Why approximate Bayesian computational (ABC) methods cannot handle model choice problems

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Abstract

Approximate Bayesian computation (ABC), also known as likelihood-free methods, have become a favourite tool for the analysis of complex stochastic models, primarily in population genetics but also in financial analyses. We advocated in Grelaud et al. (2009) the use of ABC for Bayesian model choice in the specific case of Gibbs random fields (GRF), relying on a sufficiency property mainly enjoyed by GRFs to show that the approach was legitimate. Despite having previously suggested the use of ABC for model choice in a wider range of models in the DIY ABC software (Cornuet et al., 2008), we present theoretical evidence that the general use of ABC for model choice is fraught with danger in the sense that no amount of computation, however large, can guarantee a proper approximation of the posterior probabilities of the models under comparison.

Keywords: likelihood-free methods, Bayes factor, DIYABC, Bayesian model choice, sufficiency.

1 Introduction

Inference on population genetic models such as coalescent trees is one representative example of cases when statistical analyses like Bayesian inference cannot operate because the likelihood function associated with the data is not completely known, i.e. cannot be computed in a manageable time (Tavaré et al. 1997, Beaumont et al. 2002, Cornuet et al. 2008). The fundamental reason for this impossibility is that the statistical model associated with coalescent data needs to integrate over trees of extreme complexity.

In such settings, traditional approximation tools based on Monte Carlo simulation (Robert and Casella 2004) from the Bayesian posterior distribution are unavailable for all practical purposes. Indeed, due to the complexity of the latent structures defining the
likelihood (such as the coalescent tree), simulation of those structures is too unstable to be trusted to bring a reliable approximation in a manageable time. Such complex models call for a practical if cruder approximation method, the ABC methodology being a serious contender, where ABC stands for \textit{approximate Bayesian computation}. Tavaré et al. (1997) and Pritchard et al. (1999) introduced ABC methods as a rejection technique bypassing the computation of the likelihood function via a simulation from the corresponding distribution. For recent reviews on ABC, see Beaumont (2010) and Lopes and Beaumont (2010). The wide and successful array of applications based on implementations of ABC in genomics and ecology is covered by Csilléry et al. (2010a), while the number of publications relying on this technique runs in the hundreds.

Pritchard et al. (1999) describe the use of model choice based on ABC for distinguishing between different mutation models. The intuition behind the method is that the average ABC acceptance rate associated with a given model is proportional to the marginal likelihood corresponding to this approximative model, when identical summary statistics, distance, and tolerance level are used for all models. In practice, an estimate of the ratio of marginal likelihoods is given by the ratio of observed acceptance rates. Using Bayes formula, estimates of the posterior probabilities are straightforward to derive. This approach has been widely used in the literature (see, e.g., Estoup et al., 2004, Miller et al., 2005, and Pascual et al., 2007, Sainudiin et al., 2011). Note that Miller et al. (2005) is particularly influential for the conclusion it derives from the ABC analysis: the focus of this \textit{Science} paper is the European invasion of the western corn rootworm, which is North America’s most destructive corn pest. Because this pest was initially introduced in Central Europe, it was believed that subsequent outbreaks in Western Europe originated from this area. Based on this ABC model choice analysis of the genetic variability of the rootworm, the authors conclude that this belief is false: There have been at least three independent introductions from North America during the past two decades.

An improvement to the above estimate is due to Fagundes et al. (2007), thanks to a regression regularisation. In this approach, model indices are processed as categorical variables in a formal multinomial (polychotomous) regression. For instance, when comparing two models, this leads to a standard logistic regression. Rejection-based approaches were lately introduced by Cornuet et al. (2008), Grelaud et al. (2009) and Toni et al. (2009), in a Monte Carlo perspective simulating model indices as well as model parameters. Those more recent extensions are already widely in use by the population genetics community, as exemplified by Belle et al. (2008), Cornuet et al. (2010), Excoffier et al. (2009), Ghirotto et al. (2010), Guillemaud et al. (2009), Leuenberger and Wegmann (2010), Patin et al. (2009), Ramakrishnan and Hadly (2009), Verdu et al. (2009), or Wegmann and Excoffier (2010). Another illustration of the popularity of this approach is given by the availability of three three softwares implementing an ABC model choice methodology:
• ABC-SysBio\(^1\) developed by the Theoretical Systems Biology Group at Imperial College London, which implements a SMC-based ABC for inference in system biology, including model-choice (Toni et al., 2009).

• DIYABC\(^2\) developed by the Centre de Biologie et de Gestion des Populations, at INRA Montpellier, which implements a regularised ABC-MC algorithm on population history using molecular markers (Cornuet et al., 2008).

• PopABC\(^3\) developed by the School of Biological Sciences at the University of Reading, which implements a regular ABC-MC algorithm for genealogical simulation (Lopes et al., 2009).

Grelaud et al. (2009) process via ABC the specific case of Gibbs random fields with missing normalising constants. They establish that exact Bayesian model selection can be implemented in this setting, deriving this result from the property that the concatenation of the sufficient statistics across models is also sufficient for model comparison. In a subsequent paper, Didelot et al. (2010) advocate the role of ABC approximations in general Bayesian model choice. The issue of sufficiency is covered in this paper, with a generic cross-model sufficiency completion leading the authors to validate the method in full generality, including in-sufficient cases.

In this paper, we argue that ABC is a valid approximation method for conducting Bayesian inference in complex stochastic models, barring the limitation that it cannot discriminate between those complex stochastic models when based on summary statistics. In essence, we highlight the fact that, since ABC is conducting model choice based on in-sufficient statistics, the resulting inference is flawed in that the loss of information is severe to the point of inconsistency, namely that the ABC model selection cannot recover the proper model, even with an infinite amount of observation and computation. We demonstrate this inconsistency in the limiting (and more favourable) case of sufficient statistics.

The conclusion of the current paper are thus quite negative in that we consider that conducting testing or model comparison using ABC does not carry any reliable weight of evidence and therefore should not be trusted. More empirical measures such as those proposed in Ratmann et al. (2009) and Drovandi et al. (2011) seem to be the only possibility at the current time for conducting model comparison. We are therefore at odds with the positive conclusion found in Didelot et al. (2010), as discussed below.

We stress here that, while Templeton (2008, 2010) repeatedly expressed reservations about the formal validity of the ABC approach in statistical testing, those criticisms were addressed at the Bayesian paradigm per se rather than at the approximation method.

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\(^1\)http://abc-sysbio.sourceforge.net
\(^2\)http://www1.montpellier.inra.fr/CBGP/diyabc
\(^3\)http://code.google.com/p/popab
Quite clearly, Templeton’s criticisms got rebutted in Beaumont et al. (2010), Csilléry et al. (2010b), Berger et al. (2010) and are not relevant for the current paper.

The plan of the paper is as follows: in Section 2 we recall the basics of ABC as well as its justification; Section 4 exposes why a Bayes factor based on an ABC approximation is not converging to the true Bayes factor as the computational effort increases; Section 5 explains the specificity of MRFs in this regard, while Section 6 illustrates the potential for divergence in examples. Section 7 concludes the paper.

2 The ABC approach and its justifications

The setting in which ABC operates is the approximation of the simulation from the posterior distribution

$$\pi(\theta | y) \propto \pi(\theta) f(y | \theta)$$

when both distributions associated with $\pi$ and $f$ can be simulated. The first ABC algorithm was introduced by Pritchard et al. (1999) in a genetic setting, as follows: given a sample $y$ from a sample space $\mathcal{D}$,

| Algorithm 1 ABC sampler |
|-------------------------|
| for $i = 1$ to $N$ do |
| repeat |
| Generate $\theta'$ from the prior distribution $\pi(\cdot)$ |
| Generate $z$ from the likelihood $f(\cdot | \theta')$ |
| until $\rho\{\eta(z), \eta(y)\} \leq \epsilon$ |
| set $\theta_i = \theta'$, |
| end for |

The parameters of the ABC algorithm are the statistic $\eta$, the distance $\rho\{\cdot, \cdot\} \geq 0$, and the tolerance level $\epsilon > 0$. The approximation of the posterior distribution provided by the algorithm is that it samples from the marginal in $\theta$ of the joint distribution

$$\pi_\epsilon(\theta, z | y) = \frac{\pi(\theta) f(z | \theta) \mathbb{1}_{A_{\epsilon,y}}(z)}{\int_{A_{\epsilon,y} \times \Theta} \pi(\theta) f(z | \theta) dz d\theta},$$

(1)

where $\mathbb{1}_B(\cdot)$ denotes the indicator function of the set $B$ and where

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

The basic justification of the ABC approximation is that, when using a sufficient statistic $\eta$ and a small (enough) tolerance $\epsilon$, we have

$$\pi_\epsilon(\theta | y) = \int \pi_\epsilon(\theta, z | y) dz \approx \pi(\theta | y),$$

the (correct) posterior distribution $\pi(\theta | y)$ being the limit as $\epsilon$ goes to zero of $\pi_\epsilon(\theta | y)$. 4
In practice, the statistic $\eta$ is not sufficient and the approximation then converges to $\pi(\theta | \eta(y))$. This fact is appreciated by users in the field who see this loss of information as an unavoidable price to pay for the access to computable quantities. While acknowledging the gain brought by ABC in handling Bayesian inference in complex models, we will demonstrate below that the loss due to the ABC approximation may be arbitrary in the specific setting of Bayesian model choice and testing, whether or not $\eta$ is sufficient.

3 ABC and model choice

Testing and model choice constitute a highly specific domain of Bayesian analysis that involves conceptual and computational complexification since several models are simultaneously considered (Robert 2001, Marin and Robert 2010). Given that both inferential problems are processed the same way in a Bayesian perspective, we will only mention model choice in the remainder of the paper, but the reader must bear in mind that we cover testing as a particular case. The standard tool on which a Bayesian approach relies is the evidence (Jeffreys 1939), also called the marginal likelihood,

$$w(y) = \int_{\Theta} \pi(\theta)f(y | \theta) \, d\theta,$$

that leads to the Bayes factor for comparing the evidences brought by the data on models with likelihoods $f_1(z | \theta_1)$ and $f_2(z | \theta_2)$,

$$B_{12}(y) = \frac{w_1(y)}{w_2(y)} = \frac{\int_{\Theta_1} \pi_1(\theta_1)f_1(y | \theta_1) \, d\theta_1}{\int_{\Theta_2} \pi_2(\theta_2)f_2(y | \theta_2) \, d\theta_2}.$$

As detailed in the Bayesian literature (Berger 1985, Robert 2001, MacKay 2002, Marin and Robert 2010), this ratio provides an absolute criterion for model comparison that is naturally penalised for model complexity (Beaumont et al. 2010, Berger et al. 2010) and whose first order approximation is the Bayesian information criterion (BIC).

Given that this issue is fundamental to our point, we recall that Bayesian model choice proceeds by creating a probability structure across models (or likelihoods). Namely, in addition to the parameters associated with each model, a Bayesian inference introduces the model index $M$ as an extra parameter. It is associated with its own prior distribution, $\pi(M = m)$ ($m = 1, \ldots, M$), while the prior distribution on the parameter is conditional on the value $m$ of the model index, denoted by $\pi_m(\theta_m)$ and defined on the parameter space $\Theta_m$. The choice between those models is then driven by the posterior distribution of $M$,

$$\mathbb{P}(M | y) = \frac{\pi(M = m)w_m(y)}{\sum_k \pi(M = k)w_k(y)},$$

where $w_k(y)$ denotes the marginal likelihood of $y$ for model $k$. 
While this distribution is well-defined and straightforward to interpret, it offers a challenging computational conundrum in Bayesian analysis. Moreover, the solutions found in the literature (Chen et al., 2000, Marin and Robert, 2010) do not handle the case when the likelihood is not available and ABC represents the almost unique alternative.

As exposed in e.g. Grelaud et al. (2009), Toni and Stumpf (2010), and Didelot et al. (2010), once $M$ is incorporated within the parameters, the ABC approximation to the posterior follows from the same principles as regular ABC. The corresponding implementation is as follows, using for the tolerance region a statistic $\eta(z) = (\eta_1(z), \ldots, \eta_M(z))$ that is the concatenation of the summary statistics used for all models (with an obvious elimination of duplicates).

Algorithm 2 ABC model choice sampler (ABC-MC)

\begin{verbatim}
for i = 1 to N do
    repeat
        Generate $m$ from the prior $\pi(M = m)$
        Generate $\theta_m$ from the prior $\pi_m(\theta_m)$
        Generate $z$ from the model $f_m(z|\theta_m)$
    until $\rho(\eta(z), \eta(y)) \leq \epsilon$
    Set $m(i) = m$ and $\theta(i) = \theta_m$
end for
\end{verbatim}

The ABC estimate of the posterior probability $\pi(M = m|y)$ is then the frequency of acceptances from model $m$ in the above simulation

$$\hat{P}(M|y) = \frac{1}{N} \sum_{i=1}^{N} I_{m(i)=m}.$$ 

This also corresponds to the frequency of simulated pseudo-dataset from model $m$ that are closer to the data $y$ than the tolerance $\epsilon$. In order to improve the estimation by smoothing, Cornuet et al. (2008) follow the rationale that motivated the use of a local linear regression in Beaumont et al. (2002) and rely on a weighted polychotomous logistic regression to estimate $\pi(M = m|y)$. This modelling is implemented in the DIYABC software.

4 The difficulty with ABC-MC

Most perspectives on ABC do not question the role of the ABC distance nor of the statistic $\eta$ in model choice settings. There is however a much stronger discrepancy between the genuine Bayes factor / posterior probability and the approximations resulting from ABC.
The ABC approximation to a Bayes factor, $B_{12}$ say, resulting from Algorithm 2 is

$$
\hat{B}_{12}(y) = \frac{\pi(M = 2)}{\pi(M = 1)} \frac{\sum_{t=1}^{N} \mathbb{1}_{m^{t}=1}}{\sum_{t=1}^{N} \mathbb{1}_{m^{t}=2}}
$$

An alternative representation is given by

$$
\hat{B}_{12}(y) = \frac{\pi(M = 2)}{\pi(M = 1)} \frac{\sum_{t=1}^{T} \mathbb{1}_{m^{t}=1} \mathbb{1}_{\rho(\eta(z'), \eta(y)) \leq \epsilon}}{\sum_{t=1}^{T} \mathbb{1}_{m^{t}=2} \mathbb{1}_{\rho(\eta(z'), \eta(y)) \leq \epsilon}},
$$

where the pairs $(m^{t}, z^{t})$ are simulated from the (joint) prior and $T$ is the total number of simulations that are necessary for $N$ acceptances in Algorithm 2. In order to study the limiting behaviour of this approximation, we first let $T$ go to infinity. (For simplification purposes and without loss of generality, we choose a uniform prior on the model index.) The limit of $\hat{B}_{12}(y)$ is then

$$
B_{12}(y) = \frac{\mathbb{P}[M = 1, \rho(\eta(z), \eta(y)) \leq \epsilon]}{\mathbb{P}[M = 2, \rho(\eta(z), \eta(y)) \leq \epsilon]} = \frac{\int \mathbb{1}_{\rho(\eta(z), \eta(y)) \leq \epsilon} \pi_1(\theta_1) f_1(z | \theta_1) \, dz \, d\theta_1}{\int \mathbb{1}_{\rho(\eta(z), \eta(y)) \leq \epsilon} \pi_2(\theta_2) f_2(z | \theta_2) \, dz \, d\theta_2} = \frac{\int \mathbb{1}_{\rho(\eta(y)) \leq \epsilon} \pi_1(\theta_1) f_1^{\eta}(\eta | \theta_1) \, d\eta \, d\theta_1}{\int \mathbb{1}_{\rho(\eta(y)) \leq \epsilon} \pi_2(\theta_2) f_2^{\eta}(\eta | \theta_2) \, d\eta \, d\theta_2},
$$

where $f_1^{\eta}(\eta | \theta_1)$ and $f_2^{\eta}(\eta | \theta_2)$ denote the distributions of $\eta(z)$ when $z \sim f_1(z | \theta_1)$ and $z \sim f_2(z | \theta_2)$, respectively. By L’Hospital formula, if we let $\epsilon$ go to zero, the above converges to

$$
B_{12}^{\eta}(y) = \frac{\int \pi_1(\theta_1) f_1^{\eta}(\eta(y) | \theta_1) \, d\theta_1}{\int \pi_2(\theta_2) f_2^{\eta}(\eta(y) | \theta_2) \, d\theta_2},
$$

which is precisely and exactly the Bayes factor for testing model 1 versus model 2 based on the sole observation of $\eta(y)$. This result is completely coherent with the current perspective on ABC, namely that the inference derived from the ideal ABC output when $\epsilon = 0$ only uses the information contained in $\eta(y)$. Thus, in the limiting case, i.e. when the ABC algorithm uses an infinite computing power, the ABC odds ratio does not take into account the features of the data besides the value of $\eta(y)$, which is why the limiting Bayes factor only depends on the distributions of $\eta$ under both models.

In contrast with point estimation—where using a sufficient statistic has no impact on the inference in the limiting case—, the loss of information resulting from considering solely $\eta$ seriously impacts the resulting inference on which model is best supported by the data. Indeed, as exhibited in a special case by Grelaud et al. (2009), the information contained in $\eta(y)$ is almost always smaller than the information contained in $y$ and this
even in the case $\eta(y)$ is a sufficient statistic for both models. In other words, $\eta(y)$ being sufficient for both $f_1(y|\theta_1)$ and $f_2(y|\theta_2)$ does not usually imply that $\eta(y)$ is sufficient for $\{m, f_m(y|\theta_m)\}$. To see why this is the case, consider the most favourable case, namely when $\eta(y)$ is a sufficient statistic for both models. We then have by the factorisation theorem (Lehmann and Casella, 1998) that $f_i(y|\theta_i) = g_i(y)f_i(\eta(y)|\theta_i)$, therefore that

$$B_{12}(y) = \frac{w_1(y)}{w_2(y)} = \frac{\int_{\Theta_1} \pi(\theta_1)g_1(y)f_1^\eta(\eta(y)|\theta_1)\,d\theta_1}{\int_{\Theta_2} \pi(\theta_2)g_2(y)f_2^\eta(\eta(y)|\theta_2)\,d\theta_2} = \frac{g_1(y)}{g_2(y)}B_{12}^\eta(y).$$

Therefore, unless $g_1(y) = g_2(y)$, the two Bayes factors differ by this ratio, $g_1(y)/g_2(y)$, which is only equal to one in a very small number of known cases. This decomposition is a straightforward proof that a model-wise sufficient statistic is usually not sufficient across models, i.e. for model comparison. An immediate corollary is that the ABC-MC approximation does not converge to the exact Bayes factor.

The discrepancy between the limiting ABC inference and the genuine Bayesian inference does not completely come as a surprise, because ABC is indeed an approximation method. Users of ABC algorithms are therefore prepared for some degree of imprecision in their final answer, a point stressed by Wilkinson (2008) or Fearnhead and Prangle (2010) when they qualify ABC as exact inference on a wrong model. However, the magnitude of the difference between $B_{12}(y)$ and $B_{12}^\eta(y)$ expressed by (2) is such that there is no direct connection between both answers. In a general setting, if $\eta$ has the same dimension as one component of the $n$ components of $y$, the ratio $g_1(y)/g_2(y)$ is equivalent to a density ratio for a sample of size $O(n)$, hence it can be arbitrarily small or arbitrarily large when $n$ grows. On the opposite, the Bayes factor $B_{12}^\eta(y)$ is based on what is equivalent to a single observation, hence does not necessarily converge with $n$, as shown by the Poisson and normal examples below. The conclusion derived from one Bayes factor may therefore completely differ from the conclusion derived from other one and there is no possibility of a generic agreement between both, or even of a manageable correction factor.

For this reason, we conclude that the ABC approach cannot be used for testing nor for model choice, with the exception of Gibbs random fields as explained in the next section. In all cases when $g_1(y)/g_2(y)$ is different from one and impossible to approximate, no inference on the true Bayes factor can be made based on the ABC-MC approximation without further information on the ratio $g_1(y)/g_2(y)$, which is most often unavailable.

We note that Didelot et al. (2010) also derived this relation between both Bayes factors.
in their formula (18) but surprisingly concluded on advocating the use of ABC in complex models, where there are no sufficient statistics. We disagree with this perspective for reasons that will be made clear in the following sections.

5 The special case of Gibbs random fields

Grelaud et al. (2009) showed that, for Gibbs random fields and in particular for Potts models, when the goal is to compare several neighbourhood structures, the computation of the posterior probabilities of the models/structures under competition can be operated by likelihood-free simulation techniques, in the sense that there exists a converging approximation to the true Bayes factor. The reason for this property is that, in the above ratio, $g_1(y) = g_2(y)$ in this special model.

Indeed, if we consider a Gibbs random field given by the likelihood function

$$f(y|\theta) = \frac{1}{Z_\theta} \exp\{\theta^T \eta(y)\},$$

where $\mathbf{y}$ is a vector of dimension $n$ taking values over the finite set $\mathcal{X}$ (possibly a lattice), $\eta(\cdot)$ is the potential function defining the random field, taking values in $\mathbb{R}^p$, $\theta \in \mathbb{R}^p$ is the associated parameter, and $Z_\theta$ is the corresponding normalising constant, the potential function $\eta$ is a sufficient statistic for the model. For instance, in Potts models, the sufficient statistic is the number of neighbours,

$$\eta(y) = \sum_{i' \sim i} 1\{y_i = y_{i'}\},$$

associated with a neighbourhood structure denoted by $i \sim i'$ (meaning that $i$ and $i'$ are neighbours).

The property that validates an ABC resolution for the comparison of Gibbs random fields is that, due to their specific structure, there exists a sufficient statistic vector that runs across models and which allows for an exact (when $\epsilon = 0$) simulation from the posterior probabilities of the models. More specifically, consider $M$ Gibbs random fields in competition, each one being associated with a potential function $\eta_m$ ($1 \leq m \leq M$), i.e. with corresponding likelihood

$$f_m(y|\theta_m) = \exp\{\theta_m^T \eta_m(y)\} / Z_{\theta_m,m},$$

where $\theta_m \in \Theta_m$ and $Z_{\theta_m,m}$ is the unknown normalising constant. A Bayesian analysis operates on the extended parameter space $\Theta = \bigcup_{m=1}^M \{m\} \times \Theta_m$ that includes both the model index $\mathcal{M}$ and the corresponding parameter space $\Theta_m$. The inferential target is thus the model posterior probability

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

9
i.e. the marginal in $M$ of the posterior distribution on $(M, \theta_1, \ldots, \theta_M)$ given $y$. Each model has its own sufficient statistic $\eta_m(\cdot)$. Then, for each model, the vector of statistics $\eta(\cdot) = (\eta_1(\cdot), \ldots, \eta_M(\cdot))$ is clearly sufficient; furthermore [Grelaud et al. (2009)] exposed the fact that $\eta$ is also sufficient for the joint parameter $(M, \theta_1, \ldots, \theta_M)$. That this concatenation of sufficient statistics is jointly sufficient across models is a property that is rather specific to Gibbs random field models, at least from a practical perspective (see below). Figure 1 shows an experiment from [Grelaud et al. (2009)] concluding rightly at the agreement between the exact Bayes factor and an ABC approximation.

Figure 1: Comparison between the true Bayes factor and the ABC approximation in a Markov model selection of [Grelaud et al. (2009)], based on 2,000 simulated sequences and $4 \times 10^6$ proposals from the prior. The solid/red line is the diagonal. *(Source: Grelaud et al., 2009.)*

[Didelot et al.] (2010) point out that this specific property of Gibbs random fields can be extended to any exponential family (hence to any setting enjoying sufficient statistics, see e.g. [Casella and Berger (2001)]. Their argument is an encompassing property: by including all sufficient statistics and all dominating measure statistics in an encompassing model, models under comparison become submodels of the encompassing model. They then conclude that the concatenation of those statistics is jointly sufficient across models. While this encompassing principle holds in full generality, in particular when comparing
models that are already embedded, we think it leads to a biased perspective about the merits of ABC for model choice: in practice, complex models do not enjoy sufficient statistics (if only because they are not exponential families). As demonstrated in the next section, there is more than a mere loss of information due to the use of insufficient statistics and looking at what happens in the limiting case when one is relying on a common sufficient statistic is a formal study that brings light on the potentially huge discrepancy between the ABC-based Bayes factor and the true Bayes factor. To study a solution to the problem in the formal case of the exponential families does not help in the understanding of the discrepancy in non-exponential models.

6 Arbitrary ratios

The difficulty with the arbitrary discrepancy between $B_{12}(y)$ and $B_{12}^\eta(y)$ is that it is impossible to evaluate in a general setting, while there is no reason to expect a reasonable agreement between both quantities. A first illustration was produced by Marin et al. (2011) in the setting of $MA(q)$ time series: a simulation experiment showed that, when comparing an $MA(2)$ with an $MA(1)$ model, the ABC approximation to the Bayes factor was stable (around 2.3) as $\epsilon$ decreases, remaining far from the true Bayes factor 17.7 for an $MA(2)$ simulated sample, while the approximation was 0.25 against a true value of 0.004 in the case of a simulated $MA(1)$ sample.

6.1 A Poisson-negative binomial illustration

As a first illustration of the discrepancy due to the use of a sufficient statistic, consider the simple case when a sample $y = (y_1, \ldots, y_n)$ could come from either a Poisson $\mathcal{P}(\lambda)$ distribution or from a geometric $\mathcal{G}(p)$ distribution, already introduced in Grelaud et al. (2009) as a counter-example to Gibbs random fields and later reprocessed in Didelot et al. (2010) to support their sufficiency argument. In this setting, the sum $S = \sum_{i=1}^n y_i = \eta(y)$ is a sufficient statistic for both models but not across models. The distribution of the sample given $S$ is a multinomial $\mathcal{M}(S, 1/n, \ldots, 1/n)$ distribution when the data is Poisson, since $S$ is then a Poisson $\mathcal{P}(n\lambda)$ variable, while it is the uniform distribution with constant probability

$$\frac{1}{(n+S-1)^n} \sum_{y_i=S} = \frac{S!(n-1)!}{(n+S-1)!} \sum_{y_i=S}$$

in the geometric case, since $S$ is then a negative binomial $\mathcal{N}(n, p)$ variable. The discrepancy ratio is therefore

$$\frac{g_1(y)}{g_2(y)} = \frac{S!n^{-S}/\prod_i y_i!}{1/(n+S-1)}$$
When simulating $n$ Poisson or geometric variables and using prior distributions

$$\lambda \sim \mathcal{E}(1), \quad p \sim \mathcal{U}(0, 1),$$

on the respective models, the exact Bayes factor can be evaluated and the range and distribution of the discrepancy are therefore available. Figure 2 gives the range of $B_{12}(y)$ versus $B_{12}^n(y)$, showing that $B_{12}^n(y)$ is in this case absolutely un-related with $B_{12}(y)$: The values produced by both approaches simply have nothing in common. As noted above, the approximation $B_{12}^n(y)$ based on the sufficient statistic $S$ is producing figures of the magnitude of a single observation, while the true Bayes factor is of the order of the sample size.

Figure 2: Comparison between the true log-Bayes factor (first axis) for the comparison of a Poisson model versus a negative binomial model and of the log-Bayes factor based on the sufficient statistic $\sum_i y_i$ (second axis), for Poisson (left) and negative binomial (left) samples of size $n = 50$, based on $T = 10^4$ replications.

The discrepancy between both Bayes factors is in fact increasing with the sample size, as shown by the following result:

**Lemma 1.** Consider performing model selection between model 1: $\mathcal{P}(\lambda)$ with prior distribution $\pi_1(\lambda)$ equal to an $\mathcal{E}(1)$ distribution and model 2: $\mathcal{G}(p)$ with a uniform prior
distribution $\pi_2$ when the observed data $y$ consists of iid observations with $E[y_i] = \theta_0 > 0$. Then $S(y) = \sum_{i=1}^n y_i$ is the minimal sufficient statistic for both models and the Bayes factor based on the sufficient statistic $S(y)$, $B^n_{12}(y)$, satisfies

$$\lim_{n \to \infty} B^n_{12}(y) = \frac{(\theta_0 + 1)^2}{\theta_0} e^{-\theta_0} \text{ a.s.}$$

Therefore, the Bayes factor based on the sufficient statistic $S(y)$ is not consistent; it converges to a non-zero, finite value almost surely.

Proof. Under model 1, we have $S \sim P(n\lambda)$, with corresponding likelihood

$$f_1^S(S|\lambda) = \frac{1}{\Gamma(S + 1)} (n\lambda)^S e^{-n\lambda}.$$

The marginal likelihood of $S$ under the prior $\pi_1$ is then

$$\int_0^\infty \frac{\lambda^S e^{-\lambda}}{\Gamma(S + 1) n^{-S}} e^{-\lambda} d\lambda = \frac{1}{S} \int_0^\infty \frac{\lambda^S e^{-(n+1)\lambda}}{\Gamma(S) n^{-S}} d\lambda = \frac{1}{S} \frac{n^S}{(n+1)^S} = \frac{1}{S} \left(1 + \frac{1}{n}\right)^{-S}.$$

Under model 2, the sufficient statistic has a negative binomial distribution, $S \sim \text{Neg}(n,p)$ and thus

$$f_2^S(S|p) = \left(\frac{n + S - 1}{S}\right) p^S (1-p)^n = \frac{\Gamma(S + n)}{\Gamma(S + 1) \Gamma(n)} p^S (1-p)^n.$$

The corresponding marginal likelihood under the prior $\pi_2$ is

$$\frac{\Gamma(S + n)}{\Gamma(S + 1) \Gamma(n)} \int_0^1 p^S (1-p)^n dp = \frac{\Gamma(S + n)}{\Gamma(S + 1) \Gamma(n)} \text{Beta}(S + 1, n + 1) = \frac{n}{(S + n + 1)(S + n)}.$$

Therefore from (3) and (4), the Bayes factor based on the sufficient statistic is given by

$$B^n_{12}(y) = \left(1 + \frac{1}{n}\right)^{-S} \times \frac{(S + n) (S + n + 1)}{S n} \left(\frac{1}{\theta_0}\right)^S$$

Since the $y_i$'s are iid with mean $\theta_0$, the Law of Large Numbers implies that $S/n \to \theta_0$ almost surely, thus

$$\lim_{n \to \infty} \frac{(S + n) (S + n + 1)}{S n} = \frac{(\theta_0 + 1)^2}{\theta_0}$$
since $\theta_0 > 0$. Furthermore,

$$
\lim_{n \to \infty} \left(1 + \frac{1}{n}\right)^{-S} = \lim_{n \to \infty} e^{-S \log(1+1/n)} = e^{-\theta_0}.
$$

Thus from (3)–(5) we deduce that

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

proving the result.

In this specific setting, Didelot et al. (2010) show that adding $P = \prod_i y_i!$ to the sufficient statistic $S$ induces a statistic $(S, P)$ that is sufficient across both models. While this is a mathematically correct observation, we think it is not helpful for the understanding of the behaviour of ABC-model choice in realistic settings: outside toy examples as the one above and well-structured although complex exponential families like Gibbs random fields, it is not possible to come up with completion mechanisms that ensure sufficiency across models and it is therefore more fruitful to consider the diverging behaviour of the ABC approximation as given, rather than attempting at solving the problem.

### 6.2 A normal illustration

First, note that, given a one-dimensional sufficient statistic $S = \eta(y)$, the functions $g_1(y)$ and $g_2(y)$ can on principle be anything. For instance,

$$
g_1(y) = \prod_{i=1}^{n} \varphi(y_i - S|\sigma_1^2) \mathbb{I}_{\sum_i y_i = nS}
$$

and

$$
g_2(y) = \prod_{i=1}^{n} \varphi(y_i - S|\sigma_2^2) \mathbb{I}_{\sum_i y_i = nS}
$$

is a possible model. In other words, by a reparameterisation of the models, we could observe $y = (y_1, \ldots, y_{n-1}, S)$ with

$$
y_1, \ldots, y_{n-1}|S \overset{\text{iid}}{\sim} \mathcal{N}(S, \sigma_1^2) \quad \text{and} \quad y_1, \ldots, y_{n-1}|S \overset{\text{iid}}{\sim} \mathcal{N}(S, \sigma_2^2),
$$

this independently of the distributions of $S$ under both models. (This means that we can find two competing models where the distributions of $S$ are not connected with $\sigma_1$ nor with $\sigma_2$.) Because they depend on the choice of those distributions, the true Bayes factor and the ABC-Bayes factor are unrelated and may as well diverge from one another. Admittedly, this construct is artificial in that there is no clear statistical setting when this
could occur, but the construct is both mathematically valid and informative about the lack of control over the diverging factor \( g_1(y) / g_2(y) \).

If we look at a fully normal \( \mathcal{N}(\mu, \sigma^2) \) setting, we have

\[
f(y|\mu) \propto \exp \left\{ -n\sigma^{-2}(\bar{y} - \mu)^2 / 2 - \sigma^{-2} \sum_{i=1}^{n} (y_i - \bar{y})^2 / 2 \right\} \sigma^{-n}
\]

hence

\[
f(y|\bar{y}) \propto \exp \left\{ -\sigma^{-2} \sum_{i=1}^{n} (y_i - \bar{y})^2 / 2 \right\} \sigma^{-n} \sum_{y_i = n\bar{y}}.
\]

If we reparameterise the observations into \( u = (y_1 - \bar{y}, \ldots, y_{n-1} - \bar{y}, \bar{y}) \), we do get

\[
f(u|\mu) \propto \sigma^{-n} \exp \left\{ -n\sigma^{-2}(\bar{y} - \mu)^2 / 2 \right\} \times \exp \left\{ -\sigma^{-2} \sum_{i=1}^{n-1} u_i^2 / 2 - \sigma^{-2} \left[ \sum_{i=1}^{n-1} u_i \right]^2 / 2 \right\}
\]

since the Jacobian is 1. Hence

\[
f(u|\bar{y}) \propto \exp \left\{ -\sigma^{-2} \sum_{i=1}^{n-1} u_i^2 / 2 - \sigma^{-2} \left[ \sum_{i=1}^{n-1} u_i \right]^2 / 2 \right\} \sigma^{-n}
\]

Considering both models

\[ y_1, \ldots, y_n \overset{iid}{\sim} \mathcal{N}(\mu, \sigma_1^2) \quad \text{and} \quad y_1, \ldots, y_n \overset{iid}{\sim} \mathcal{N}(\mu, \sigma_2^2), \]

the discrepancy ratio is then given by

\[
g_1(y) = \frac{\exp \left\{ -\sigma_1^{-2} \sum_{i=1}^{n-1} (y_i - \bar{y})^2 / 2 - \sigma_1^{-2} \left[ \sum_{i=1}^{n-1} (y_i - \bar{y}) \right]^2 / 2 \right\} \sigma_1^{-n+1}}{\exp \left\{ -\sigma_2^{-2} \sum_{i=1}^{n-1} (y_i - \bar{y})^2 / 2 - \sigma_2^{-2} \left[ \sum_{i=1}^{n-1} (y_i - \bar{y}) \right]^2 / 2 \right\} \sigma_2^{-n+1}}
\]

\[
= \frac{\sigma_2^{n-1}}{\sigma_1^{n-1}} \exp \left\{ \frac{\sigma_2^2 - \sigma_1^2}{2} \left( \sum_{i=1}^{n-1} (y_i - \bar{y})^2 + \sum_{i=1}^{n-1} (y_i - \bar{y})^2 \right) \right\}
\]

and is connected with the lack of consistency of the Bayes factor:

**Lemma 2.** Consider performing model selection between model 1: \( \mathcal{N}(\mu, \sigma_1^2) \) and model 2: \( \mathcal{N}(\mu, \sigma_2^2) \), \( \sigma_1 \) and \( \sigma_2 \) being given, with prior distributions \( \pi_1(\mu) = \pi_2(\mu) \) equal to a \( \mathcal{N}(0, a^2) \) distribution and when the observed data \( \mathbf{y} \) consists of iid observations with finite mean and
variance. Then \( S(y) = \sum_{i=1}^{n} y_i \) is the minimal sufficient statistic for both models and the Bayes factor based on the sufficient statistic \( S(y) \), \( B_{12}^n(y) \), satisfies

\[
\lim_{n \to \infty} B_{12}^n(y) = 1 \quad \text{a.s.}
\]

**Proof.** The marginal likelihood associated with \( S(y) \) and the prior \( \mu \sim \mathcal{N}(0, a^2) \) is

\[
m^n(S) \propto \sqrt{n}\sigma_1^{-1} \int e^{-n(y-\mu)^2/2\sigma_1^2} e^{-\mu^2/2a^2} d\mu
\]

\[
= \sqrt{n}\sigma_1^{-1} \exp \left\{ -\frac{\bar{y}^2}{2(a^2 + \sigma_1^2/n)} \right\} / \sqrt{n\sigma_1^{-1} + a^{-2}},
\]

hence leading to the Bayes factor

\[
B_{12}^n(y) = \frac{\sigma_2}{\sigma_1} \exp \left\{ -\frac{\bar{y}^2}{2(a^2 + \sigma_1^2/n)} \right\} \sqrt{\frac{n\sigma_1^{-1} + a^{-2}}{n\sigma_1^{-1} + a^{-2}}},
\]

which indeed converges to 1 as \( n \) goes to infinity. \( \square \)

Figure 3 illustrates the behaviour of the discrepancy ratio when \( \sigma_1 = 0.1 \) and \( \sigma_2 = 10 \), for datasets of size \( n = 15 \) simulated according to both models. The discrepancy (expressed on a log scale) is once again dramatic, in concordance with the above lemma.

If we now turn to an alternative choice of sufficient statistic, using the pair \((\bar{y}, S^2)\) with

\[
S^2 = \sum_{i=1}^{n} (y_i - \bar{y})^2,
\]

we follow the solution of Didelot et al. (2010). Using a conjugate prior \( \mu \sim \mathcal{N}(0, a^2) \), the true Bayes factor is given by

\[
B_{12}(y) = \frac{\sigma_2^{-n}}{\sigma_1^{-n}} \frac{\exp\{-S^2/2\sigma_1^2\}}{\exp\{-S^2/2\sigma_2^2\}} \frac{\exp\{-\bar{y}^2/2(a^2 + \sigma_1^2/n)\}}{\exp\{-\bar{y}^2/2(a^2 + \sigma_2^2/n)\}} \sqrt{\frac{a^{-2} + \sigma_2^{-2}n}{a^{-2} + \sigma_1^{-2}n}}.
\]

and it is equal to the Bayes factor based on the corresponding distributions of the pair \((\bar{y}, S^2)\) in the respective models. Again, we do not think this coincidence brings the proper light on the behaviour of the ABC approximations in realistic settings.
Figure 3: Empirical distributions of the log discrepancy \( \log g_1(y)/g_2(y) \) for datasets of size \( n = 15 \) simulated from \( \mathcal{N}(\mu, \sigma_1^2) \) (left) and \( \mathcal{N}(\mu, \sigma_2^2) \) (right) distributions when \( \sigma_1 = 0.1 \) and \( \sigma_2 = 10 \), based on \( 10^4 \) replications and a flat prior.
7 Conclusion

Since its introduction by Tavaré et al. (1997) and Pritchard et al. (1999), ABC has been extensively used in several areas involving complex likelihoods, primarily in population genetics. In those domains, ABC has been used both for point estimation and testing of hypotheses. In realistic settings, with the exception of Gibbs random fields that satisfy a resilience property with respect to their sufficient statistics, the conclusions drawn on model comparison cannot alas be trusted \textit{per se} but require further analyses as to the pertinence of the (ABC) Bayes factor based on the summary statistics. This paper has only examined in details the case when the summary statistics are sufficient for both models, while practical situations imply the use of in-sufficient statistics, and further research is needed for the latter case. However, this practical situation implies a wider loss of information compared with the exact inferential approach, hence a wider discrepancy between the exact Bayes factor and the quantity produced by an ABC approximation. It thus appears to us an urgent duty to warn the community about the dangers of this approximation, especially when considering the rapidly increasing number of applications using ABC for conducting model choice and hypothesis testing. As a final (and negative) point, we unfortunately do not see an immediate and generic alternative for the approximation of Bayes factors because importance sampling techniques are suffering from the same difficulty, namely they only depend on the summary statistics.

As a final remark, we note that Sousa et al. (2009) advocate the use of full allelic distributions in an ABC framework, instead of resorting to summary statistics. They show that it is possible to apply ABC using allele frequencies to draw inferences in cases where it is difficult to select a set of suitable summary statistics (and when the complexity of the model or the size of dataset makes it computationally prohibitive to use full-likelihood methods). In such settings, were we to consider a model choice problem, the divergence exhibited in the current paper would not occur because the measure of distance does not rely on a reduction of the sample.

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