

# **Quantitative Genetics, Prediction and Selection Theory**

**SELECTION INDICES**

**BLUP and REML**

**BAYESIAN INFERENCE**

**GENOMIC SELECTION**

# Bayesian Methods

## 1. Bayesian inference

Bayes' theorem

Prior probability

Probability density functions

## 2. The mixed model in Bayesian inference

Predicting additive values and estimating genetic parameters

Marginalization

### *Interlude: MCMC*

BLUP and REML considered as Bayesian methods

### *Interlude: Inference on breeding values and genetic parameters under selection*

## 3. The multitrait model

Traits having the same model

Data augmentation

# Bayes theorem

$A$ : to be man

$B$ : to be British

$N$ : Total number of individuals

$N_A$ : number of men

$N_B$ : number of British people

$N_{AB}$ : number of British men

$$P(A, B) = \frac{N_{AB}}{N}$$

But if we take only the British people, the probability of being a man is

$$P(A | B) = \frac{N_{AB}}{N_B}$$

# Bayes theorem

$$\begin{aligned} P(A, B) &= \frac{N_{AB}}{N} = \frac{N_{AB}}{N_B} \cdot \frac{N_B}{N} = \\ &= P(A | B) \cdot P(B) \end{aligned}$$

# Bayes theorem

$$\begin{aligned} P(A,B) &= P(A|B) \cdot P(B) \\ &= P(B|A) \cdot P(A) \end{aligned}$$

$$P(A|B) = P(B|A) \cdot P(A) / P(B)$$

# Bayes theorem

**Model:**  $y = \text{Group} + e$

Group: Selected line (**S**)  
Control line (**C**)

~~Question~~ Is  $S \neq C$  ?

# Bayes theorem

**Model:**  $y = \text{Group} + e$

**Group:** Selected line (**S**)  
Control line (**C**)

**Question:** Is  $S > C$  ?

$P(S > C)$  ? or  $P(S - C > 0)$  ?

# Bayes theorem

$$P(A|B) = P(B|A) \cdot P(A) / P(B)$$

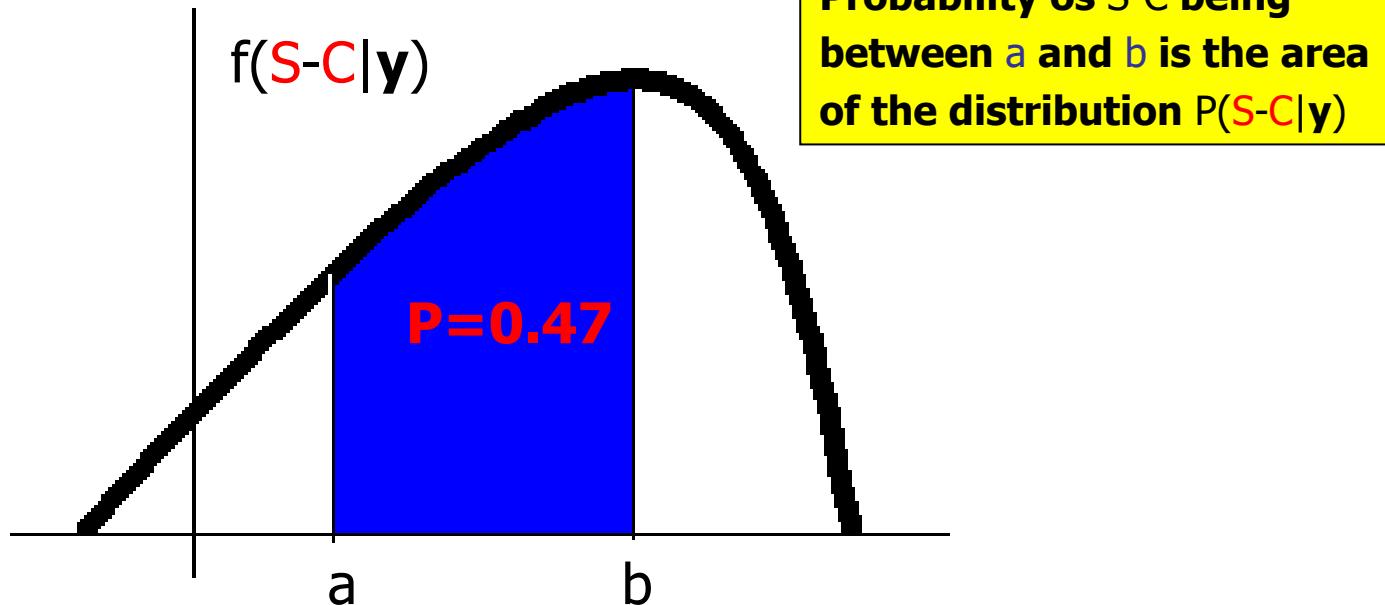
$$P(S-C|y) = P(y|S-C) \cdot P(S-C) / P(y)$$

**S**: Selected line

**C**: Control line

**y**: data

# Density functions



# Prior information

- 4.1. Exact prior information
- 4.2. Vague prior information
- 4.3. No prior information
- 4.4. Improper priors
- 4.5. The Achilles heel of Bayesian inference

# Exact Prior information



**Black**

**AA**

**Black**

**Aa**

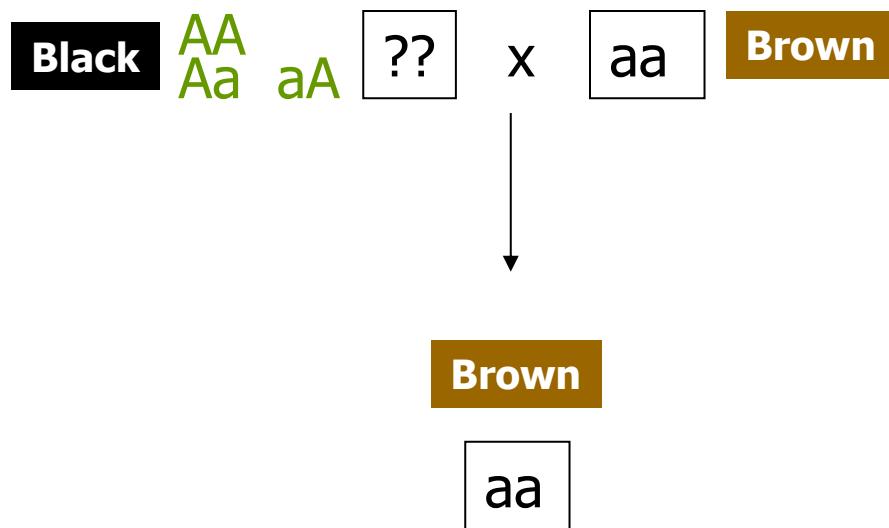
**Black**

**aA**

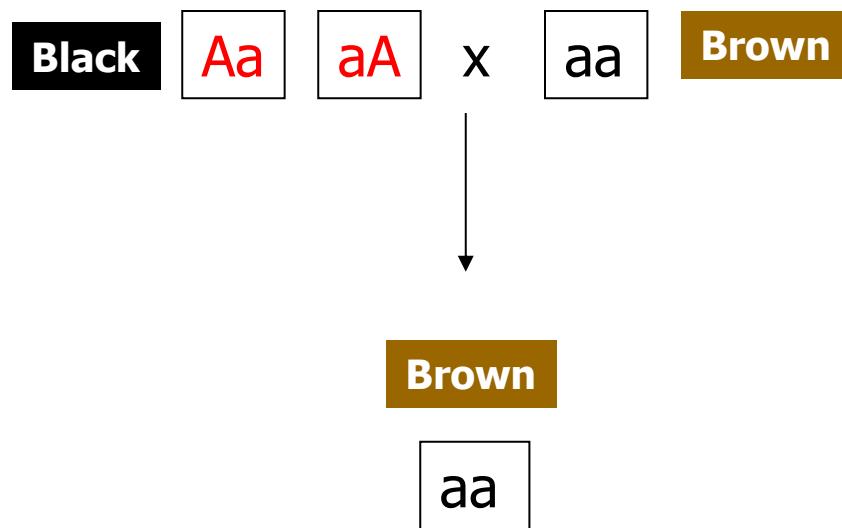
**Brown**

**aa**

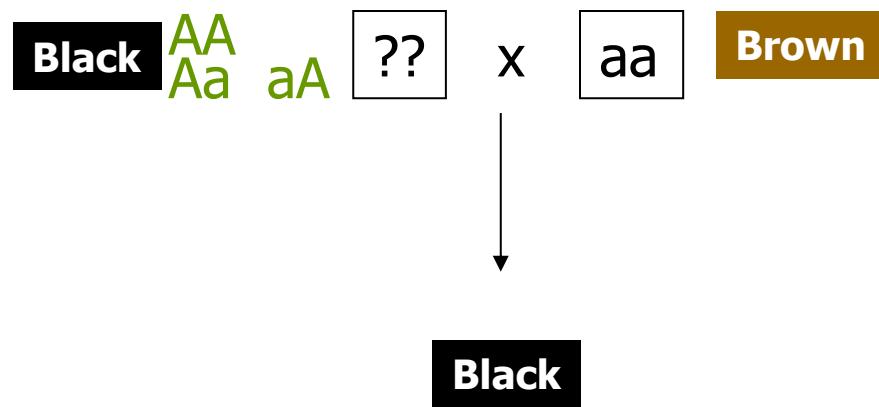
# Exact Prior information



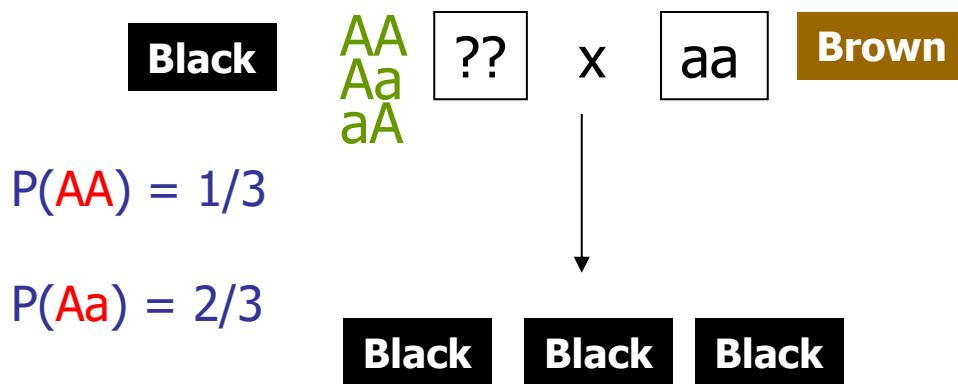
# Exact Prior information



# Exact Prior information



# Exact Prior information



# Exact Prior information

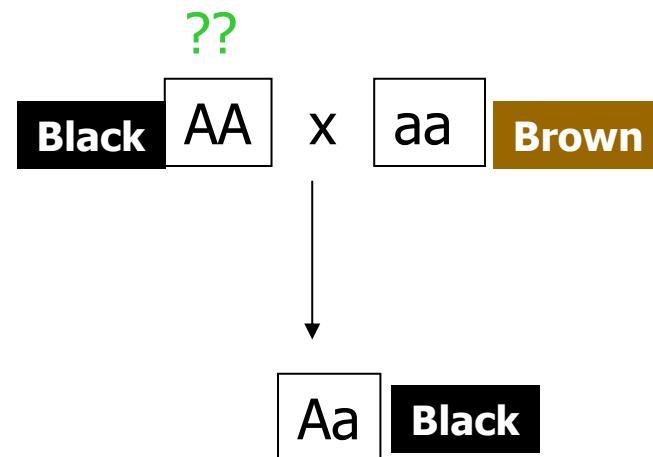
$$P(A|B) = P(B|A) P(A) / P(B)$$

$$P(\text{AA} | y=3\mathbf{B}) = P(y=3\mathbf{B} | \text{AA}) \cdot P(\text{AA}) / P(y=3\mathbf{B})$$

- $P(y=3\mathbf{B} | \text{AA}) = 1$

- $P(\text{AA}) = 1/3$

- $P(y=3\mathbf{B})$



# Exact Prior information

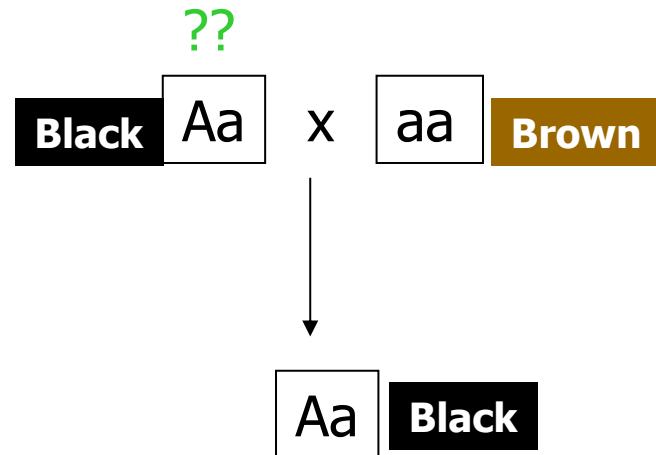
$$P(A|B) = P(B|A) P(A) / P(B)$$

$$P(Aa \mid y=3B) = P(y=3B \mid Aa) \cdot P(Aa) / P(y=3B)$$

- $P(y=3B \mid Aa) = (1/2)^3$

- $P(Aa) = 2/3$

- $P(y=3B)$



# Exact Prior information

$$P(A, B) = P(A | B) P(B)$$

$$P(y=3B) = (y= 3B \text{ & AA}) + P(y=3B \text{ & Aa}) =$$

$$P(y= 3B | AA) P(AA) + P(y= 3B | Aa) P(Aa) =$$

$$1 \cdot 1/3 + (1/2)^3 \cdot 2/3 =$$

$$= 5/12 = \mathbf{0.42}$$

# Exact Prior information

$$P(\text{AA} \mid y=3\mathbf{B}) = P(y=3\mathbf{B} \mid \text{AA}) \cdot P(\text{AA}) / P(y=3\mathbf{B})$$

- $P(y=3\mathbf{B} \mid \text{AA}) = 1$
- $P(\text{AA}) = 1/3$
- $P(y=3\mathbf{B}) = 5/12$

$$P(\text{AA} \mid y=3\mathbf{B}) = 1 \cdot (1/3) / (5/12) = \mathbf{0.80}$$

# Exact Prior information

$$P(Aa \mid y=3B) = P(y=3B \mid Aa) \cdot P(Aa) / P(y=3B)$$

- $P(y=3B \mid Aa) = (1/2)^3$

- $P(Aa) = 2/3$

??

- $P(y=3B) = 5/12$

Black Aa x aa Brown

$$P(Aa \mid y=3B) = (1/2)^3 \cdot (2/3) / (5/12) = 0.20$$

Aa Black

# Exact Prior information

Notice that

$$P(\text{AA} \mid y=3\mathbf{B}) = 0.80$$

$$\underline{P(\text{Aa} \mid y=3\mathbf{B}) = 0.20}$$

$$1.00$$

However, the likelihoods

$$P(y=3\mathbf{B} \mid \text{AA}) = 1$$

$$P(y=3\mathbf{B} \mid \text{Aa}) = (1/2)^3 = 0.125$$

By ML we choose **AA** without a measure of uncertainty

# Exact Prior information

## WITH FLAT PRIOR INFORMATION

$$P(AA) = 1/2$$

$$P(Aa) = 1/2$$

$$P(A? | y=3B) = P(y= 3B | A?) \cdot P(A?) / P(y=3B)$$

$$\begin{aligned} P(y=3B) &= P(y= 3B | AA) P(AA) + P(y= 3B | Aa) P(Aa) = \\ &= 1 \cdot 1/2 + (1/2)^3 \cdot 1/2 = 9/16 = 0.56 \end{aligned}$$

$$P(AA | y=3B) = 1 \cdot (1/2) / (9/16) = 0.89$$

$$P(Aa | y=3B) = (1/2)^3 \cdot (1/2) / (9/16) = 0.11$$

# Exact Prior information

**WITH HIGH PRIOR INFORMATION**

$$P(AA) = 0.002$$

$$P(Aa) = 0.998$$

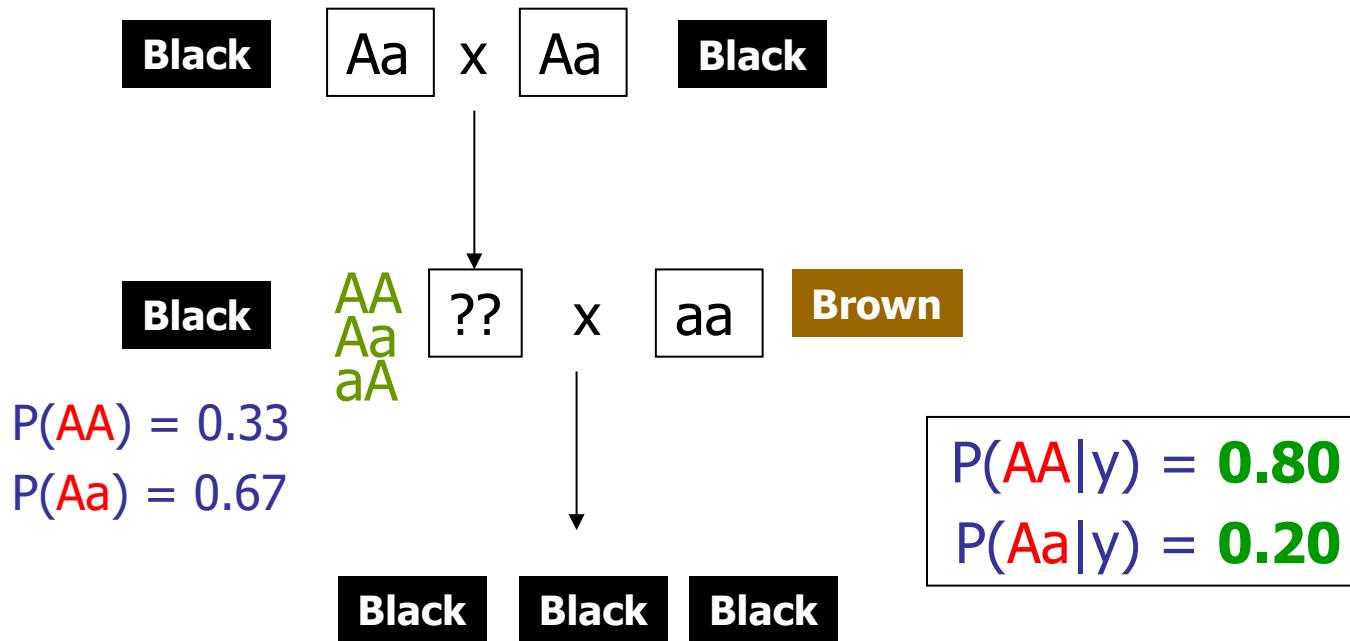
$$P(A? | y=3B) = P(y= 3B | A?) \cdot P(A?) / P(y=3B)$$

$$\begin{aligned} P(y=3B) &= P(y= 3B | AA) P(AA) + P(y= 3B | Aa) P(Aa) = \\ &= 1 \cdot 0.002 + (1/2)^3 \cdot 0.998 = 0.13 \end{aligned}$$

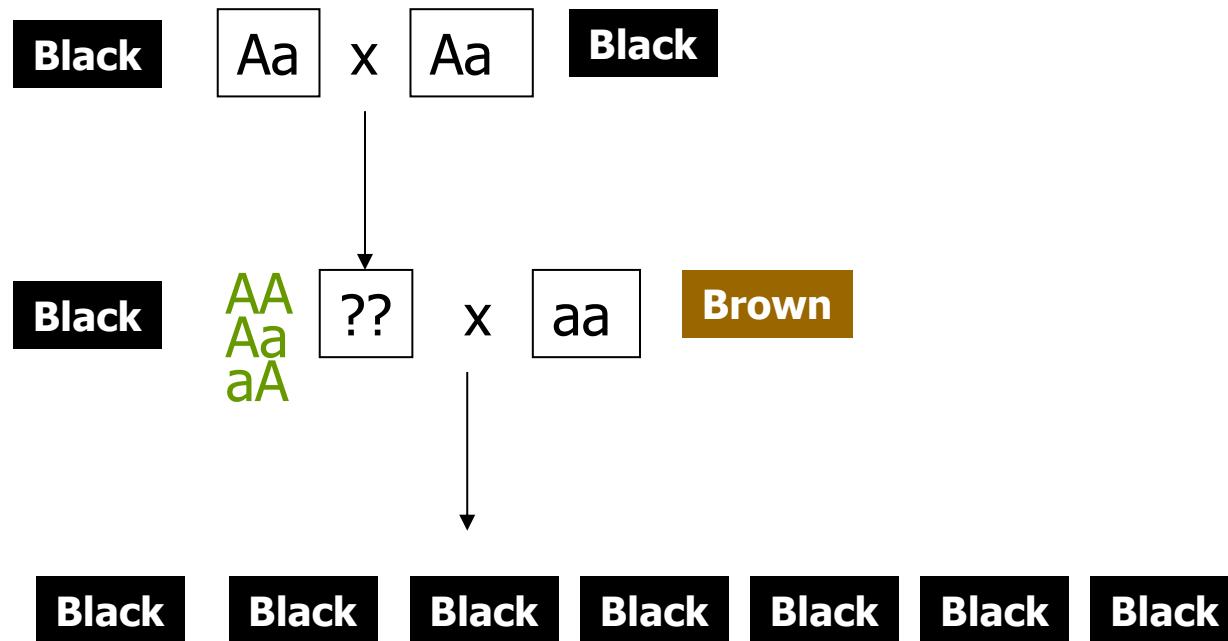
$$P(AA | y=3B) = 1 \cdot 0.002 / 0.13 = \mathbf{0.02}$$

$$P(Aa | y=3B) = (1/2)^3 \cdot 0.998 / 0.13 = \mathbf{0.98}$$

# Exact Prior information



# Exact Prior information



# Exact Prior information

$$P(AA) = 0.33$$

$$P(Aa) = 0.67$$

$$P(AA|y=3B) = 0.80$$

$$P(Aa|y=3B) = 0.20$$

$$P(AA|y=7B) = 0.99$$

$$P(Aa|y=7B) = 0.01$$

# Exact Prior information

$$P(AA) = 0.33$$

$$P(Aa) = 0.67$$

$$P(AA|y=3\mathbf{B}) = 0.80$$
$$P(Aa|y=3\mathbf{B}) = 0.20$$

$$P(AA) = 0.50$$

$$P(Aa) = 0.50$$

$$P(AA|y=3\mathbf{B}) = 0.89$$
$$P(Aa|y=3\mathbf{B}) = 0.11$$

$$P(AA) = 0.33$$

$$P(Aa) = 0.67$$

$$P(AA|y=7\mathbf{B}) = 0.99$$
$$P(Aa|y=7\mathbf{B}) = 0.01$$

$$P(AA) = 0.50$$

$$P(Aa) = 0.50$$

$$P(AA|y=7\mathbf{B}) = 0.99$$
$$P(Aa|y=7\mathbf{B}) = 0.01$$

When  
more  
data,  
prior is  
irrelevant

# Exact Prior information

**When more data, prior becomes irrelevant**

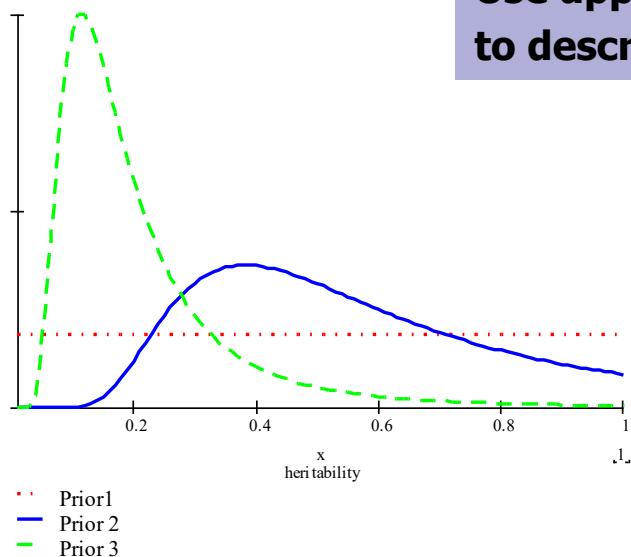
$$\begin{aligned} f(\theta | \mathbf{y}) \propto f(\mathbf{y} | \theta) f(\theta) &= f(y_1, y_2, \dots, y_n | \theta) f(\theta) = \\ &= f(y_1 | \theta) f(y_2 | \theta) \dots f(y_n | \theta) \boxed{f(\theta)} \end{aligned}$$

$$\log f(\theta | \mathbf{y}) \propto \log f(y_1 | \theta) + \log f(y_2 | \theta) + \dots + \log f(y_n | \theta) + \boxed{\log f(\theta)}$$

# Vague prior information

- PROBABILITY describes BELIEFS
  - Subjective probability is not arbitrary
  - It should be vague (otherwise, no reason to perform an experiment)
  - When not vague, make conditional inferences (avoid problems)
- USE APPROPRIATE PRIOR DENSITIES
  - Linear beliefs (for effects, etc.) are symmetrical: Normal for example.
  - Quadratic beliefs (for variances,  $h^2$ , etc.) are assymetrical. I-gamma for example
- TRY SEVERAL PRIORS
  - If posteriors are almost the same, prior information is irrelevant

# Vague prior information



**Use appropriate functions  
to describe vague prior knowledge**

**Blasco et al. 1998  
Genetics 143: 301-306**

# Vague prior information

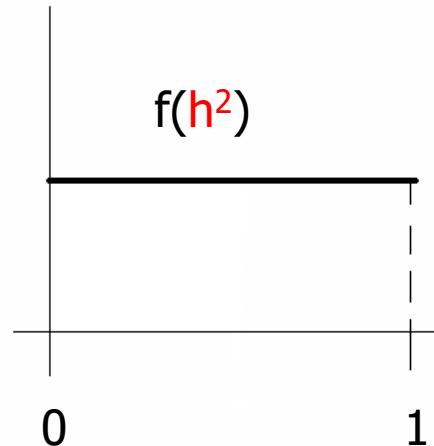
## PROBLEMS

- How can be integrated information from other experiments?
  - Is your experiment fully comparable with other experiments?
  - Do you believe in ALL published results?
- How can you define multivariate beliefs?
- The posterior of today is tomorrow's prior

Bayesian  
propaganda !!

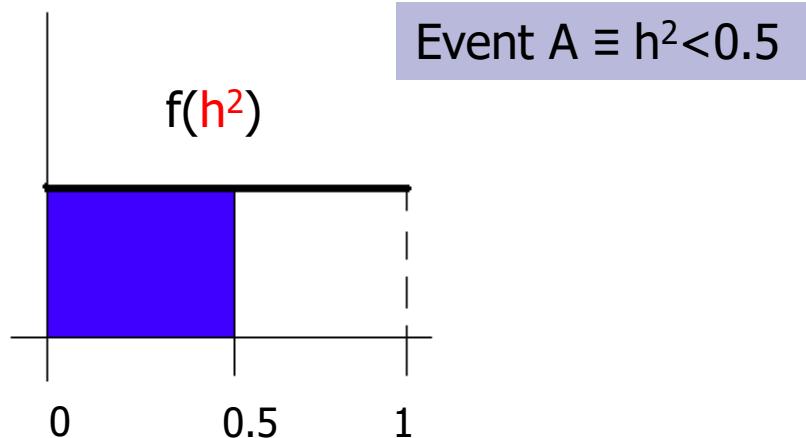
# No Prior information

**FLAT PRIORS**



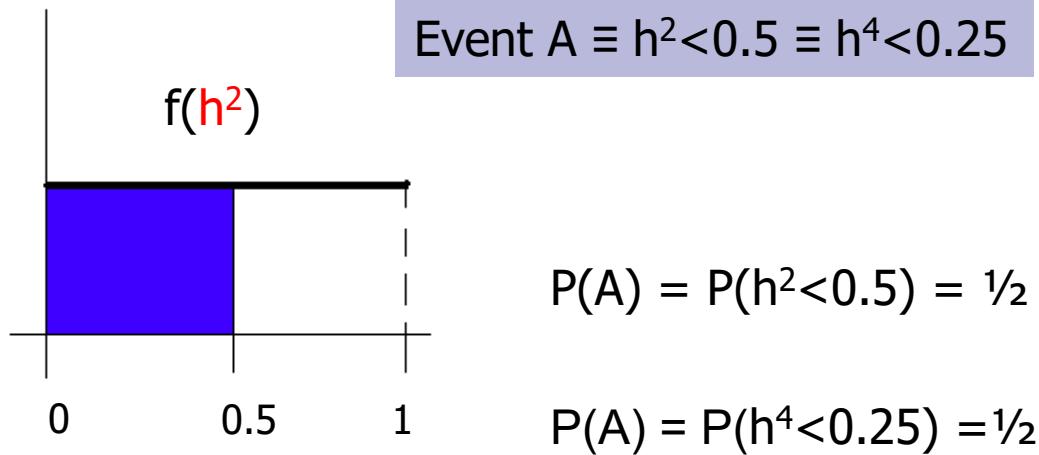
# No Prior information

## FLAT PRIORS

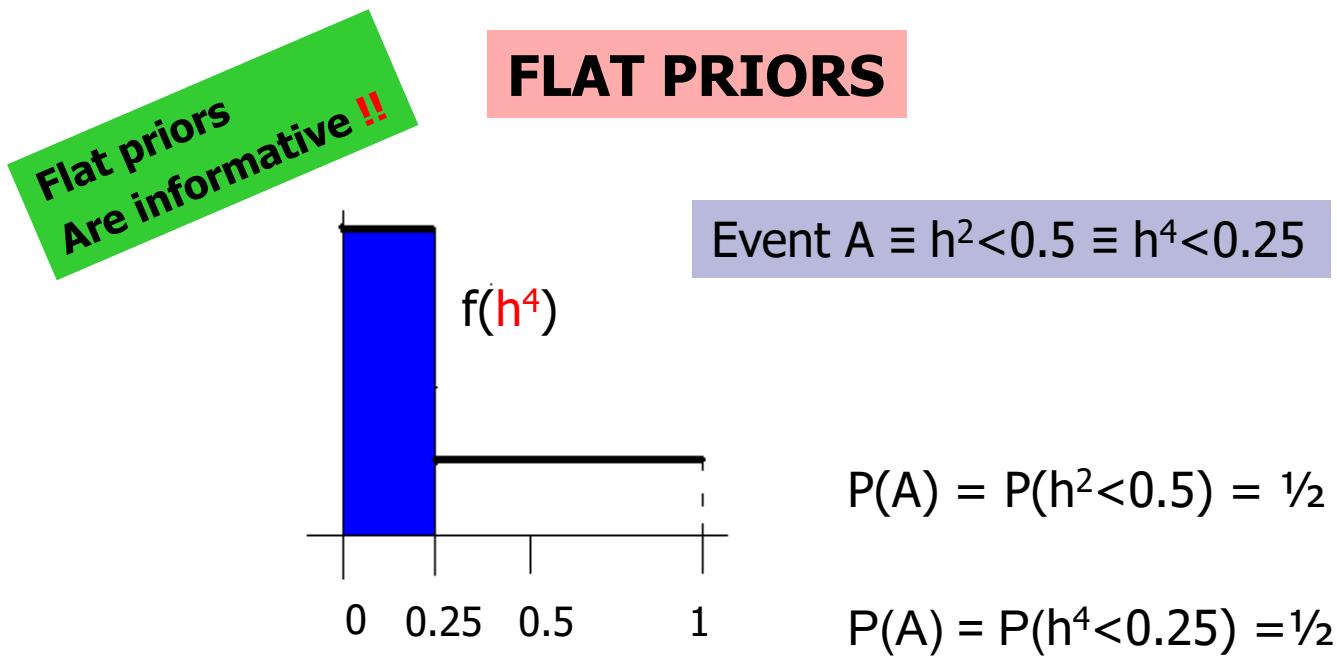


# No Prior information

## FLAT PRIORS



# No Prior information



# No Prior information

- Non informative priors are informative
- Thus, we introduce information we do not know where it comes from
- Some non-informative priors minimize the information introduced
- We should avoid (in general) improper priors
- We should check how results are affected by using a prior, even if this prior is non-informative
- ... but we do not know how to do this in the multivariate case

# No Prior information

- Other alternatives have been proposed:
  - **Jeffrey's priors:**  
They are invariant to transformations
  - **Bernardo's Reference priors:**  
Minimum prior information
  - **Maximum entropy prior information:**  
Minimum prior information with some subjective informative restrictions
- However, all of them have problems in the multivariate case

# No Prior information

## MULTIVARIATE PRIORS

- We cannot have subjective multivariate priors
  - Subjective priors: hire a psicoanalist
- We cannot have 'objective' multivariate priors !!
  - Do not use big flat priors
  - Do not use almost big flat priors!!
  - Be careful with some common priors like inverted Wishart !!
- A practical solution:
  - Flat priors with sound limits
  - Vague Informative priors with sound limits

# Improper priors

- Some priors are not densities
  - Example:  $f(\theta) = k$        $k$ : arbitrary constant
$$\int f(\theta) d\theta = \infty$$
- They can produce improper posterior densities
- They lead to proper posterior densities when
$$f(y) = \int f(y|\theta) f(\theta) d\theta < \infty$$

# Improper priors

- Sometimes they are innocuous

Example:  $y \sim N(\mu, 1)$        $\mu \sim k$

$$\begin{aligned} f(y) &= \int_{-\infty}^{\infty} f(y | \mu) f(\mu) d\mu = \int_{-\infty}^{\infty} f(y | \mu) k d\mu = k \int_{-\infty}^{\infty} f(y | \mu) d\mu = \\ &= k \int \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{(y-\mu)^2}{2}\right] d\mu = k \int \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{(\mu-y)^2}{2}\right] d\mu = k \end{aligned}$$

$$f(\mu | y) = \frac{f(y | \mu) f(\mu)}{f(y)} = \frac{f(y | \mu) \cdot k}{k} = f(y | \mu)$$

**But sometimes they are not !**

# Improper priors

- Improper priors may lead to improper posteriors
- When using MCMC improper posteriors may not be detected
- Do not use improper priors !!
  - Do not use big flat priors
  - Do not use almost big flat priors!! E.g.:  $f(\theta) \sim N(0, 10^6)$   
(they behave as improper priors and give a false sense of safety)
- A practical solution:
  - Flat priors with sound limits
  - Vague Informative priors with sound limits

# No Prior information

- Modern Bayesians consider prior information as just a mathematical artefact that allow us to work with probabilities

... but  $\text{PROBABILITY} \times \text{ARTEFACT} \neq \text{PROBABILITY}$

$\text{PROBABILITY} \times \text{ARTEFACT} = \text{ARTEFACT}$

- If we **behave** as if it is a probability, the distortion is not high

**... and we can enjoy the advantages of working with probabilities**

# The Bayesian choice

## SOME DISSAPOINTMENTS ALONG YOUR LIFE:

- Father Christmas are mum and dad
- In the improbable case of the existence of the Heaven, nobody has make a reservation for you there
- Bayesian methods have concentual problems as the frequentists ones, and it is

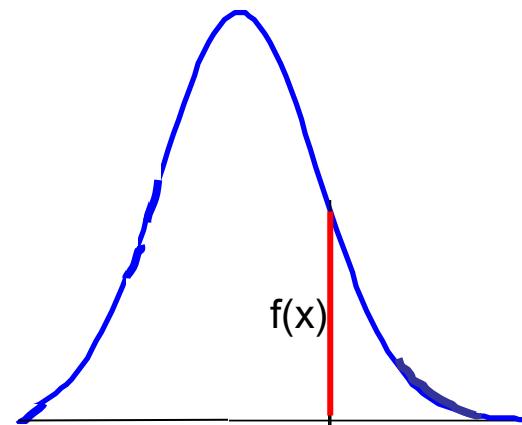
My opinion  
straightforward  
better what y

**The great advantage  
is to work with  
Probabilities**

...s have a more  
can understand

# Density function

$f(x)$  is **not** a probability

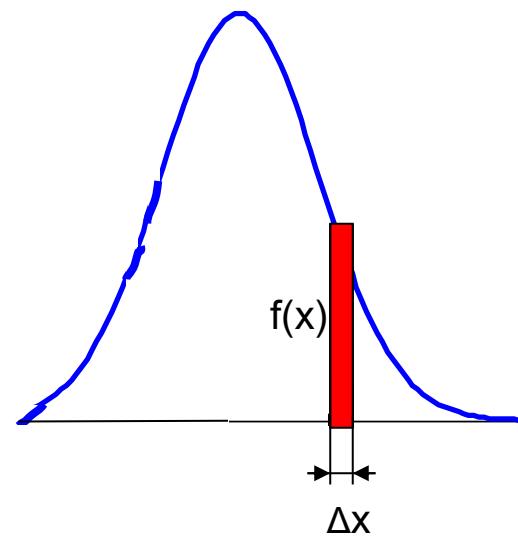


# Density function

$f(x)$  is **not** a probability

$f(x) \cdot \Delta x$  is approx. a probability

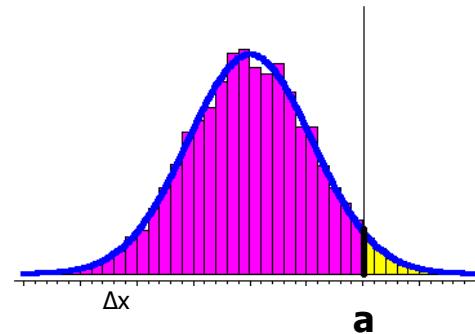
$f(x) \cdot dx$  is a probability



# Density function

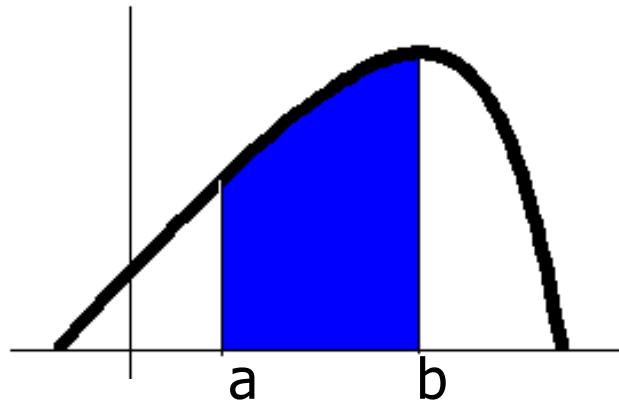
$f(x) \cdot dx$  is a probability

$\int_a^{+\infty} f(x) dx$  is a probability (a sum of probabilities)



# Density function

$$P(a \leq x \leq b) = \int_a^b f(x) dx$$



## Conditional distribution

$$P(A|B) = \frac{P(B|A) \cdot P(A)}{P(B)}$$

$$f(x|y) \Delta x = \frac{f(y|x) \Delta y \cdot f(x) \Delta x}{f(y) \Delta y}$$

$$f(x|y) = \frac{f(y|x) \cdot f(x)}{f(y)}$$

## Conditional distribution

$$f(x,y) = f(x|y) \cdot f(y)$$

$$f(x|y) = \frac{f(x,y)}{f(y)} \longrightarrow f(x|y) = \frac{f(x,y)}{f(y)}$$

$$f(x|y=y_0) = \frac{f(x,y_0)}{f(y_0)}$$

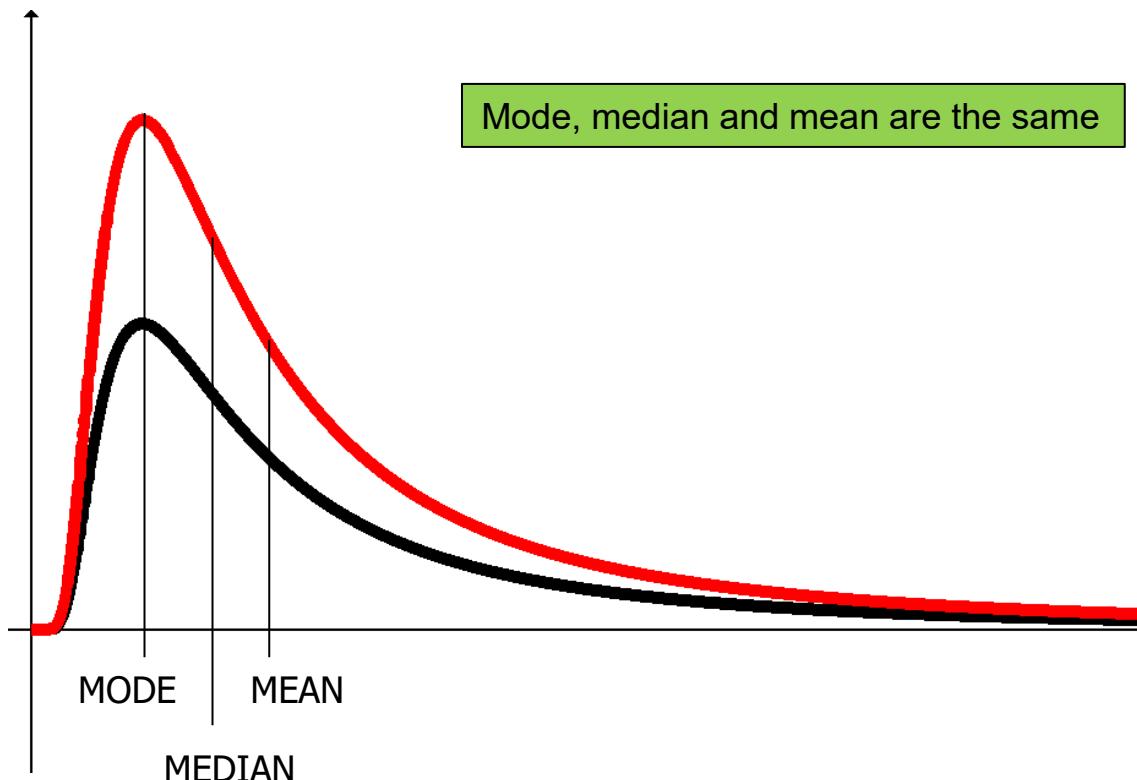
# Conditional distribution

$$f(x|y) = \frac{f(y|x) \cdot f(x)}{f(y)}$$

$$f(\textcolor{red}{x}|y) = \frac{f(y|\textcolor{red}{x}) \cdot f(\textcolor{red}{x})}{f(y)}$$

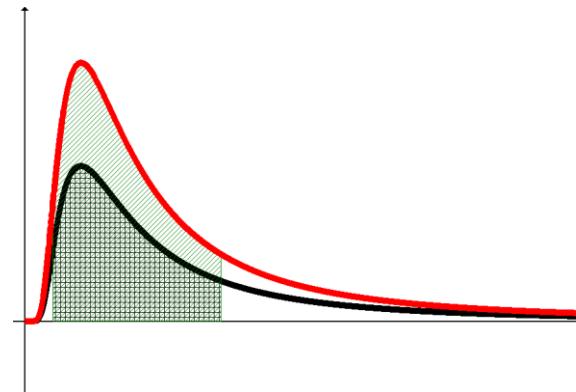
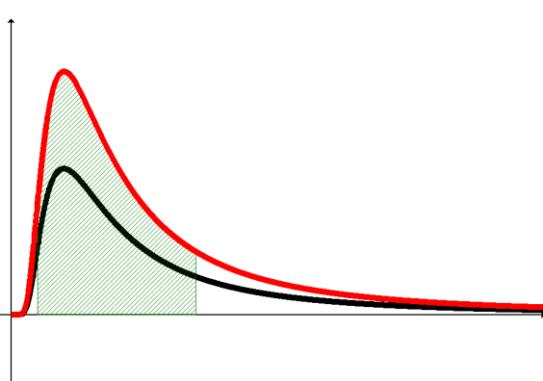
$$f(\textcolor{red}{x}|y) \propto f(y|\textcolor{red}{x}) \cdot f(\textcolor{red}{x})$$

# Working proportionally



# Working proportionally

Probabilities are the same



# Risk, bias and variance

ERROR OF ESTIMATION

$$e = u - \hat{u}$$

LOSS FUNCTION

$$l(\hat{u}, u) = e^2$$

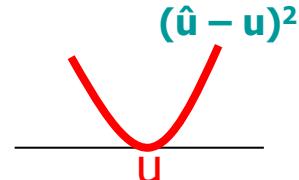
RISK

$$R(\hat{u}, u) = E[l(\hat{u}, u)] = E(e^2)$$

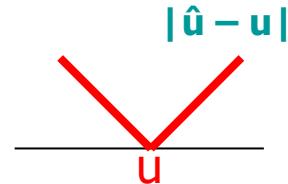
# Features of Bayesian inference

## POINT ESTIMATES

- MEAN: minimizes  $RISK = E(\hat{u} - u)^2$



- MEDIAN: minimizes  $RISK = E|\hat{u} - u|$



- MODE: is the most probable value

# Features of Bayesian inference

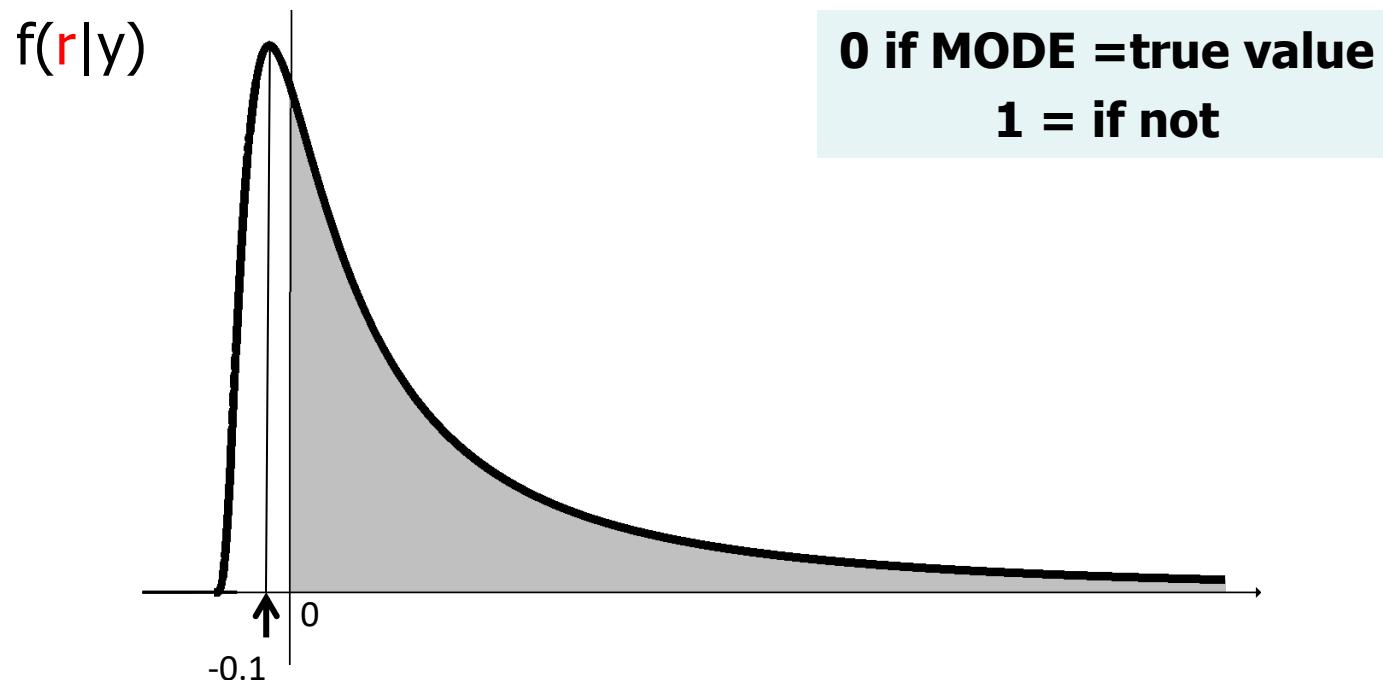
## POINT ESTIMATES

... but MODE has a horrible loss function!

**0 if MODE =true value  
1 = if not**

# Features of Bayesian inference

## POINT ESTIMATES



# Features of Bayesian inference

## POINT ESTIMATES

... but **MEAN** also has a horrible loss function!

	$x$	$x^2$
1	1	1
2	2	4
3	3	9
Mean	2	4.7

**$(\hat{u} - u)^2$  is NOT invariant  
to transformations !!**

i.e.: the loss of  $u^2$  is not  
the square of the loss of  $u$  !!

$$2^2 \neq 4.7$$

i.e.: the MEAN for  $\sigma^2$  is not  
the square of the MEAN of  $\sigma$

# Features of Bayesian inference

## POINT ESTIMATES

Only the **MEDIAN** is invariant

$x = 1 1 1 2 2 3 4 4 5 5 5$

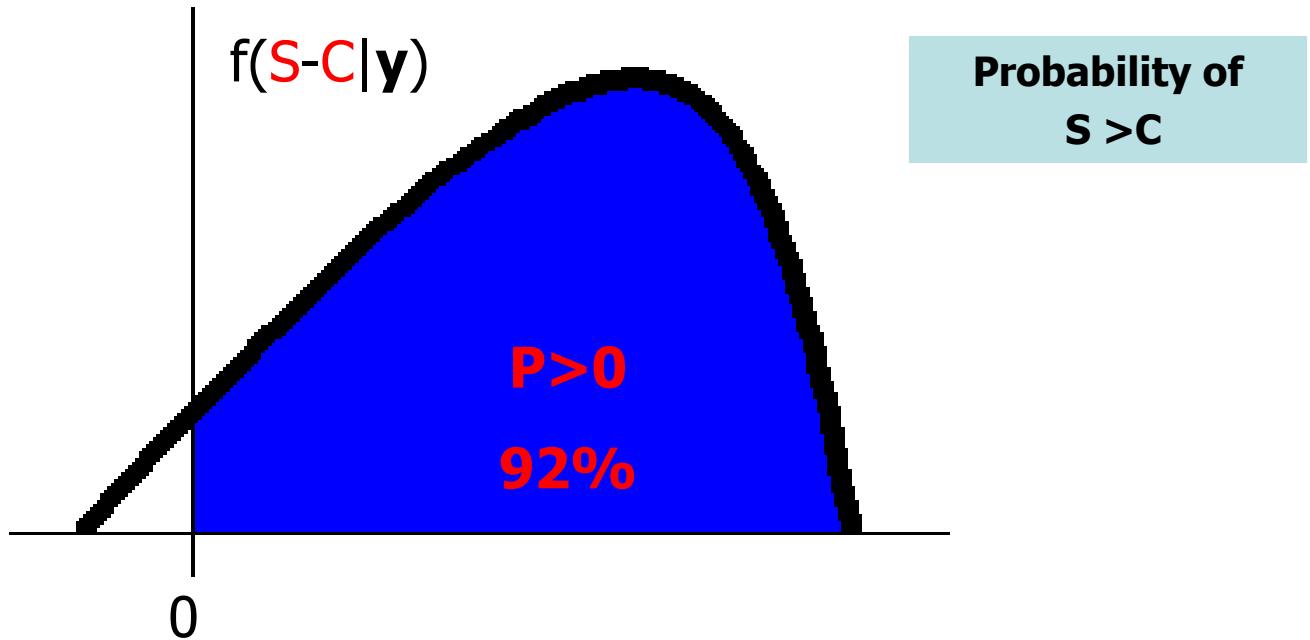
**median  $x = 3$**

$x^2 = 1 1 1 4 4 9 16 16 25 25 25$

**median  $x = 9$**

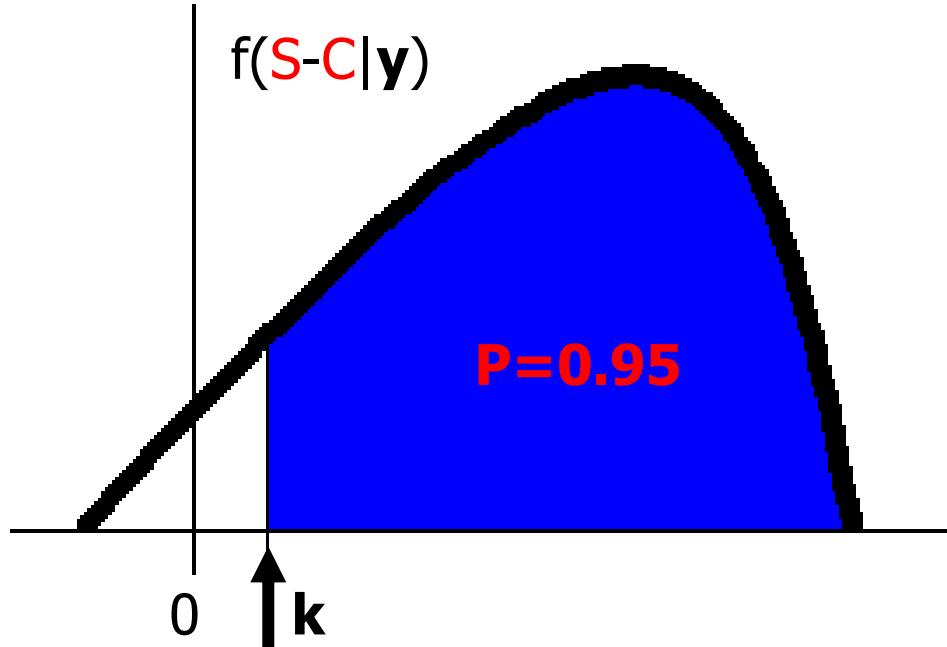
# Features of Bayesian inference

## CREDIBILITY INTERVALS



# Features of Bayesian inference

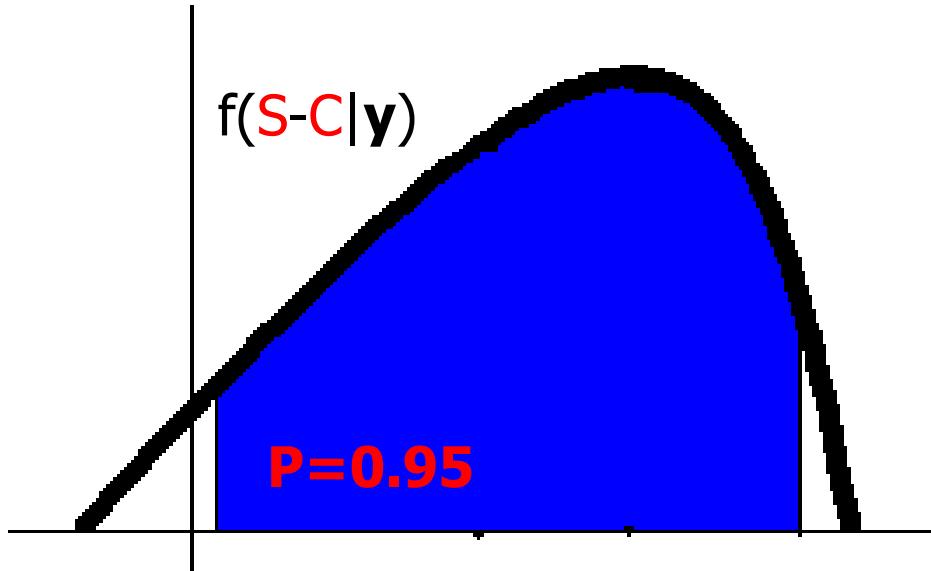
## CREDIBILITY INTERVALS



k is a guaranteed value  
for  $P=95\%$  or for  $P=80\%$ ,  
or for other  $P$

# Features of Bayesian inference

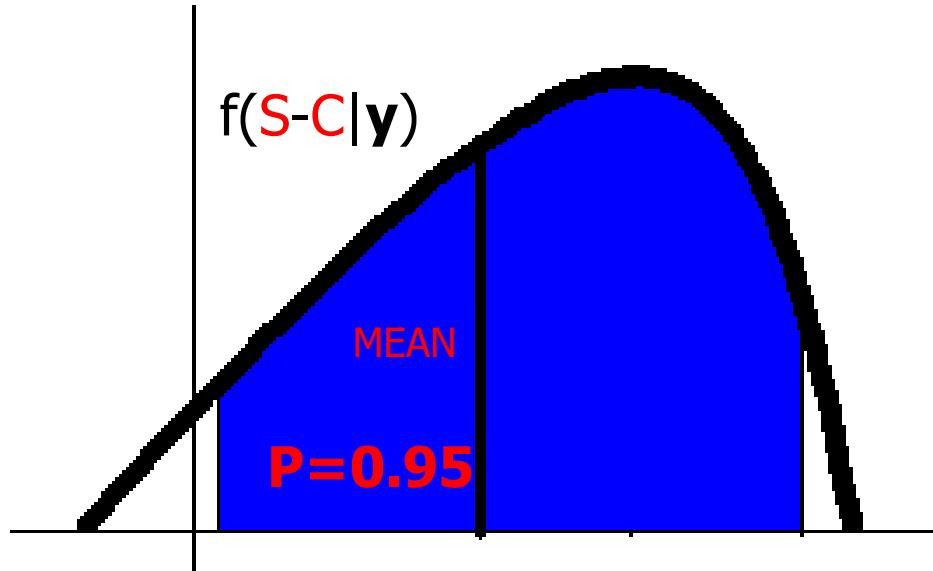
## CREDIBILITY INTERVALS



Shortest interval with  $P=0.95$

# Features of Bayesian inference

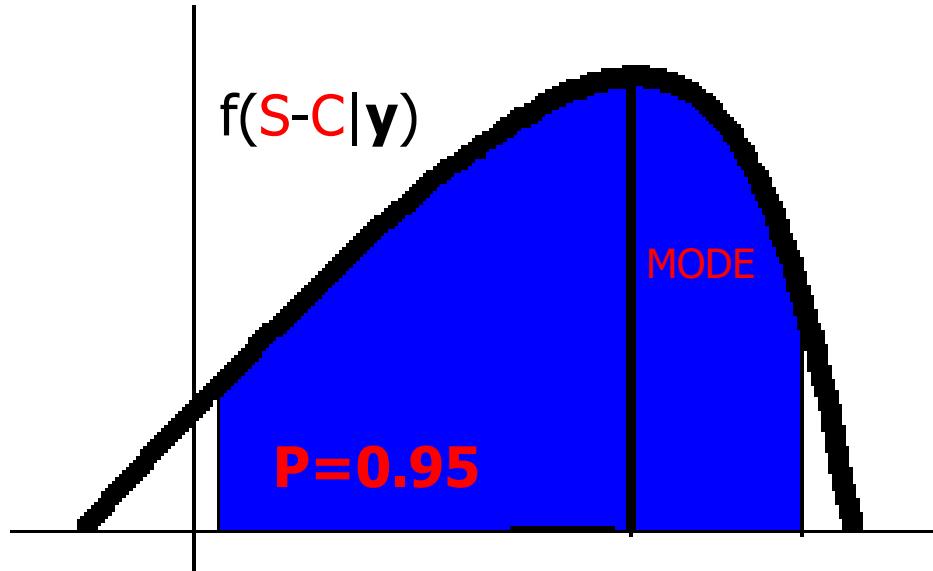
## CREDIBILITY INTERVALS



Shortest interval with  $P=0.95$

# Features of Bayesian inference

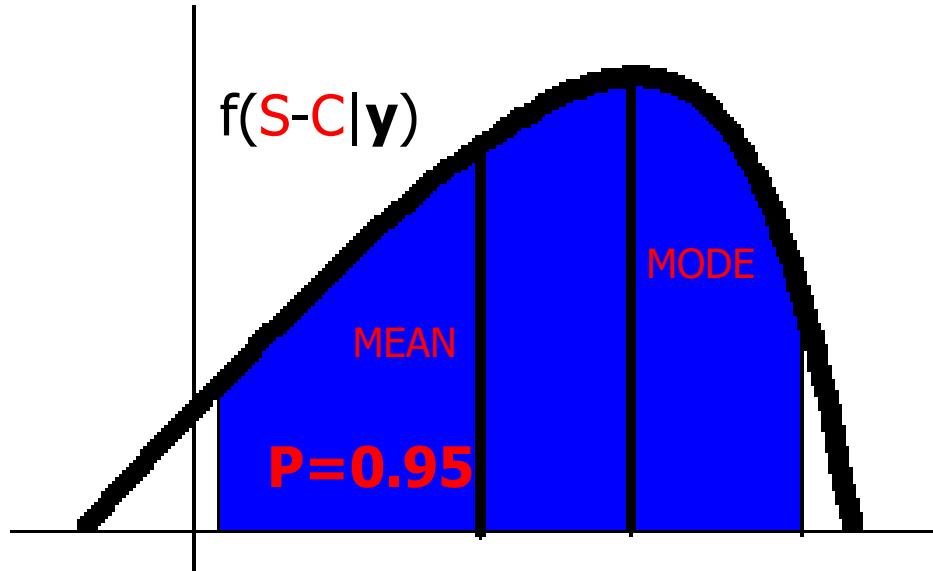
## CREDIBILITY INTERVALS



Shortest interval with  $P=0.95$

# Features of Bayesian inference

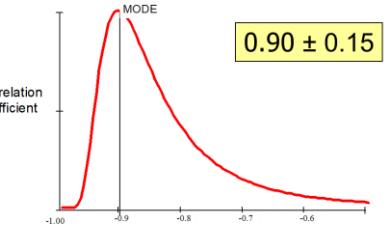
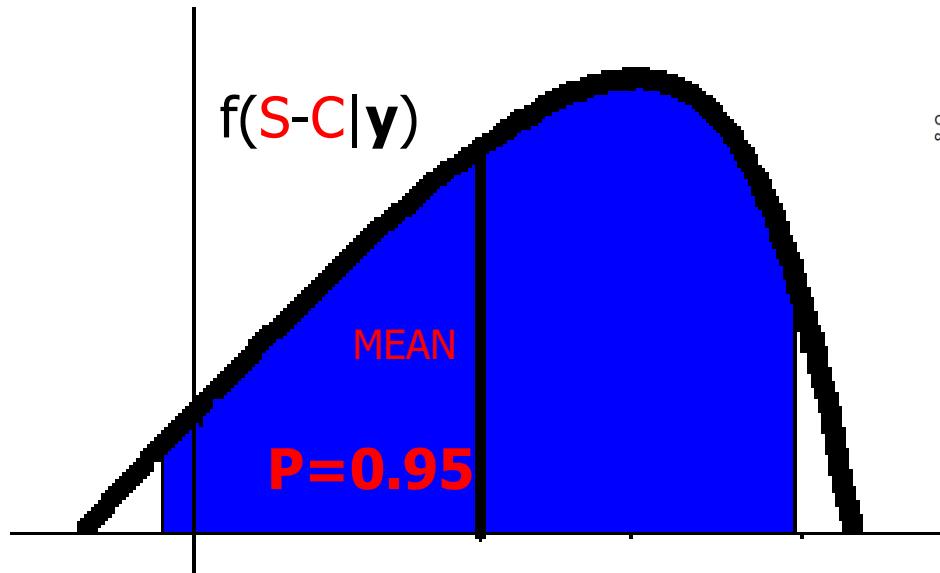
## CREDIBILITY INTERVALS



Shortest interval with  $P=0.95$

# Features of Bayesian inference

## CREDIBILITY INTERVALS



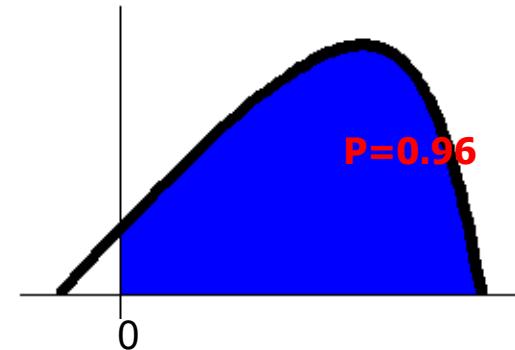
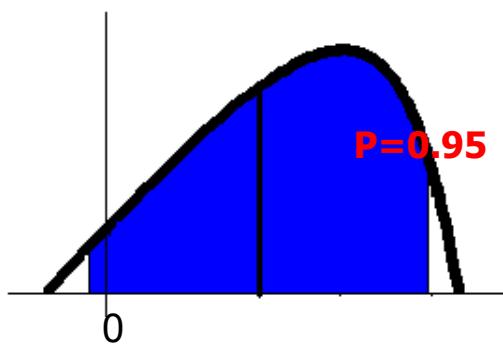
Symmetric interval with  $P=0.95$

# Features of Bayesian inference

## CREDIBILITY INTERVALS

Notice that zero can be within the confidence interval and still  $P(S-C>0)$  can be  $>0.95$

If 0 is within the HPD interval, this does not mean that there are no “significant differences”



# Features of Bayesian inference

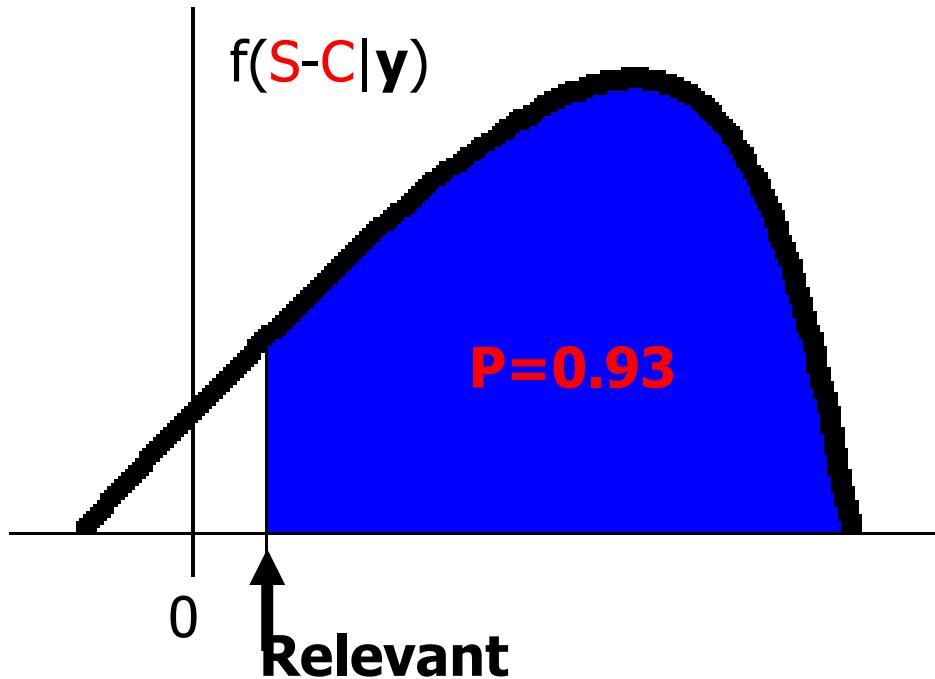
## CREDIBILITY INTERVALS

**Relevant value:** the **minimum difference** between S and C having an economical or biological meaning

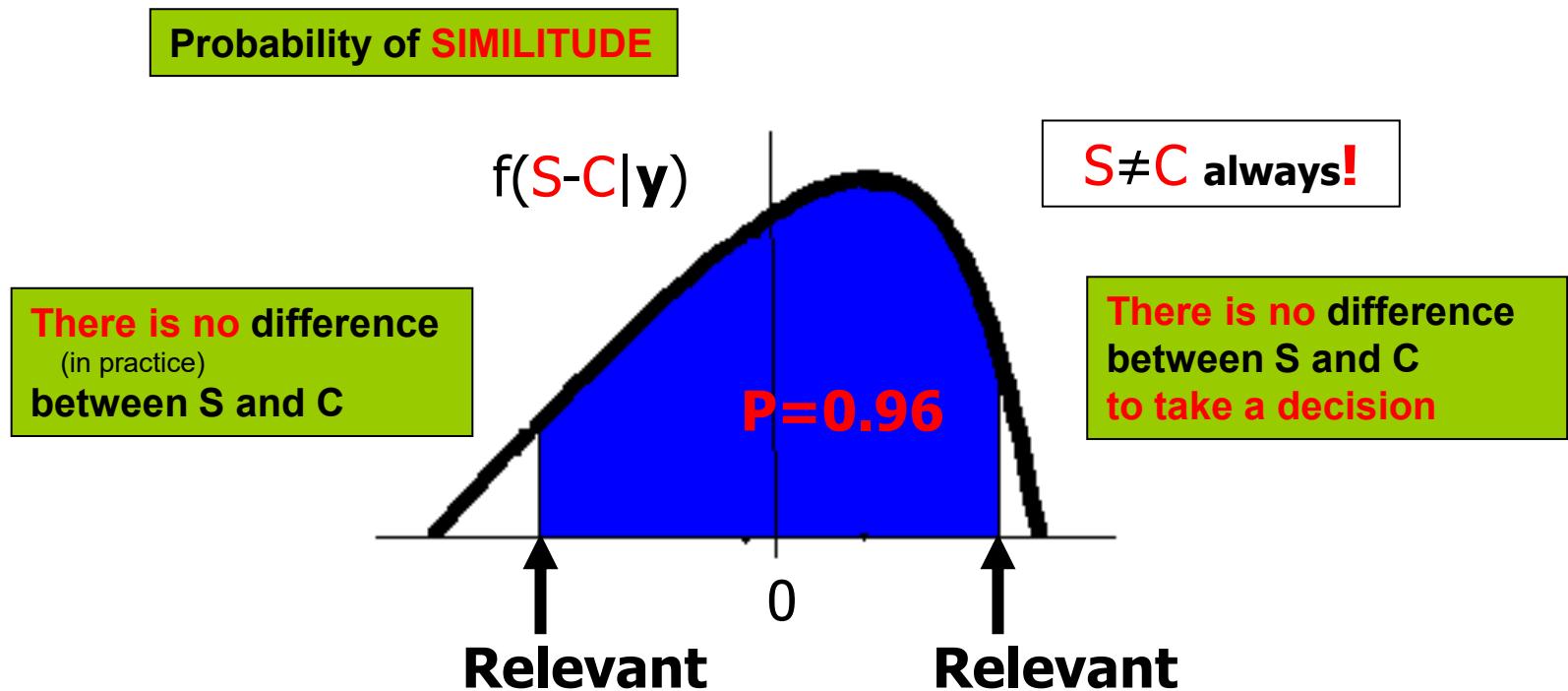
- It is the minimum value from which we take a decision
- It is the value used for experimental designs
- It should be proposed for each trait based on biological or economical arguments
- When no clues, use a fraction of the standard deviation
- In animal production, most economical relevant values go from **1/2 to 1/3 s.d.** of the trait

# Features of Bayesian inference

Probability of RELEVANCE



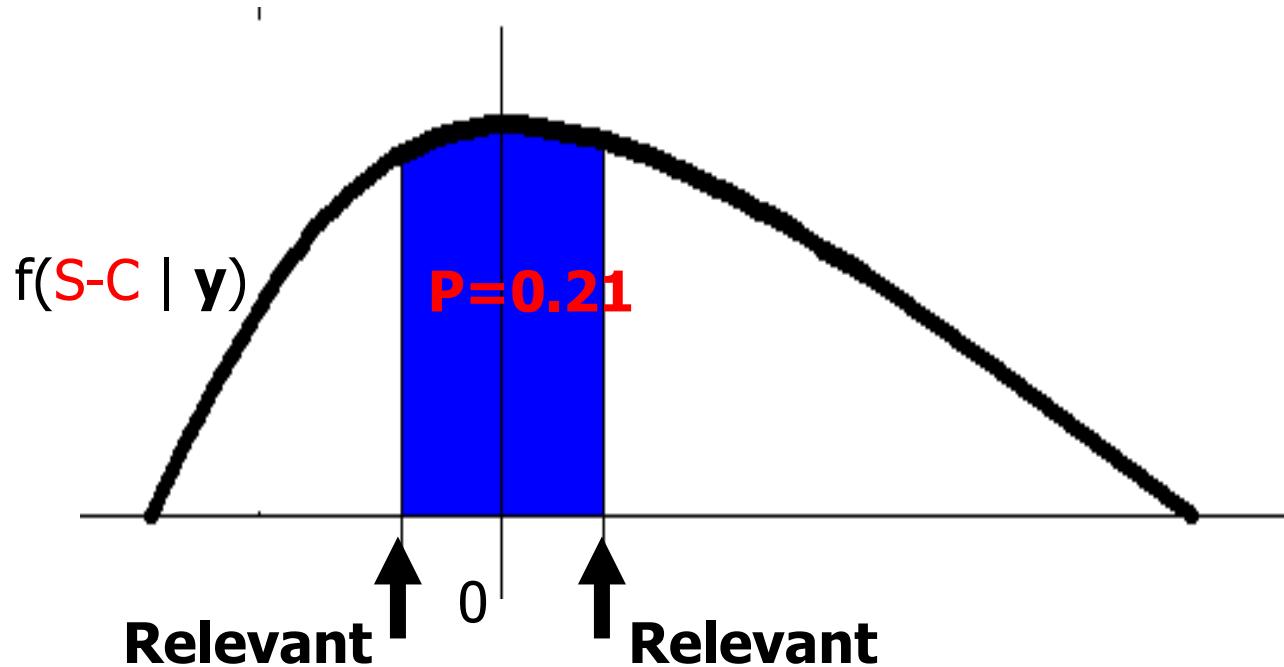
# Features of Bayesian inference



# Features of Bayesian inference

Probability of **SIMILITUDE**

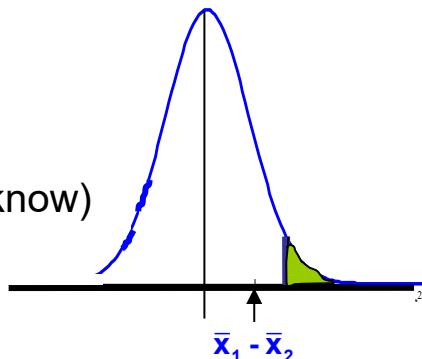
For my decision, I do not know whether  $S > C$  or  $S < C$



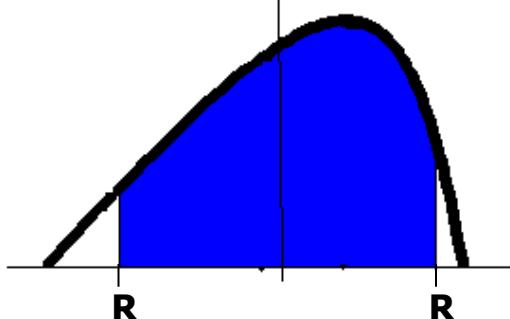
# Features of Bayesian inference

Before being Bayesian

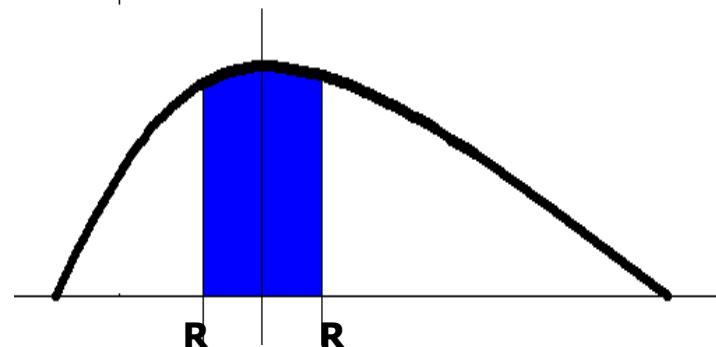
n.s. = no sé (I do not know)



After being Bayesian



There are no differences  
(in practice)



I do not know

# Features of Bayesian inference

## CREDIBILITY INTERVALS

We still have the problem of which difference is “**relevant**” for many traits:

FLAVOUR: metallic, liver, grass, sweet, etc.

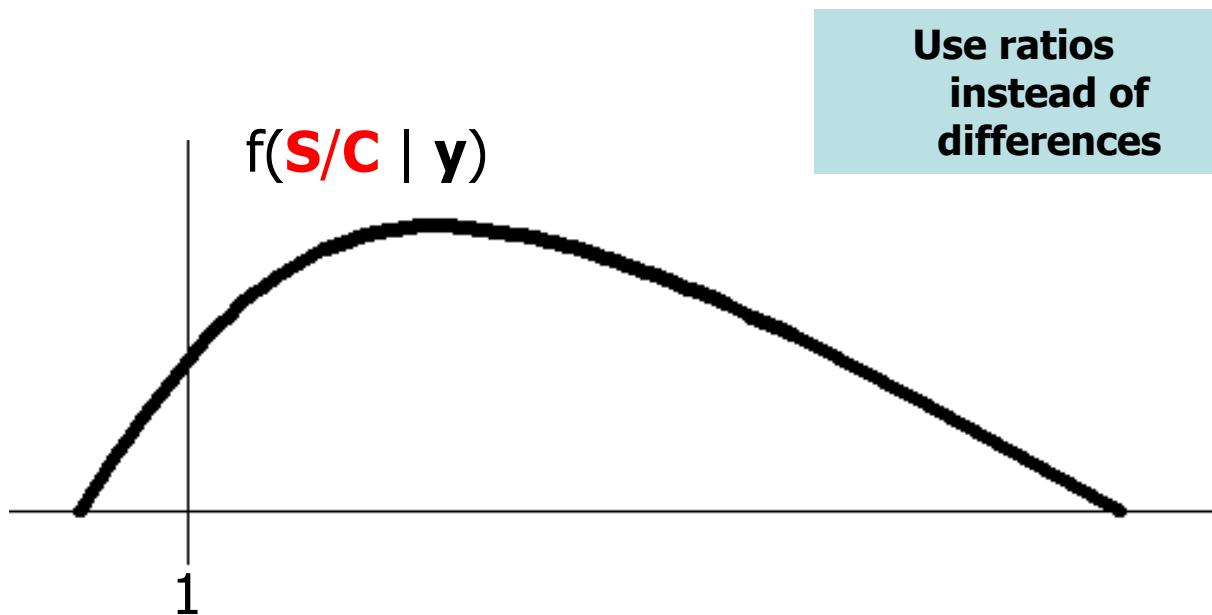
ENZYMES ACTIVITY, WHC, COLOUR, etc.

Relevant value: **1/2 or 1/3 SD** of the trait

Relevant value: **5% or 10%** higher (or lower)

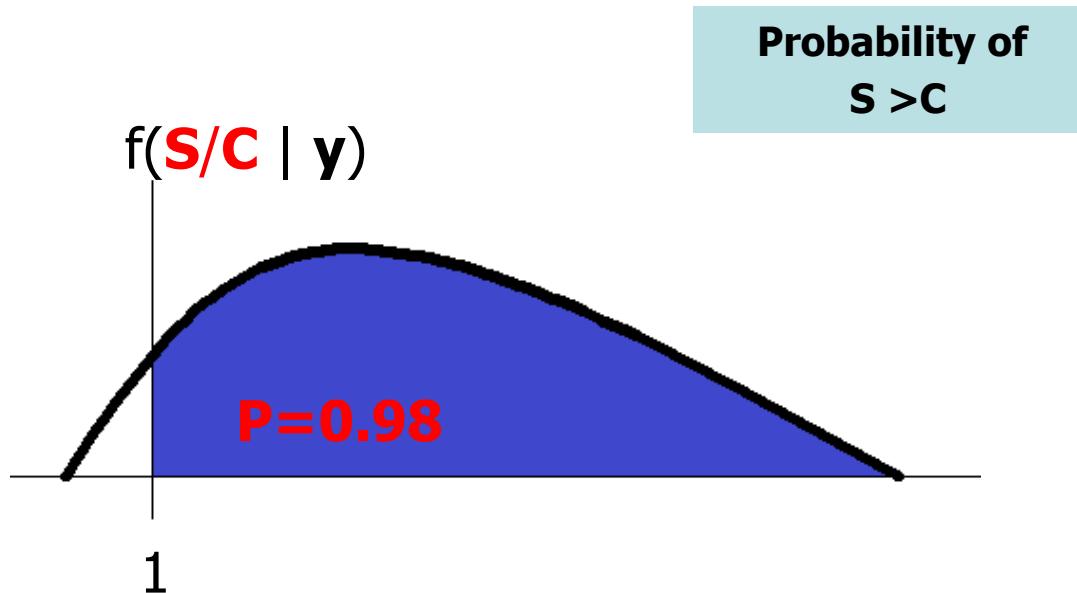
# Features of Bayesian inference

## CREDIBILITY INTERVALS



# Features of Bayesian inference

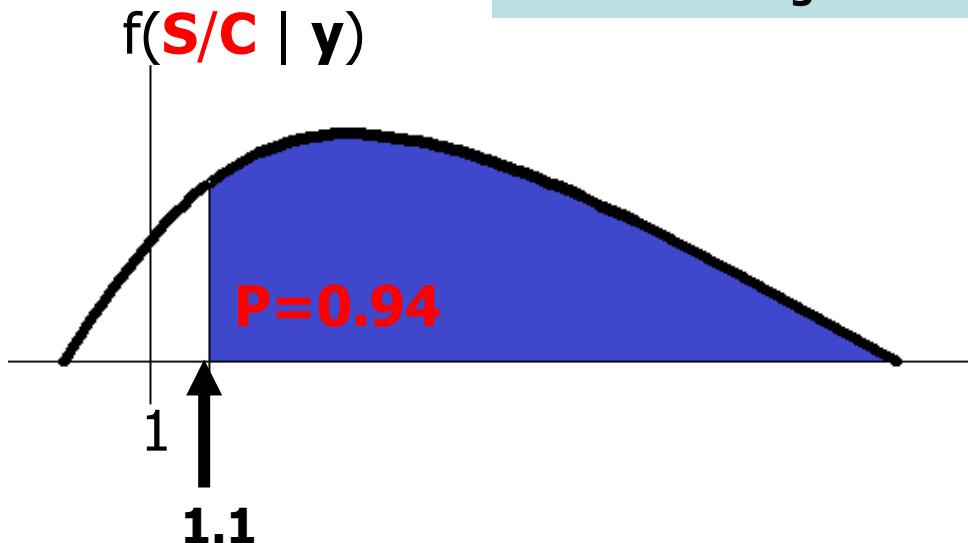
## CREDIBILITY INTERVALS



# Features of Bayesian inference

## CREDIBILITY INTERVALS

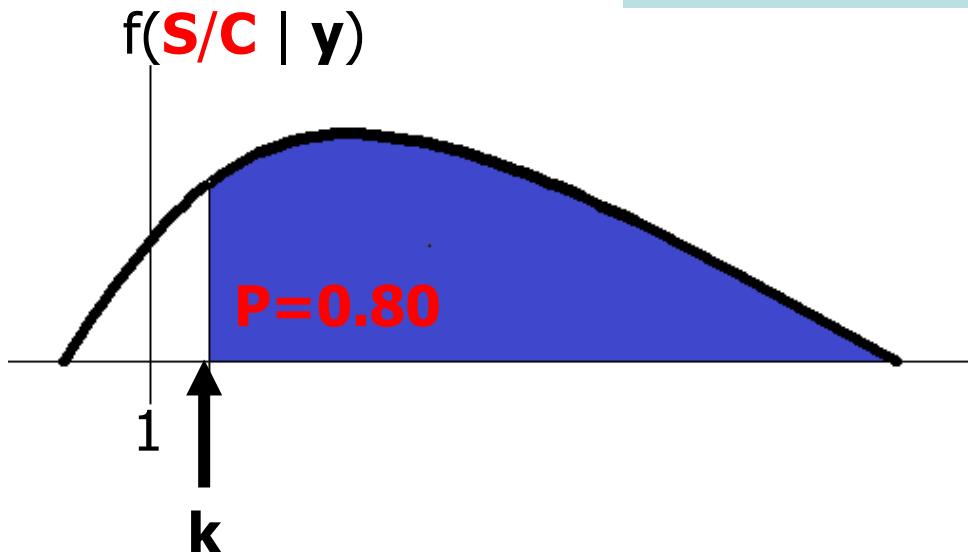
Probability of S being at least  
a 10% higher than C



# Features of Bayesian inference

## CREDIBILITY INTERVALS

**S is k times higher than C  
with a probability of 80%**



# The Bayesian choice

2.1. Bayes theorem

2.2. Features of Bayesian inference

## **2.3. Marginalisation**

2.4. Bayesian Hypothesis tests

2.5. Advantages of Bayesian inference

# Marginalisation

SALARY	British <b>B</b>	Spanish <b>S</b>
Men <b>M</b>	36 (40%)	26 (10%)
Women <b>W</b>	30 (20%)	20 (30%)

$$f(M, B) = f(M | B) \cdot f(B) \rightarrow f(H | B) = \frac{f(M, B)}{f(B)} = \frac{0.4}{0.6} = \frac{2}{3}$$

$$f(W, B) = f(W | B) \cdot f(B) \rightarrow f(W | B) = \frac{f(W, B)}{f(B)} = \frac{0.2}{0.6} = \frac{1}{3}$$

$$\text{British salary} = 36 \cdot \frac{2}{3} + 30 \cdot \frac{1}{3} = 34$$

$$\text{Spanish salary} = 26 \cdot \frac{0.3}{0.3 + 0.1} + 20 \cdot \frac{0.1}{0.3 + 0.1} = 24.5$$

# Marginalisation

SALARY	British	Spanish
Men	36 (40%)	26 (10%)
Women	30 (20%)	20 (30%)

SALARY	British	Spanish
	34 (60%)	24.5 (40%)

# Marginalisation

## EXAMPLE

$$A = b \cdot y + e = h^2 \cdot y + e$$

unknowns:  $A$  and  $h^2$       data:  $y$

Example:  $h^2$  can only take two values: 0.1 or 0.2

$$f(A | y) = f(A | h^2=0.1, y) P(h^2=0.1) + f(A | h^2=0.2, y) P(h^2=0.2)$$

When estimating  $A$ , we take into account the error of estimation of  $h^2$   
(its probability of being 0.1 or 0.2)

# Marginalisation

$$f(\mathbf{x}) = \int f(\mathbf{x}, y) dy = \int f(\mathbf{x} | y) f(y) dy$$

Summed up

Each value of  $y$

by its probability

$$A = b \cdot y + e = h^2 \cdot y + e$$

$h^2$  can take *any value* between 0 and 1

$$f(A | y) = \int_0^1 f(A | h^2, y) f(h^2) dh^2$$

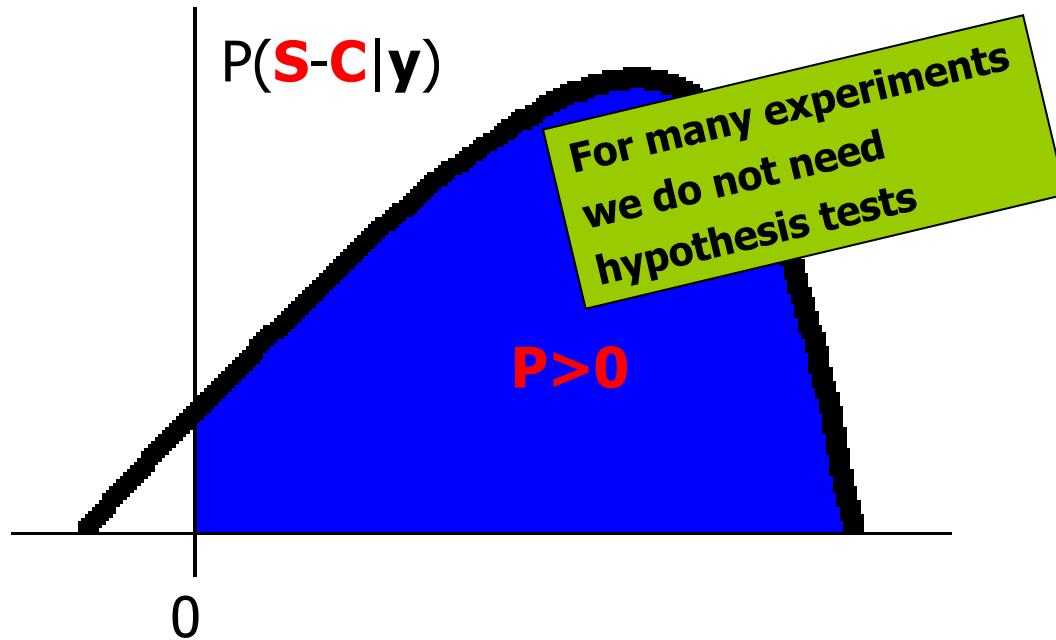
all possible values of  $h^2$  (which is 'given'), weighted by their probabilities  $f(h^2)dh^2$

# The Bayesian choice

- 2.1. Bayes theorem
- 2.2. Features of Bayesian inference
- 2.3. Marginalisation
- 2.4. Bayesian Hypothesis tests**
- 2.5. Advantages of Bayesian inference

# Hypothesis test

This is **NOT** a hypothesis test



# Hypothesis test

Calculate the probability of each hypothesis

$$P(M_1 | \mathbf{y}), P(M_2 | \mathbf{y}), P(M_3 | \mathbf{y}), \dots$$

... and choose the  $M_i$  more probable

$$P(M_1 | \mathbf{y}) = \frac{P(\mathbf{y} | M_1) \cdot P(M_1)}{P(\mathbf{y})} = \frac{P(\mathbf{y} | M_1) \cdot P(M_1)}{P(\mathbf{y} | M_1) + P(\mathbf{y} | M_2) + \dots}$$

$$M_1: \mathbf{y} = f(\boldsymbol{\theta}) + \mathbf{e}$$

$$P(\mathbf{y} | M_1) = \int f(\mathbf{y} | \boldsymbol{\theta}) \cdot f(\boldsymbol{\theta}) \cdot d\boldsymbol{\theta}$$

# The Bayesian solution

## BAYES FACTORS

$$\frac{P(M_0 | y)}{P(M_1 | y)} = \frac{P(y | M_0) \cdot P(M_0)}{P(y | M_1) \cdot P(M_1)} = BF \cdot \frac{P(M_0)}{P(M_1)}$$

**THEY ARE SENSITIVE TO PRIORS**

$$BF = \frac{P(y | M_0)}{P(y | M_1)}$$

$$\frac{P(M_0 | y)}{P(M_1 | y)} = BF$$

Moreover, often  $P(M_0) \neq P(M_1)$   
Be careful !!

If  $P(M_0) = P(M_1)$

# The Bayesian choice

- 2.1. Bayes theorem
- 2.2. Features of Bayesian inference
- 2.3. Marginalisation
- 2.4. Bayesian Hypothesis tests
- 2.5. Advantages of Bayesian inference**

# Advantages of Bayesian Inference

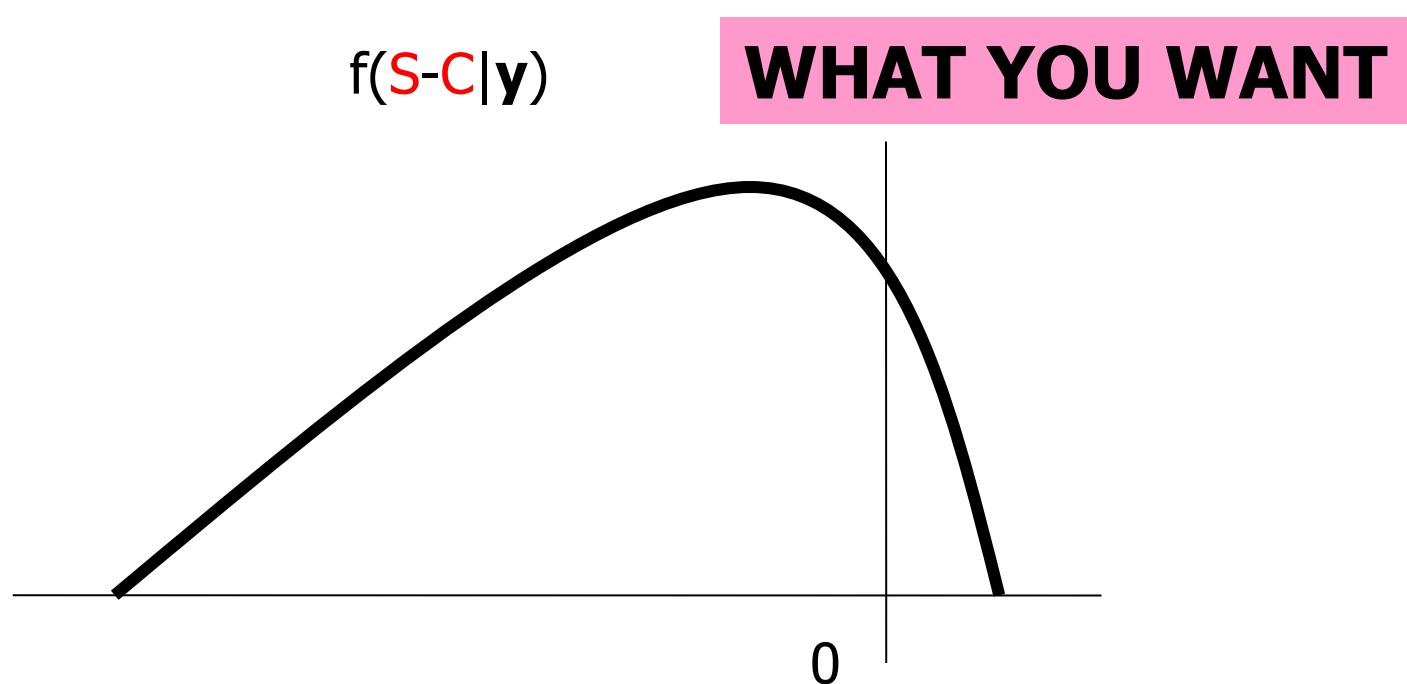
- We are not worried about bias (there is nothing like bias in a Bayesian context)
- We should not decide whether an effect is fixed or random (all of them are random)
- We normally do not need Hypothesis tests
- We have a **measure of uncertainty** for both hypothesis tests and credibility intervals, we work with Probabilities
- We work with marginal probabilities: i.e., all multivariate problems are converted in **univariate**.
- We have a method for inferences, **a path to be followed**.

# *Interlude*

*MCMC*

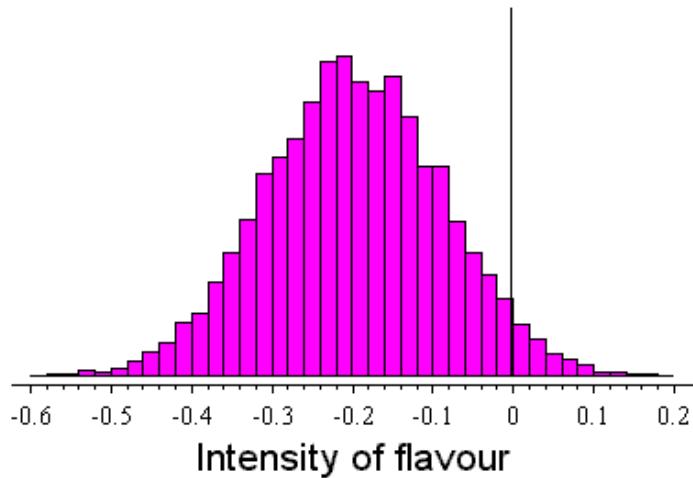
**MCMC light**  
**(without MCMC)**

# MCMC



# MCMC

**WHAT YOU GET**



# MCMC

- You get a sample of the marginal posterior distribution for each level of each effect in the model
- You can create new samples as functions of the samples  
(for example, S-C or S/C)

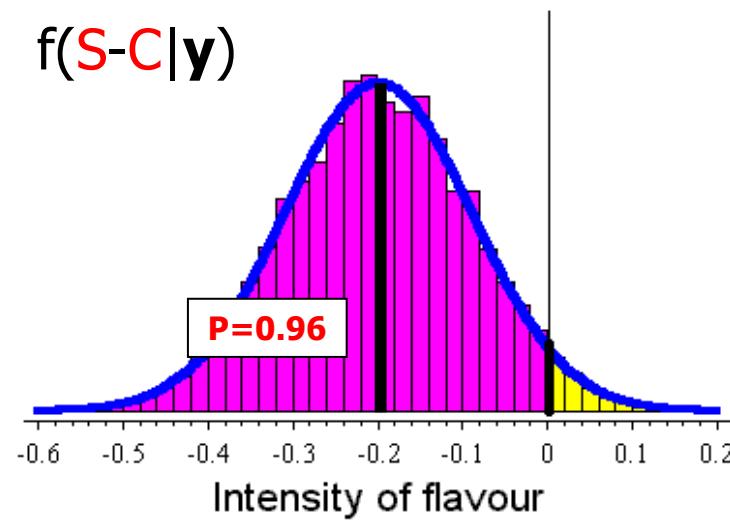
**S:** [3.1, 3.3, 4.1, 4.8, 4.9,.....]

**C:** [2.4, 2.6, 2.6, 2.6, 2.8,.....]

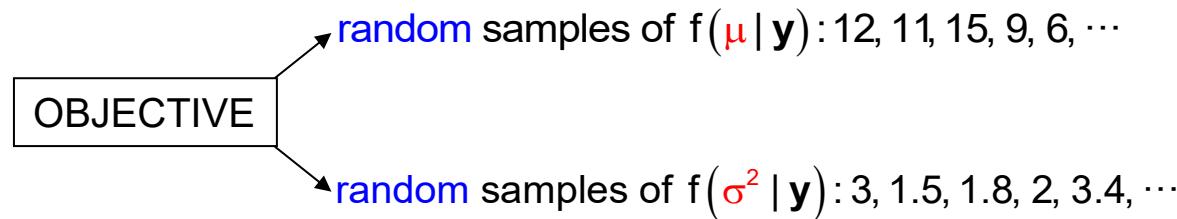
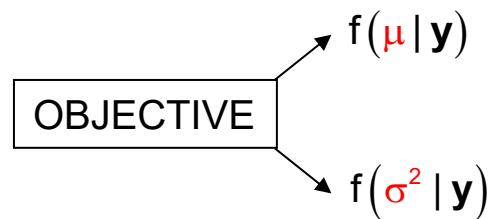
**S-C:** [0.7, 0.7, 1.5, 2.2, 2.1,.....]

**S/C:** [1.3, 1.3, 1.6, 1.8, 1.7,.....]

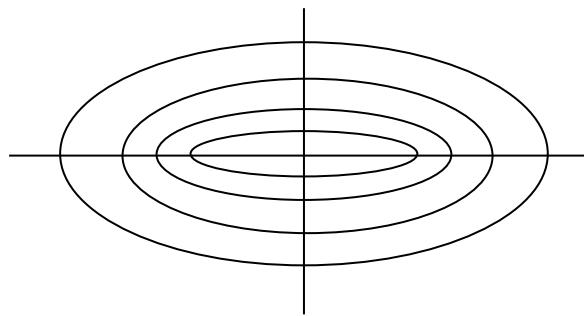
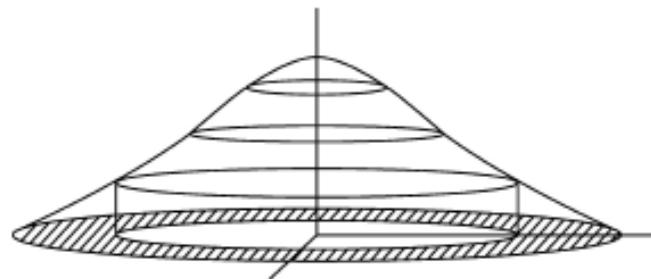
# Marginal posterior distribution



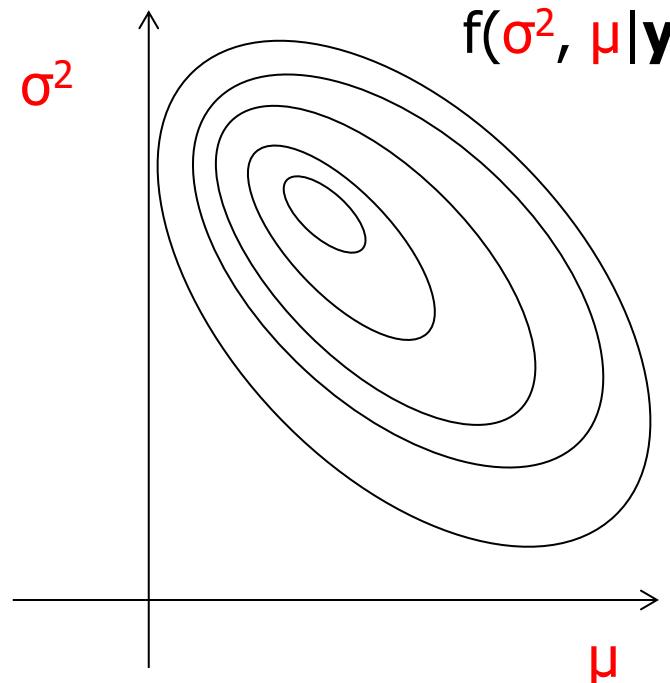
# Marginal posterior distribution



# Gibbs sampling



# Gibbs sampling



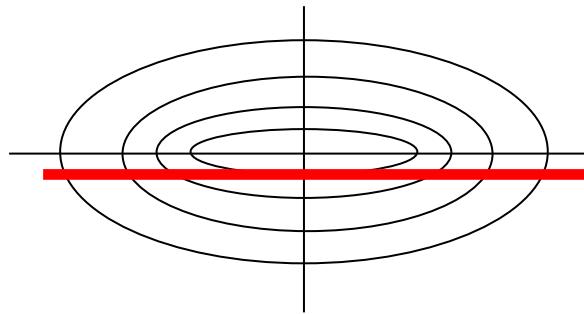
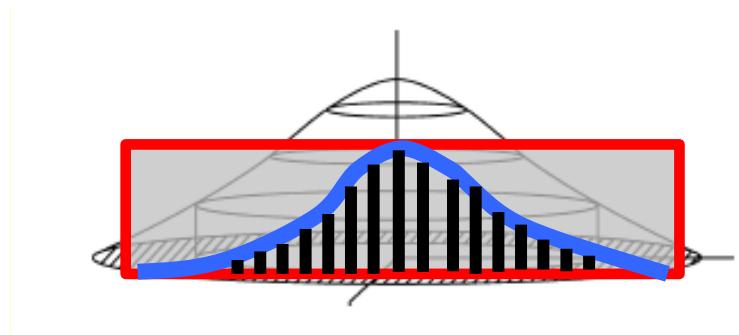
OBJECTIVE:  
Random samples  
from  $f(\sigma^2, \mu | \mathbf{y})$

$\sigma^2$	$\mu$
3	12
1.5	18
2	11
...	...
...	...

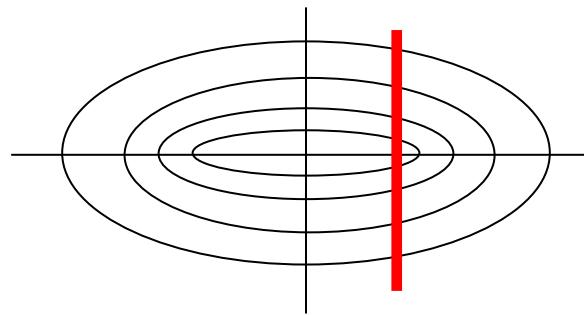
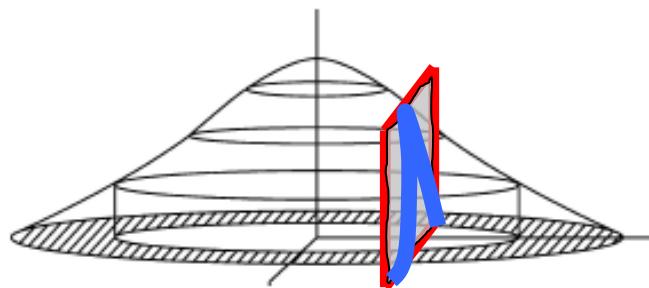
Random  
samples of  
 $f(\sigma^2 | \mathbf{y})$

Random  
samples of  
 $f(\mu | \mathbf{y})$

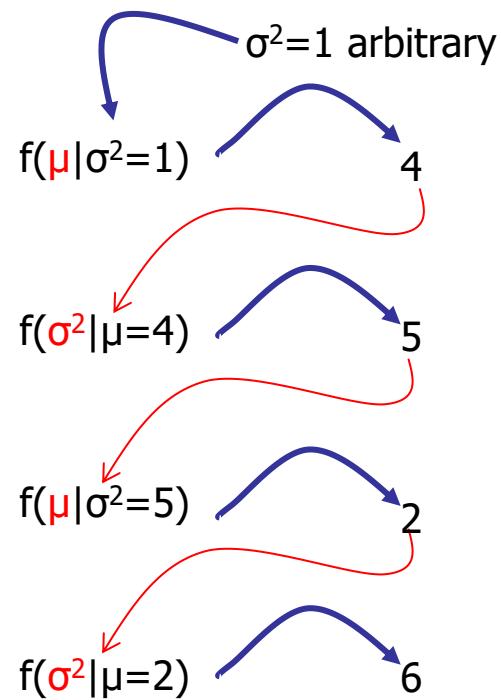
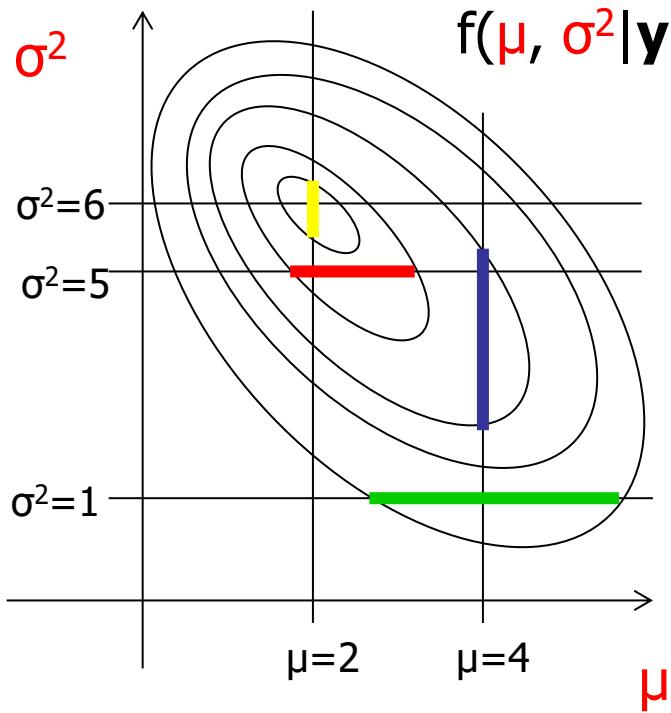
# Gibbs sampling



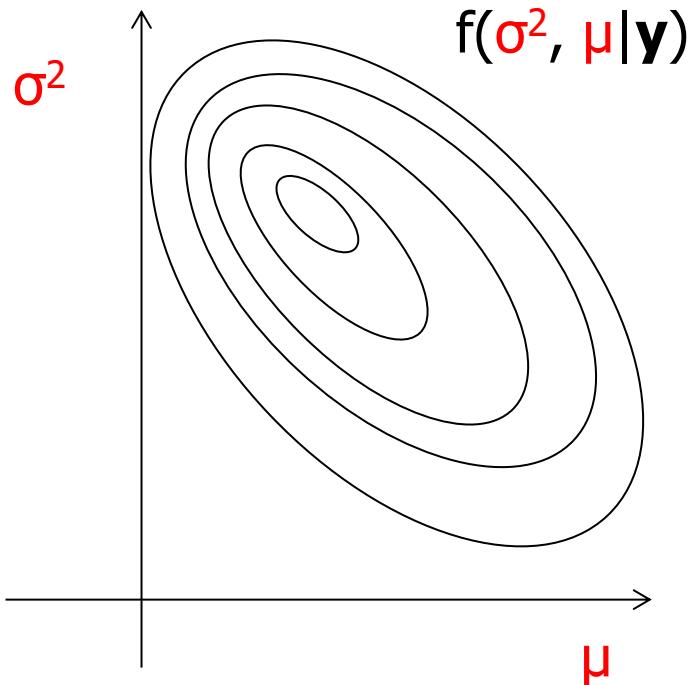
# Gibbs sampling



# Gibbs sampling



# Gibbs sampling



OBJECTIVE:  
Random samples  
from  $f(\sigma^2, \mu | \mathbf{y})$

$\sigma^2$	$\mu$
3	12
1.5	18
2	11
...	...
...	...

Random  
samples of  
 $f(\sigma^2 | \mathbf{y})$

Random  
samples of  
 $f(\mu | \mathbf{y})$

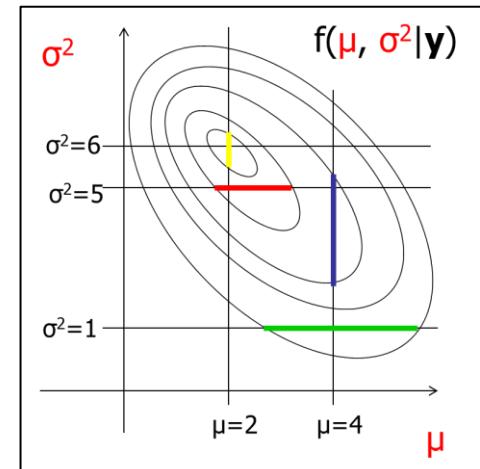
# Gibbs sampling

$$f(\mu | \sigma^2, \mathbf{y}) : [4, 3, 3.3, 4.1, 4.8, 4.9, \dots]$$

$$f(\mu | \mathbf{y}) : [4.8, 4.9, \dots]$$

$$f(\sigma^2 | \mu, \mathbf{y}) : [2, 5, 3, 3, 2.6, 2.6, 2.8, \dots]$$

$$f(\sigma^2 | \mathbf{y}) : [2.6, 2.8, \dots]$$



# Inferences

**Throw the burn-up & Sort the chain**

$f(\mu | \mathbf{y}) : [-5, -4.8, -3.9, -3.9, -1, 0.1, 1, 1.8, 3.3, 4.1, 4.9, \dots]$

$P(\mu > 0)$

**Find the % of positive samples**

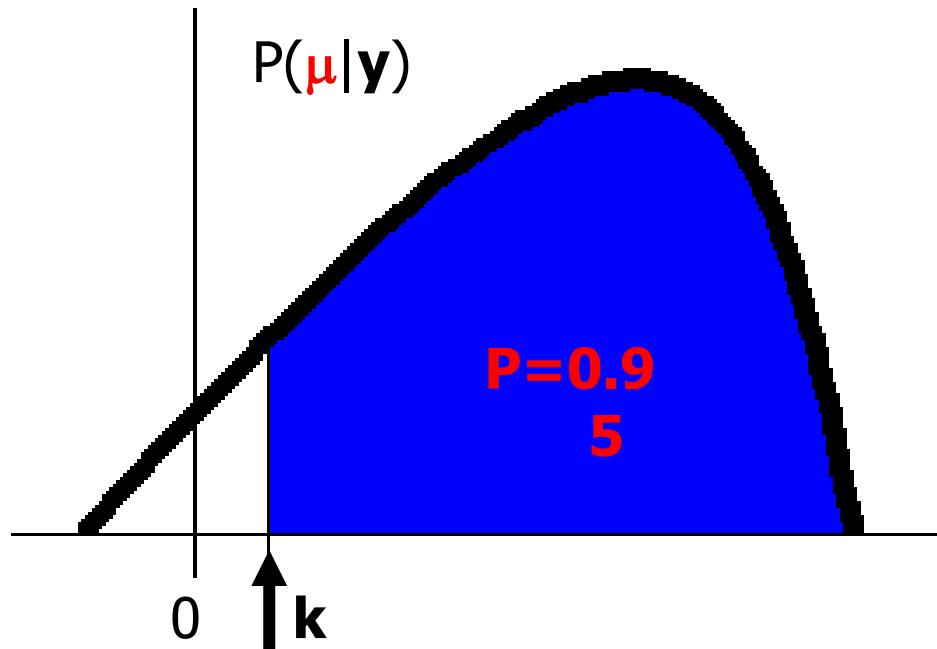
$f(\mu | \mathbf{y}) : [-5, -4.8, -3.9, -3.9, -1, 0.1, 1, 1.8, 3.3, 4.1, 4.9, \dots]$

$P(1 \leq \mu \leq 4)$

**Find the % of samples  
between 1 and 4**

$f(\mu | \mathbf{y}) : [-5, -4.8, -3.9, -3.9, -1, 0.1, 1, 1.8, 3.3, 4.1, 4.9, \dots]$

# Credibility intervals



# Inferences

$$P[k, +\infty) = 95\%$$

Find the 5 % of the first samples

$$f(\mu | \mathbf{y}) : [-5, -4.8, -3.9, -3.9, -1, 0.1, 1, 1.8, 3.3, 4.1, 4.9, \dots]$$

$$k=3.3$$

HPD(95%)

Try intervals with 95 % of samples.  
Choose the shortest one

$$f(\mu | \mathbf{y}) : [-5, -4.8, -3.9, -3.9, -1, 0.1, 1, 1.8, 3.3, 4.1, 4.9, \dots]$$

# Inferences

$$P[k, +\infty) = 95\%$$

Find the 5 % of the first samples

$$f(\mu | \mathbf{y}) : [-5, -4.8, -3.9, -3.9, -1, 0.1, 1, 1.8, 3.3, 4.1, 4.9, \dots]$$

$$k=3.3$$

HPD(95%)

Try intervals with 95 % of samples.  
Choose the shortest one

$$f(\mu | \mathbf{y}) : [-5, -4.8, -3.9, -3.9, -1, 0.1, 1, 1.8, 3.3, 4.1, 4.9, \dots]$$

# Inferences

Probability of relevance

Define the minimum relevant quantity  $R$   
Find the % of samples higher than  $R$

$f(\mu|y) : [-5, -4.8, -3.9, -3.9, -1, 0.1, \dots, 1.8, 3.3, 4.1, 4.9, \dots]$

Relevant quantity  $R = 0.5$

NO NEED OF  
INTEGRALS !!

$P(\mu \geq R) = 0.89$

**Gibbs sampling**  
**is not a method of estimation**  
**it is a numerical procedure**  
**to obtain**  
**MARGINAL POSTERIOR**  
**DISTRIBUTIONS**  
**used for Bayesian estimation**

# Gibbs sampling

- We transform a multivariate problem in several univariate problems
- We do not accept the first samples because they are not taken at random ([burn-in](#)).
- All samples are correlated. We have a [Monte Carlo](#) error

# Gibbs sampling

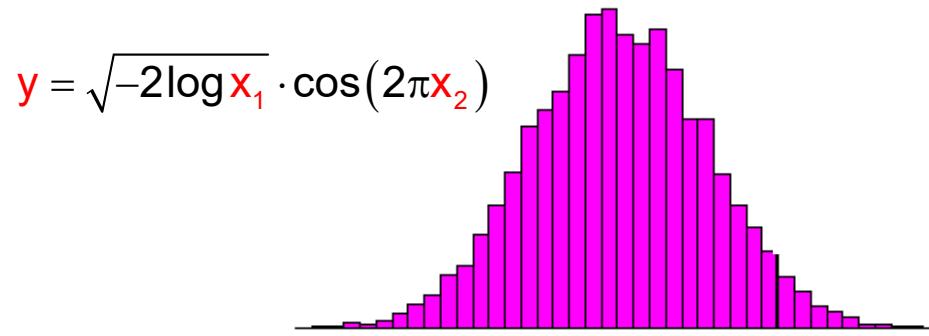
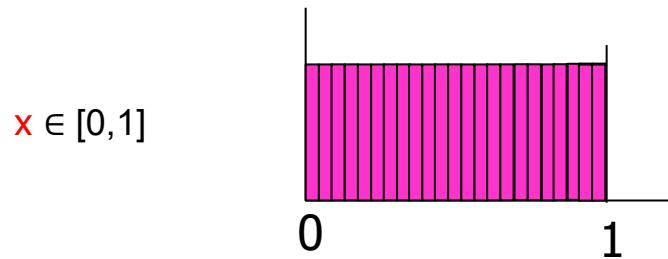
- We always accept the samples, but **we should know how to sample**
- There are algorithms to sample from known functions

FOR EXAMPLE: How to sample from a  $N(0,1)$  distribution:

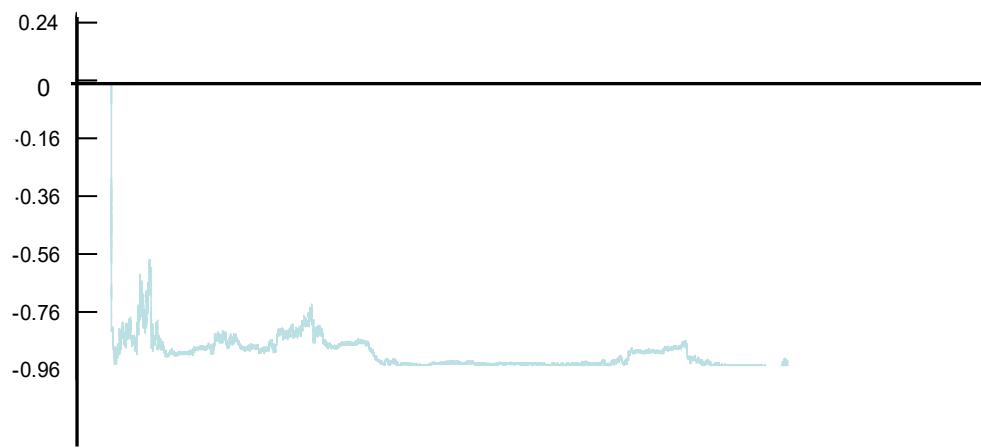
- 1) Take two random samples  $x \in [0,1]$  from a random number generator
- 2) Calculate  $y = \sqrt{-2\log x_1} \cdot \cos(2\pi x_2)$

$y$  is then a random sample from a  $N(0,1)$

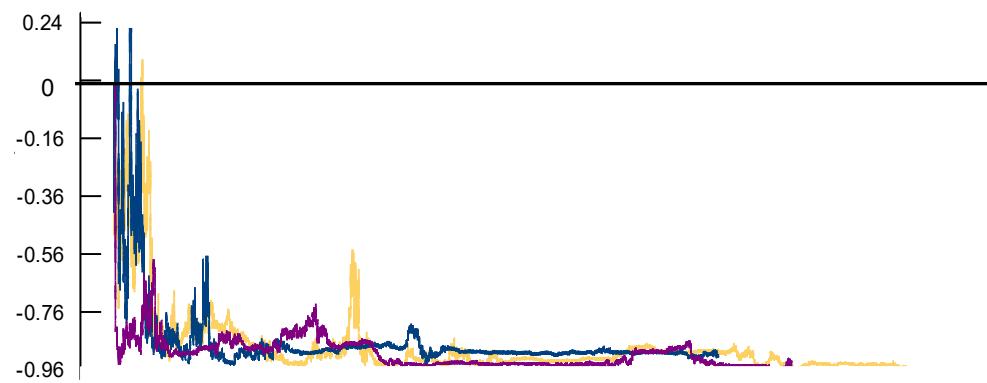
# Gibbs sampling



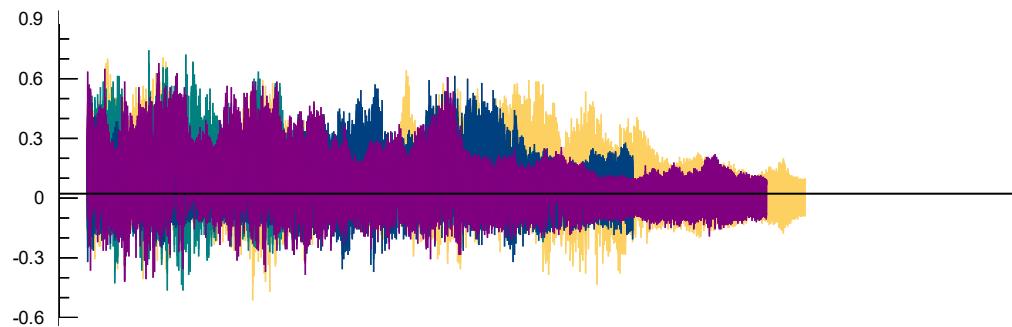
# Convergence



# Convergence



# Gibbs sampling



# Convergence tests

- GELMAN & RUBIN
  - The variance between chains is not higher than the variance within chains
- GEWEKE
  - The first half of the chain has the same average as the second part of the chain
- JOHNSON
  - Chains with the same random seed and different initial values should converge

**...they never assure convergence !!**

# Burn-in

- VISUAL INSPECTION
  - Usually it works, but it can give surprises in complicated models
- RAFTERY & LEWIS METHOD
  - It requires your chain to have some properties you do not know whether it has. It is commonly cited, mainly because it gives very low values of burn-in.
- JOHNSON COUPLED CHAINS
  - Chains with the same random seed and different initial values should converge. You decide when.

**...they never assure convergence !!**

# Monte Carlo s.e.

- We estimate the posterior distribution, we have an error of estimation called Monte Carlo s.e.
- We can make it as small as we want, taking more samples
- Samples can be highly correlated. Effective sample size is the size of a uncorrelated sample giving the same Monte Carlo s.e.
- Usually it is not a worth to take two consecutive samples, e.g., we take one each 20 or one each 50. This is called the sampling lag
- We shall calculate autocorrelation between two consecutive samples

# Other sampling methods

**WE DO NOT KNOW HOW TO SAMPLE**

- ACCEPTANCE-REJECTION SAMPLING
- METROPOLIS-HASTINGS
- IMPORTANCE SAMPLING

... etc

*End of the Interlude*