Goodness-of-fit statistics for approximate Bayesian computation.

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Running head  Goodness-of-fit with ABC
Abstract

Approximate Bayesian computation is a statistical framework that uses numerical simulations to calibrate and compare models. Instead of computing likelihood functions, Approximate Bayesian computation relies on numerical simulations, which makes it applicable to complex models in ecology and evolution. As usual for statistical modeling, evaluating goodness-of-fit is a fundamental step for Approximate Bayesian Computation.

Here, we introduce a goodness-of-fit approach based on hypothesis-testing. We introduce two test statistics based on the mean distance between numerical summaries of the data and simulated ones. One test statistic relies on summaries simulated with the prior predictive distribution whereas the other one relies on simulations from the posterior predictive distribution. For different coalescent models, we find that the statistics are well calibrated, meaning that the type I error can be controlled. However, the statistical power of the two statistics is extremely variable across models ranging from 20% to 100%. The difference of power between the two statistics is negligible in models of demographic inference but substantial in an additional and purely statistical example. When analyzing resequencing data to evaluate models of human demography, the two statistics provide similar results and confirm that an out-of-Africa bottleneck cannot be rejected for Asiatic and European data. We also consider two speciation models in the context of a butterfly species complex. One goodness-of-fit statistic indicates a poor fit for both models, and the numerical summaries causing the poor fit were identified using posterior predictive checks.

Statistical tests for goodness-of-fit should foster evaluation of model fit in Approximate Bayesian Computation. The test statistic based on simulations from the prior predictive distribution is implemented in the gfit function of the R abc package.
Introduction

Evaluating the goodness-of-fit of a statistical model is part of statistical modeling. Evaluating to what extent a model fit the data is a prerequisite before model improvement, which is the third step of Bayesian data analysis following model formulation and model fitting (Gelman et al., 2014). Approximate Bayesian computation (ABC) follows the rules of Bayesian data analysis and should also encompass goodness-of-fit evaluation (Csilléry et al., 2010).

Ecological or evolutionary models fitted and compared with ABC are usually introduced for explanatory purposes. The objective is to explain the data in terms of ecological and evolutionary processes that arose in the past. Typical questions addressed with ABC are related to historical processes of speciation (Roux et al., 2013), processes of divergence and migration between populations (Laval et al., 2010; Pelletier and Carstens, 2014), processes of biological adaptation (Peter et al., 2012), or ecological dynamics of natural ecosystems (Hartig et al., 2014; Lagarrigues et al., 2015). There is another use of statistical modeling in ecology that seeks a predictive goal instead of an explanatory one. Species distribution models are examples of statistical models introduced for sake of prediction (Elith and Leathwick, 2009). Models designed for a predictive purpose can be evaluated using cross-validation techniques to measure predictive accuracy (Hijmans, 2012). However, there are no measures of predictive accuracy for explanatory models. The impossibility to evaluate prediction ability makes goodness-of-fit evaluation all the more important for models introduced for explanatory purposes.

Evaluating goodness-of-fit in Bayesian analysis is usually performed with graphical checks such as posterior predictive checks (Gelman et al., 2014; Grunenstaeudl et al., 2015). It consists in simulating the parameter \( \theta \) according to the posterior distribution \( p(\theta | s) \), where \( s \) denotes the observed summary statistics...
computed from the data, and then to generate replicated summary statistics $s^{rep}$ based on the generating mechanism $p(s|\theta)$. Summary statistics simulated with this mechanism are sampled according to the posterior predictive distribution that is denoted $p(s|\theta)$ (Gelman et al., 2014). Observed summary statistics $s$ are then compared to the one-dimensional histograms of these replicated summary statistics. Finding an observed summary statistic outside of the range of the posterior predictive distribution is an indication of poor fit. It is also possible to compute the fraction of times posterior predictive simulations are larger (or lower) than the observed summary statistic to obtain posterior predictive P-values (Meng, 1994). Posterior predictive checks are well-suited to Approximate Bayesian Computation for at least two reasons. First, parameter inference is based on summary statistics $s$, which provide straightforward test statistics for posterior predictive checks. Second, the simulation mechanism, which consists of simulating statistics according to $p(s|\theta)$, is already used for parameter inference and can be recycled for goodness-of-fit. Applications of ABC in ecology and evolution have used posterior predictive checks to evaluate model fit in different fields such as demographic inferences in population genetics (Li et al., 2014), taxonomy and systematics (Dong et al., 2014), or ecosystem modeling (Morales et al., 2015).

However, one major concern about posterior predictive P-values is that they are not properly calibrated. Posterior predictive P-values are not uniformly distributed when the data are realizations of the investigated model (i.e., when the null hypothesis is true). Posterior predictive P-values are more concentrated around 1/2 than expected under a uniform distribution (Robins et al., 2000). To provide well-calibrated P-values, we introduce an alternative approach for performing goodness-of-fit in ABC. The objective of the proposed goodness-of-fit (GOF) statistics is to provide an assessment of model fit based on a classi-
cal hypothesis testing framework, where each investigated model serves as the
null hypothesis. Providing well-calibrated P-values allows for its common in-
terpretation across statistical problems in ecology. In Bayesian statistics, there
have been already several attempts at providing well-calibrated P-values, includ-
ing conditional predictive P-values or partial posterior predictive P-values but
they are difficult to compute in complex statistical models (Bayarri and Berger,
2000). Another proposition includes a Bayesian chi-square statistic for GOF
but it is limited to uni-dimensional data or summary statistic (Johnson, 2004).
To provide well-calibrated P-values, we introduce two GOF test statistics whose
computations are straightforward with ABC algorithms. P-values are evaluated
based on the histogram that is constructed by repeatedly computing the GOF
statistics on pseudo-observed data. After providing definitions of the two GOF
statistics, we evaluate their statistical properties in different models of interest
in population genetics, and we compute the statistics in the context of human
and butterfly molecular data.

Methods

A goodness-of-fit statistic based on the prior predictive dis-
tribution

The objective is to test a null hypothesis that assumes that the data are real-
izations of a statistical model denoted $M_0$. The statistical model $M_0$ is defined
by a possibly multivariate parameter denoted $\theta$. In order to introduce the
goodness-of-fit statistic, we recall what is the rejection algorithm. The rejection
algorithm is the basic algorithm to produce samples from a distribution that
approximates the posterior distribution of $\theta$ (Pritchard et al., 1999). First, pa-
parameter values, $\theta_i$, $i = 1, \ldots, n$, are sampled from the prior distribution $p(\theta)$.
Then, summary statistics, $s_i$, are simulated using the generating mechanism $p(s|\theta_i)$. The resulting distribution with which summary statistics are simulated is named as the prior predictive distribution (Gelman et al., 2014). Simulated summary statistics are compared to the observed ones using a distance measure $d$, such as the Euclidean distance. The rejection algorithm rejects all simulations that are too far from the simulations based on the distance measure $d$. In practice, the percentage $\tilde{n}/n$ of accepted simulations, coined as the acceptance rate, is set to a given value (e.g. 1%). The goodness-of-fit statistic is defined as the mean distance between the observed summary statistics and the $\tilde{n}$ simulated statistics that have been accepted (Figure 1)

$$D_{\text{prior}} = \frac{1}{\tilde{n}} \sum_{i=1}^{\tilde{n}} d(s_{\text{accept},i}, s),$$

where $s_{\text{accept}, 1}, \ldots, s_{\text{accept}, \tilde{n}}$ denote the $\tilde{n}$ accepted simulated summary statistics.

To compute the distance $d$, we assume that each one-dimensional summary statistic has been standardized using the median absolute deviation, which is a robust estimate of the standard deviation (Csilléry et al., 2012). The median absolute deviation is computed based on summary statistics simulated from the prior predictive distribution.

To obtain the null distribution of the test statistic $D_{\text{prior}}$, we consider pseudo-observed data sets (Bertorelle et al., 2010). A simulation from model $M_0$ is discarded and considered as the observed data. The remaining $n-1$ simulations are then used to perform the rejection algorithm and to compute the test statistic. Repeating this process $M$ times, we obtain a vector of test statistics $D_{\text{prior}, 1}, \ldots, D_{\text{prior}, M}$. The P-value $P$ of the goodness-of-fit procedure is computed as the proportion of test statistics obtained under model $M_0$ that are larger than the observed one.
\[ P = \frac{1}{M} \sum_{j=1}^{M} \mathbb{1}_{D_{\text{prior}} \geq D_{\text{prior}}}, \]  

where \( \mathbb{1} \) denotes the indicator function. By construction, P-values will be uniformly distributed for summary statistics simulated under the prior predictive distribution, which is defined by the prior distribution of the parameters \( p(\theta) \) and the generating mechanism for the summary statistics \( p(s|\theta) \).

Because computing the goodness-of-fit statistic of equation (1) and its corresponding P-value does not require new simulations in addition to the ones performed for parameter inference, it was possible to implement it in the \texttt{abc R} package, and the name of the \texttt{R} function is \texttt{gfit} (Csilléry et al., 2012).

An alternative goodness-of-fit statistic based on the posterior predictive distribution

We derive an alternative statistic based on summary statistics simulated with the posterior predictive distribution. The alternative statistic denoted as \( D_{\text{post}} \) measures the mean distance between observed summary statistics and statistics simulated based on parameters sampled from the posterior distribution. An advantage of \( D_{\text{post}} \) is that it can make use of regression-adjustments that improve the estimation of the posterior distribution (Beaumont et al., 2002; Blum and François, 2010). The statistic \( D_{\text{post}} \) is defined as follows

\[ D_{\text{post}} = \frac{1}{n'} \sum_{i=1}^{n'} d(s_{\text{rep}}^i, s), \]  

where \( n' \) denotes the number of posterior replicates, and where the summary statistics \( s_{\text{rep}}^i, i = 1, \ldots, n' \), have been sampled according to the posterior predictive distribution \( p(s|s) \). To obtain the null distribution, the test statistic \( D_{\text{post}} \) is computed for \( M \) pseudo-observed data sets, and P-values are obtained...
similarly to equation (2). The computation of the null distribution is computationally intensive. Computing one P-value requires $M \times n'$ times call to the generating mechanism $p(s|\theta)$ that returns a set of summary statistics based on an input value of the parameter $\theta$. Again, P-values will be uniformly distributed for summary statistics simulated under the prior predictive distribution.

**Examples**

**An example of statistical model**

To evaluate type I error and statistical power, we start by considering a toy statistical model. The objective is to test the goodness-of-fit of a Gaussian distribution and of a Laplace distribution when data were simulated with one of these two possible distributions (François and Laval, 2011). For each possible distribution, we simulated 10,000 samples, each of them consisting of a sample of size 50 or 100 summarized by its mean, variance, skewness and kurtosis. For the Gaussian samples, we consider a uniform prior between $-10$ and 10 for the mean parameter and an inverse chi square parameter with 3 degrees of freedom for the variance parameter. For Laplace samples, we consider the same prior for the location parameter. We simulated the scale parameter so that the theoretical variance is also an inverse chi square parameter with 3 degrees of freedom. Detailed aspects of the simulations can be found in the R file that contains a script to generate the simulations and evaluate type I and II errors (Supplementary file 1).

**Examples of demographic inference**

Then, we consider two biologically relevant problems of statistical inference, one related to demographic inference and another to model speciation processes. In the first problem, we test if population genetic data are compatible with a model
of historical bottleneck or of population expansion (Figure 2). For this problem, we consider data simulated with two different coalescent models for which we also used different sets of summary statistics.

The first set of simulations was performed with ms (Hudson, 2002) and consists of 50,000 bp sequences that have been sequenced from 10 diploid individuals. Prior distributions and further details can be found in the R file that contains a script to generate the simulations (Supplementary file 2). A total of 60,000 simulations was performed for each demographic model. Data were summarized using three summary statistics: average nucleotide diversity, and the mean and variance (over loci) of Tajima’s D (Voight et al., 2005). Goodness-of-fit was evaluated based on $D_{\text{prior}}$ and $D_{\text{post}}$.

The second set of simulations was generated using fastsimcoal2 (Excoffier et al., 2013) and consists of a total of 100 independent stretches of the genomes for 10 diploid individuals. Prior distributions are given in the supplementary text. Data were summarized with the total number of SNPs and the unfolded site-frequency-spectrum, defined as the vector counting the number of mutations carried by $i$ chromosomes, for $i$ ranging from 1 to 19. Because this simulation framework is computationally intensive, we evaluated its fit only based on the $D_{\text{prior}}$ statistic.

Examples of speciation models

In the second problem, we consider two models of divergence and admixture that correspond to hypothesized scenarios of speciation in the butterfly species complex Coenonympha (Capblancq et al., 2015). Two species from this complex, C. arcania and C. gardetta, are assumed to have diverged 1.5 to 4 millions years ago (Kodandaramaiah and Wahlberg, 2009), while a third species C. darwiniana is assumed to be the result of admixture between the two ancestral populations (Capblancq et al., 2015). Based on samples from four populations
(one population of *C. arcana*, one of *C. gardetta*, and two populations of *C. darwiniana* sampled in France and Switzerland), we test the fit of two alternative models. The first model assumes that the same admixture event is at the origin of two populations of *C. darwiniana*, and the second model assumes independent admixture events (Figure 2). The prior distributions are given in the supplementary text. We computed with DIYABC a total of 16 summary statistics corresponding to the genetic diversity in each population and to the pairwise $F_{st}$ and Nei’s distances between populations (Cornuet et al., 2010). We generated 1,000,000 simulations for each admixture model. Because this simulation framework is computationally intensive, we evaluated its fit only based on the $D_{prior}$ statistic.

**Application to real data**

We applied the goodness-of-fit statistics $D_{prior}$ and $D_{post}$ to human data consisting of 50 2,000 bp sequence data sampled in 10 individuals coming from three different populations: Africa (Hausa), Asia (Chinese), and Europe (Italian) (Voight et al., 2005). The summary statistics are the average nucleotide diversity and the mean and variance (over loci) of Tajima’s D for three human samples coming from Africa (Hausa), Asia (Chinese), and Europe (Italian). The simulations used to evaluate goodness-of-fit are the simulations of bottleneck and of expansion performed with *ms*.

We also applied the goodness-of-statistics $D_{prior}$ to the dataset of SNPs sampled in the four butterfly species. A total of 139 individuals were genotyped, including 33 individuals of *C. arcana*, 52 individuals of *C. gardetta*, 35 individuals of Swiss *C. Darwiniana*, and 19 individuals of French *C. darwiniana* (Capblancq et al., 2015). The final data set used to compute the 16 summary statistics contains 510 polymorphic loci.
Parameter settings of the GOF statistics

When computing the GOF statistic $D_{\text{prior}}$ of equation (1), the percentage of accepted simulations for the rejection algorithm was set to $\tilde{n}/n = 1\%$. P-values were computed using equation (2) with a total of $M = 1,000$ replicates. When computing the GOF statistic $D_{\text{post}}$ of equation (3), we again consider the Euclidean distance for $d$ and assume that summary statistics have been scaled using median absolute deviations estimated based on the $M \times n'$ posterior replicates. To evaluate $D_{\text{post}}$, the percentage of accepted simulations is set to 1%, a linear adjustment is used for parameter inference (Beaumont et al., 2002), and the number $n'$ of posterior replicates is of 100. Each P-value is evaluated using a total of $M = 200$ replicates.

Results

Simulation study of a toy model

We set the expected type I error at 5% by rejecting the null model when P-values are smaller than 5%. For the toy model, tests based on $D_{\text{prior}}$ or $D_{\text{post}}$ are well calibrated with type I error ranging from 4% to 6% when the nominal type I error is of 5%. However, the power to reject the null is very weak for the statistic $D_{\text{prior}}$ of equation (1). When rejecting the Gaussian distribution, the power is of 9.5% and when rejecting the Laplace model, the power is of 6.5%. When considering the alternative statistic $D_{\text{post}}$ based on the posterior predictive distribution, the power is of 51.5% when rejecting the Gaussian distribution and of 5% when rejecting the Laplace distribution. Increasing the sample size from $n = 50$ to $n = 100$ shows again that the power to reject the Gaussian distribution is increased when using $D_{\text{post}}$ (power of 78%) instead of $D_{\text{prior}}$ (power of 11%).
Distributions of P-values for different evolutionary models

Using the first set of simulations for demographic inference, there are two possible null models (bottleneck or expansion) and two possible models for simulating the data (bottleneck or expansion), which results in four different distributions of P-values. When the null model is used for the simulations, the P-values are uniformly distributed (Figure 3). When the two models are different, the distributions of P-values are shifted towards zero. Moreover, there is a clear asymmetry when performing model fit. P-values obtained when testing the bottleneck model for simulations of expansion are more shifted towards zero than when testing the expansion model for simulations of bottleneck (Figure 3). The distributions of P-values are similar when considering the statistic $D_{post}$ instead of $D_{prior}$ (Figure 3).

Using the second set of simulations based on the site-frequency-spectrum (SFS) and the simulations of speciation models, we again find that P-values are uniformly distributed when simulations are performed using the null model (Supp Info Figure 1 and Figure 4). For the SFS based simulations, there is also an asymmetry in the distributions of P-values. P-values obtained when testing the bottleneck model for simulations of expansion are more shifted towards zero than when testing the expansion model for simulations of bottleneck (Supp Info Figure 1). For the speciation models and when the null model is different from the simulation model, P-values obtained when testing the model with one event of admixture are more shifted towards zero than when testing the model with two events of admixture (Figure 4).

Statistical power

The power of the test statistic $D_{prior}$ is asymmetric (Table 1). It is more difficult to reject an expansion model (power of 18% or 21.5% depending on the summary
statistics) than to reject a bottleneck model (power of 67% or of 53% depending on the summary statistics). Finding asymmetric statistical power is expected because P-values obtained when testing the bottleneck model for simulations of expansion are more shifted toward 0 than when testing the opposite (Figure 3). By contrast to the toy example, considering the $D_{\text{post}}$ statistic instead of $D_{\text{prior}}$ hardly changes statistical power (Table 1). For speciation models, we also find asymmetric statistical power. The power is of 99% when rejecting the one-event admixture model whereas it is of 19.5% when rejecting the two-event admixture model. Again, observing asymmetric power is expected because of the shapes of the distributions of P-values (Figure 4).

**Application to human data**

We apply the goodness-of-statistics $D_{\text{prior}}$ and $D_{\text{post}}$ to the human resequencing data (Table 2). The African dataset is compatible with a constant-population size ($P = 0.21$), a bottleneck ($P = 0.17$), and an expansion model ($P = 0.55$). The Asiatic dataset is compatible with a constant-population size and a bottleneck model ($P = 0.10$ and $P = 0.86$), but not with an expansion model ($P = 0.01$). Finally, the European dataset is compatible with a bottleneck model ($P = 0.60$), but both the constant-population size and the expansion models can be rejected ($P = 0.02$ and $P < 10^{-2}$). Using the goodness-of-fit statistics $D_{\text{post}}$ based on posterior replicates leads to similar conclusions (Table 2). Analysis of the resequencing data with the goodness-of-fit statistics confirms that the out-of-Africa bottleneck cannot be rejected for the Asiatic and the European data (Voight et al. 2005).
Application to study models of speciation in a butterfly species complex

We first consider a visualization routine to investigate model fit with ABC. For the two competing models, we computed principal component analysis (PCA) based on the set of 1 million simulations performed under each model and we displayed the envelope containing 90% of the points in the space defined by the first two PCs [Cornuet et al. 2010; Sjödin et al. 2013]. Figure 5 shows that the model with one admixture event is able to reproduce the summary statistics when summarized by the first two PCs, since the projection of the observed data falls into the 90% envelope. For the two-event admixture model, observed data are outside but nearby the 90% envelope. As a conclusion, the visualization routine based on PCA does not indicate a poor fit of any of the two different admixture models to the polymorphism data of the butterfly Coenonympha species complex.

By contrast, test of GOF based on $D_{prior}$ shows that both models do not provide a good fit to the 16 summary statistics ($P < 10^{-4}$). Performing posterior predictive checks confirms the poor fit because 3 out of 16 summary statistics cannot be reproduced with any of the two admixture models. In 3 out of 4 populations, the simulated mean genetic diversities across all loci are always smaller than the observed values. Thus, we replace in each population the mean genetic diversity across all loci by the mean genetic diversity across variable loci. After replacement of these 4 summary statistics, the $D_{prior}$ statistic does not indicate a poor fit anymore and both speciation models are able to reproduce the 16 observed summary statistics ($P = 0.25$ and $P = 0.28$).
Discussion

We propose two goodness-of-fit statistics to evaluate model fit in Approximate Bayesian Computation. The first goodness-of-fit statistic $D_{\text{prior}}$ is equal to the mean distance between observed summary statistics and the closest simulated ones where summary statistics were simulated with the prior predictive distribution. P-values are estimated based on Monte Carlo replicates by repeatedly computing the goodness-of-fit statistic on pseudo-observed data or summary statistics simulated from the null model. Based on simulations, we confirm that the statistic is well-calibrated because P-values are uniformly distributed when parameters are simulated with the prior distribution and when summary statistic are simulated with the investigated model. However, its statistical power is extremely variable ranging from 20% to 100% in the simulations we investigated.

Observing variable statistical power is expected for admixture models. For instance, the model that comprises of two admixture events is more flexible than the evolutionary model with one admixture event only. As a consequence, it is more difficult to reject the two-admixture model (power of 19.5%) than the one-admixture model (power of 99%) because most of the simulations obtained with one admixture event can be reproduced with two admixture events but the reverse is not true.

We propose a second goodness-of-fit statistic $D_{\text{post}}$ based on posterior replicates. It has several advantages. A conceptual advantage is that it is less dependent on the prior that the $D_{\text{prior}}$ statistic. When using $D_{\text{prior}}$, a good model or evolutionary scenario can come under suspicion with a poor choice of prior distribution. Same arguments were advanced to criticize prior predictive P-values ([Bayarri and Berger 2000](#)). Another difference between the two goodness-of-fit statistics concerns statistical power. When using uninformative prior distributions, as for the toy statistical model we considered, the
$D_{\text{prior}}$ statistic has a weak statistical power compared to $D_{\text{post}}$. However, the statistic $D_{\text{post}}$ has an important drawback related to its computational burden. When using for instance $n' = 100$ posterior replicates to evaluate the statistic and $M = 1,000$ pseudo observed data to compute the null distribution, a total of $100,000 = 1,000 \times 100$ additional simulations are required to evaluate P-values whereas the $D_{\text{prior}}$ statistic does not require simulations in addition to the ones performed for parameter inference. Simulation-based comparisons between $D_{\text{prior}}$ and $D_{\text{post}}$ are equivocal. For the simple toy model, the statistical power of $D_{\text{post}}$ is $5 - 7$ times larger than $D_{\text{prior}}$ whereas there was no substantial difference for the examples of evolutionary scenarios.

Compared to model comparison, which is a common step in ABC, goodness-of-fit has been too neglected. Goodness-of-fit and model comparisons are two different aspects of statistical analysis that should not be confused. Goodness-of-fit tests the absolute fit of a statistical model and do not seek to compare models. The fact that goodness-of-fit provides an absolute measure is valid when considering $D_{\text{prior}}$ and $D_{\text{post}}$ because they rely on Fisher’s approach of significance testing, which requires only one hypothesis, and not on Neyman-Pearson’s approach of hypothesis testing (e.g. likelihood-ratio test) that would require two hypotheses (Lehmann 1993; Beaumont et al. 2010). By contrast, model selection provides statistical measures that are relative to the set of models to be compared (Hickerson 2014; Pelletier and Carstens 2014). Model selection does not test models and do not evaluate model fit. If all candidate models provide a poor fit, model selection will not provide any statistical warning, and that should be a strong endeavor to evaluate model fit.

How should we evaluate model fit based on test statistics and corresponding P-values? Using a standard P-value cutoff of 0.05, there are two options whether or not the P-value is smaller than the cutoff value. The first option is when the
null model cannot be rejected ($P > 0.05$). If the model passes the test, it does not either certify the ‘truth’ of a current scientific theory. Rykiel (1996) coins the validation procedure as operational validation, which is defined as a test protocol to check that the model is an adequate representation of the system. However, he stresses that an adequate representation is not a ‘guarantee that the scientific basis of the model and its internal structure correspond to the actual processes or cause-effect relationships operating in the real system’. Following Popperian philosophy, a P-value larger than 0.05 is not an indication that the tested model is true but that it can not be rejected. A null model may not be rejected for many reasons including lack of power, which can be due to a poor choice of summary statistics or a small sample size.

When the proposed model does not pass the test ($P < 0.05$), poorly fitted summary statistics can be identified using prior or posterior predictive checks. For instance, with the genetic markers of the butterfly species complex, we identified that mean genetic diversity over all loci including SNPs that do not vary within the population is responsible for the poor fit of the investigated models. This suggests potential model improvements such as including gene flow following admixture, which would increase the mean genetic diversity over all loci by decreasing the number of private SNPs. The example of the speciation models shows that having a single and well-calibrated P-value, rather than using graphical routines, such as the PCA-based graphical routine of Figure 5, offers the opportunity for a convenient evaluation of fit. Providing a single well-calibrated P-value for each model is especially useful when there are many summary statistics as it can occur when reconstructing historical demography with molecular data (Robinson et al., 2014). Posterior predictive checks are useful as a second step to detect the summary statistics that explain a poor fit.

The proposed goodness-of-fit statistics seek to foster evaluation of model fit
in ABC. However, the proposed test statistics should not encourage black-box analyses with ABC where decision to reject or not a model relies exclusively on the returned P-value. We view the goodness-of test statistics and corresponding P-values as useful diagnostic devices, particularly when screening models with many summary statistics. P-values are one of many ways to quickly alert oneself to some of the important features of a data set (Gelman et al., 1996). To encourage goodness-of-fit evaluation, the abc R package includes the gfit function that evaluates statistical significance based on the $D_{\text{prior}}$ statistic of equation (1).

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References

Bayarri, M. and J. O. Berger, 2000. P values for composite null models. Journal of the American Statistical Association 95:1127–1142.

Beaumont, M. A., R. Nielsen, C. Robert, J. Hey, O. Gaggiotti, L. Knowles, A. Estoup, M. Panchal, J. Corander, M. Hickerson, et al., 2010. In defence of model-based inference in phylogeography. Molecular Ecology 19:436–446.

Beaumont, M. A., W. Zhang, and D. J. Balding, 2002. Approximate Bayesian computation in population genetics. Genetics 162:2025–2035.

Bertorelle, G., A. Benazzo, and S. Mona, 2010. ABC as a flexible framework to estimate demography over space and time: some cons, many pros. Molecular Ecology 19:2609–2625.

Blum, M. G. B. and O. François, 2010. Non-linear regression models for Approximate Bayesian Computation. Statistics and Computing 20:63–73.

Capblancq, T., L. Després, D. Rioux, and J. Mavarez, 2015. Hybridization promotes speciation in coenonympha butterflies. Molecular Ecology 24:6209–6222.

Cornuet, J.-M., V. Ravigne, and A. Estoup, 2010. Inference on population history and model checking using DNA sequence and microsatellite data with the software DIYABC (v1.0). BMC Bioinformatics 11:401.

Csilléry, K., M. G. B. Blum, O. E. Gaggiotti, and O. François, 2010. Approximate Bayesian Computation in practice. Trends Ecol Evol 25:410–418.

Csilléry, K., O. François, and M. G. B. Blum, 2012. abc: an R package for approximate Bayesian computation (abc). Methods in ecology and evolution 3:475–479.
Dong, F., F.-S. Zou, F.-M. Lei, W. Liang, S.-H. Li, and X.-J. Yang, 2014. Testing hypotheses of mitochondrial gene-tree paraphyly: unravelling mitochondrial capture of the streak-breasted scimitar babbler (Pomatorhinus ruficollis) by the taiwan scimitar babbler (Pomatorhinus musicus). Molecular ecology 23:5855–5867.

Elith, J. and J. R. Leathwick, 2009. Species distribution models: ecological explanation and prediction across space and time. Annual Review of Ecology, Evolution, and Systematics 40:677.

Excoffier, L., I. Dupanloup, E. Huerta-Sánchez, V. C. Sousa, and M. Foll, 2013. Robust demographic inference from genomic and snp data. PLoS Genetics 9:e1003905.

François, O. and G. Laval, 2011. Deviance information criteria for model selection in approximate Bayesian computation. Statistical Applications in Genetics and Molecular Biology 10:1–25.

Gelman, A., J. B. Carlin, H. S. Stern, and D. B. Rubin, 2014. Bayesian data analysis, vol. 2. Taylor & Francis.

Gelman, A., X.-L. Meng, and H. Stern, 1996. Discussion of ‘posterior predictive assessment of model fitness via realized discrepancies’. Statistica sinica 6:767–773.

Gruenstaeudl, M., N. M. Reid, G. L. Wheeler, and B. C. Carstens, 2015. Posterior predictive checks of coalescent models: P2c2m, an r package. Molecular Ecology Resources .

Hartig, F., C. Dislich, T. Wiegand, and A. Huth, 2014. Technical note: Approximate Bayesian parameterization of a process-based tropical forest model. Biogeosciences 11.
Hickerson, M. J., 2014. All models are wrong. Molecular ecology 23:2887–2889.

Hijmans, R. J., 2012. Cross-validation of species distribution models: removing spatial sorting bias and calibration with a null model. Ecology 93:679–688.

Hudson, R. R., 2002. Generating samples under a Wright-Fisher neutral model of genetic variation. Bioinformatics 18:337–338.

Johnson, V. E., 2004. A bayesian chi2 test for goodness-of-fit. Annals of Statistics Pp. 2361–2384.

Kodandaramaiah, U. and N. Wahlberg, 2009. Phylogeny and biogeography of coenonympha butterflies (nymphalidae: Satyrinae)–patterns of colonization in the holarctic. Systematic Entomology 34:315–323.

Lagarrigues, G., F. Jabot, V. Lafond, and B. Courbaud, 2015. Approximate Bayesian computation to recalibrate individual-based models with population data: Illustration with a forest simulation model. Ecological Modelling 306:278–286.

Laval, G., E. Patin, L. B. Barreiro, and L. Quintana-Murci, 2010. Formulating a historical and demographic model of recent human evolution based on resequencing data from noncoding regions. PloS one 5:e10284.

Lehmann, E. L., 1993. The fisher, neyman-pearson theories of testing hypotheses: One theory or two? Journal of the American Statistical Association 88:1242–1249.

Li, S., C. Schlebusch, and M. Jakobsson, 2014. Genetic variation reveals large-scale population expansion and migration during the expansion of bantu-speaking peoples. Proceedings of the Royal Society of London B: Biological Sciences 281:20141448.
Meng, X.-L., 1994. Posterior predictive p-values. The Annals of Statistics Pp. 1142–1160.

Morales, J. M., M. Mermoz, J. H. Gowda, and T. Kitzberger, 2015. A stochastic fire spread model for north patagonia based on fire occurrence maps. Ecological Modelling 300:73–80.

Pelletier, T. A. and B. C. Carstens, 2014. Model choice for phylogeographic inference using a large set of models. Molecular ecology 23:3028–3043.

Peter, B. M., E. Huerta-Sanchez, and R. Nielsen, 2012. Distinguishing between selective sweeps from standing variation and from a de novo mutation.

Pritchard, J. K., M. T. Seielstad, A. Perez-Lezaun, and M. W. Feldman, 1999. Population growth of human Y chromosomes: a study of Y chromosome microsatellites. Molecular Biology and Evolution 16:1791–1798.

Robins, J. M., A. van der Vaart, and V. Ventura, 2000. Asymptotic distribution of p values in composite null models. Journal of the American Statistical Association 95:1143–1156.

Robinson, J. D., L. Bunnefeld, J. Hearn, G. N. Stone, and M. J. Hickerson, 2014. Abc inference of multi-population divergence with admixture from unphased population genomic data. Molecular ecology 23:4458–4471.

Roux, C., G. Tsagkogeorga, N. Bierne, and N. Galtier, 2013. Crossing the species barrier: genomic hotspots of introgression between two highly divergent ciona intestinalis species. Molecular Biology and Evolution 30:1574–1587.

Rykiel, E. J., 1996. Testing ecological models: the meaning of validation. Ecological modelling 90:229–244.
Sjödin, P., A. E. Sjöstrand, M. Jakobsson, and M. G. B. Blum, 2013. Resequencing data provide no evidence for a human bottleneck in Africa during the penultimate glacial period. Molecular Biology and Evolution 30:513–525.

Voight, B. F., A. M. Adams, L. A. Frisse, Y. Qian, R. R. Hudson, and A. Di Rienzo, 2005. Interrogating multiple aspects of variation in a full resequencing data set to infer human population size changes. Proc Natl Acad Sci USA 102:18508–18513.
Simulate summary statistics from the prior predictive distribution.

Accept the \( n \) summary statistics \( s_{\text{accept}} \) that are the closest to the observed one.

OR

Simulate \( n' \) additional summary statistics \( s_{\text{rep}} \) from the posterior predictive distribution.

Repeat \( M \) times the computation of \( D_{\text{prior}} \) (resp. \( D_{\text{post}} \)) by replacing \( s \) (ie. \( \star \)) by randomly chosen \( s \) simulated from the prior predictive distribution (ie. \( \circ \)).

Build histogram from \( D_{\text{prior}}^1 \) ... \( D_{\text{prior}}^M \) (resp. \( D_{\text{post}}^1 \) ... \( D_{\text{post}}^M \)).

\[
D_{\text{prior}} = \frac{1}{n} \sum_i d(s_{\text{accept}}^i, s)
\]

\[
D_{\text{post}} = \frac{1}{n'} \sum_i d(s_{\text{rep}}^i, s)
\]

\[
P = \frac{1}{M} \sum_j \text{Ind}(D_{\text{prior}}^j \geq D_{\text{prior}}) = \text{card}(\star)/M
\]

Expected distribution of \( D_{\text{prior}} \)

Figure 1: Graphical description of the two goodness-of-fit statistics. The number of accepted summary statistics is denoted as \( n \), the observed summary statistic is denoted as \( s \), the accepted summary statistics are denoted as \( s_{\text{accept}}^1, \ldots, s_{\text{accept}}^n \), the summary statistics simulated with the posterior predictive distribution are denoted as \( s_{\text{rep}}^1, \ldots, s_{\text{rep}}^n \), the number of posterior replicates is denoted as \( n' \), the number of pseudo-observed datasets used to compute \( P \)-values is denoted as \( M \), and the indicator function is denoted as \( \text{Ind} \).
Figure 2: Graphical description of the two examples used to evaluate type I error and power with the goodness-of-fit statistics.
Figure 3: Distribution of P-values for a bottleneck and an expansion model. Data are summarized using three summary statistics, which are the average nucleotide diversity and the mean and variance (over loci) of Tajima’s D. When using $D_{\text{prior}}$ (resp. $D_{\text{post}}$), a total of 1,000 (resp. 200) P-values are computed for each combination of null model and of model used for the simulations.
Inferring modes of speciation

Figure 4: Distribution of P-values based on $D_{\text{prior}}$ for models with one and two events of admixture. Data are summarized using 16 summary statistics corresponding to the genetic diversity in each population and to the pairwise $F_{st}$ and Nei distances between pairs of populations. P-values are computed for each combination of null model and of model used for the simulations.
Figure 5: Visual evaluation of the goodness-of-fit of the two admixture scenarios. Principal component analysis applied to the 16 summary statistics simulated based on the prior predictive distribution. The cross corresponds to observed data. The envelopes are obtained using the gfitpca routine of the abc package and contain 90% of the simulated data points.
Table 1: Statistical power of the goodness-of-fit statistics $D_{prior}$ for different problems of inference in evolutionary biology. The numbers given in parenthesis correspond to the statistical power obtained with $D_{post}$. SFS stands for the site frequency spectrum, which is used as summary statistics and 3 stats. stands for the 3 statistics consisting of the average nucleotide diversity and the mean and variance (over loci) of Tajima’s D.

| Truth                      | Bott. (SFS) | Exp. (SFS) | Bott (3 stat.) | Exp. (3 stat.) | 1 admix. | 2 admix. |
|----------------------------|-------------|------------|----------------|----------------|----------|----------|
| Bott. (SFS)                | 21.5%       |            |                |                |          |          |
| Exp. (SFS)                 | 53%         |            |                |                |          |          |
| Bott. (3 stat.)            |             |            | 18% (17%)      |                |          |          |
| Exp. (3 stat.)             |             |            | 67% (72%)      |                |          |          |
| 1 admix.                   |             |            |                |                |          | 19.5%    |
| 2 admix.                   |             |            |                |                |          | 99%      |
|       | Africa       | Asia         | Europe       |
|-------|--------------|--------------|--------------|
| const.| 0.21 (0.38)  | 0.10 (0.07)  | 0.02 (0.02)  |
| bott. | 0.17 (0.43)  | 0.86 (0.80)  | 0.60 (0.50)  |
| exp.  | 0.55 (0.60)  | 0.01 (0.02)  | 0.00 (0.00)  |

Table 2: P-values obtained with the goodness-of-fit statistics $D_{prior}$ and $D_{post}$ (in parenthesis) for sequence data coming from 3 different populations (Voight et al., 2005). Data consist of the average nucleotide diversity and the mean and variance (over loci) of Tajima’s D. Const. stands for constant population size, bott. stands for the bottleneck model, and exp. stands for the model of demographic expansion.