

# ABC Methods for Bayesian Model Choice

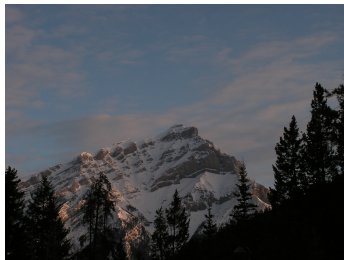
Christian P. Robert

Université Paris-Dauphine, IuF, & CREST  
<http://www.ceremade.dauphine.fr/~xian>

BIRS 12w5105

Joint work with J.-M. Cornuet, A. Grelaud,  
J.-M. Marin, N. Pillai, & J. Rousseau

# Outline



Approximate Bayesian computation

ABC for model choice

Gibbs random fields

Generic ABC model choice

Model choice consistency

# Approximate Bayesian computation

Approximate Bayesian computation

ABC for model choice

Gibbs random fields

Generic ABC model choice

Model choice consistency

## Regular Bayesian computation issues

When faced with a non-standard posterior distribution

$$\pi(\theta|\mathbf{y}) \propto \pi(\theta)L(\theta|\mathbf{y})$$

the standard solution is to use simulation (Monte Carlo) to produce a sample

$$\theta_1, \dots, \theta_T$$

from  $\pi(\theta|\mathbf{y})$  (or approximately by Markov chain Monte Carlo methods)

[Robert & Casella, 2004]

## Untractable likelihoods

Cases when the likelihood function  $f(\mathbf{y}|\theta)$  is unavailable and when the completion step

$$f(\mathbf{y}|\theta) = \int_{\mathcal{Z}} f(\mathbf{y}, \mathbf{z}|\theta) d\mathbf{z}$$

is impossible or too costly because of the dimension of  $\mathbf{z}$

© MCMC cannot be implemented!

# The ABC method

Bayesian setting: target is  $\pi(\theta)f(x|\theta)$

# The ABC method

**Bayesian setting:** target is  $\pi(\theta)f(x|\theta)$

When likelihood  $f(x|\theta)$  not in closed form, likelihood-free rejection technique:

# The ABC method

**Bayesian setting:** target is  $\pi(\theta)f(x|\theta)$

When likelihood  $f(x|\theta)$  not in closed form, likelihood-free rejection technique:

## ABC algorithm

For an observation  $\mathbf{y} \sim f(\mathbf{y}|\theta)$ , under the prior  $\pi(\theta)$ , keep *jointly* simulating

$$\theta' \sim \pi(\theta), \mathbf{z} \sim f(\mathbf{z}|\theta'),$$

*until* the auxiliary variable  $\mathbf{z}$  is **equal to the observed value**,  $\mathbf{z} = \mathbf{y}$ .

[Rubin, 1984; Tavaré et al., 1997]



## A as approximative

When  $y$  is a continuous random variable, equality  $\mathbf{z} = \mathbf{y}$  is replaced with a **tolerance** condition,

$$\varrho(\mathbf{y}, \mathbf{z}) \leq \epsilon$$

where  $\varrho$  is a distance

## A as approximative

When  $y$  is a continuous random variable, equality  $\mathbf{z} = \mathbf{y}$  is replaced with a **tolerance** condition,

$$\varrho(\mathbf{y}, \mathbf{z}) \leq \epsilon$$

where  $\varrho$  is a distance

Output distributed from

$$\pi(\theta) P_{\theta}\{\varrho(\mathbf{y}, \mathbf{z}) < \epsilon\} \propto \pi(\theta | \varrho(\mathbf{y}, \mathbf{z}) < \epsilon)$$

# ABC algorithm

---

**Algorithm 1** Likelihood-free rejection sampler

---

**for**  $i = 1$  to  $N$  **do**

**repeat**

        generate  $\theta'$  from the prior distribution  $\pi(\cdot)$

        generate  $\mathbf{z}$  from the likelihood  $f(\cdot|\theta')$

**until**  $\rho\{\eta(\mathbf{z}), \eta(\mathbf{y})\} \leq \epsilon$

    set  $\theta_i = \theta'$

**end for**

---

where  $\eta(\mathbf{y})$  defines a (maybe in-sufficient) statistic

# Output

The likelihood-free algorithm samples from the marginal in  $\mathbf{z}$  of:

$$\pi_{\epsilon}(\theta, \mathbf{z}|\mathbf{y}) = \frac{\pi(\theta)f(\mathbf{z}|\theta)\mathbb{I}_{A_{\epsilon,\mathbf{y}}}(\mathbf{z})}{\int_{A_{\epsilon,\mathbf{y}} \times \Theta} \pi(\theta)f(\mathbf{z}|\theta)d\mathbf{z}d\theta},$$

where  $A_{\epsilon,\mathbf{y}} = \{\mathbf{z} \in \mathcal{D} | \rho(\eta(\mathbf{z}), \eta(\mathbf{y})) < \epsilon\}$ .

## Output

The likelihood-free algorithm samples from the marginal in  $\mathbf{z}$  of:

$$\pi_{\epsilon}(\theta, \mathbf{z}|\mathbf{y}) = \frac{\pi(\theta)f(\mathbf{z}|\theta)\mathbb{I}_{A_{\epsilon,\mathbf{y}}}(\mathbf{z})}{\int_{A_{\epsilon,\mathbf{y}} \times \Theta} \pi(\theta)f(\mathbf{z}|\theta)d\mathbf{z}d\theta},$$

where  $A_{\epsilon,\mathbf{y}} = \{\mathbf{z} \in \mathcal{D} | \rho(\eta(\mathbf{z}), \eta(\mathbf{y})) < \epsilon\}$ .

The idea behind ABC is that the summary statistics coupled with a small tolerance should provide a good approximation of the posterior distribution:

$$\pi_{\epsilon}(\theta|\mathbf{y}) = \int \pi_{\epsilon}(\theta, \mathbf{z}|\mathbf{y})d\mathbf{z} \approx \pi(\theta|\eta(\mathbf{y})).$$

[Not guaranteed!]

# ABC for model choice

Approximate Bayesian computation

ABC for model choice

Gibbs random fields

Generic ABC model choice

Model choice consistency

# Bayesian model choice

## Principle

Several models

$$M_1, M_2, \dots$$

are considered simultaneously for dataset  $\mathbf{y}$  and model index  $\mathcal{M}$  central to inference.

Use of a prior  $\pi(\mathcal{M} = m)$ , plus a prior distribution on the parameter conditional on the value  $m$  of the model index,  $\pi_m(\boldsymbol{\theta}_m)$

Goal is to derive the posterior distribution of  $\mathcal{M}$ ,

$$\pi(\mathcal{M} = m | \text{data})$$

a challenging computational target when models are complex.

## Generic ABC for model choice

---

**Algorithm 2** Likelihood-free model choice sampler (ABC-MC)

---

**for**  $t = 1$  to  $T$  **do**

**repeat**

    Generate  $m$  from the prior  $\pi(\mathcal{M} = m)$

    Generate  $\boldsymbol{\theta}_m$  from the prior  $\pi_m(\boldsymbol{\theta}_m)$

    Generate  $\mathbf{z}$  from the model  $f_m(\mathbf{z}|\boldsymbol{\theta}_m)$

**until**  $\rho\{\eta(\mathbf{z}), \eta(\mathbf{y})\} < \epsilon$

  Set  $m^{(t)} = m$  and  $\boldsymbol{\theta}^{(t)} = \boldsymbol{\theta}_m$

**end for**

---

[Grelaud & al., 2009; Toni & al., 2009]



## ABC estimates

Posterior probability  $\pi(\mathcal{M} = m | \mathbf{y})$  approximated by the frequency of acceptances from model  $m$

$$\frac{1}{T} \sum_{t=1}^T \mathbb{I}_{m^{(t)}=m}.$$

Early issues with implementation:

- ▶ should tolerances  $\epsilon$  be the same for all models?
- ▶ should summary statistics vary across models? incl. their dimension?
- ▶ should the distance measure  $\rho$  vary across models?

## ABC estimates

Posterior probability  $\pi(\mathcal{M} = m|\mathbf{y})$  approximated by the frequency of acceptances from model  $m$

$$\frac{1}{T} \sum_{t=1}^T \mathbb{I}_{m^{(t)}=m} .$$

Extension to a weighted polychotomous logistic regression estimate of  $\pi(\mathcal{M} = m|\mathbf{y})$ , with non-parametric kernel weights

[Cornuet et al., DIYABC, 2009]

# Potts model

▸ Skip MRFs

## Potts model

Distribution with an energy function of the form

$$\theta S(\mathbf{y}) = \theta \sum_{l \sim i} \delta_{y_l = y_i}$$

where  $l \sim i$  denotes a neighbourhood structure

# Potts model

▸ Skip MRFs

## Potts model

Distribution with an energy function of the form

$$\theta S(\mathbf{y}) = \theta \sum_{l \sim i} \delta_{y_l = y_i}$$

where  $l \sim i$  denotes a neighbourhood structure

In most realistic settings, summation

$$Z_\theta = \sum_{\mathbf{x} \in \mathcal{X}} \exp\{\theta S(\mathbf{x})\}$$

involves too many terms to be manageable and numerical approximations cannot always be trusted

# Neighbourhood relations

## Setup

Choice to be made between  $M$  neighbourhood relations

$$i \stackrel{m}{\sim} i' \quad (0 \leq m \leq M - 1)$$

with

$$S_m(\mathbf{x}) = \sum_{i \stackrel{m}{\sim} i'} \mathbb{I}_{\{x_i = x_{i'}\}}$$

driven by the posterior probabilities of the models.

# Model index

Computational target:

$$\mathbb{P}(\mathcal{M} = m | \mathbf{x}) \propto \int_{\Theta_m} f_m(\mathbf{x} | \theta_m) \pi_m(\theta_m) \mathrm{d}\theta_m \pi(\mathcal{M} = m)$$

# Model index

Computational target:

$$\mathbb{P}(\mathcal{M} = m | \mathbf{x}) \propto \int_{\Theta_m} f_m(\mathbf{x} | \theta_m) \pi_m(\theta_m) d\theta_m \pi(\mathcal{M} = m)$$

If  $S(\mathbf{x})$  **sufficient statistic** for the joint parameters  
 $(\mathcal{M}, \theta_0, \dots, \theta_{M-1})$ ,

$$\mathbb{P}(\mathcal{M} = m | \mathbf{x}) = \mathbb{P}(\mathcal{M} = m | S(\mathbf{x})).$$

## Sufficient statistics in Gibbs random fields

Each model  $m$  has its own sufficient statistic  $S_m(\cdot)$  and  $S(\cdot) = (S_0(\cdot), \dots, S_{M-1}(\cdot))$  is also (model-)sufficient.



## Sufficient statistics in Gibbs random fields

Each model  $m$  has its own sufficient statistic  $S_m(\cdot)$  and  $S(\cdot) = (S_0(\cdot), \dots, S_{M-1}(\cdot))$  is also (model-)sufficient.

**Explanation:** For Gibbs random fields,

$$\begin{aligned} x|\mathcal{M} = m \sim f_m(\mathbf{x}|\theta_m) &= f_m^1(\mathbf{x}|S(\mathbf{x}))f_m^2(S(\mathbf{x})|\theta_m) \\ &= \frac{1}{n(S(\mathbf{x}))} f_m^2(S(\mathbf{x})|\theta_m) \end{aligned}$$

where

$$n(S(\mathbf{x})) = \#\{\tilde{\mathbf{x}} \in \mathcal{X} : S(\tilde{\mathbf{x}}) = S(\mathbf{x})\}$$

©  $S(\mathbf{x})$  is sufficient for the joint parameters

## More about sufficiency

If  $\eta_1(\mathbf{x})$  sufficient statistic for model  $m = 1$  and parameter  $\theta_1$  and  $\eta_2(\mathbf{x})$  sufficient statistic for model  $m = 2$  and parameter  $\theta_2$ ,  
 $(\eta_1(\mathbf{x}), \eta_2(\mathbf{x}))$  is not always sufficient for  $(m, \theta_m)$

## More about sufficiency

If  $\eta_1(\mathbf{x})$  sufficient statistic for model  $m = 1$  and parameter  $\theta_1$  and  $\eta_2(\mathbf{x})$  sufficient statistic for model  $m = 2$  and parameter  $\theta_2$ ,  $(\eta_1(\mathbf{x}), \eta_2(\mathbf{x}))$  is not always sufficient for  $(m, \theta_m)$

© Potential loss of information at the testing level

## Limiting behaviour of $B_{12}$ ( $T \rightarrow \infty$ )

ABC approximation

$$\widehat{B}_{12}(\mathbf{y}) = \frac{\sum_{t=1}^T \mathbb{I}_{m^t=1} \mathbb{I}_{\rho\{\eta(\mathbf{z}^t), \eta(\mathbf{y})\} \leq \epsilon}}{\sum_{t=1}^T \mathbb{I}_{m^t=2} \mathbb{I}_{\rho\{\eta(\mathbf{z}^t), \eta(\mathbf{y})\} \leq \epsilon}},$$

where the  $(m^t, z^t)$ 's are simulated from the (joint) prior

## Limiting behaviour of $B_{12}$ ( $T \rightarrow \infty$ )

ABC approximation

$$\widehat{B}_{12}(\mathbf{y}) = \frac{\sum_{t=1}^T \mathbb{I}_{m^t=1} \mathbb{I}_{\rho\{\eta(\mathbf{z}^t), \eta(\mathbf{y})\} \leq \epsilon}}{\sum_{t=1}^T \mathbb{I}_{m^t=2} \mathbb{I}_{\rho\{\eta(\mathbf{z}^t), \eta(\mathbf{y})\} \leq \epsilon}},$$

where the  $(m^t, z^t)$ 's are simulated from the (joint) prior

As  $T$  go to infinity, limit

$$\begin{aligned} B_{12}^\epsilon(\mathbf{y}) &= \frac{\int \mathbb{I}_{\rho\{\eta(\mathbf{z}), \eta(\mathbf{y})\} \leq \epsilon} \pi_1(\boldsymbol{\theta}_1) f_1(\mathbf{z}|\boldsymbol{\theta}_1) \, d\mathbf{z} \, d\boldsymbol{\theta}_1}{\int \mathbb{I}_{\rho\{\eta(\mathbf{z}), \eta(\mathbf{y})\} \leq \epsilon} \pi_2(\boldsymbol{\theta}_2) f_2(\mathbf{z}|\boldsymbol{\theta}_2) \, d\mathbf{z} \, d\boldsymbol{\theta}_2} \\ &= \frac{\int \mathbb{I}_{\rho\{\eta, \eta(\mathbf{y})\} \leq \epsilon} \pi_1(\boldsymbol{\theta}_1) f_1^\eta(\eta|\boldsymbol{\theta}_1) \, d\eta \, d\boldsymbol{\theta}_1}{\int \mathbb{I}_{\rho\{\eta, \eta(\mathbf{y})\} \leq \epsilon} \pi_2(\boldsymbol{\theta}_2) f_2^\eta(\eta|\boldsymbol{\theta}_2) \, d\eta \, d\boldsymbol{\theta}_2}, \end{aligned}$$

where  $f_1^\eta(\eta|\boldsymbol{\theta}_1)$  and  $f_2^\eta(\eta|\boldsymbol{\theta}_2)$  distributions of  $\eta(\mathbf{z})$

## Limiting behaviour of $B_{12}$ ( $\epsilon \rightarrow 0$ )

When  $\epsilon$  goes to zero,

$$B_{12}^{\eta}(\mathbf{y}) = \frac{\int \pi_1(\boldsymbol{\theta}_1) f_1^{\eta}(\eta(\mathbf{y})|\boldsymbol{\theta}_1) d\boldsymbol{\theta}_1}{\int \pi_2(\boldsymbol{\theta}_2) f_2^{\eta}(\eta(\mathbf{y})|\boldsymbol{\theta}_2) d\boldsymbol{\theta}_2}$$

## Limiting behaviour of $B_{12}$ ( $\epsilon \rightarrow 0$ )

When  $\epsilon$  goes to zero,

$$B_{12}^{\eta}(\mathbf{y}) = \frac{\int \pi_1(\boldsymbol{\theta}_1) f_1^{\eta}(\eta(\mathbf{y})|\boldsymbol{\theta}_1) d\boldsymbol{\theta}_1}{\int \pi_2(\boldsymbol{\theta}_2) f_2^{\eta}(\eta(\mathbf{y})|\boldsymbol{\theta}_2) d\boldsymbol{\theta}_2}$$

© Bayes factor based on the sole observation of  $\eta(\mathbf{y})$

## Limiting behaviour of $B_{12}$ (under sufficiency)

If  $\eta(\mathbf{y})$  sufficient statistic in both models,

$$f_i(\mathbf{y}|\boldsymbol{\theta}_i) = g_i(\mathbf{y})f_i^\eta(\eta(\mathbf{y})|\boldsymbol{\theta}_i)$$

Thus

$$\begin{aligned} B_{12}(\mathbf{y}) &= \frac{\int_{\Theta_1} \pi(\boldsymbol{\theta}_1)g_1(\mathbf{y})f_1^\eta(\eta(\mathbf{y})|\boldsymbol{\theta}_1) d\boldsymbol{\theta}_1}{\int_{\Theta_2} \pi(\boldsymbol{\theta}_2)g_2(\mathbf{y})f_2^\eta(\eta(\mathbf{y})|\boldsymbol{\theta}_2) d\boldsymbol{\theta}_2} \\ &= \frac{g_1(\mathbf{y}) \int \pi_1(\boldsymbol{\theta}_1)f_1^\eta(\eta(\mathbf{y})|\boldsymbol{\theta}_1) d\boldsymbol{\theta}_1}{g_2(\mathbf{y}) \int \pi_2(\boldsymbol{\theta}_2)f_2^\eta(\eta(\mathbf{y})|\boldsymbol{\theta}_2) d\boldsymbol{\theta}_2} = \frac{g_1(\mathbf{y})}{g_2(\mathbf{y})} B_{12}^\eta(\mathbf{y}). \end{aligned}$$

[Didelot, Everitt, Johansen & Lawson, 2011]



## Limiting behaviour of $B_{12}$ (under sufficiency)

If  $\eta(\mathbf{y})$  sufficient statistic in both models,

$$f_i(\mathbf{y}|\boldsymbol{\theta}_i) = g_i(\mathbf{y})f_i^\eta(\eta(\mathbf{y})|\boldsymbol{\theta}_i)$$

Thus

$$\begin{aligned} B_{12}(\mathbf{y}) &= \frac{\int_{\Theta_1} \pi(\boldsymbol{\theta}_1)g_1(\mathbf{y})f_1^\eta(\eta(\mathbf{y})|\boldsymbol{\theta}_1) d\boldsymbol{\theta}_1}{\int_{\Theta_2} \pi(\boldsymbol{\theta}_2)g_2(\mathbf{y})f_2^\eta(\eta(\mathbf{y})|\boldsymbol{\theta}_2) d\boldsymbol{\theta}_2} \\ &= \frac{g_1(\mathbf{y}) \int \pi_1(\boldsymbol{\theta}_1)f_1^\eta(\eta(\mathbf{y})|\boldsymbol{\theta}_1) d\boldsymbol{\theta}_1}{g_2(\mathbf{y}) \int \pi_2(\boldsymbol{\theta}_2)f_2^\eta(\eta(\mathbf{y})|\boldsymbol{\theta}_2) d\boldsymbol{\theta}_2} = \frac{g_1(\mathbf{y})}{g_2(\mathbf{y})} B_{12}^\eta(\mathbf{y}). \end{aligned}$$

[Didelot, Everitt, Johansen & Lawson, 2011]

© No discrepancy only when cross-model sufficiency

## Poisson/geometric example

Sample

$$\mathbf{x} = (x_1, \dots, x_n)$$

from either a Poisson  $\mathcal{P}(\lambda)$  or from a geometric  $\mathcal{G}(p)$

Sum

$$S = \sum_{i=1}^n x_i = \eta(\mathbf{x})$$

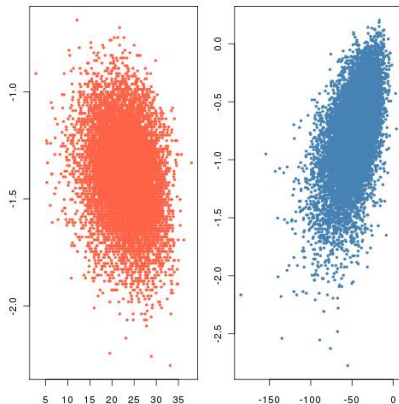
sufficient statistic for either model **but not simultaneously**

Discrepancy ratio

$$\frac{g_1(\mathbf{x})}{g_2(\mathbf{x})} = \frac{S!n^{-S} / \prod_i x_i!}{1 / \binom{n+S-1}{S}}$$

## Poisson/geometric discrepancy

Range of  $B_{12}(\mathbf{x})$  versus  $B_{12}^{\eta}(\mathbf{x})$ : The values produced have nothing in common.



## Formal recovery

Creating an encompassing exponential family

$$f(\mathbf{x}|\theta_1, \theta_2, \alpha_1, \alpha_2) \propto \exp\{\theta_1^T \eta_1(\mathbf{x}) + \theta_2^T \eta_2(\mathbf{x}) + \alpha_1 t_1(\mathbf{x}) + \alpha_2 t_2(\mathbf{x})\}$$

leads to a sufficient statistic  $(\eta_1(\mathbf{x}), \eta_2(\mathbf{x}), t_1(\mathbf{x}), t_2(\mathbf{x}))$

[Didelot, Everitt, Johansen & Lawson, 2011]

## Formal recovery

Creating an encompassing exponential family

$$f(\mathbf{x}|\theta_1, \theta_2, \alpha_1, \alpha_2) \propto \exp\{\theta_1^\top \eta_1(\mathbf{x}) + \theta_2^\top \eta_2(\mathbf{x}) + \alpha_1 t_1(\mathbf{x}) + \alpha_2 t_2(\mathbf{x})\}$$

leads to a sufficient statistic  $(\eta_1(\mathbf{x}), \eta_2(\mathbf{x}), t_1(\mathbf{x}), t_2(\mathbf{x}))$

[Didelot, Everitt, Johansen & Lawson, 2011]

In the Poisson/geometric case, if  $\prod_i x_i!$  is added to  $S$ , no discrepancy

## Formal recovery

Creating an encompassing exponential family

$$f(\mathbf{x}|\theta_1, \theta_2, \alpha_1, \alpha_2) \propto \exp\{\theta_1^T \eta_1(\mathbf{x}) + \theta_2^T \eta_2(\mathbf{x}) + \alpha_1 t_1(\mathbf{x}) + \alpha_2 t_2(\mathbf{x})\}$$

leads to a sufficient statistic  $(\eta_1(\mathbf{x}), \eta_2(\mathbf{x}), t_1(\mathbf{x}), t_2(\mathbf{x}))$

[Didelot, Everitt, Johansen & Lawson, 2011]

Only applies in genuine sufficiency settings...

© Inability to evaluate loss brought by summary statistics

## Meaning of the ABC-Bayes factor

The ABC approximation to the Bayes Factor is based solely on the summary statistics....

## Meaning of the ABC-Bayes factor

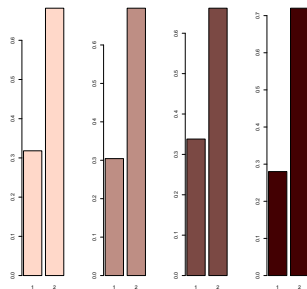
The ABC approximation to the Bayes Factor is based solely on the summary statistics....

In the Poisson/geometric case, if  $\mathbb{E}[y_i] = \theta_0 > 0$ ,

$$\lim_{n \rightarrow \infty} B_{12}^{\eta}(\mathbf{y}) = \frac{(\theta_0 + 1)^2}{\theta_0} e^{-\theta_0}$$

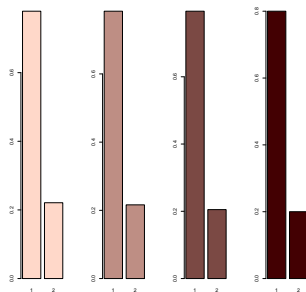


# MA example



Evolution [against  $\epsilon$ ] of ABC Bayes factor, in terms of frequencies of visits to models MA(1) (left) and MA(2) (right) when  $\epsilon$  equal to 10, 1, .1, .01% quantiles on insufficient autocovariance distances. Sample of 50 points from a MA(2) with  $\theta_1 = 0.6$ ,  $\theta_2 = 0.2$ . True Bayes factor equal to 17.71.

## MA example



Evolution [against  $\epsilon$ ] of ABC Bayes factor, in terms of frequencies of visits to models MA(1) (left) and MA(2) (right) when  $\epsilon$  equal to 10, 1, .1, .01% quantiles on insufficient autocovariance distances. Sample of 50 points from a MA(1) model with  $\theta_1 = 0.6$ . True Bayes factor  $B_{21}$  equal to .004.

# A population genetics evaluation

Population genetics example with

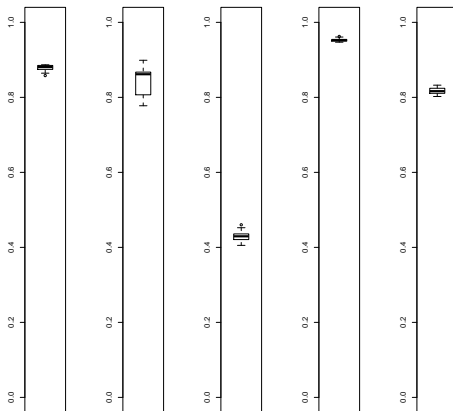
- ▶ 3 populations
- ▶ 2 scenari
- ▶ 15 individuals
- ▶ 5 loci
- ▶ single mutation parameter

# A population genetics evaluation

Population genetics example with

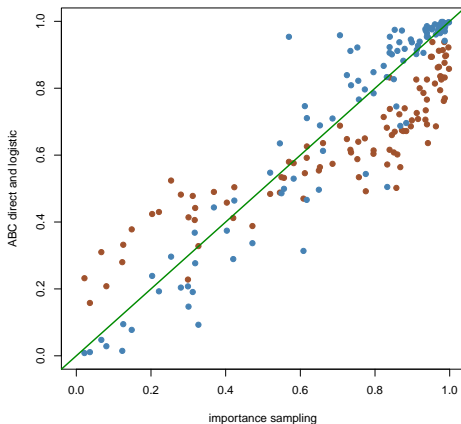
- ▶ 3 populations
- ▶ 2 scenari
- ▶ 15 individuals
- ▶ 5 loci
- ▶ single mutation parameter
- ▶ 24 summary statistics
- ▶ 2 million ABC proposal
- ▶ importance [tree] sampling alternative

# Stability of importance sampling



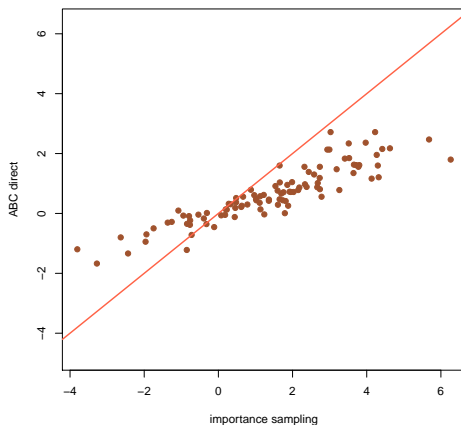
# Comparison with ABC

Use of 24 summary statistics and DIY-ABC logistic correction



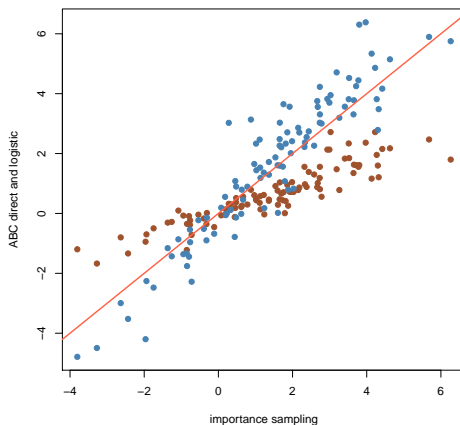
# Comparison with ABC

Use of 15 summary statistics and DIY-ABC logistic correction



# Comparison with ABC

Use of 15 summary statistics and DIY-ABC logistic correction





## The only safe cases???

Besides specific models like Gibbs random fields,  
using distances over the data itself escapes the discrepancy...

[Toni & Stumpf, 2010; Sousa & al., 2009]

## The only safe cases???

Besides specific models like Gibbs random fields,  
using distances over the data itself escapes the discrepancy...

[Toni & Stumpf, 2010; Sousa & al., 2009]

...and so does the use of more informal model fitting measures

[Ratmann & al., 2009]

# ABC model choice consistency

Approximate Bayesian computation

ABC for model choice

Gibbs random fields

Generic ABC model choice

**Model choice consistency**

# The starting point

Central question to the validation of ABC for model choice:

**When is a Bayes factor based on an insufficient statistic  $T(\mathbf{y})$  consistent?**

# The starting point

Central question to the validation of ABC for model choice:

**When is a Bayes factor based on an insufficient statistic  $T(\mathbf{y})$  consistent?**

**Note:** © drawn on  $T(\mathbf{y})$  through  $B_{12}^T(\mathbf{y})$  necessarily differs from © drawn on  $\mathbf{y}$  through  $B_{12}(\mathbf{y})$

## A benchmark if toy example

Comparison suggested by referee of **PNAS** paper [thanks]:

[X, Cornuet, Marin, & Pillai, Aug. 2011]

Model  $\mathfrak{M}_1$ :  $\mathbf{y} \sim \mathcal{N}(\theta_1, 1)$  opposed

to model  $\mathfrak{M}_2$ :  $\mathbf{y} \sim \mathcal{L}(\theta_2, 1/\sqrt{2})$ , Laplace distribution with mean  $\theta_2$  and scale parameter  $1/\sqrt{2}$  (variance one).

## A benchmark if toy example

Comparison suggested by referee of PNAS paper [thanks]:

[X, Cornuet, Marin, & Pillai, Aug. 2011]

Model  $\mathfrak{M}_1$ :  $\mathbf{y} \sim \mathcal{N}(\theta_1, 1)$  opposed

to model  $\mathfrak{M}_2$ :  $\mathbf{y} \sim \mathcal{L}(\theta_2, 1/\sqrt{2})$ , Laplace distribution with mean  $\theta_2$  and scale parameter  $1/\sqrt{2}$  (variance one).

Four possible statistics

1. sample mean  $\bar{\mathbf{y}}$  (sufficient for  $\mathfrak{M}_1$  if not  $\mathfrak{M}_2$ );
2. sample median  $\text{med}(\mathbf{y})$  (insufficient);
3. sample variance  $\text{var}(\mathbf{y})$  (ancillary);
4. median absolute deviation  $\text{mad}(\mathbf{y}) = \text{med}(\mathbf{y} - \text{med}(\mathbf{y}))$ ;

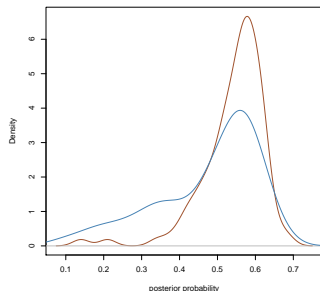
## A benchmark if toy example

Comparison suggested by referee of PNAS paper [thanks]:

[X, Cornuet, Marin, & Pillai, Aug. 2011]

Model  $\mathfrak{M}_1$ :  $\mathbf{y} \sim \mathcal{N}(\theta_1, 1)$  opposed

to model  $\mathfrak{M}_2$ :  $\mathbf{y} \sim \mathcal{L}(\theta_2, 1/\sqrt{2})$ , Laplace distribution with mean  $\theta_2$  and scale parameter  $1/\sqrt{2}$  (variance one).





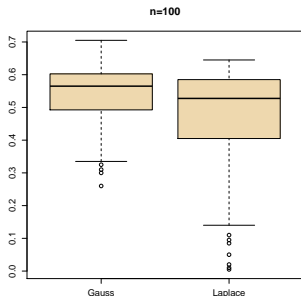
## A benchmark if toy example

Comparison suggested by referee of PNAS paper [thanks]:

[X, Cornuet, Marin, & Pillai, Aug. 2011]

Model  $\mathfrak{M}_1$ :  $\mathbf{y} \sim \mathcal{N}(\theta_1, 1)$  opposed

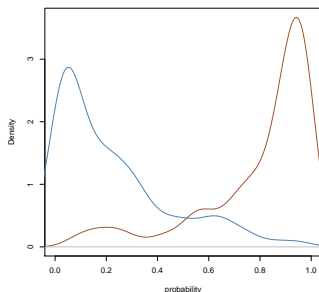
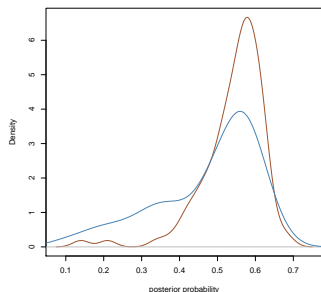
to model  $\mathfrak{M}_2$ :  $\mathbf{y} \sim \mathcal{L}(\theta_2, 1/\sqrt{2})$ , Laplace distribution with mean  $\theta_2$  and scale parameter  $1/\sqrt{2}$  (variance one).



## A benchmark if toy example

Comparison suggested by referee of PNAS paper [thanks]:  
 [X, Cornuet, Marin, & Pillai, Aug. 2011]

Model  $\mathfrak{M}_1$ :  $\mathbf{y} \sim \mathcal{N}(\theta_1, 1)$  opposed  
 to model  $\mathfrak{M}_2$ :  $\mathbf{y} \sim \mathcal{L}(\theta_2, 1/\sqrt{2})$ , Laplace distribution with mean  $\theta_2$   
 and scale parameter  $1/\sqrt{2}$  (variance one).



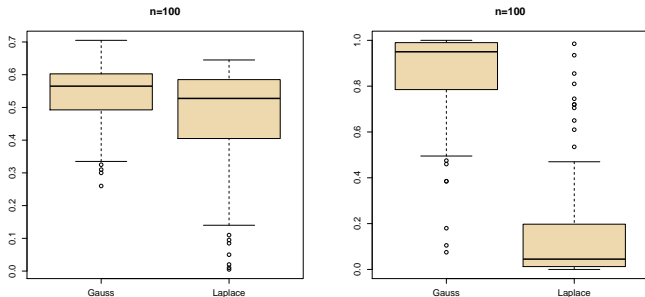
## A benchmark if toy example

Comparison suggested by referee of **PNAS** paper [thanks]:

[X, Cornuet, Marin, & Pillai, Aug. 2011]

Model  $\mathfrak{M}_1$ :  $\mathbf{y} \sim \mathcal{N}(\theta_1, 1)$  opposed

to model  $\mathfrak{M}_2$ :  $\mathbf{y} \sim \mathcal{L}(\theta_2, 1/\sqrt{2})$ , Laplace distribution with mean  $\theta_2$  and scale parameter  $1/\sqrt{2}$  (variance one).



# Framework

Starting from sample

$$\mathbf{y} = (y_1, \dots, y_n)$$

the observed sample, not necessarily iid with *true* distribution

$$\mathbf{y} \sim \mathbb{P}^n$$

Summary statistics

$$\mathbf{T}(\mathbf{y}) = \mathbf{T}^n = (T_1(\mathbf{y}), T_2(\mathbf{y}), \dots, T_d(\mathbf{y})) \in \mathbb{R}^d$$

with *true* distribution  $\mathbf{T}^n \sim G_n$ .

# Framework

## © Comparison of

- under  $\mathfrak{M}_1$ ,  $\mathbf{y} \sim F_{1,n}(\cdot|\theta_1)$  where  $\theta_1 \in \Theta_1 \subset \mathbb{R}^{p_1}$
- under  $\mathfrak{M}_2$ ,  $\mathbf{y} \sim F_{2,n}(\cdot|\theta_2)$  where  $\theta_2 \in \Theta_2 \subset \mathbb{R}^{p_2}$

turned into

- under  $\mathfrak{M}_1$ ,  $\mathbf{T}(\mathbf{y}) \sim G_{1,n}(\cdot|\theta_1)$ , and  $\theta_1|\mathbf{T}(\mathbf{y}) \sim \pi_1(\cdot|\mathbf{T}^n)$
- under  $\mathfrak{M}_2$ ,  $\mathbf{T}(\mathbf{y}) \sim G_{2,n}(\cdot|\theta_2)$ , and  $\theta_2|\mathbf{T}(\mathbf{y}) \sim \pi_2(\cdot|\mathbf{T}^n)$

# Assumptions

A collection of asymptotic “standard” assumptions:

**[A1]–[A2]** are standard central limit theorems (**[A1]** redundant when one model is “true”)

**[A3]** controls the large deviations of the estimator  $T^n$  from the estimand  $\mu(\theta)$

**[A4]** is the standard prior mass condition found in Bayesian asymptotics ( $d_i$  effective dimension of the parameter)

**[A5]** controls more tightly convergence esp. when  $\mu_i$  is not one-to-one

# Assumptions

A collection of asymptotic “standard” assumptions:

**[A1]** There exist a sequence  $\{v_n\}$  converging to  $+\infty$ ,  
 an a.c. distribution  $Q$  with continuous bounded density  $q(\cdot)$ ,  
 a symmetric,  $d \times d$  positive definite matrix  $V_0$   
 and a vector  $\mu_0 \in \mathbb{R}^d$  such that

$$v_n V_0^{-1/2} (\mathbf{T}^n - \mu_0) \overset{n \rightarrow \infty}{\rightsquigarrow} Q, \text{ under } G_n$$

and for all  $M > 0$

$$\sup_{v_n | t - \mu_0 | < M} \left| |V_0|^{1/2} v_n^{-d} g_n(t) - q(v_n V_0^{-1/2} \{t - \mu_0\}) \right| = o(1)$$

# Assumptions

A collection of asymptotic “standard” assumptions:

**[A2]** For  $i = 1, 2$ , there exist  $d \times d$  symmetric positive definite matrices  $V_i(\theta_i)$  and  $\mu_i(\theta_i) \in \mathbb{R}^d$  such that

$$v_n V_i(\theta_i)^{-1/2} (\mathbf{T}^n - \mu_i(\theta_i)) \overset{n \rightarrow \infty}{\rightsquigarrow} Q, \quad \text{under } G_{i,n}(\cdot | \theta_i).$$



# Assumptions

A collection of asymptotic “standard” assumptions:

**[A3]** For  $i = 1, 2$ , there exist sets  $\mathcal{F}_{n,i} \subset \Theta_i$  and constants  $\epsilon_i, \tau_i, \alpha_i > 0$  such that for all  $\tau > 0$ ,

$$\begin{aligned} \sup_{\theta_i \in \mathcal{F}_{n,i}} G_{i,n} \left[ |\mathbf{T}^n - \mu(\theta_i)| > \tau |\mu_i(\theta_i) - \mu_0| \wedge \epsilon_i \mid \theta_i \right] \\ \lesssim v_n^{-\alpha_i} (|\mu_i(\theta_i) - \mu_0| \wedge \epsilon_i)^{-\alpha_i} \end{aligned}$$

with

$$\pi_i(\mathcal{F}_{n,i}^c) = o(v_n^{-\tau_i}).$$

# Assumptions

A collection of asymptotic “standard” assumptions:

**[A4]** For  $u > 0$

$$S_{n,i}(u) = \{\theta_i \in \mathcal{F}_{n,i}; |\mu(\theta_i) - \mu_0| \leq u v_n^{-1}\}$$

if  $\inf\{|\mu_i(\theta_i) - \mu_0|; \theta_i \in \Theta_i\} = 0$ , there exist constants  $d_i < \tau_i \wedge \alpha_i - 1$  such that

$$\pi_i(S_{n,i}(u)) \sim u^{d_i} v_n^{-d_i}, \quad \forall u \lesssim v_n$$

# Assumptions

A collection of asymptotic “standard” assumptions:

**[A5]** If  $\inf\{|\mu_i(\theta_i) - \mu_0|; \theta_i \in \Theta_i\} = 0$ , there exists  $U > 0$  such that for any  $M > 0$ ,

$$\sup_{v_n |t - \mu_0| < M} \sup_{\theta_i \in S_{n,i}(U)} \left| |V_i(\theta_i)|^{1/2} v_n^{-d} g_i(t|\theta_i) - q(v_n V_i(\theta_i)^{-1/2} (t - \mu(\theta_i))) \right| = o(1)$$

and

$$\lim_{M \rightarrow \infty} \limsup_n \frac{\pi_i \left( S_{n,i}(U) \cap \{ \|V_i(\theta_i)^{-1}\| + \|V_i(\theta_i)\| > M \} \right)}{\pi_i(S_{n,i}(U))} = 0.$$

# Assumptions

A collection of asymptotic “standard” assumptions:

**[A1]–[A2]** are standard central limit theorems (**[A1]** redundant when one model is “true”)

**[A3]** controls the large deviations of the estimator  $T^n$  from the estimand  $\mu(\theta)$

**[A4]** is the standard prior mass condition found in Bayesian asymptotics ( $d_i$  effective dimension of the parameter)

**[A5]** controls more tightly convergence esp. when  $\mu_i$  is not one-to-one

# Effective dimension

**[A4]** Understanding  $d_1, d_2$  : defined **only when**

$\mu_0 \in \{\mu_i(\theta_i), \theta_i \in \Theta_i\}$ ,

$$\pi_i(\theta_i : |\mu_i(\theta_i) - \mu_0| < n^{-1/2}) = O(n^{-d_i/2})$$

is the effective dimension of the model  $\Theta_i$  around  $\mu_0$

## Asymptotic marginals

Asymptotically, under **[A1]–[A5]**

$$m_i(t) = \int_{\Theta_i} g_i(t|\theta_i) \pi_i(\theta_i) d\theta_i$$

is such that

(i) if  $\inf\{|\mu_i(\theta_i) - \mu_0|; \theta_i \in \Theta_i\} = 0$ ,

$$C_l v_n^{d-d_i} \leq m_i(\mathbf{T}^n) \leq C_u v_n^{d-d_i}$$

and

(ii) if  $\inf\{|\mu_i(\theta_i) - \mu_0|; \theta_i \in \Theta_i\} > 0$

$$m_i(\mathbf{T}^n) = o_{\mathbb{P}^n} [v_n^{d-\tau_i} + v_n^{d-\alpha_i}].$$

## Within-model consistency

Under same assumptions,

$$\text{if } \inf\{|\mu_i(\theta_i) - \mu_0|; \theta_i \in \Theta_i\} = 0,$$

the posterior distribution of  $\mu_i(\theta_i)$  given  $\mathbf{T}^n$  is consistent at rate  $1/v_n$  provided  $\alpha_i \wedge \tau_i > d_i$ .

## Within-model consistency

Under same assumptions,

$$\text{if } \inf\{|\mu_i(\theta_i) - \mu_0|; \theta_i \in \Theta_i\} = 0,$$

the posterior distribution of  $\mu_i(\theta_i)$  given  $\mathbf{T}^n$  is consistent at rate  $1/v_n$  provided  $\alpha_i \wedge \tau_i > d_i$ .

**Note:**  $d_i$  can truly be seen as an effective dimension of the model under the posterior  $\pi_i(\cdot|\mathbf{T}^n)$ , since if  $\mu_0 \in \{\mu_i(\theta_i); \theta_i \in \Theta_i\}$ ,

$$m_i(\mathbf{T}^n) \sim v_n^{d-d_i}$$



## Between-model consistency

Consequence of above is that asymptotic behaviour of the Bayes factor is driven by the asymptotic mean value of  $\mathbf{T}^n$  under both models. **And only by this mean value!**

## Between-model consistency

Consequence of above is that asymptotic behaviour of the Bayes factor is driven by the asymptotic mean value of  $\mathbf{T}^n$  under both models. **And only by this mean value!**

Indeed, if

$$\inf\{|\mu_0 - \mu_2(\theta_2)|; \theta_2 \in \Theta_2\} = \inf\{|\mu_0 - \mu_1(\theta_1)|; \theta_1 \in \Theta_1\} = 0$$

then

$$C_l v_n^{-(d_1-d_2)} \leq m_1(\mathbf{T}^n)/m_2(\mathbf{T}^n) \leq C_u v_n^{-(d_1-d_2)},$$

where  $C_l, C_u = O_{\mathbb{P}^n}(1)$ , irrespective of the true model.

© Only depends on the difference  $d_1 - d_2$

## Between-model consistency

Consequence of above is that asymptotic behaviour of the Bayes factor is driven by the asymptotic mean value of  $\mathbf{T}^n$  under both models. **And only by this mean value!**

Else, if

$$\inf\{|\mu_0 - \mu_2(\theta_2)|; \theta_2 \in \Theta_2\} > \inf\{|\mu_0 - \mu_1(\theta_1)|; \theta_1 \in \Theta_1\} = 0$$

then

$$\frac{m_1(\mathbf{T}^n)}{m_2(\mathbf{T}^n)} \geq C_u \min \left( v_n^{-(d_1 - \alpha_2)}, v_n^{-(d_1 - \tau_2)} \right),$$

# Consistency theorem

If

$$\inf\{|\mu_0 - \mu_2(\theta_2)|; \theta_2 \in \Theta_2\} = \inf\{|\mu_0 - \mu_1(\theta_1)|; \theta_1 \in \Theta_1\} = 0,$$

Bayes factor

$$B_{12}^T = O(v_n^{-(d_1-d_2)})$$

irrespective of the true model. It is consistent iff  $P_n$  is within the model with the smallest dimension

## Consistency theorem

If  $\mathbb{P}^n$  belongs to one of the two models and if  $\mu_0$  cannot be attained by the other one :

$$\begin{aligned} 0 &= \min (\inf \{|\mu_0 - \mu_i(\theta_i)|; \theta_i \in \Theta_i\}, i = 1, 2) \\ &< \max (\inf \{|\mu_0 - \mu_i(\theta_i)|; \theta_i \in \Theta_i\}, i = 1, 2), \end{aligned}$$

then the Bayes factor  $B_{12}^T$  is consistent

## Consequences on summary statistics

Bayes factor driven by the means  $\mu_i(\theta_i)$  and the relative position of  $\mu_0$  wrt both sets  $\{\mu_i(\theta_i); \theta_i \in \Theta_i\}$ ,  $i = 1, 2$ .

For ABC, this implies the **most likely statistics  $T^n$**  are ancillary statistics with different mean values under both models

## Consequences on summary statistics

Bayes factor driven by the means  $\mu_i(\theta_i)$  and the relative position of  $\mu_0$  wrt both sets  $\{\mu_i(\theta_i); \theta_i \in \Theta_i\}$ ,  $i = 1, 2$ .

For ABC, this implies the **most likely statistics  $T^n$  are ancillary statistics with different mean values under both models**

Else, if  $T^n$  asymptotically depends on some of the parameters of the models, it is quite likely that there exists  $\theta_i \in \Theta_i$  such that  $\mu_i(\theta_i) = \mu_0$  even though model  $\mathfrak{M}_1$  is misspecified

## Toy example: Laplace versus Gauss [1]

If

$$\mathbf{T}^n = n^{-1} \sum_{i=1}^n X_i^4, \quad \mu_1(\theta) = 3 + \theta^4 + 6\theta^2, \quad \mu_2(\theta) = 6 + \dots$$

and the true distribution is Laplace with mean  $\theta_0 = 1$ , under the Gaussian model the value  $\theta^* = 2\sqrt{3} - 3$  leads to  $\mu_0 = \mu(\theta^*)$   
[here  $d_1 = d_2 = d = 1$ ]



## Toy example: Laplace versus Gauss [1]

If

$$\mathbf{T}^n = n^{-1} \sum_{i=1}^n X_i^4, \quad \mu_1(\theta) = 3 + \theta^4 + 6\theta^2, \quad \mu_2(\theta) = 6 + \dots$$

and the true distribution is Laplace with mean  $\theta_0 = 1$ , under the Gaussian model the value  $\theta^* = 2\sqrt{3} - 3$  leads to  $\mu_0 = \mu(\theta^*)$

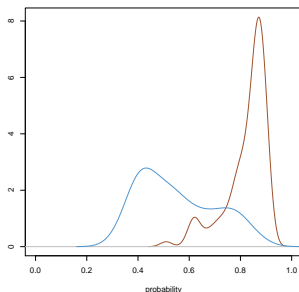
[here  $d_1 = d_2 = d = 1$ ]

© a Bayes factor associated with such a statistic is inconsistent

# Toy example: Laplace versus Gauss [1]

If

$$\mathbf{T}^n = n^{-1} \sum_{i=1}^n X_i^4, \quad \mu_1(\theta) = 3 + \theta^4 + 6\theta^2, \quad \mu_2(\theta) = 6 + \dots$$

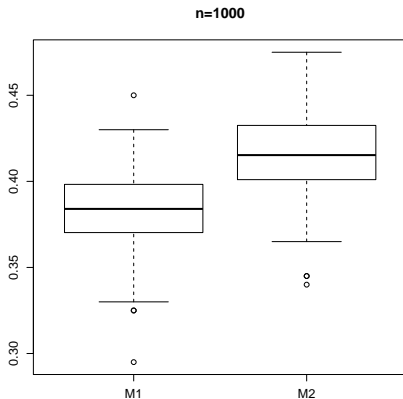


**Fourth moment**

# Toy example: Laplace versus Gauss [1]

If

$$\mathbf{T}^n = n^{-1} \sum_{i=1}^n X_i^4, \quad \mu_1(\theta) = 3 + \theta^4 + 6\theta^2, \quad \mu_2(\theta) = 6 + \dots$$



## Toy example: Laplace versus Gauss [1]

If

$$\mathbf{T}^n = n^{-1} \sum_{i=1}^n X_i^4, \quad \mu_1(\theta) = 3 + \theta^4 + 6\theta^2, \quad \mu_2(\theta) = 6 + \dots$$

**Caption:** Comparison of the distributions of the posterior probabilities that the data is from a normal model (as opposed to a Laplace model) with unknown mean when the data is made of  $n = 1000$  observations either from a normal (M1) or Laplace (M2) distribution with mean one and when the summary statistic in the ABC algorithm is restricted to the empirical fourth moment. The ABC algorithm uses proposals from the prior  $\mathcal{N}(0, 4)$  and selects the tolerance as the 1% distance quantile.

## Toy example: Laplace versus Gauss [0]

When

$$\mathbf{T}(\mathbf{y}) = \left\{ \bar{y}_n^{(4)}, \bar{y}_n^{(6)} \right\}$$

and the true distribution is Laplace with mean  $\theta_0 = 0$ , then

$$\mu_0 = 6, \mu_1(\theta_1^*) = 6 \text{ with } \theta_1^* = 2\sqrt{3} - 3$$

$$[d_1 = 1 \text{ and } d_2 = 1/2]$$

thus

$$B_{12} \sim n^{-1/4} \rightarrow 0 : \text{ consistent}$$

## Toy example: Laplace versus Gauss [0]

When

$$\mathbf{T}(\mathbf{y}) = \left\{ \bar{y}_n^{(4)}, \bar{y}_n^{(6)} \right\}$$

and the true distribution is Laplace with mean  $\theta_0 = 0$ , then

$$\mu_0 = 6, \mu_1(\theta_1^*) = 6 \text{ with } \theta_1^* = 2\sqrt{3} - 3$$

$$[d_1 = 1 \text{ and } d_2 = 1/2]$$

thus

$$B_{12} \sim n^{-1/4} \rightarrow 0 : \text{ consistent}$$

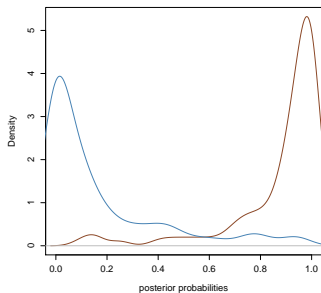
Under the Gaussian model  $\mu_0 = 3 \mu_2(\theta_2) \geq 6 > 3 \forall \theta_2$

$$B_{12} \rightarrow +\infty : \text{ consistent}$$

# Toy example: Laplace versus Gauss [0]

When

$$\mathbf{T}(\mathbf{y}) = \left\{ \bar{y}_n^{(4)}, \bar{y}_n^{(6)} \right\}$$



**Fourth AND sixth moments**

# Embedded models

When  $\mathfrak{M}_1$  submodel of  $\mathfrak{M}_2$ , and if the true distribution belongs to the smaller model  $\mathfrak{M}_1$ , Bayes factor is of order

$$v_n^{-(d_1-d_2)}$$



## Embedded models

When  $\mathfrak{M}_1$  submodel of  $\mathfrak{M}_2$ , and if the true distribution belongs to the smaller model  $\mathfrak{M}_1$ , Bayes factor is of order

$$v_n^{-(d_1-d_2)}$$

If summary statistic only informative on a parameter that is the same under both models, i.e if  $d_1 = d_2$ , then

© the Bayes factor is not consistent

## Embedded models

When  $\mathfrak{M}_1$  submodel of  $\mathfrak{M}_2$ , and if the true distribution belongs to the smaller model  $\mathfrak{M}_1$ , Bayes factor is of order

$$v_n^{-(d_1-d_2)}$$

Else,  $d_1 < d_2$  and Bayes factor is consistent under  $\mathfrak{M}_1$ . If true distribution not in  $\mathfrak{M}_1$ , then

© Bayes factor is consistent only if  $\mu_1 \neq \mu_2 = \mu_0$

## Another toy example: Quantile distribution

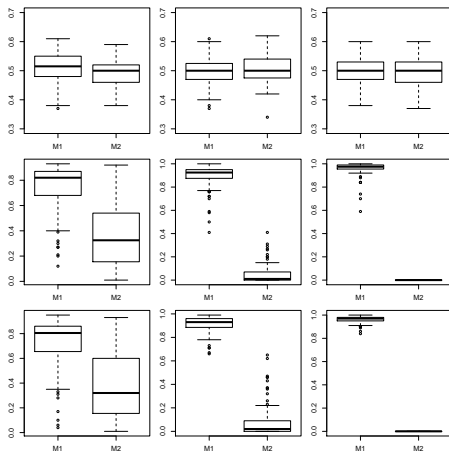
$$Q(p; A, B, g, k) = A + B \left[ 1 + \frac{1 - \exp\{-gz(p)\}}{1 + \exp\{-gz(p)\}} \right] [1 + z(p)^2]^k z(p)$$

$A, B, g$  and  $k$ , location, scale, skewness and kurtosis parameters

Embedded models:

- ▶  $\mathfrak{M}_1 : g = 0$  and  $k \sim \mathcal{U}[-1/2, 5]$
- ▶  $\mathfrak{M}_2 : g \sim \mathcal{U}[0, 4]$  and  $k \sim \mathcal{U}[-1/2, 5]$ .

# Consistency [or not]



## Consistency [or not]

**Caption:** *Comparison of the distributions of the posterior probabilities that the data is from model  $\mathfrak{M}_1$  when the data is made of 100 observations (left column), 1000 observations (central column) and 10,000 observations (right column) either from  $\mathfrak{M}_1$  (M1) or  $\mathfrak{M}_2$  (M2) when the summary statistics in the ABC algorithm are made of the empirical quantile at level 10% (first row), the empirical quantiles at levels 10% and 90% (second row), and the empirical quantiles at levels 10%, 40%, 60% and 90% (third row), respectively. The boxplots rely on 100 replicas and the ABC algorithms are based on  $10^4$  proposals from the prior, with the tolerance being chosen as the 1% quantile on the distances.*

# Conclusions

- Model selection feasible with ABC
- Choice of summary statistics is paramount
- At best, ABC  $\rightarrow \pi(\cdot | \mathbf{T}(\mathbf{y}))$  which concentrates around  $\mu_0$

# Conclusions

- Model selection feasible with ABC
- Choice of summary statistics is paramount
- At best, ABC  $\rightarrow \pi(\cdot | \mathbf{T}(\mathbf{y}))$  which concentrates around  $\mu_0$
- For estimation :  $\{\theta; \mu(\theta) = \mu_0\} = \theta_0$
- For testing  $\{\mu_1(\theta_1), \theta_1 \in \Theta_1\} \cap \{\mu_2(\theta_2), \theta_2 \in \Theta_2\} = \emptyset$