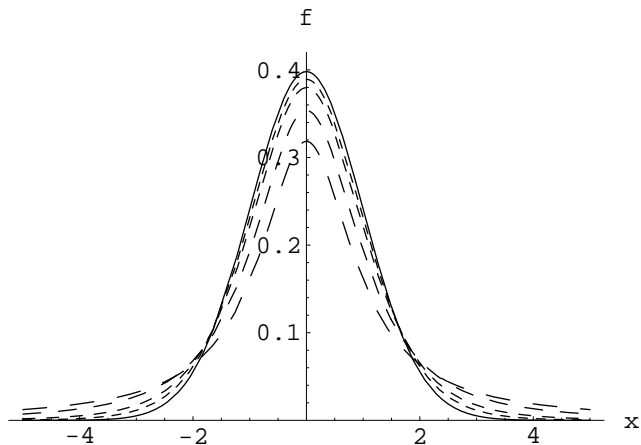
$$\begin{aligned}\nu &= n - 2 \\ t &= \frac{\mu - \bar{x}}{s/\sqrt{n-2}},\end{aligned}$$

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  $\nu$  equal to 1 , 2, 5, 10 and 100 ( $\approx$  “ $\infty$ ”).

# Inferring $\mu$ and $\sigma$ from a sample

(Gaussian, independent observations – prior uniform on  $\mu$  and  $\sigma$ )

In summary,

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

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The uncertainty on  $\sigma$  increases the probability of the values of  $\mu$  far from  $\bar{x}$ :

- ▶ 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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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 $\mu$ and $\sigma$ from a sample

Misunderstandings and 'myths' related to the Student  $t$  distribution

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

$$\begin{aligned} E(\mu) &\stackrel{(n>3)}{=} \bar{x} \\ \sigma(\mu) &\stackrel{(n>4)}{=} \frac{s}{\sqrt{n-4}}. \end{aligned}$$

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

---

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# Inferring $\mu$ and $\sigma$ from a sample

(Gaussian, independent observations – prior uniform on  $\mu$  and  $\sigma$ )

► Large  $n$  limit:

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

# Inferring $\mu$ and $\sigma$ from a sample

(Gaussian, independent observations – prior uniform on  $\mu$  and  $\sigma$ )

**Marginal**  $f(\sigma)$

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

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## Marginal $f(\sigma)$

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

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That is... (no special function)

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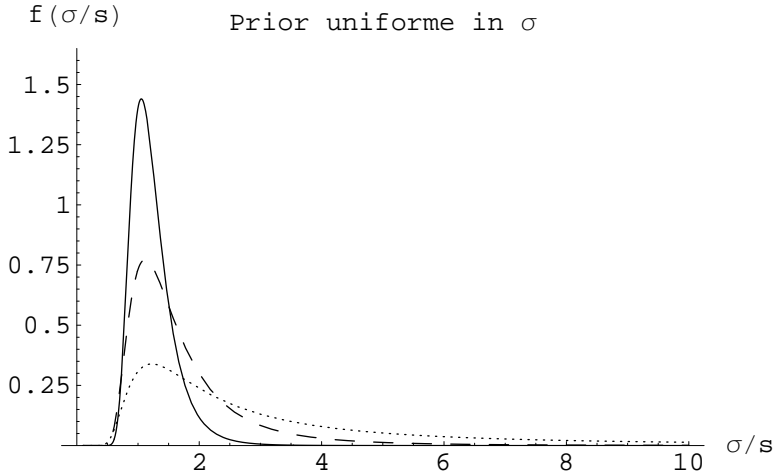
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[But if we would use  $\tau = 1/\sigma^2$  we would recognize a Gamma...]

# Inferring $\mu$ and $\sigma$ from a sample

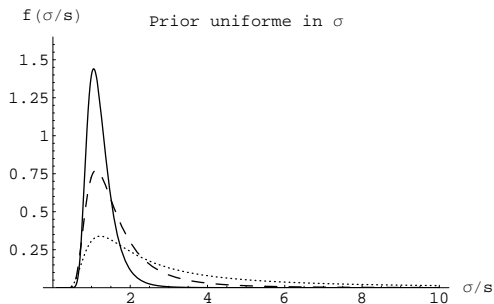
(Gaussian, independent observations – prior uniform on  $\mu$  and  $\sigma$ )



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

# Inferring $\mu$ and $\sigma$ from a sample

(Gaussian, independent observations – prior uniform on  $\mu$  and  $\sigma$ )



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

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

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

# Inferring $\mu$ and $\sigma$ from a sample

(Gaussian, independent observations – prior uniform on  $\mu$  and  $\sigma$ )

**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)

$$E(\mu) = \bar{x}$$

$$E(\sigma) = s$$

(They are indeed the modes!)

# Inferring $\mu$ and $\sigma$ from a sample

(Gaussian, independent observations – prior uniform on  $\mu$  and  $\sigma$ )

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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reobtaining the large number limit.

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reobtaining the large number limit. And, notice,  $\rho(\mu, \sigma) = 0$ .

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reobtaining the large number limit. And, notice,  $\rho(\mu, \sigma) = 0$ .

Q.: Are they independent?

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

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For a **fixed**  $\mu$  (and observed  $s$  and  $\bar{x}$ )

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

## Inferring $\mu$ and $\sigma$ from a sample

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

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

It is **technically** convenient to use  $\tau = 1/\sigma^2$ :

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

For a **fixed**  $\mu$  (and observed  $s$  and  $\bar{x}$ )

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

Do you recognize a *famous* mathematical form?

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On the other way around, for a **fixed**  $\tau$ ,

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



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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.