

An introduction to Approximate Bayesian Computation methods

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Valencia, January 28, 2015



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Introduction: why do we need ABC? ABC algorithm Extensions to ABC ABC with quasi-likelihoods GOF ABC models

1 Introduction: why do we need ABC?

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Introduction to Approximate Bayesian Computation (ABC)

- ABC is a relative recent computational technique to approximate posterior distributions with the only requirement of being able to sample from the model (likelihood):

$$f(\cdot | \theta)$$

- First ABC ideas were mentioned by Donal Rubin (Annals of Statistics, 1984), also Diggle and Gratton in 1984 (JRSS B) proposed to use systematic simulation to approximate the likelihood function.
- The first paper proposing ABC to approximate posterior distributions in a Bayesian context, was in the field of population genetics about 18 years ago (Tavaré et al., 1997, Genetics).

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Computation in Bayesian Inference

- Bayesian inference involves the estimation of a conditional probability density.
- The expert defines a model for observable given parameters (parametric inference): $f(\mathbf{y} | \theta)$, and a prior distribution for parameters, $\pi(\theta)$.
- Using Bayes Theorem, the aim is to compute the **posterior distribution for θ**

$$\pi(\theta | \mathbf{y}) = \frac{f(\mathbf{y} | \theta)\pi(\theta)}{f(\mathbf{y})},$$

where $f(\mathbf{y}) = \int f(\mathbf{y} | \theta)\pi(\theta)d\theta$.

Such marginal density in general is difficult to be calculated, because it is a high dimensional integral.

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Methods of computation in Bayesian Inference

Different computation/simulation methods have been proposed in literature to approximate posterior and marginal distributions* :

- Monte Carlo methods, such as Markov Chain Monte Carlo (MCMC);
- Importance sampling (IS);
- Sequential Monte Carlo (SMC)

When the likelihood is intractable, it is not possible to evaluate $L(\boldsymbol{\theta} | \mathbf{y}) = f(\mathbf{y} | \boldsymbol{\theta})$, these standard Monte Carlo techniques do not apply.

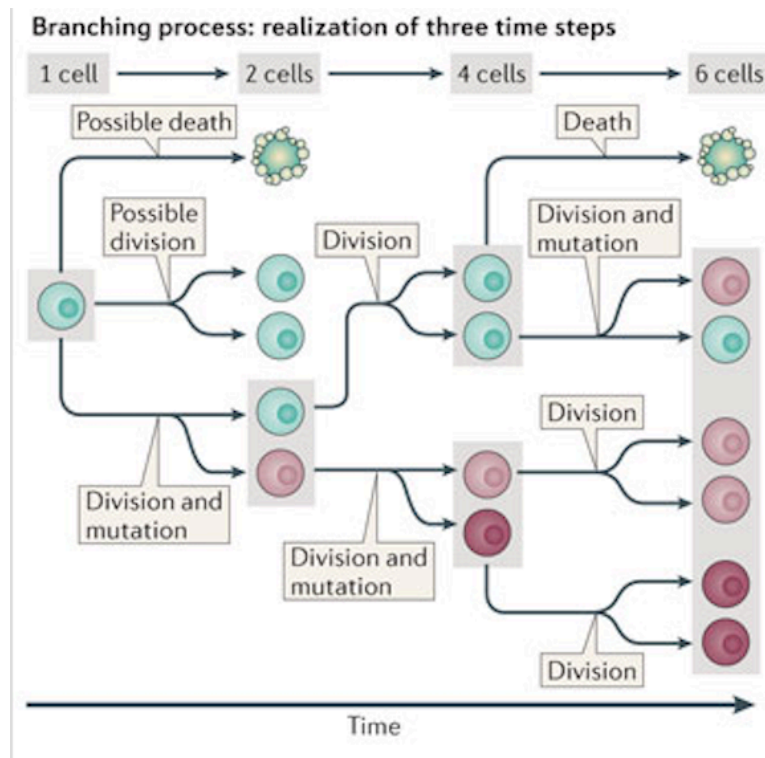
ABC methods are Monte Carlo techniques developed for use with completely intractable likelihood, that is when $f(\mathbf{y} | \boldsymbol{\theta})$ can not be evaluated.

*Robert and Casella, 2004

Example: birth-death-mutation process

- Many epidemic transmission process can be represented by a **birth-death-mutation process** (Tanaka et al. 2006).
- It consists on a continuous-time stochastic model describing the growth in the number of infectious cases of a disease over time.
 - Birth:** represents the occurrence of a new infection;
 - Death:** corresponds to death of the host;
 - Mutation:** allows different genotypes of the pathogen.
- Assuming some epidemiological properties, it is possible to describe the probabilities of transition in the continuous-time process, using three rates: **Birth rate**, α ; **death rate**, δ ; and **mutation rate**, θ (per unit of time).

Example: birth-death-mutation process



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Example: birth-death-mutation process

- Let the observable variable be $X_i(t)$ = number of infected with genotype i and:
- Let be $P_{i,x}(t) = P(X_i(t) = x)$
- It is possible to express the time evolution of $P_{i,x}(t)$ through the differential equation:

$$\frac{dP_{i,x}(t)}{dt} = -(\alpha + \delta + \theta)xP_{i,x}(t) + \alpha(x-1)P_{i,x-1}(t) + (\delta + \theta)(x+1)P_{i,x+1}(t)$$

- Similar equations account for the creation of new genotypes, or the total number of cases.

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Example: Simulation of the birth-death-mutation process

- $G(t)$ is the number of distinct genotypes at current time t .
- $N(t) = \sum_{i=1}^{G(t)} X_i(t)$ is the total number of infected.
- Type of event simulation:

$$P(\text{birth} \mid \text{event}) = \frac{\alpha}{\alpha + \delta + \theta}$$

$$P(\text{death} \mid \text{event}) = \frac{\delta}{\alpha + \delta + \theta}$$

$$P(\text{mutation} \mid \text{event}) = \frac{\theta}{\alpha + \delta + \theta}$$

If event = mutation, $G(t) = G(t) + 1$, and $X_{G(t)} = 1$.

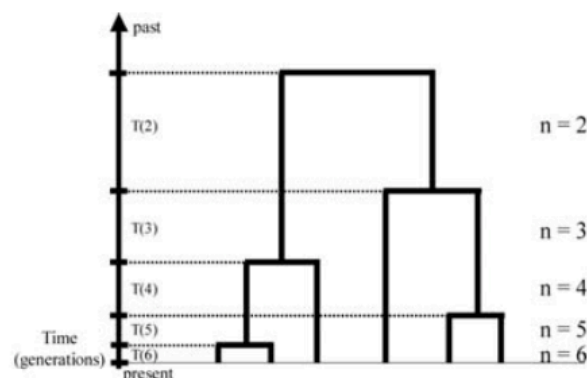
- Given an event of the three types,

$$P(\text{occurrence in genotype } i \mid \text{event}) = \frac{X_i(t)}{N(t)}$$

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Other Example: Coalescent Model

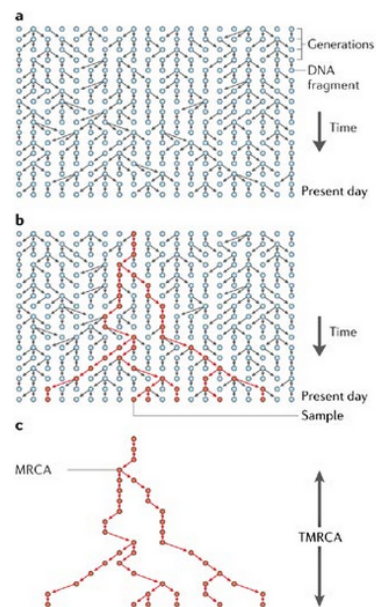
- This is a model used in population genetics.
- Given a sample of n genes, this model could be used to know how long we must go backward in generations (6 in the figure) to share a common ancestor (TMRCA).



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Example: Coalescent Model

This model is used to estimate the time to the common ancestor, but also other characteristics as the effective mutation rate, θ , from the observed data, as the number of segregating sites.



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Estimation the mutation rate

- Using recombination rules from genetics, then random fluctuation in allele frequencies can be expressed in terms of probability.
- For a set of n DNA sequences, where the aim is the **estimation of the effective mutation rate $\theta > 0$** , under the infinitely-many-sites model assumption.
- In this model, mutations occur at rate θ at DNA sites that have not been hit by mutation before.
- If a site is affected by mutation, it is said to be segregating in the sample.
- Data consists in $s =$ number of segregating sites.

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Estimation the mutation rate. Computer Model

- The generating mechanism for s , under the assumptions above, is the following:
 1. Generate L_n , the total length of the branches in the genealogical tree, with $L_n = \sum_{j=2}^n jT_j$.
 2. In a wide range of models in population genetics, the inter-coalescence times, T_j , can be expressed as independent random variables distributed exponential with rate $\mu_j = j(j-1)/2$, so L_n has

$$E(L_n) = 2 \sum_{j=1}^{n-1} \frac{1}{j}$$

$$Var(L_n) = 4 \sum_{j=1}^{n-1} \frac{1}{j^2}$$

3. Generate $(S \mid \theta, L_n) \sim \text{Poisson}(\theta L_n/2)$.
The election of this rate in the Poisson is to verify that $E(S \mid \theta) = \theta \sum_{j=1}^{n-1} \frac{1}{j}$

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Example: Coalescent Model. Likelihood

- The likelihood $f(\cdot \mid \theta)$ is given by the marginal density of $(S \mid \theta)$ with respect to L_n , which has a closed form only for $n = 2$ as $T_2 \sim \text{Exp}(1/2)$.
- For large n , it is easy simulate from the model, but there is no closed expression of the likelihood.
- Once s is observed, we can do inference about θ , using ABC methods.

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Original ABC works as follows:

Target: To approximate via simulation $\pi(\boldsymbol{\theta} | \mathbf{y}) \propto \pi(\boldsymbol{\theta})f(\mathbf{y} | \boldsymbol{\theta})$.

When $f(\mathbf{y} | \boldsymbol{\theta})$ has not closed expression, then original version of ABC can be used:

ABC algorithm

Suppose data is \mathbf{y} from model $f(\mathbf{y} | \boldsymbol{\theta})$. Under the prior $\pi(\boldsymbol{\theta})$, simulate jointly

$$\boldsymbol{\theta}^* \sim \pi(\boldsymbol{\theta}), \mathbf{z} \sim f(\mathbf{z} | \boldsymbol{\theta}^*)$$

until $\mathbf{z} = \mathbf{y}$.

(Tavaré et al. 1997)

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ABC works:

It is based on Acceptance-Rejection:

$$\begin{aligned} p(\theta_i) &= \sum_{\mathbf{z} \in \mathcal{D}} \pi(\theta_i) f(\mathbf{z} | \theta_i) \mathbb{I}_{\mathbf{y}}(\mathbf{z}) = \\ &= \pi(\theta_i) f(\mathbf{y} | \theta_i) = \pi(\theta_i | \mathbf{y}) \end{aligned}$$

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Approximate in ABC because...

When \mathbf{y} is a continuous random variable, the event $\mathbf{z} = \mathbf{y}$ has probability zero! So, the equality is replaced with a tolerance condition:

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

where ρ is a distance.

In this case, simulations are distributed according to:

$$\pi(\boldsymbol{\theta})P(\rho(\mathbf{y}, \mathbf{z}) \leq \epsilon | \boldsymbol{\theta}) \propto \pi(\boldsymbol{\theta} | \rho(\mathbf{y}, \mathbf{z}) \leq \epsilon)$$

(Pritchard et al. 1999)

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ABC algorithm

- 1 $\boldsymbol{\theta} \sim \pi(\boldsymbol{\theta})$
 - 2 $\mathbf{z} | \boldsymbol{\theta} \sim f(\mathbf{y} | \boldsymbol{\theta})$
 - 3 if $\rho(\mathbf{z}, \mathbf{y}) < \epsilon$, retain $\boldsymbol{\theta}$ (indirect evaluation of the likelihood)
- If $\epsilon = 0$ this algorithm is exact and gives draws from the posterior distribution.
 - Whereas as $\epsilon \rightarrow \infty$, the algorithm gives draws from the prior.
 - Smaller values of ϵ produce samples that approximate better the posterior, but,
 - It results in lower acceptance rates in step 3, that using larger values.

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Extensions to use summary statistics

- When data is high dimensional, a standard change is to summarize the model output and data, using a **summary statistic $s(\cdot)$** to work in a low dimensional space.
- In this case the step 3 is:
 - 3** if $\rho(s(\mathbf{z}), s(\mathbf{y})) < \epsilon$, retain θ .

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How are distributed the simulations?...

Denote $\mathbf{s} = s(\mathbf{z})$ and the observed statistic $\mathbf{s}_{obs} = s(\mathbf{y})$.

The above ABC algorithm samples from the joint distribution:

$$\pi^\epsilon(\theta, \mathbf{s} \mid \mathbf{s}_{obs}) \propto \pi(\theta) f(\mathbf{s} \mid \theta) \mathbb{I}_{\rho(\mathbf{s}, \mathbf{s}_{obs}) < \epsilon}$$

where $\mathbb{I}_{\rho(\mathbf{s}, \mathbf{s}_{obs}) < \epsilon}$ is the indicator for the event

$$\{\mathbf{s} \in \mathcal{S} \mid \rho(\mathbf{s}_{obs}, \mathbf{s}) < \epsilon\}$$

So ABC algorithm approximates the posterior for θ using:

$$\pi^\epsilon(\theta \mid \mathbf{s}_{obs}) = \int_{\mathcal{S}} \pi^\epsilon(\theta, \mathbf{s} \mid \mathbf{s}_{obs}) d\mathbf{s} \approx \pi(\theta \mid \mathbf{y})$$

The idea is that a small ϵ coupled with suitable summary statistics provide a good approximation of the posterior

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Some comments about $s(\cdot)$

- Ideally, $s(\cdot)$ should be **sufficient for θ** .
- But, in real problems, if the likelihood is unknown, sufficient statistics cannot be identified.
- Summarizing the data and model output through **non-sufficient summaries** adds another layer of approximation.
- It is not known what effect any given choice for $s(\cdot)$ has on the approximation.

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Extensions to basic ABC

- As simulating from the prior is often poor in efficiency, [Marjoram et al, 2003](#) extend the rejection algorithm to MCMC algorithms.
- [Sisson et al., 2007](#) propose the use of approximate sequential Monte Carlo algorithms.
- [Beaumont et al., 2002](#) extend the ABC using a weighting scheme instead of the 0-1 of the acceptance-rejection method. Then the weighted sample is used to train a local-linear regression to model the posterior distribution.

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Introduction: The MCMC ABC

The MCMC-ABC ** works as follows for a certain proposal $q(\cdot)$ at step t :

- 1 $\theta^* \sim q(\theta^{(t)} | \theta^{(t-1)});$
- 2 $\mathbf{s} | \theta^* \sim f(\mathbf{s}(y) | \theta^*)$
- 3 accept θ^* with probability

$$\max \left\{ \frac{\pi(\theta^*) q(\theta^{(t-1)} | \theta^*)}{\pi(\theta^{(t-1)}) q(\theta^* | \theta_{t-1})} \mathbb{I}_{\rho(\mathbf{s}_{obs}, \mathbf{s}) < \epsilon}, 1 \right\},$$

which:

- does not involve direct evaluation of the likelihood $f(\mathbf{y} | \theta)$.
- works with $\pi(\theta)$ improper.

Our aim is to find *automatically* a good proposal $q(\cdot)$.

** Marjoram et al. (PNAS, 2003)

Our proposal ***: Construction of an automatic proposal, using a type of pseudo-likelihood.

Set

$$q(\theta) \propto L_Q(\theta)$$

where $L_Q(\theta)$ is the Quasi Likelihood function for θ .

*** Cabras, Castellanos and Ruli (Bayesian Analysis, 2015)

Quasi Likelihood for $p = 1$

- Let $\Psi = \Psi(\mathbf{y}; \theta) = \sum_{i=1}^n \psi(y_i; \theta)$ be an unbiased estimating function $E(\Psi|\theta) = 0$
- A quasi likelihood is defined as

$$L_Q(\theta) = \exp \left\{ \sum_{i=1}^n \int_{c_0}^{\theta} A(t) \psi(y_i; t) dt \right\},$$

where c_0 is an arbitrary constant and $A(\theta) = \Omega(\theta)^{-1} M(\theta)$ with:

- $M(\theta) = -E \left(\frac{\partial \Psi}{\partial \theta} \mid \theta \right);$
- $\Omega(\theta) = E(\Psi^2 \mid \theta) = \text{Var}(\Psi|\theta).$

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Quasi Likelihood for $p = 1$ (Proposition)

Suppose:

- $f(\theta) = E(s|\theta)$ is a bounded regression function with $|f'(\theta)| < \infty$
- $\sigma_R^2 = \text{Var}(s|\theta)$ be the conditional variance.
- For $\psi(s_{obs}; \theta) = s_{obs} - f(\theta)$

THEN

$$L_Q(\theta) = \phi \left(\frac{f(\theta) - s_{obs}}{\sigma_R} \right),$$

where $\phi(\cdot)$ is the density of the standard normal.

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Tools to estimate

In order to complete our definition we need to estimate:

- $f(\theta)$ with $\hat{f}(\theta)$ (e.g. a spline, GAM, ...);
- σ_R^2 with the residual regression variance $\hat{\sigma}_R^2$.
- In the algorithm, the variance could be also no constant, $\sigma_R^2(\theta)$, it can be estimated as well as $f(\theta)$.

We use a **pilot run** to calculate these estimators:

- 1 draw M values of $s \mid \theta \sim f(\mathbf{y} \mid \theta)$ for θ in a certain regular grid;
- 2 regressed s on θ , obtaining $\hat{f}(\theta)$ and $\hat{\sigma}_R^2(\theta)$.

The $\text{ABC}_{q/}$ is an ABC-MCMC algorithm with proposal:

$$q^Q(\theta \mid \theta^{(t-1)}) = \phi \left(\frac{f(\theta) - f(\theta^{(t-1)})}{\sigma_R(\theta^{(t-1)})} \right) \mid f'(\theta) \mid .$$

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ABC-MCMC with Pseudo-likelihoods ($p = 1$)

Require: f , $f'(\theta)$, $\sigma_R^2(\theta)$, or their estimates $(\hat{f}, \hat{f}'(\theta), \hat{\sigma}_R^2(\theta))$.

For $t = 1$ to T

- 1 Simulate

$$f^* \sim N(f(\theta^{(t-1)}), \sigma_R^2(\theta^{(t-1)}));$$

- 2 Set $\theta^* = \{\theta : f^{-1}(f^*) = \theta\}$;
- 3 Generate $s \sim f(s(y) \mid \theta^*)$;
- 4 Calculate $\rho = \rho(s_{\text{obs}}, s)$;
- 5 Calculate the derivative, $f'(\theta)$, of $f(\theta)$, at $\theta^{(t-1)}$ and θ^* ;
- 6 With probability

$$\min \left\{ 1, \frac{\pi(\theta^*) q^Q(\theta^{(t-1)} \mid \theta^*)}{\pi(\theta^{(t-1)}) q^Q(\theta^* \mid \theta^{(t-1)})} \mathbb{I}_{\rho < \epsilon} \right\}$$

accept θ^* and set $\theta^{(t)} = \theta^*$, otherwise $\theta^{(t)} = \theta^{(t-1)}$

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Calculating estimators: \hat{f} , $\hat{f}'(\theta)$, $\hat{\sigma}_R^2(\theta)$

- 1 Consider M values $\tilde{\theta} = (\tilde{\theta}_1, \dots, \tilde{\theta}_M)$ taken in a regular spaced grid of a suitable large subset $\tilde{\Theta} \subseteq \Theta$;
- 2 Generate $\tilde{s} = (\tilde{s}_1, \dots, \tilde{s}_M)$ where $\tilde{s}_m \sim f(s(y) \mid \tilde{\theta}_m)$;
- 3 Regress \tilde{s} on $\tilde{\theta}$ obtaining $\hat{f}(\theta)$ and $\hat{f}'(\theta)$ (using Splines, GAM, etc.);
- 4 Regress $\left\{ \log \left(\hat{f}(\tilde{\theta}_m) - \tilde{s}_m \right)^2 \right\}_{m=1, \dots, M}$ on $\tilde{\theta}$ obtaining $\hat{\sigma}_R^2(\theta)$.

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Example: Coalescent Model (revisited)

This model assigns, for a certain DNA sequence of length n , the probability to have y mutations given an unknown mutation rate $\theta > 0$.

Remember that the simulation model (computer model) is:

- $T_j \sim \text{Exp}(\text{mean} = 2/j(j-1))$ is the **unobservable** time;
- $L_n = \sum_{j=2}^n jT_j$ is the total length of the genealogical tree;
- $(Y \mid \theta, L_n) \sim \text{Poisson}(\theta L_n/2)$.

$L_N(\theta)$ has a closed form only for $n = 2$.

We apply ABC_{qI} considering $s = \log(1 + y)$ and parametrization in $\log(\theta)$.

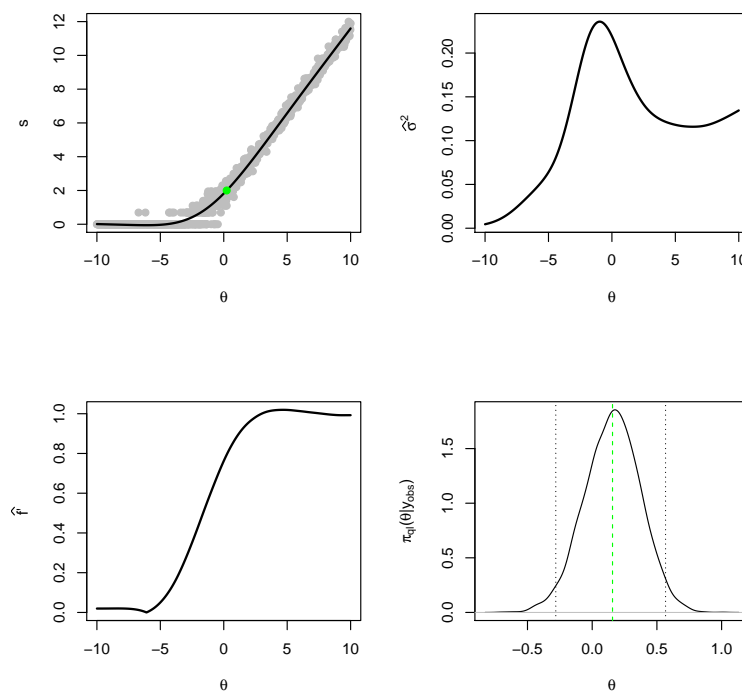
For purposes of comparison, with $n > 2$ we consider:

- A parametric approximation $\pi_{ap}(\theta \mid s)$ using the Poisson likelihood;
- $\pi(\theta) = \text{Exp}(1)$.

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Example: Coalescent Model (cont.)

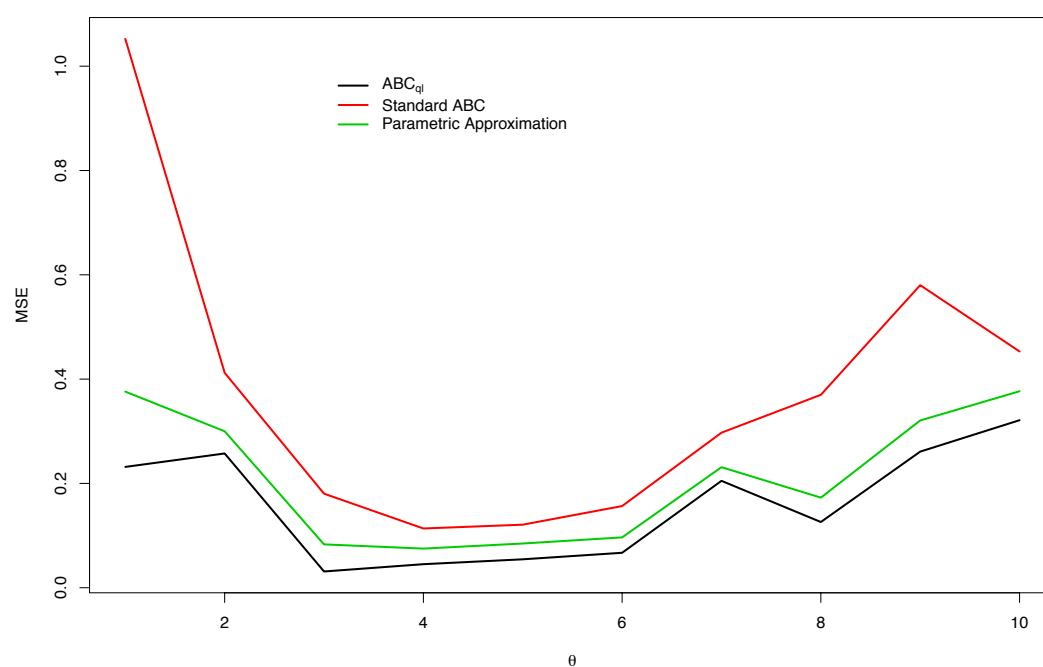
Estimation of $f(\theta)$, $f'(\theta)$, $\sigma_R^2(\theta)$:



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Example: Coalescent Model (cont.)

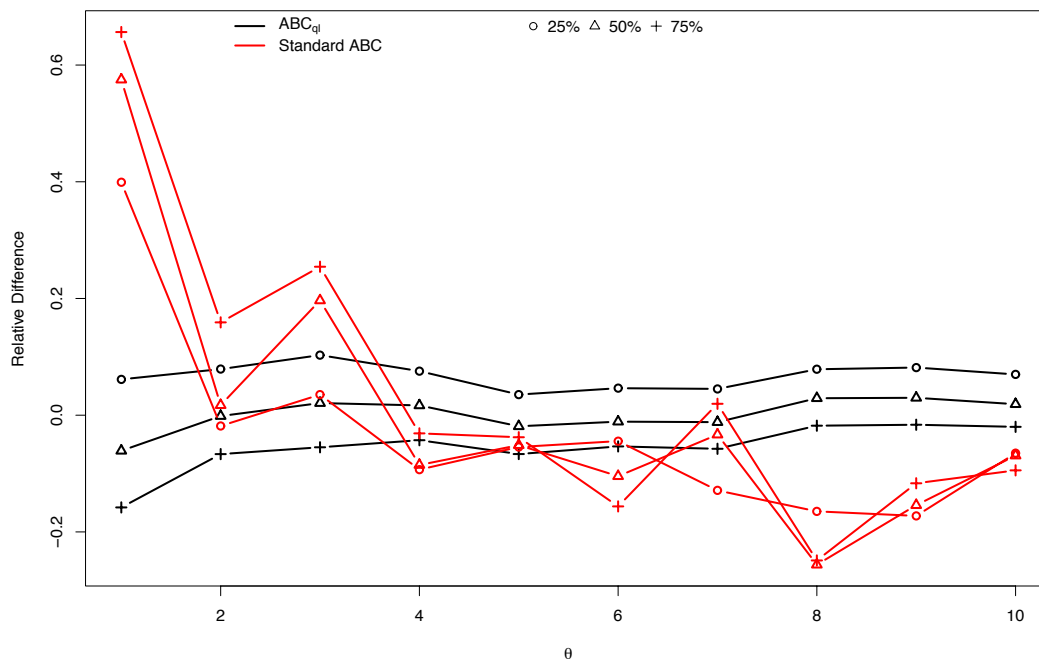
Comparison in terms of Mean Squared Error for θ for $n = 100$.



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Example: Coalescent Model (cont.)

Comparison in terms of Quantile Relative Difference $(Q_p - Q_p^0)/Q_p^0$ where Q_p and Q_p^0 are the p -th quantiles of the ABC posterior and the parametric approximation.



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Goodness of fit ABC models

- 1 GOF uses **calibrated** p -values,

$$(P - \text{value} | \text{Null Model}) \sim U(0, 1).$$

- 2 GOF focuses on evaluating particular a given model feature:
diagnostic statistic $T = t(\mathbf{y})$
 (large values \Rightarrow incompatibilities) and T possibly not ancillary w.r.t. θ .
- 3 The model under GOF is not $\pi(\theta | \mathbf{y})$, but $\pi^\epsilon(\theta | \mathbf{s}_{obs})$
 (it is the one we deal with).

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The GOF ABC evaluation: implementation

- Recall: a p -value is

$$p - value = Pr^{h(t)}(T \geq t_{obs}),$$

- $H(T)$ is the sampling distribution of T under the model.
- $H(T)$ is usually not known exactly;
 - we approximate it by drawing T in ABC algorithm.
 - How ?

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The GOF ABC evaluation: implementation

In the original ABC:

- 1 $\theta \sim \pi(\theta)$;
- 2 $\mathbf{y}|\theta \sim f(\mathbf{y} | \theta)$ and calculate $\mathbf{s}(\mathbf{y})$;
- 3 if $\rho(\mathbf{s}_{obs}, \mathbf{s}) < \epsilon$ retain θ and $t(\mathbf{y})$.

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The GOF ABC evaluation: rationale

The **conditional predictive** p -value****

$$p_{cpred} = Pr^{m(\cdot | \mathbf{s}_{obs})}(T(\mathbf{y}) \geq t_{obs}),$$

where

$$m(t | \mathbf{s}) = \int f(t | \mathbf{s}, \boldsymbol{\theta}) \pi(\boldsymbol{\theta} | \mathbf{s}) d\boldsymbol{\theta},$$

$$\pi(\boldsymbol{\theta} | \mathbf{s}) = \frac{f(\mathbf{s} | \boldsymbol{\theta}) \pi(\boldsymbol{\theta})}{\int f(\mathbf{s} | \boldsymbol{\theta}) \pi(\boldsymbol{\theta}) d\boldsymbol{\theta}}.$$

**** Bayarri and Berger, (JASA, 2000)

The GOF ABC evaluation: rationale

Applying the above ABC algorithm, we are using

$$m(t | \mathbf{s})$$

where \mathbf{s} are the statistics used in ABC. So, we are approximating p_{cpred} , and:

- 1 Fact: $p_{cpred} \sim U(0, 1)$ for $n \rightarrow \infty$ if $\mathbf{s}_{obs} = \hat{\boldsymbol{\theta}}$;*****
- 2 if \mathbf{s} not ancillary $\Rightarrow \mathbf{s}$ is sufficient for model $f(\mathbf{s} | \boldsymbol{\theta})$;
- 3 for $\epsilon \rightarrow 0$

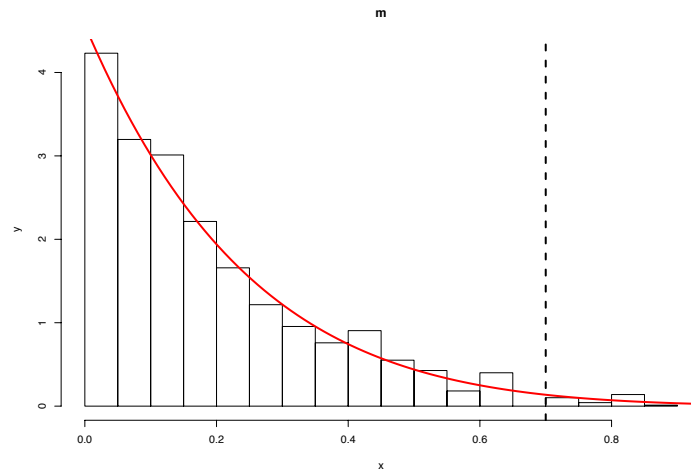
$$\Rightarrow f(\mathbf{s} | \boldsymbol{\theta}) \mathbb{I}\{\mathbf{s} \in B_{\epsilon}(\mathbf{s}_{obs})\} \rightarrow f(\mathbf{s}_{obs} | \boldsymbol{\theta}).$$

- 4 $\Rightarrow \mathbf{s}_{obs} = \hat{\boldsymbol{\theta}} \Rightarrow$ We are in step 1.

***** Fraser and Rousseau (Biometrika, 2008)

Exponential distribution

$Y \sim \text{Exp}(\theta)$, $\pi(\theta) \propto 1/\theta$, $S = 10 \cdot \bar{\mathbf{y}}$, $T = \min(\mathbf{y})$, $n = 10$
 Exact $m(t|\hat{\theta})$ (red line) and approximated $m(t|s)$ (simulations) with MCMC-ABC

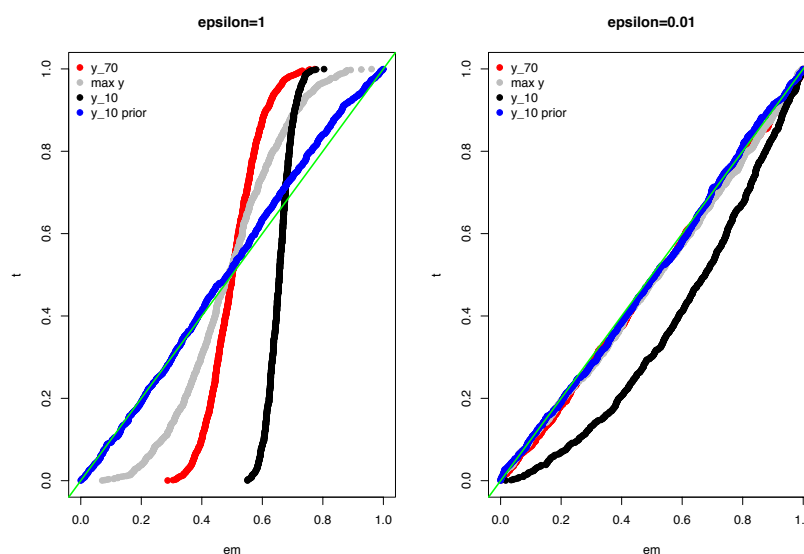


ABC: $p_{cpred} = 0.015$ (Exact: 0.019), $p_{post} = 0.048$.

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Uniform model. Effect of non sufficient statistics

$Y \sim U(0, \theta)$, $\pi(\theta) = U(0, 10)$, $T = \bar{\mathbf{y}}$, $n = 20$



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Remarks (1/2)

- 1 Since we are able to simulate from $f(y | \theta)$ then $\hat{f}(\theta)$ and $\hat{\sigma}_R^2$ can be practically estimated at a desired precision;
- 2 More precision can be achieved by making wider the regular grid/lattice;
- 3 With $p > 1$ large values of M are needed because of the curse of dimensionality;
- 4 The grid/lattice should be always enough to include the observed \mathbf{s}_{obs}
- 5 $\hat{f}(\theta)$ can be any estimator which provides smooth functions.

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Remarks (2/2)

- 1 For not injective $f(\theta)$ one could consider to estimate it, separately, on those subspaces of $\mathbb{R} \times \Theta$ in which it is monotone;
- 2 The inverse $\hat{f}^{-1}(f^*)$ can be either obtained analytically or with the bisection method on $\hat{f}'(\theta) = f^*$ or by numerical minimization of $(\hat{f}'(\theta) - f^*)^2$, e.g. by a Newton-Rapson algorithm;
- 3 In order to fix ϵ it would be enough to draw samples of θ from $q(\theta)$ and set ϵ as some percentile of the empirical distribution of the distances $\rho(s_1, s_{obs}), \dots, \rho(s_K, s_{obs})$.

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Conclusions

- ABC_{qI} relies on the reparametrization $f(\theta)$ which relates θ with \mathbf{s} .
 - ...other authors^{*****} suggest that $f(\theta)$ should be the posterior quantities of interest as $E_{\pi_N(\theta|y)}(\theta)$.
- ABC_{qI} mitigates the importance of the choice of \mathbf{s} .
- To implement ABC_{qI} we need just basic knowledge of regression analysis to: have a sensible choice of \mathbf{s} (at least avoid ancillaries).
- We need just standard numerical routines to calculate inverse and Jacobian.
- The only important tuning parameter remains ϵ .

*****Fearnhead, P. and D. Prangle (JRRS-B, 2012).

Thanks !!!

Main References - ABC

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