



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 $i=1:N$

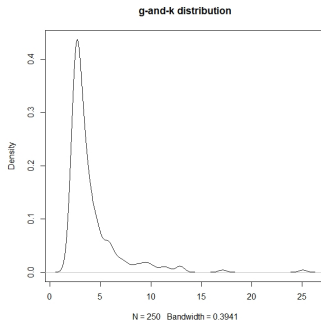
1. Generate $\theta^{(i)} \sim g(\theta)$
2. Generate $y \sim p(y|\theta^{(i)})$
3. Compute summary statistic $s = S(y)$
 - if $d(s, s_{obs}) \leq h$ then accept $\theta^{(i)}$ with probability $\frac{\pi(\theta^{(i)})}{Kg(\theta^{(i)})}$
where $K \geq \max_{\theta} \frac{\pi(\theta)}{g(\theta)}$, otherwise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

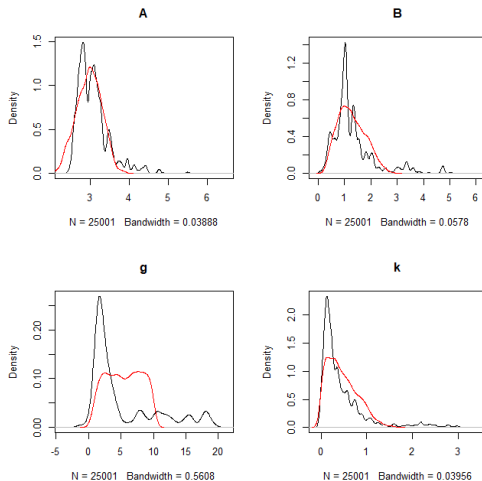


Figure: Posterior distribution estimate, **WABC approximation**

WABC

► 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 θ_i is the i th parameter and ϵ_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 β_0 can be neglected and the summary statistic for ABC is just $\hat{\beta}^{(i)}f(y)$.

Semi-automatic ABC

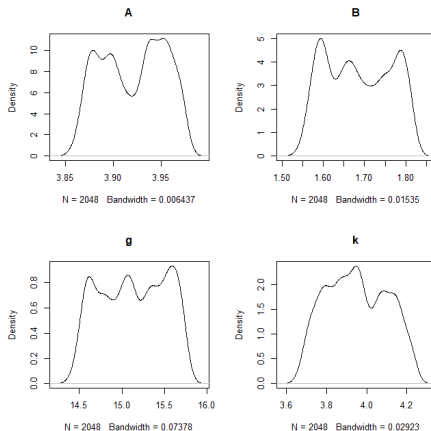


Figure: WABC semi-automatic approximation

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 θ' 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

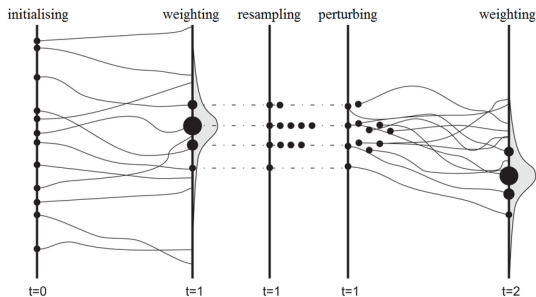


Figure: D. Alvares, "Sequential Monte Carlo methods in Bayesian joint models for longitudinal and time-to-event data" (2017).

ABC SMC

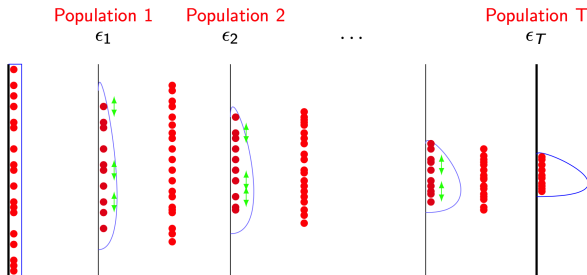


Figure: T. Toni, M. Stumpf, "Tutorial on ABC rejection and ABC SMC for parameter estimation and model selection" (2009).

WABC SMC

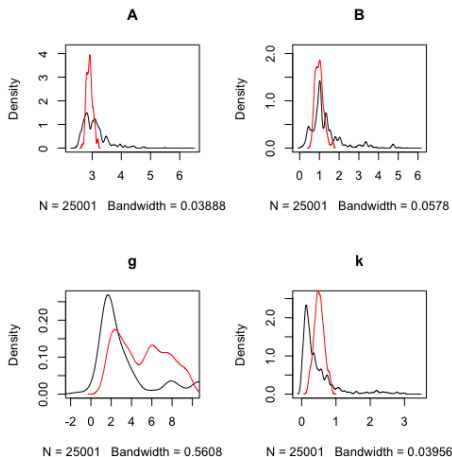
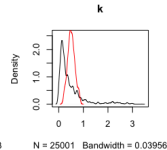
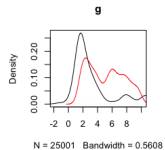
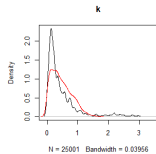
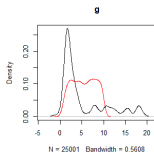
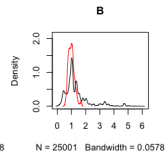
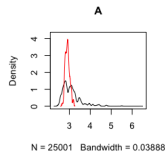
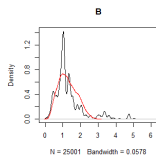
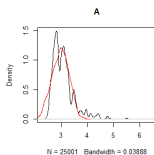


Figure: Posterior distribution estimate, WABC-SMC approximation

Comparison

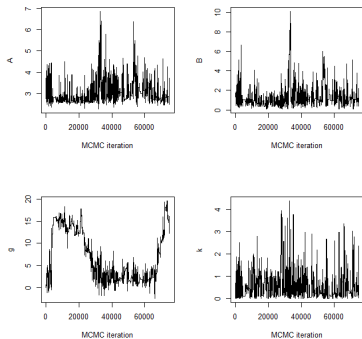


(a) WABC

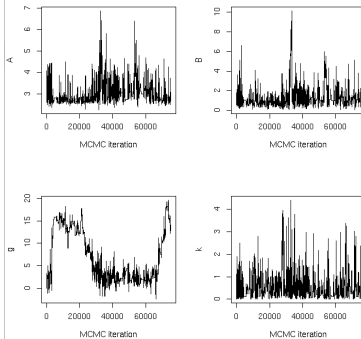
(b) WABC-SMC

Conclusion

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






(c) WABC



(d) WABC-SMC

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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