Evaluation of Tolerance Selection Strategies and Multifidelity Techniques in ABC Methods

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Introducing Our Problem

Some context

- Mathematical models are essential tools for understanding complex systems and predicting outcomes.
- Standard Bayesian inference:
  - Posterior simulation algorithms (MCMC, importance sampling, etc).
- Computational intractability of $L(y|\theta)$.
- Unable to numerically evaluate likelihood for any θ.

Approximate Bayesian Computation

Approximate Bayesian Computation (ABC) methods effectively approximate posterior distribution to make model calibration.

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Objectives

This work focuses on the analysis of the tolerance techniques choice and the application of multifidelity process in ABC methodology.

- Compare three different **tolerance strategies** within ABC-SMC.
- Explore the integration of **multifidelity techniques** to reduce computational costs while maintaining or improving result accuracy.

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In Bayesian framework:

$$p(\theta|y) \propto \mathcal{L}(y|\theta)\pi(\theta). \tag{1}$$

In ABC framework:

$$p(\theta|y) \propto p(\theta|\rho(y, y_{obs}) \leq \epsilon), \tag{2}$$

where,

- $\rho(.)$: some distance measure;
- y: simulated value;
- y_{obs}: observed value,
- ϵ: tolerance value.

How Does ABC Work?

Simple ABC Mechanism:

1. Sample θ^* from the prior distribution $p(\theta)$;
2. Simulate data set from the model, using parameter θ^*, to get D^*;
3. If D is "close enough" of D^*, accept θ^*; otherwise, reject,
4. Repeat until N particles (the parameter values or parameter sets) $\Theta^* = \{\theta_i^*; i = 1, \ldots, N\}$ are accepted.

Note: *"close enough" could be if $\|D - D^*\| \leq \epsilon$ for small ϵ.*

Note: *Computation increases exponentially as accuracy increases (i.e. as $\epsilon \to 0$).*

- **Sequential Monte Carlo Approximate Bayesian Computation** (ABC SMC):
  - The algorithm starts with a **higher tolerance level** and **gradually decreases it over iterations**.
  - Each particle (sample) has a **weight**, allowing the method to prioritize particles that better represent the posterior distribution in subsequent iterations.
  - **Kernel functions** are applied to **perturb particles** to create diversity.

ABC Basics

Choice of Tolerances

One fundamental point is the **choice of tolerances** ϵ for ABC

$$\|D - D^*\| \leq \epsilon \tag{3}$$

- Choosing an appropriate tolerance level is crucial for balancing accuracy and computational efficiency in ABC.
  - The choice of tolerance may be using predetermined vectors (trial and error).
  - Or from adaptive methods.

Another fundamental challenge in ABC methods is the need for a large number of simulations

- One way to overcome this is using models that can be simulated more cheaply through the multifidelity technique.
- Combines simulation with different levels of fidelity to improve the efficiency of the inference process.

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Tolerance Strategies in ABC

The Choice of Tolerances

- The choice of tolerance values significantly impacts the computational efficiency of ABC methods.
  - Fixed.
  - Percentile-based.
  - Percentage-based.

Tolerance Choice Implemented

- Fixing values in advance:
  - Based in prior knowledge and **empirical tests** performed with the model.

Tolerance Choice Implemented

- Adaptive percentile and percentage selection:
  - Using the value corresponding to the percentile or percentage in the ordered distance vector (d^T_{t-1}) accepted in the previous iteration $t-1$.

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Multifidelity Technique

in ABC context

- One way to improving the efficiency is the use of multifidelity models:
  - Combines less expensive models with more costly ones.

Numerical Methods

- **Euler Method**
- **Richardson Extrapolation**

Multifidelity Cost Comparative

in ABC-SMC with Multifidelity

By using this multifidelity strategy, the computational cost becomes proportional to the total number of Euler evaluations.

Evaluation of the Euler function with **step size h** → Additional evaluation with **step size h/2** → Number of samples + 2 x number of accepted particles

$$\text{Total Cost} = N_{h_{samples}} + 2 \cdot N_{\text{accepted}} \tag{4}$$

$$\text{Total Savings} = \left(N_{h_{samples}} + 2 \cdot N_{\text{accepted}}\right) - 2 \cdot N_{samples\frac{h}{2}} \tag{5}$$

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Epidemiological Models

Susceptible - Infected - Recovery

- β: infection rate.
- γ: recovery rate.

SIR model ODE's

$$\begin{aligned} \frac{dS}{dt} &= -\beta S I \, , \\ \frac{dI}{dt} &= \beta S I - \gamma I \, , \\ \frac{dD}{dt} &= \gamma I \, . \end{aligned} \tag{6}$$

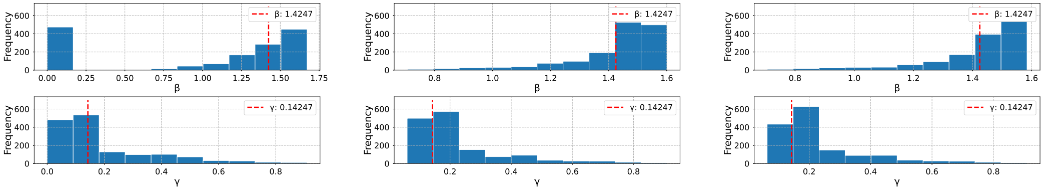
Contents

- Fixed.
- Percentile-based.
- Percentage-based.

Results

Tolerances Strategies with SIR model

Figure: Comparison of histograms for the posterior distribution of β and γ for each tolerance strategy with $pop = 5$ and $h = 0.25$.



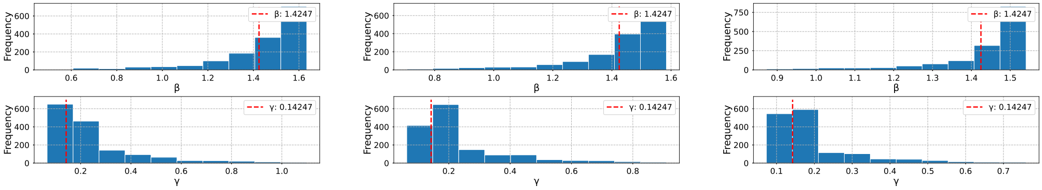
(a) Fixed tolerance method.   (b) Percentile tolerance method.   (c) Percentage tolerance method.

- We utilized our proposed approach with a **multifidelity** and **percentile-based** tolerance selection strategy.

Results

Multifidelity Techniques and Percentile-based Tolerance Strategy with SIR model

Figure: Comparison of the histograms of β and γ for percentile tolerance strategies with multifidelity techniques for $pop = 5$ and $h = 0.5, 0.25, 0.125$.

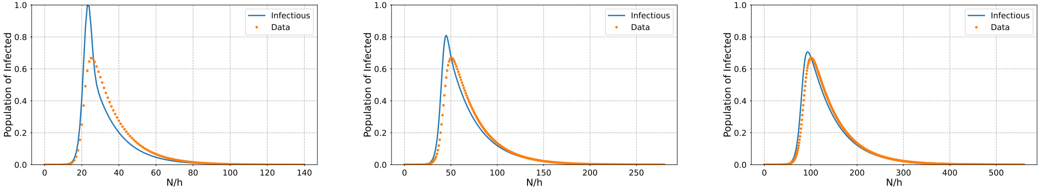


(a) $h = 0.5$.

(b) $h = 0.25$.

(c) $h = 0.125$.

Figure: Comparison of the infects population curve of SIR model for percentile tolerance strategies with multifidelity techniques for $pop = 5$, $N = 70$, $h = 0.5, 0.25, 0.125$, line in blue, and the observed data, orange dots.



(a) $h = 0.5$. (b) $h = 0.25$. (c) $h = 0.125$.

Strategies for $h = 0.5, 0.25, 0.125$

- Initially, all methods yield good results;

Table: Parameters with smallest distance with step size of $h = 0.5, 0.25$ and 0.125, and $pop = 5$.

	β	γ	dmin
$h = 0.5$	1.6333	0.1482	1.4247
$h = 0.25$	1.5832	0.1385	0.3901
$h = 0.125$	1.5176	0.1421	0.1610
$h = 0.167$	1.5516	0.1432	0.1868
$h = 0.083$	1.4855	0.1428	0.1310
$h = 0.042$	1.4538	0.1425	0.0972

- **Reference Parameter**:
  - Transmission rate: $\beta = 1.4247$
  - Recovery rate: $\gamma = 0.14286$

Table: Number of samples necessary for each population in $pop = 5$ round, with $h = 0.5, 0.25$ and 0.125.

	$pop1$	$pop2$	$pop3$	$pop4$	$pop5$
$h = 0.5$	1181	1121	892	923	915
$h = 0.25$	1770	925	848	1127	989
$h = 0.125$	2657	1117	926	1328	1157

Table: Number of samples necessary for each population in $pop = 5$ round, with $h = 0.5, 0.25$ and 0.125.

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Table: Cost comparison between $h = 0.5$ and $h = 0.25$, and between $h = 0.25$ and $h = 0.125$, for Euler and multifidelity.

	$pop1$	$pop2$	$pop3$	$pop4$	$pop5$
$0.5/0.25$	-1759	-129	-204	-731	-463
$0.25/0.125$	-2944	-709	-404	-929	-725

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8 Conclusions

Conclusions

- The adaptive strategies provide the best results.
- Initial analysis indicates that these strategies do not produce significant variations in the parameter estimates.
- The adjustment of the step size h present improvements.
- The implementation of multifidelity technique provides a more efficient calibration.

To be investigate is:

- Check how the other parameters are correlated.
- Application to complex and high-dimensional models.

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Thank you all for your attention!