



**POLITECNICO**  
MILANO 1863

# How approximate is ABC?

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## ABC

## ► Inputs

- $N > 0$  integer
- $\pi(\theta|y_{obs}) \propto p(y_{obs}|\theta)\pi(\theta)$  target posterior density
- $g(\theta)$  proposal density
- $h > 0$  scale parameter
- $s = S(y)$  summary statistic

## ► Sampling

For  $i=1:N$

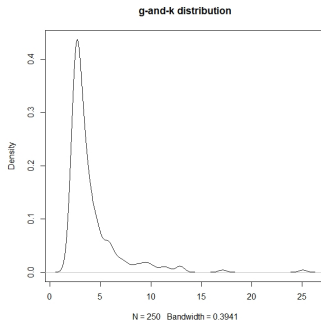
1. Generate  $\theta^{(i)} \sim g(\theta)$
2. Generate  $y \sim p(y|\theta^{(i)})$
3. Compute summary statistic  $s = S(y)$ 
  - if  $d(s, s_{obs}) \leq h$  then accept  $\theta^{(i)}$  with probability  $\frac{\pi(\theta^{(i)})}{Kg(\theta^{(i)})}$   
where  $K \geq \max_{\theta} \frac{\pi(\theta)}{g(\theta)}$ , otherwise go to 1.

## g-and-k distribution

It's a classical example of ABC because it is a flexible shaped distribution and, for this reason, **it is used to model non-standard data through a small number of parameters.**

$$q \in (0, 1) \mapsto A + B(1 + 0.8 \frac{1 - e^{-g * z(q)}}{1 + e^{-g * z(q)}})(1 + z(q)^2)^k z(q)$$

- $n = 250$
- $A = 3$
- $B = 1$
- $g = 2$
- $k = 0.5$



## Wasserstein distance

A natural approach to **reduce the variance of the distance while avoiding loss of information**, caused by the use of summary statistics, is to consider the following distance:

$$\mathcal{W}(y_{1:n}, z_{1:n}) = \inf_{\sigma \in \mathcal{S}_n} \frac{1}{n} \sum_{i=1}^n |y_i - z_{\sigma(i)}|$$

where  $\mathcal{S}_n$  is the permutation of  $\{1, \dots, n\}$ .

Since observations are univariate, the infimum is reached when  $y_{1:n}$  and  $z_{1:n}$  are sorted in increasing order and matching the order statistics.

## Numerical experiment

We estimate the **posterior distribution** by running 5 **Metropolis–Hastings chains** for 75000 iterations and discard the first 50000 as burn-in.

For the **WABC approximation**, we use the **MCMC sampler** with  $N = 2048$  particles, for a total of  $2,4 * 10^6$  simulations from the model.

## WABC

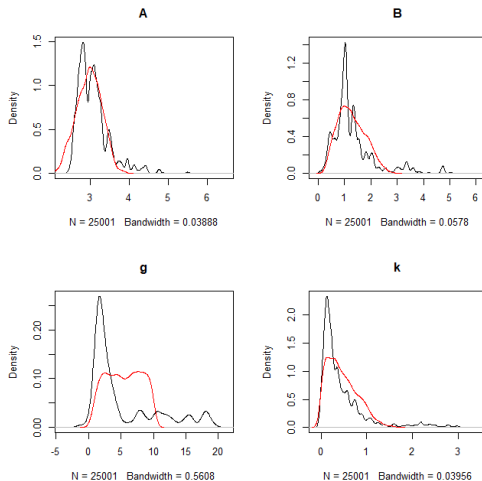


Figure: Posterior distribution estimate, **WABC approximation**

# Semi-automatic ABC

## ► Inputs

- $N > 0$  integer
- $\pi(\theta|y_{obs}) \propto p(y_{obs}|\theta)\pi(\theta)$  target posterior density
- $gk(\theta)$  *univariate g-and-k distribution* as proposal density
- $h > 0$  scale parameter
- $s = S(y)$  summary statistic

## ► Sampling

For  $i=1:N$

1. Generate  $\theta^{(i)} \sim gk(\theta)$
2. Generate  $y \sim p(y|\theta^{(i)})$
3. Compute summary statistic  $s = S(y)$

- if  $\mathcal{W}(s, s_{obs}) \leq h$  then accept  $\theta^{(i)}$  with probability  $\frac{\pi(\theta^{(i)})}{Kg(\theta^{(i)})}$   
where  $K \geq \max_{\theta} \frac{\pi(\theta)}{g(\theta)}$ , otherwise go to 1.

## Semi-automatic ABC

The core idea behind semi-automatic ABC is that we can use simulation to estimate appropriate summary statistics that are equal to posterior means.

### Steps

1. *simulate sets of parameter values and data*
2. *use the simulated sets of parameter values and data to estimate the summary statistics*
3. *run ABC with this choice of summary statistics*



## Semi-automatic ABC

1. Simulate  $M$  sets of parameter values from the prior and for each of them we simulate an artificial dataset.
2. Consider a vector of **linear transformation of the data**  $f(y) = (y, y^2)$  and fit the model

$$\theta_i = E(\theta_i|y) + \epsilon_i = \beta_0^{(i)} + \beta^{(i)}f(y) + \epsilon_i$$

where  $\theta_i$  is the  $i$ th parameter and  $\epsilon_i$  is some mean-zero noise.  
 $E(\theta_i|y)$  is estimated by the fitted function  $\beta_0^{(i)} + \beta^{(i)}f(y)$ .

3. ABC uses only the **difference in summary statistics** so  $\beta_0$  can be neglected and the summary statistic for ABC is just  $\hat{\beta}^{(i)}f(y)$ .

# Semi-automatic ABC

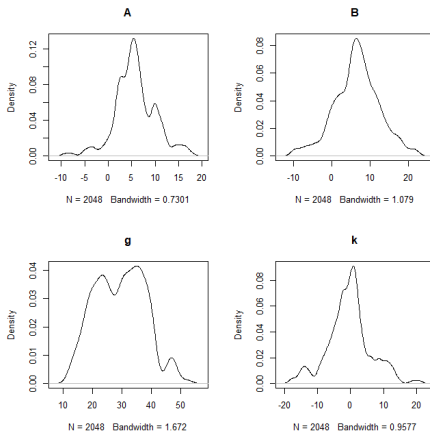


Figure: ABC semi-automatic approximation

# ABC SMC

ABC method based on sequential Monte Carlo is an alternative approach to estimate dynamical models' parameters.

## Why should we use ABC SMC?

- ▶ Information about the inferability of parameters
- ▶ Information about model sensitivity
- ▶ **Better performances** with respect to other ABC approaches
- ▶ Developed as a tool for model selection, it's able to choose the best model using the standard Bayesian model selection apparatus.

## ABC SMC

For  $i=1, \dots, N$

1. Generate  $\theta_0^{(i)} \sim g(\theta)$
2. Generate  $y_0^{(i)}(t) \sim p(y|\theta_0^{(i)})$  and compute  $s_0^{(i)}(t) = S(y_0^{(i)}), \forall t = 1, \dots, T$
3. Compute weights  $w_0^{(i)} = \pi(\theta_0^{(i)})/g(\theta_0^{(i)})$  and set  $m = 1$
4. **Sampling**

► **Reweighth**

Determine

$h_m : ESS(w_m^{(m)}, \dots, w_m^{(N)}) = \alpha ESS(w_{m-1}^{(m)}, \dots, w_{m-1}^{(N)})$  where

$w_m^{(i)} = w_{m-1}^{(i)} \frac{\sum_{t=1}^T K_{h_m}(\|s_{m-1}^{(i)}(t) - s_{obs}\|) \pi(\theta_m^{(i)})}{\sum_{t=1}^T K_{h_{m-1}}(\|s_{m-1}^{(i)}(t) - s_{obs}\|) \pi(\theta_{m-1}^{(i)})}$ , then compute

new particle weights and set  $\theta_m^{(i)} = \theta_{m-1}^{(i)}, s_m^{(i)} = s_{m-1}^{(i)}$

$\forall i = 1 : n \forall t = 1 : T$

## ABC SMC

## ► Resample

If  $ESS(w_m^{(m)}, \dots, w_m^{(N)}) < E$  then resample  $N$  particles from  $\{\theta_m^{(i)}, s_m^{(i)}(1), \dots, s_m^{(i)}(T), w_m^{(i)} / \sum_{j=1}^N w_m^{(j)}\}$  and set  $w_m^{(i)} = 1/N$

## ► Move

For  $i=1, \dots, N$

If  $w_m^{(i)} > 0$

(a) Generate  $\theta' \sim g_m(\theta_m^{(i)}, \theta)$ ,  $y'(t) \sim p(y|\theta_m^{(i)})$  and compute  $s'(t) = S(y'(t)) \forall t = 1, \dots, T$

(b) Accept  $\theta'$  with probability

$$\min\left\{1, \frac{\sum_{t=1}^T K_{h_m}(\|s_{m-1}^{(i)}(t) - s_{obs}\|) \pi(\theta_m^{(i)}) g(\theta', \theta_m^{(i)})}{\sum_{t=1}^T K_{h_{m-1}}(\|s_{m-1}^{(i)}(t) - s_{obs}\|) \pi(\theta_{m-1}^{(i)}) g(\theta_m^{(i)}, \theta')}\right\} \text{ and set}$$

$$\theta_m^{(i)} = \theta', s_m^{(i)}(t) = s'(t) \forall t = 1, \dots, T$$

(c) Increment  $m = m + 1$ .

If stopping rule is not satisfied, go to (a)

## ABC SMC

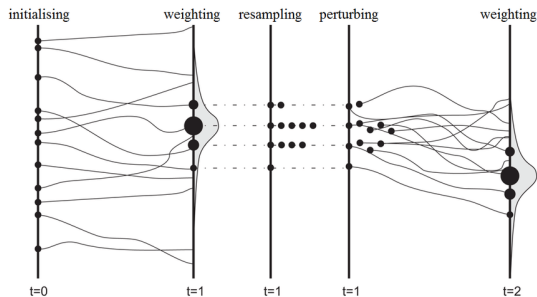


Figure: D. Alvares, "Sequential Monte Carlo methods in Bayesian joint models for longitudinal and time-to-event data" (2017).

## ABC SMC

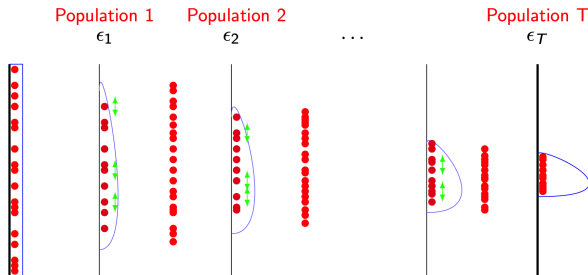


Figure: T. Toni, M. Stumpf, "Tutorial on ABC rejection and ABC SMC for parameter estimation and model selection" (2009).

## WABC SMC

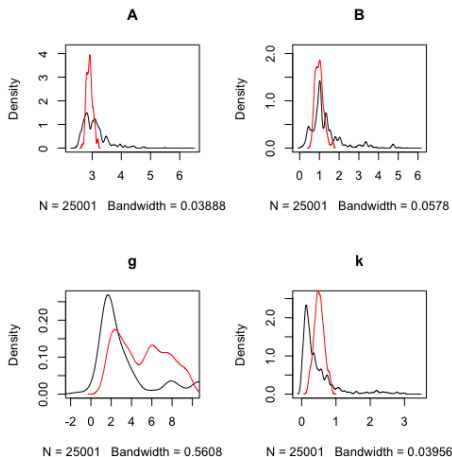
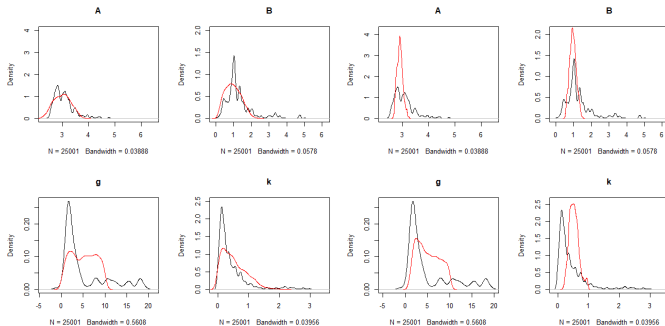


Figure: Posterior distribution estimate, WABC-SMC approximation



# Comparison

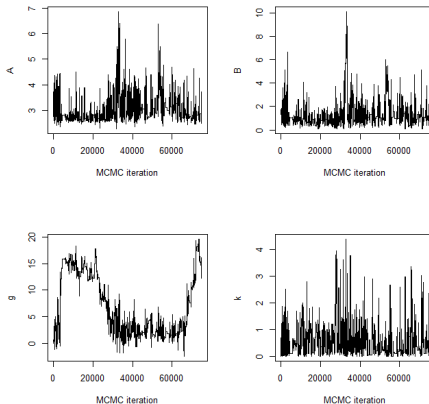


(a) WABC




(b) WABC-SMC

## Conclusion

- ▶ WABC-SMC posteriors are closer to the target distributions
- ▶ Neither method captures the marginal posterior of  $g$  well



## References

-  **S.A. Sisson, Y. Fan and M. Beaumont**, "Handbook of Approximate Bayesian Computation", *Chapman and Hall/CRC*, Chapter 1, pp. 3-44, (2018).
-  **E. Bernton, P.E. Jacob, M. Gerber, C.P. Robert**, "Approximate Bayesian computation with the Wasserstein distance", *Journal of the Royal Statistical Society: Series B*, Volume 81, Issue 2, pp. 235-269, (2019).
-  **P. Del Moral, A. Doucet, A. Jasra**, "An adaptive sequential Monte Carlo method for approximate Bayesian computation", *Statistics and Computing*, 22 pp. 1009–1020, (2012).

## References



**T. Toni, D. Welch, N. Strelkowa, A. Ipsen and M. Stumpf**, "Approximate Bayesian Computation scheme for parameter inference and model selection in dynamical systems", *Journal of the Royal Statistical Society*, Volume 6, Number 31, pp. 187-202, (2008).



**P. Fearnhead and D. Prangle**, "Constructing summary statistics for approximate Bayesian computation: semi-automatic approximate Bayesian computation", *Journal of the Royal Statistical Society: Series B*, Volume 74, Number 3, pp. 419-474, (2012).

# Repository on GitHub

README.md

## HowApproximateIsABC

Project of the Bayesian Statistics's course at Politecnico di Milano A.Y. 2020/2021

### 1stPresentation

Introduction to the ABC algorithm.

### 2ndPresentation

Practical difficulties on implementing ABC.

#### ReachDataset

Analyzing practical difficulties in ABC algorithm: how to choose *acceptance rate* and *tolerance*.

#### GenusDataset

Analyzing practical difficulties in ABC algorithm: how to choose *summary statistics* and *kernel*.

#### DarwinDataset

Analyzing practical difficulties in ABC algorithm: how to choose the *proposal*.

### 3rdPresentation

Example with the *univariate g-and-k* distribution based on <https://github.com/pierrejacob/winference> and <https://github.com/dennisprangle/abctools>



#### Contributors 3



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#### Languages



• R 100.0%

<https://github.com/marikadimarcantonio/HowApproximateIsABC>

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