Batch simulations and uncertainty quantification in Gaussian process surrogate-based approximate Bayesian computation

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Abstract

Surrogate models such as Gaussian processes (GP) have been proposed to accelerate approximate Bayesian computation (ABC) when the statistical model of interest is expensive-to-simulate. In one such promising framework the discrepancy between simulated and observed data is modelled with a GP. So far principled strategies have been proposed only for sequential selection of the simulation locations. To address this limitation, we develop Bayesian optimal design strategies to parallelise the expensive simulations. Current surrogate-based ABC methods also produce only a point estimate of the ABC posterior while there can be substantial additional uncertainty due to the limited budget of simulations. We also address the problem of quantifying the uncertainty of ABC posterior and discuss the connections between our resulting framework called Bayesian ABC, Bayesian quadrature (BQ) and Bayesian optimisation (BO). Experiments with several toy and real-world simulation models demonstrate advantages of the proposed techniques.

1 Introduction

Approximate Bayesian computation (Beaumont et al., 2002; Marin et al., 2012; Lintusaari et al., 2017) has become an essential tool for Bayesian inference when the likelihood function of a statistical model of interest is intractable, i.e. when the analytical form of the likelihood is either unavailable or too costly to evaluate, but simulating the model is feasible. The main idea of the ABC rejection sampler (Pritchard et al., 1999) is to draw a parameter from the prior, use it to simulate one pseudo-data set and finally accept the parameter as a draw from an approximate posterior if the discrepancy between the simulated and observed data sets is small enough. While the computational efficiency of this basic ABC algorithm has been improved in several ways, many models e.g. in genomics and epidemiology (Numminen et al., 2013; Marttinen et al., 2015; McKinley et al., 2018), astronomy (Rogers et al., 2019) and climate science (Holden et al., 2018) are very costly to simulate making sampling-based ABC inference algorithms infeasible. To increase sample-efficiency of ABC, various methods using surrogate models such as neural networks (Papamakarios and Murray, 2016; Papamakarios et al., 2019; Lueckmann et al., 2019; Greenberg et al., 2019) and Gaussian processes (Meeds and Welling, 2014; Wilkinson, 2014; Gutmann and Corander, 2016; McKinley et al., 2018; Järvenpää et al., 2018, 2019a,b) have been proposed.

In one promising surrogate-based ABC framework the discrepancy between the observed and simulated data, a key quantity in ABC, is modelled with a GP (Gutmann and Corander, 2016; Järvenpää et al., 2018, 2019a). Principled sequential Bayesian experimental design (also known as active learning) methods to select the simulation locations so as to maximise the sample-efficiency were proposed by Järvenpää et al. (2019a). However, current principled methods allow to run only one simulation at a time while in practice one often has access to multiple computers to run some of the simulations in parallel. In this work, motivated by the related problem of batch BO (Ginsbourger et al., 2010; Desautels et al., 2014; Shah and Gharrahamani, 2015; Wu and Frazier, 2016; Wilson et al., 2018) and the parallel GP-accelerated synthetic likelihood method by Järvenpää et al. (2019b), we resolve this limitation by developing principled batch simulation methods which are then shown to considerably decrease the wall-time needed for ABC inference.

In practice the posterior distribution is often summarised for further decision making using e.g. expectation and variance. When the computational resources for ABC inference are limited, it would be important to assess the accuracy of such summaries, but this has not been explicitly acknowledged in earlier work. As an additional contribution of this paper, we devise an approximate numerical method to propagate the uncer-
tainty of the discrepancy, represented by the GP model, to the resulting ABC posterior summaries. Such uncertainty estimates are useful for assessing the accuracy of the inference and can also guide the termination of the inference algorithm. We call the resulting framework as *Bayesian ABC*\(^1\) and discuss its connection to BQ and BO methods.

To summarise, we make the following contributions:

- We develop Bayesian experimental design strategies for principled parallelisation of the potentially expensive simulations in the Bayesian ABC framework (Section 3).
- We propose an approximate method to quantify the uncertainty in the moments and marginals of the ABC posterior (Section 4).
- Connections between Bayesian ABC, Bayesian quadrature and Bayesian optimisation are discussed to improve understanding of these conceptually similar GP-surrogate methods (Section 5).
- Experiments with several toy models and three real-world simulation models are used to demonstrate the ABC posterior uncertainty quantification and to show that Bayesian ABC framework is well-suited for parallel simulations (Section 6).

## 2 Bayesian ABC

### 2.1 Brief background on ABC

Suppose our initial knowledge about the (continuous) parameters \( \theta \in \Theta \subset \mathbb{R}^p \) of a statistical model of interest is coded into a prior density \( \pi(\theta) \). If the likelihood function \( \pi(x_0 | \theta) \) is available, the posterior distribution describing our knowledge of \( \theta \) given the observed data \( x_0 \in \mathcal{X} \), can be computed using Bayes’ theorem

\[
\pi(\theta | x_0) = \frac{\pi(\theta)\pi(x_0 | \theta)}{\int_\Theta \pi(\theta)\pi(x_0 | \theta) \, d\theta}.
\]

(1)

If the likelihood function is intractable, evaluating Eq. 1 even up-to-normalisation becomes infeasible. Standard ABC algorithms such as the ABC rejection sampler instead target the approximate posterior

\[
\pi_{\text{ABC}}(\theta | x_0) \triangleq \frac{\pi(\theta)\int_{\mathcal{X}} \pi_{\varepsilon}(x_0 | x) \pi(x | \theta) \, dx}{\int_\Theta \pi(\theta)\int_{\mathcal{X}} \pi_{\varepsilon}(x_0 | x) \pi(x' | \theta) \, dx' \, d\theta},
\]

(2)

where \( \pi_{\varepsilon}(x_0 | x) = \mathbb{I}_{\Delta(x_0, x) \leq \varepsilon} \). Other choices of kernel \( \pi_{\varepsilon} \) are also possible (Wilkinson, 2013). Above, \( \Delta : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}_+ \) is a discrepancy function used to compare the similarity of the data sets and \( \varepsilon \) is a threshold parameter. Small \( \varepsilon \) produces good approximations but renders sampling-based ABC methods inefficient. A well-constructed discrepancy function is an important ingredient of accurate ABC inference (Marin et al., 2012; Fearnhead and Prangle, 2012). In this paper we assume a suitable discrepancy function is already available (e.g. constructed based on expert opinion, earlier analyses on other similar models, pilot runs or distance measures between raw data sets (Park et al., 2016; Jiang et al., 2018; Bernton et al., 2019)) and focus on approximating any given ABC posterior in Eq. 2 as well as possible given only a limited budget of simulations (e.g. less than a thousand).

### 2.2 Bayesian ABC framework

The main idea of Bayesian ABC is to explicitly use another layer of Bayesian inference to estimate the ABC posterior in Eq. 2. The previously simulated discrepancy-parameter-pairs are treated as data to learn a surrogate model, which will predict the discrepancy for a given parameter value. The surrogate model is further used to form an estimator for the ABC posterior (Section 4).

We assume each discrepancy evaluation denoted by \( \Delta_i \) at corresponding parameter \( \theta_i \), is generated as

\[
\Delta_i = f(\theta_i) + \nu_i, \quad \nu_i \sim \mathcal{N}(0, \sigma_n^2),
\]

(3)

where \( \sigma_n^2 > 0 \) is the variance of the discrepancy assumed here constant over \( \Theta \).\(^2\) To encode the assumptions of smoothness and e.g. potential quadratic shape of the discrepancy \( \Delta_0 \), its unknown mean function \( f \) is given a hierarchical GP prior

\[
f | \gamma \sim \mathcal{GP}(m_0(\theta), k_\phi(\theta, \theta')), \quad m_0(\theta) \triangleq \sum_{i=1}^t \gamma_i h_i(\theta), \quad \gamma \sim \mathcal{N}(b, B),
\]

(4)

where \( k_\phi : \Theta^2 \rightarrow \mathbb{R} \) is a covariance function with hyperparameters \( \phi \) and \( h_i : \Theta \rightarrow \mathbb{R} \) are basis functions (both assumed continuous). We marginalise \( \gamma \) in Eq. 4, as in O’Hagan and Kingman (1978), and Riihimäki and Vehtari (2014), to obtain the GP prior

\[
f \sim \mathcal{GP}(h(\theta)^\top b, k_\phi(\theta, \theta') + h(\theta)^\top Bh(\theta')), \quad (5)
\]

where \( h(\theta) \in \mathbb{R}^r \) is a column vector consisting of the basis functions \( h_i \) evaluated at \( \theta \). For now, we assume the GP hyperparameters \( \psi \triangleq (\sigma_n^2, \phi) \) are fixed and omit \( \psi \) from our notation for brevity.

Given any \( t \) discrepancy-parameter-pairs \( D_t \triangleq \{ (\Delta_i, \theta_i) \}_i=1 \) we can obtain \( f | D_t \sim \mathcal{GP}(m_t(\theta), c_t(\theta, \theta')) \),

\[
m_t(\theta) \triangleq k_t(\theta)K_t^{-1}\Delta_t + R_t^{\top} \hat{\gamma}_t,
\]

(6)

\(^1\)We use this name in analogy with the related problems of Bayesian quadrature and Bayesian optimisation.

\(^2\)We justify this seemingly strong modelling assumption in the Appendix A.2.
where \( [K_i]_{ij} \triangleq k(\theta_i, \theta_j) + 1_{i=j} \sigma_n^2 \), \( k(\theta, \theta) \triangleq (k(\theta, \theta_1), \ldots, k(\theta, \theta_t))^{\top} \), \( \Delta_t \triangleq (\Delta_1, \ldots, \Delta_t)^{\top} \) and

\[
\gamma_i \triangleq [B^{-1} + H_i K_i^{-1} H_i^{\top}]^{-1}(H_i K_i^{-1} \Delta_i + B^{-1} b), \quad R_i(\theta) \triangleq H_i^{-1} K_i^{-1} k_i^\top(\theta),
\]

Above \( \gamma_i \) is the generalised least-squares estimate, \( H_i \) is the \( r \times t \) matrix whose columns consist of basis function values evaluated at \( \theta_{1:t}, \theta_{1:t} \) is a \( p \times t \) matrix, and \( H(\theta) \in \mathbb{R}^r \) is the corresponding vector of test point \( \theta \). We also define \( s_{i}^2(\theta) \triangleq c_i(\theta, \theta) \) and \( \Pi_{D_i}^f \triangleq \mathcal{GP}(\mu_i(\theta), c_i(\theta, \theta')) \). For further details of GP regression, see e.g. Rasmussen and Williams (2006).

If the true discrepancy mean function \( f \) and the variance of the discrepancy \( \sigma_n^2 \) were known, the ABC posterior could be obtained from Eq. 2 as

\[
\pi_{ABC}^f(\theta) \triangleq \frac{\pi(\theta) \Phi((\varepsilon - f(\theta))/\sigma_n)}{\int_{\Theta} \pi(\theta') \Phi((\varepsilon - f(\theta'))/\sigma_n) \, d\theta'},
\]

where \( \Phi(\cdot) \) is the Gaussian cdf. As we have only access to observations \( D_t \) our knowledge about \( f \) is represented by the Gaussian measure \( f \sim \Pi_{D_t}^f \) and ABC posterior in Eq. 10 is treated as an unknown quantity. Its posterior distribution describes the amount of uncertainty in \( \pi_{ABC}^f \) due to the limited \( t \) simulations and is obtained as the push-forward measure through the mapping \( f \mapsto \pi_{ABC}^f \) given by Eq. 10.

Computing the distribution of \( \pi_{ABC}^f \) is difficult due to its nonlinear dependence on \( f \) and because \( f \) is infinite-dimensional. However, the mean, variance and quantiles of the unnormalised ABC posterior

\[
\tilde{\pi}_{ABC}^f(\theta) \triangleq \pi(\theta) \Phi((\varepsilon - f(\theta))/\sigma_n),
\]

i.e. the numerator of Eq. 10, can be computed analytically. Formulas for these quantities were derived by Järvenpää et al. (2019a) in the case of a zero mean GP prior but they hold also for our more general GP model. For example,

\[
E_{f | D_t}(\tilde{\pi}_{ABC}^f(\theta)) = \pi(\theta) \Phi(a_t(\theta)),
\]

\[
a_t(\theta) \triangleq (\varepsilon - m_t(\theta))/\sqrt{\sigma_n^2 + s_{t}^2(\theta)},
\]

\[
\text{med}_{f | D_t}(\tilde{\pi}_{ABC}^f(\theta)) = \pi(\theta) \Phi((\varepsilon - m_t(\theta))/\sigma_n),
\]

where med denotes the marginal (i.e. elementwise) median.

### 3 Parallel simulations

#### 3.1 Decision-theoretic approach

We aim to find the most informative simulation locations for obtaining the best possible estimate of the ABC posterior \( \pi_{ABC}^f \) given the postulated GP model. Principled sequential designs, where one simulation is run at a time, were developed by Järvenpää et al. (2019a). In practice, to decrease the wall-time needed for the inference task, one could run some of the simulations in parallel. In the following, we apply Bayesian experimental design theory for the (synchronous) batch setting where \( b \) simulations are simultaneously selected to be computed in parallel.

First, consider a loss function \( l : \mathcal{G}^2 \rightarrow \mathbb{R}_+ \) so that \( l(\pi_{ABC}, d) \) quantifies the penalty of reporting \( d \in \mathcal{G} \) as our ABC posterior when the true one is \( \pi_{ABC} \in \mathcal{G} \). Given \( D_t \), the one-batch-ahead Bayes-optimal selection of the next batch of \( b \) evaluations \( \theta^{\text{opt}} = [\theta_1^{\text{opt}}, \ldots, \theta_b^{\text{opt}}] \) is then obtained as

\[
\theta^{\text{opt}} = \arg \min_{\theta^* \in \Theta^b} L_t(\theta^*), \quad \text{where}
\]

\[
L_t(\theta^*) = \mathbb{E}_{\Delta^* | \theta^*, D_t} \left( \min_{d \in \mathcal{G}} \mathbb{E}_{f | D_t \cup D^*} l(\pi_{ABC}^f, d) \right),
\]

In Eq. 16, we calculate an expectation over future discrepancy evaluations \( \Delta^* = (\Delta_1^*, \ldots, \Delta_t^*) \) at locations \( \theta^* \), assuming they follow our current GP model. The expectation is taken of the Bayes risk \( L(\Pi_{D_t \cup D^*}^f) \) resulting from the nested decision problem of choosing the estimator \( d \), assuming \( \Delta^* \) are known and merged with current data \( D_t \) via \( D^* \triangleq \{ \Delta_i^* | \theta_i \} \}_{i=1}^b \). While the main quantity of interest in the Bayesian ABC framework is the ABC posterior \( \pi_{ABC}^f \) in Eq. 10, in practice it is desirable to use a loss function \( \tilde{l} \) based on the unnormalised distribution \( \tilde{\pi}_{ABC}^f \). Such a simplification, also used by Kandasamy et al. (2017), Sinsbeck and Nowak (2017), and Järvenpää et al. (2019a,b), allows efficient computations. Furthermore, evaluations that are optimal for estimating \( \tilde{\pi}_{ABC}^f \) will be informative about the related quantity \( \pi_{ABC}^f \) as well.

Consider \( L^2 \) loss function \( \tilde{l}_q \triangleq \int_{\Theta} (\tilde{\pi}_{ABC}^f(\theta) - \tilde{d}(\theta))^q \, d\theta \) with \( q = 2 \) between the unnormalised ABC posterior \( \tilde{\pi}_{ABC}^f \) and its estimator \( \tilde{d} \) (both supposed to be square-integrable in \( \Theta \) i.e. \( \tilde{\pi}_{ABC}^f, \tilde{d} \in L^2(\Theta) \)). Then the optimal estimator is the mean in Eq. 12 (Sinsbeck and Nowak, 2017; Järvenpää et al., 2019b). If we instead consider \( L^1 \) loss \( \tilde{l}_1 \) (supposing \( \tilde{\pi}_{ABC}^f, \tilde{d} \in L^1(\Theta) \)), then the marginal median in Eq. 14 is the optimal estimator. Corresponding Bayes risks, denoted \( L^v \) and \( L^m \), respectively, can be computed as follows:

\[
L^v(\Pi_{D_t}^f) = \int_{\Theta} \pi^2(\theta) \Phi(a_t(\theta)) \Phi(-a_t(\theta))
\]

\[
-2T(a_t(\theta), \sigma_n/\sqrt{\sigma_n^2 + 2s_{t}^2(\theta)}) \, d\theta,
\]

\[
L^m(\Pi_{D_t}^f) = \int_{\Theta} \pi^2(\theta) \Phi(a_t(\theta))^q \, d\theta.
\]
\[ L^m(\Pi_{D_i}) = 2 \int_{\Theta} \pi(\theta) T(a_t(\theta), s_t(\theta)/\sigma_n) \, d\theta, \]

where \( a_t(\theta) \) is given by Eq. 13 and \( T(\cdot, \cdot) \) denotes Owen’s T function (Owen, 1956).

Note that all proofs are given in Appendix A.1. We call \( L_t(\theta^*) \) as an acquisition function. Expected integrated variance (EIV) and expected integrated MAD\(^3\) (EIMAD) acquisition functions, denoted \( L^e_1(\theta^*) \) and \( L^m_1(\theta^*) \), respectively, can be computed as follows:

**Proposition 3.2.** Consider the GP model in Section 2. The EIV and EIMAD acquisition functions are

\[
L^e_1(\theta^*) = 2 \int_{\Theta} \pi^2(\theta) \left[ T\left(a_t(\theta), \frac{\sigma_n^2 + s_n^2(\theta) - \tau^2_1(\theta; \theta^*)}{\sigma_n^2 + s_n^2(\theta) + \tau^2_1(\theta; \theta^*)}\right) - T\left(a_t(\theta), \frac{\sigma_n}{\sqrt{\sigma_n^2 + 2s_n^2(\theta)}}\right) \right] \, d\theta,
\]

\[
L^m_1(\theta^*) = 2 \int_{\Theta} \pi(\theta) T\left(a_t(\theta), \frac{s_n^2(\theta) - \tau^2_1(\theta; \theta^*)}{\sqrt{\sigma_n^2 + \tau^2_1(\theta; \theta^*)}}\right) \, d\theta,
\]

respectively, where \( a_t(\theta) \) is given by Eq. 13 and

\[
\tau^2_1(\theta; \theta^*) = c_1(\theta, \theta^*)[c_1(\theta^*, \theta^*) + \sigma_n^2 I^{-1} c_1(\theta^*, \theta)].
\]

**3.2 Optimisation of the acquisition functions**

Finding the one-batch-ahead optimal design \( \theta^*_{opt} \) requires global optimisation over \( \Theta^b \) for both EIV and EIMAD. Since this becomes infeasible with large batch size \( b \) and/or dimension \( p \) of the parameter space \( \Theta \), we use greedy optimisation as common also in batch BO (see, e.g., Ginsbourger et al., 2010; Snoek et al., 2012; Wilson et al., 2018). That is, the \( r \)-th point in the batch (\( 1 \leq r \leq b \)) is iteratively chosen by optimising the acquisition function evaluated with \( \theta^*_1, \ldots, \theta^*_r \) with respect to \( \theta^*_r \) when the other points \( \theta^*_1, \ldots, \theta^*_{r-1} \) are kept fixed to their already determined values. This simplifies the \( pb \)-dimensional optimisation problem to a sequence of easier \( p \)-dimensional problems. Theory of submodular optimisation has been used to study greedy batch designs (Krause et al., 2008; Bach, 2013; Wilson et al., 2018; Järvenpää et al., 2019b). Unfortunately, such analysis hardly extends to our case because the acquisition functions in Proposition 3.2 depend on \( \theta^* \) in a rather complex way. Using the facts that \( T(h, a) \) is non-decreasing for \( a \geq 0 \) and \( \tau^2_1(\theta; \theta^*) \) cannot decrease as more points are included to \( \theta^* \), we nevertheless see that both EIV and EIMAD are non-increasing as set functions of \( \theta^* \). For this reason, we can expect the greedy optimisation to be useful in practice as is seen empirically in Section 6.

Another potential computational difficulty is the integration over \( \Theta \) in Eq. 19 and 20. Many state-of-the-art BO methods, such as Hennig and Schuler (2012), Hernández-Lobato et al. (2014) and Wu and Frazier (2016), also require similar computations. We approximate the integral using numerical integration for \( p \leq 2 \) and self-normalised importance sampling (IS), where the current loss function interpreted as an unnormalised density is the instrumental distribution, for \( p > 2 \).

**3.3 Heuristic baseline batch methods**

We consider also a heuristic acquisition function which evaluates where the pointwise uncertainty of \( \hat{\pi}^f_{ABC}(\theta) \) is highest. Such intuitive strategy is sometimes called as uncertainty sampling and used, e.g., by Gunter et al. (2014), Järvenpää et al. (2019a) and Chai and Garnett (2019). When variance is used as the measure of uncertainty of \( \hat{\pi}^f_{ABC}(\theta) \), we call the method as MAXV and when MAD is used, we obtain an alternative strategy called analogously MAXMAD. The resulting acquisition functions can be easily computed using the integrands of Eq. 17 and Eq. 18.

Finally, we propose a heuristic approach from BO (Snoek et al., 2012) to parallellise MAXV and MAXMAD strategies: The first point in the batch is chosen as in the sequential case. The further points are iteratively selected as the locations where the expected variance (or MAD), taken with respect to the discrepancy values of the pending points, that is points that have been already chosen to the current batch, is highest. The resulting acquisition functions are immediately obtained as the integrands of Eq. 19 and 20.

**4 Uncertainty quantification of the ABC posterior**

Pointwise marginal uncertainty of the unnormalised ABC posterior \( \hat{\pi}^f_{ABC} \) was used in previous section for selecting the simulation locations. However, knowing the value of \( \hat{\pi}^f_{ABC} \) and its marginal uncertainty in some individual \( \theta \)-values is not very helpful for summarising and understanding the accuracy of the final estimate of the ABC posterior. Computing the distribution of the moments and marginals of the normalised ABC posterior \( \pi^f_{ABC} \) in Eq. 10 is clearly more intuitive. See Fig. 1 for a 1D demonstration of this approach.

To access the posterior of \( \pi^f_{ABC} \) it would be possible to fix a sample path \( f^{(i)} \sim \Pi_{D_i} \), then use it to fix a realisation of the ABC posterior \( \pi_{ABC}^{f^{(i)}} \) using Eq. 10 and finally use e.g. MCMC to sample from \( \pi_{ABC}^{f^{(i)}} \). This would be repeated \( s \) times and the resulting set of samples \( \{\{\theta^{(i,j)}\}_{1}^{s} \}_{j=1}^{n} \) (where \( n \) is the length of the

\(^3\)Mean absolute deviation (around median).
MCMC chain for each posterior realisation $i = 1, \ldots, s$ approximately describes the posterior of $\pi_{\text{ABC}}^f$ given $D_i$. The uncertainty of GP hyperparameters $\psi$ could also be taken into account by drawing $\psi^{(i)} \sim \pi(\psi | D_i)$ as the very first step but we here consider $\psi$ as known for simplicity although this causes some underestimation of the uncertainty of $\pi_{\text{ABC}}^f$. The outlined approach involves a major computational challenge as evaluating the $s$ sample paths at $n$ different sets of test points scales\footnote{Approximations such as random Fourier features (RFF) (Rahimi and Recht, 2008) and those by Pleiss et al. (2018) can be used to reduce this cost, e.g. Hernández-Lobato et al. (2014) and Wang and Jegelka (2017) used RFF to approximately optimize GP sample paths. However, this produces tradeoff between exact GP but small $n$ v.s. large $n$ but inexact GP which we do not analyse in this paper.} as $O(s(n t^2 + t n^2) + s n^3)$. In BQ literature similar computational challenges have been resolved using linearisation approximations as further discussed in Section 5.1. In our case, if both $\Psi(\cdot)$-terms in Eq. 10 were linear for $f$, then it can be shown that the numerator and denominator in Eq. 10 would have joint Gaussian density leading to tractable computations. However, we observed that such linearisation approach can result poor quality approximations in our case.

We propose the following computationally cheaper yet asymptotically exact approach: In small dimensions, when $p \leq 2$, we evaluate each sample path $f^{(i)}$, $i = 1, \ldots, s$ at $n^p$ fixed grid points and compute the required integrations numerically. This approach scales as $O((i n^p t^2 + i n^p t s + i n^p t^2 s)$. If $p > 2$, then self-normalised importance sampling is used. We draw $n$ samples from instrumental density, the $\alpha$-quantile of $\tilde{\pi}_{\text{ABC}}^f$ interpreted as a pdf and evaluated using Eq. A.23 of Appendix, with $\alpha = 0.95$. The samples are thinned and the resulting $\tilde{n} \ll n$ representative samples $\{\theta^{(i)}\}_{i=1}^{\tilde{n}}$ are used to compute the normalised importance weights $\omega^{(i,j)}$ for each sampled posterior $i = 1, \ldots, s$. The output is a set of weighted sample sets $\{\{(\omega^{(i,j)}, \theta^{(j)})\}_{j=1}^{\tilde{n}}\}_{i=1}^{s}$ from which moments and marginal densities can be computed using standard Monte Carlo estimators for each $i = 1, \ldots, s$. This approach requires only one MCMC sampling from the instrumental density which scales as $O(n t^2)$, i.e. only linearly with respect to $n$, so that $n$ can be large. Total cost is $O((n + \tilde{n}) t^2 + n^2 (t + s) + n^3)$.

5 On related GP-surrogate methods

5.1 Relation to Bayesian quadrature

In Bayesian quadrature one aims to compute integral $I = \int_{\mathbb{R}^p} f(\theta) \pi(\theta) d\theta$, where $f : \mathbb{R}^p \to \mathbb{R}$ is an expensive blackbox function and $\pi(\theta)$ is a known density, e.g. Gaussian. If a GP prior is placed on $f$, given some evaluations $\{(f_i, \theta_i)\}_{i=1}^{l}$ where $f_i = f(\theta_i)$, the posterior of $I$, describing one’s knowledge of the value of the integral, is Gaussian whose mean and variance can be computed analytically for some choices of $k(\theta, \theta')$ and $\pi(\theta)$ (for details, see O’Hagan, 1991; Karvonen et al., 2018; Briol et al., 2019). However, in Bayesian ABC, the quantity of interest is the ratio $\pi_{\text{ABC}}^f$ in Eq. 10 (or the function $\tilde{\pi}_{\text{ABC}}^f$ due to computational reasons), not merely a particular integral of $\tilde{\pi}_{\text{ABC}}^f$.

Motivated by the recent work by Chai and Garnett (2019), we can generalise Eq. 10 so that

$$\pi_{\text{ABC}}^f(\theta) = \frac{g(f(\theta)) \pi(\theta)}{\int_{\mathbb{R}^n} g(f(\theta')) \pi(\theta') d\theta'},$$

(22)

We use the “0-1 kernel” $1_{\Delta_{k \leq s}}$ in Eq. 2 corresponding to $g(f(\theta)) = \Psi((\varepsilon - f(\theta))/\sigma_n)$. Osborne et al. (2012b), Gutmann and Corander (2016), Acerbi (2018) and Järvenpää et al. (2019b) modelled the log-likelihood with GP, i.e. they used $g(f(\theta)) = \exp(f(\theta))$, to reckon the non-negativity of the liklihood and the high dynamic range of the log-likelihood. Osborne et al. (2012b), Gunter et al. (2014) and Chai and Garnett (2019) considered computation of marginal likelihoods $\int_{\mathbb{R}^n} g(f(\theta)) \pi(\theta) d\theta$ and used approximations to render this integral linear for $f$ thus allowing analytical computations as in standard BQ. Ratios of integrals but different from Eq. 22 were studied by Osborne et al. (2012a) who also used linearisation approximations. We observed empirically that Eq. 22 and its denominator can have highly non-Gaussian distribution in our case, and for this reason we do not advocate linearisation ap-
proportions, and proposed simulation-based approach in Section 4.

5.2 Relation to Bayesian optimisation

Suppose now \( f : \Theta \subset \mathbb{R}^p \rightarrow \mathbb{R} \) is an expensive, black-box function to be minimised. In BO, a GP prior is placed on \( f \) and the future locations for obtaining (possibly noisy) evaluations of \( f \) are chosen adaptively by optimising an acquisition function that, in some sense, measures the potential improvement in the knowledge of the minimum point brought by the extra evaluation. In principle, one could keep track of the posterior of \( \theta^* = \arg \min_{\theta \in \Theta} f(\theta) \) obtainable from the GP model and adaptively collect function values so as to minimise some measure of the posterior uncertainty of \( \theta^* \). While in practice simple acquisition functions including expected improvement and lower confidence bound (LCB) are often used and the posterior of \( \theta^* \) is rarely explicitly computed, some BO methods do directly target \( \theta^* \). Entropy search and predictive entropy search (Hennig and Schuler, 2012; Hernández-Lobato et al., 2014) use an acquisition function that measures the expected reduction in the differential entropy of the posterior of \( \theta^* \). Wang and Jegelka (2017) similarly considered the posterior of \( f^* = \min_{\theta \in \Theta} f(\theta) \). The important difference between these methods (or BO in general) and Bayesian ABC is that the quantity of interest of Bayesian ABC is not the minimiser of discrepancy but the full ABC posterior density \( \pi_{ABC}^f \) (or \( \pi_{ABCD}^f \)).

In the BOLFI framework (Gutmann and Corander, 2016), the function \( f \) was taken to be the ABC discrepancy \( \Delta_{\theta} \), and LCB acquisition function \( \text{LCB}(\theta) = n_i(\theta) - \beta_i s_i(\theta) \) (Srinivas et al., 2010; Shahriari et al., 2015) was used for illustrating their approach of learning the ABC posterior. This is reasonable because to learn the ABC posterior one needs to evaluate in the regions with small discrepancy. We can show that LCB is also related to our Bayesian ABC framework.

**Proposition 5.1.** If the prior is uniform over \( \Theta \) (and may be improper), i.e. if \( \pi(\theta) \propto 1_{\theta \in \Theta} \), then the point chosen by the LCB acquisition function with parameter \( \beta_i \) is the same as the point maximising the \( \Phi(\beta_i) \)-quantile of the unnormalised ABC posterior \( \tilde{\pi}_{ABC}^f(\theta) \) for any threshold \( \varepsilon \).

This result gives an interpretation for the LCB trade-off parameter \( \beta_i \) in the ABC setting. However, instead of simply using LCB in the Bayesian ABC framework, it is clearly be more reasonable to evaluate where the variance (or some other measure of uncertainty) is large as discussed e.g. by Kandasamy et al. (2017) and Järvenpää et al. (2019a,b). Järvenpää et al. (2019a) also showed empirically that EIV consistently works better than LCB in their sequential scenario when the goal is to learn the ABC posterior.

### 6 Experiments

We first consider four 2D toy problems to gain understanding on how the proposed method performs with a well-specified GP model. We then focus on more typical scenarios where the GP modelling assumptions do not hold exactly using three real-world simulation models. We compare the performance of the sequential and synchronous batch versions of the acquisition methods outlined in Section 3. As a simple baseline, we consider random points drawn from the prior (abbreviated as RAND). We also briefly demonstrate the uncertainty quantification of the ABC posterior.

Locations for fitting the initial GP model are sampled from the uniform prior in all cases. We take 10 initial points for 2D and 20 for 3D and 4D cases. We use \( b = 0 \), \( B_{ij} = 10^2 I_{i=j} \) and include basis functions of the form \( 1, \theta_i, \theta_i^2 \). The discrepancy \( \Delta_{\theta} \) is assumed smooth and we use the squared exponential covariance function \( k(\theta, \theta') = \sigma^2 \exp(-\frac{1}{2} \sum_{i=1}^p (\theta_i - \theta'_i)^2/\ell_i^2) \). GP hyper-parameters \( \psi = (\sigma_n^2, \ell_1, \ldots, \ell_p, \sigma_j^2) \) are given weakly informative priors and their values are obtained using MAP estimation at each iteration. Owen’s T function values are computed using a C-implementation of the algorithm by Patefield and Tandy (2000).

ABC-MCMC (Marjoram et al., 2003) with extensive simulations is used to compute the ground truth ABC posterior for the real-world models. For simplicity and to ensure meaningful comparisons to ground-truth, we fix \( \varepsilon \) to certain small predefined values although, in practice, its value is set adaptively (Järvenpää et al., 2019a) or based on pilot runs. We compute the estimate of the unnormalised ABC posterior using the Eq. 12 for MAXV, EIV, RAND and Eq. 14 for MAX-MAD, EIMAD. Adaptive MCMC is used to sample from the resulting ABC posterior estimates and from instrumental densities needed for IS approximations. TV denotes the median total variation distance between the estimated ABC posterior and the true one (2D) or the average TV between their marginal TV values (3D, 4D) computed numerically over 50 repeated runs. Iteration (i.e. number of batches chosen) serves as a proxy to wall-time. The number of simulations i.e. the maximum value of \( t \) is fixed in all experiments and the batch methods thus finish earlier.

In the following we present our test models and show the corresponding results which are discussed in more detail in Section 6.3. Further details, e.g., on the optimisation of the acquisition function, MCMC methods used, computational costs, and additional experimental results can be found in the Appendix. The results for our third, additional ABC benchmark scenario, g-and-k model, are shown in the Appendix D.
6.1 Toy simulation models

Fig. 2 shows the results with sequential methods ($b = 1$) and corresponding batch methods with $b = 5$ for four synthetically constructed toy models. These were taken from Järvenpää et al. (2019a) and are illustrated in the Appendix B. In Fig. 3 the effect of batch size $b$ is studied for the two best performing methods.

6.2 Real-world simulation models

Lorenz model. This modified version of the well-known Lorenz weather prediction model describes the dynamics of slow weather variables and their dependence on unobserved fast weather variables over a certain period of time. The model is represented by a coupled stochastic differential equation which can only be solved numerically resulting in an intractable likelihood function. The model has two parameters $\theta = (\theta_1, \theta_2)$ which we estimate from timeseries data generated using $\theta = (2, 0.1)$. See Thomas et al. (2018) for full details of the model and the experimental set-up that we also use here, with the exception that we use wider uniform prior $\theta \sim \mathcal{U}([0, 5] \times [0, 0.5])$. The discrepancy is formed as a Mahalanobis distance from six summary statistics proposed by Hakkarainen et al. (2012). The results are shown in Fig. 4(a). Furthermore, Fig. 4(b-c) demonstrates the uncertainty quantification of the expectation of the model-based ABC posterior. See Appendix B.1 for the details of the numerical computations used. The effect of batch size is shown in Fig. 5(c).

Bacterial infections model. This model describes transmission dynamics of bacterial infections in day care centers and features intractable likelihood function. The model has been developed by Numminen et al. (2013) and used previously by Gutmann and Corander (2016) and Järvenpää et al. (2019a) as an ABC benchmark problem. We estimate the internal, external and co-infection parameters $\beta \in [0, 11], \Lambda \in [0, 2]$ and $\theta \in [0, 1]$, respectively, using true data (Numminen et al., 2013) and uniform priors. The discrepancy is formed as in Gutmann and Corander (2016), see Appendix B.3 for details. The results with all methods are shown in Fig. 5(a) and Fig. 5(b) shows the effect of batch size for the two best performing methods.

6.3 Discussion on the experimental results

In general, we obtain reasonable posterior approximations considering the very limited budget of simulations. EIV and EIMAD tend to produce more stable, accurate but also more conservative estimates than MAXV and MAXMAD. Difference in approximation quality between EIV and EIMAD, both based on the same Bayesian decision theoretic framework but different loss functions, was small. While RAND worked well in 2D cases and is fully parallelisable, it unsurprisingly worked poorly in higher dimensional cases. In all cases, our batch strategies produced similar evalua-
Figure 4: (a) Lorenz model. The intervals show the 90% variability. See Fig. 2 for the legend. (b-c) Black line is the mean and dashed black the 95% CI of the ABC posterior expectations. Red line shows the true value.

Figure 5: (a) Bacterial infections model. The intervals show the 90% variability. (b) Bacterial infections model with different batch sizes and two chosen acquisition methods. (c) Additional experiments with Lorenz model.

Fig. 4(b-c) show the evolution of the uncertainty in the ABC posterior expectation of the Lorenz model over 800 iterations. The convergence is approximately towards the true ABC posterior expectation due to a slight GP misspecification. Similarly, the ABC posterior marginals of the bacterial infection model in Appendix C contain some uncertainty after 600 iterations which our approach allows to rigorously quantify. Our approach has nevertheless some limitations: The uncertainty quantification is only approximate because $\bar{n}$ and $s$ are finite. Also, when the uncertainty of $\pi_1^{ABC}$ is very high, choosing a good instrumental density can be difficult because some of the sampled posteriors are then necessarily quite different from any single instrumental density producing possibly poor approximation. In our scenarios this happened only with early iterations and can be detected e.g. by monitoring the distribution of effective sample sizes for $i = 1, \ldots, s$. While the proposed method allows uncertainty quantification of the ABC posterior and its summaries, it does not produce error estimates due to approximating the unknown true posterior with the ABC posterior. These reasons suggest that the uncertainty estimates should be interpreted with care. Developing more effective (analytical) methods for computing these uncertainty estimates is an interesting avenue for future work.

7 Conclusions

We considered ABC inference with a limited number of simulations ($t \lesssim 1000$). We outlined a GP surrogate modelling framework called Bayesian ABC and showed how the uncertainty of the ABC posterior distribution due to the limited computational resources can be approximately quantified. We also developed principled batch Bayesian experimental design methods to efficiently parallelise the expensive simulations. Experiments showed substantial gains in wall-time.

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Supplementary material for “Batch simulations and uncertainty quantification in Gaussian process surrogate-based approximate Bayesian computation”

A Proofs and additional analysis

A.1 Proofs

Proof of Lemma 3.1. We consider first the case of integrated variance. A result corresponding to Eq. 17 but with zero mean GP prior is shown as Lemma 3.1 in the article by Järvenpää et al. (2019a). However, its proof works as such also for our GP model in Section 2 and Eq. 17 follows immediately.

Let us now consider integrated MAD in Eq. 18. To simplify notation, we use $m_\theta$ for $m_{\epsilon}(\theta)$, $s_\theta^2$ for $s_{\epsilon}^2(\theta)$ and $f_\theta$ for $f(\theta)$. We then see that

$$\mathbb{E}_{f|D_n} \int_{\theta} |\pi(\theta)\Phi\left(\frac{\epsilon - f_\theta}{\sigma_n}\right) - \pi(\theta)\Phi\left(\frac{\epsilon - m_\theta}{\sigma_n}\right)| d\theta$$

(A.1)

For the inner integral with fixed $\theta$ we obtain

$$\int_{-\infty}^{m_\theta} \left[ \Phi\left(\frac{\epsilon - f_\theta}{\sigma_n}\right) - \Phi\left(\frac{\epsilon - m_\theta}{\sigma_n}\right) \right] N(f_\theta | m_\theta, s_\theta^2) df_\theta$$

(A.3)

$$= \int_{-\infty}^{m_\theta} \Phi\left(\frac{\epsilon - f_\theta}{\sigma_n}\right) N(f_\theta | m_\theta, s_\theta^2) df_\theta - \int_{-\infty}^{\infty} \Phi\left(\frac{\epsilon - f_\theta}{\sigma_n}\right) N(f_\theta | m_\theta, s_\theta^2) df_\theta$$

(A.4)

$$= \int_{-\infty}^{m_\theta} \Phi\left(\frac{\epsilon - f_\theta}{\sigma_n}\right) N(f_\theta | m_\theta, s_\theta^2) df_\theta - \int_{-\infty}^{\infty} \Phi\left(\frac{\epsilon - f_\theta}{\sigma_n}\right) N(f_\theta | m_\theta, s_\theta^2) df_\theta$$

(A.5)

$$= 2 \int_{-\infty}^{m_\theta} \Phi\left(\frac{\epsilon - f_\theta}{\sigma_n}\right) N(f_\theta | m_\theta, s_\theta^2) df_\theta - \Phi\left(\frac{\epsilon - m_\theta}{\sqrt{s_\theta^2 + s_n^2}}\right),$$

(A.6)

where on the last line we have used the fact

$$\int_{-\infty}^{m_\theta} \Phi\left(\frac{\epsilon - f_\theta}{\sigma_n}\right) N(f_\theta | m_\theta, s_\theta^2) df_\theta = \Phi\left(\frac{\epsilon - m_\theta}{\sqrt{s_\theta^2 + s_n^2}}\right)$$

(A.7)

shown by Järvenpää et al. (2019a). We further see that

$$\int_{-\infty}^{m_\theta} \Phi\left(\frac{\epsilon - f_\theta}{\sigma_n}\right) N(f_\theta | m_\theta, s_\theta^2) df_\theta$$

(A.8)

$$= \int_{-\infty}^{0} \left[ \Phi\left(\frac{\epsilon - m_\theta - y}{\sigma_n}\right) N(y | 0, s_\theta^2) dy \right] \text{[transformation } y = f_\theta - m_\theta]$$

(A.9)

$$= \int_{-\infty}^{0} \int_{-\infty}^{\infty} \left[ \frac{x - y}{\sigma_n^2} + y^2 \right] N(x | 0, s_\theta^2) dx dy$$

(A.10)

$$= \frac{1}{2\pi\sigma_n s_\theta} \int_{-\infty}^{0} \int_{-\infty}^{\infty} \exp\left( -\frac{1}{2} \left[ \frac{(x-y)^2}{\sigma_n^2} + y^2 \right] \right) dx dy$$

(A.11)

$$= \frac{1}{2\pi\sigma_n s_\theta} \int_{-\infty}^{0} \int_{-\infty}^{\infty} \exp\left( -\frac{1}{2} \left[ \frac{x}{y} \right] \left[ \begin{array}{cc} s_\theta^2 + \sigma_n^2 & s_\theta^2 \\ s_\theta^2 & s_\theta^2 + \sigma_n^2 \end{array} \right]^{-1} \left[ \begin{array}{c} x \\ y \end{array} \right] \right) dx dy$$

(A.12)

$$= \Phi_2 \left( \begin{array}{c} \epsilon - m_\theta \\ 0 \end{array} \left| \begin{array}{cc} 0 \\ 0 \end{array} \right., \left[ \begin{array}{cc} s_\theta^2 + \sigma_n^2 & s_\theta^2 \\ s_\theta^2 & s_\theta^2 + \sigma_n^2 \end{array} \right] \right)$$

(A.13)
When we combine the equations, we see that the \( \Phi \)-terms cancel out and we obtain Eq. 20.

**Proof of Proposition 3.2.** The formula for the EIV can be derived in a straightforward manner by using the GP lookahead formulas given by Lemma 5.1 by Järvenpää et al. (2019b) in the proof of Proposition 3.2 by Järvenpää et al. (2019a).

The case of EIMAD requires some extra work. First, using an equation from the proof of Lemma 3.1, we obtain

\[
\mathbb{E}_{\Delta^*|\theta^*, \mathcal{D}_t} \mathcal{L}^m(\Pi_{D_t|\theta^*}) = \mathbb{E}_{\Delta^*|\theta^*, \mathcal{D}_t} \int_{\Theta} \pi(\theta) \left[ 2 \int_{-\infty}^0 \Phi \left( \frac{\varepsilon - m_{t+b}(\theta) - y}{\sigma_n} \right) N(y \mid 0, s_{t+b}^2(\theta)) \, dy - \Phi \left( \frac{\varepsilon - m_{t+b}(\theta)}{\sqrt{\sigma_n^2 + s_{t+b}^2(\theta)}} \right) \right] \, d\theta
\]

Note that \( \Phi(\cdot) \)-terms cancel out and we obtain Eq. 20. □

**Proof of Proposition 5.1.** Järvenpää et al. (2019a) showed that the \( \alpha \)-quantile for \( \hat{\pi}_{ABC} \) at any fixed \( \theta \in \Theta \) is given by

\[
z_{t,\alpha}(\theta) = \pi(\theta) \Phi \left( \frac{s_t(\theta)\Phi^{-1}(\alpha) - m_t(\theta) + \varepsilon}{\sigma_n} \right).
\]

Using this fact when \( \pi(\theta) \) is assumed a constant in \( \Theta \) shows that

\[
\theta_{\text{opt}} = \arg \max_{\theta^* \in \Theta} z_{t,\alpha}(\theta^*)
\]
\[ \Delta_{\theta} = \sqrt{(s_o - s_{\theta})^\top W (s_o - s_{\theta})}, \]  
(A.27)

where \( W \in \mathbb{R}^{d \times d} \) is a positive definite matrix, \( s_o \triangleq s(x_o), s_{\theta} \triangleq s(x_{\theta}) \), and \( s : \mathcal{X} \to \mathbb{R}^d \) is the summary statistics function usually with \( d \geq p \). Recall that \( p \) is the dimension of the parameter space \( \Theta \). If we assume\(^5\) \( s_{\theta} \) is jointly Gaussian for each \( \theta \), some \( \theta' \) in the posterior modal area satisfies \( s_{\theta'} \sim N(s_o, \Sigma_{\theta'}) \) with positive definite \( \Sigma_{\theta'} \) and if we further choose \( W = \Sigma_{\theta'}^{-1} \), then \( \Delta_{\theta'}^2 \sim \chi^2(d) \), the chi-squared distribution with degree of freedom \( d \). This follows by noticing that there exists \( L_{\theta'} \in \mathbb{R}^{d \times d} \) such that \( \Sigma_{\theta} = L_{\theta'} L_{\theta'}^\top \), because \( L_{\theta'}^{-1} (s_o - s_{\theta}) \sim N(0, I) \) which is easy to show and because the chi-squared distribution \( \chi^2(d) \) can be characterised as a sum of squares of \( d \) independent standard Normal random variables. Further, using the last-mentioned fact, the central limit theorem (CLT) and the delta method (with the obvious fact that the square root is a smooth function), one can reason that \( \Delta_{\theta'} = (\Delta_{\theta'}^2)^{1/2} \) is approximately Gaussian for large enough \( d \). In fact, \( \Delta_{\theta'} \sim \chi(d) \), the chi distribution with degree of freedom \( d \), which is fairly close to Gaussian distribution already with \( d = 5 \).

If \( s_{\theta'} - s_o \) is nonzero mean and/or \( W \neq \Sigma_{\theta'}^{-1} \), then \( \Delta_{\theta'}^2 \) is no longer chi-squared distributed but follows generalised chi-squared distribution. Detailed analysis of this general case is difficult. However, if we further assume that the summaries in \( s_{\theta'} \) are independent, and if \( W \) is diagonal and scales \( s_{\theta'} - s_o \), so that its elements do not have too variable means and variances which are requirements for a sensible discrepancy function (Prangle, 2017), then CLT (with Lindeberg or Lyapunov condition) and delta method might apply so that the approximate Gaussianity still holds for large enough \( d \). In this case, the Gaussianity assumption of \( s_{\theta'} \) is in fact not necessary.

Furthermore, while \( \sigma_{\theta'}^2 \) can be heteroscedastic, i.e. depend on \( \theta \) as empirically investigated by Järvenpää et al. (2018), we can expect by continuity that it often is approximately constant on the modal area of the posterior where the GP fit only needs to be accurate. Also, while the discrepancy is not exactly Gaussian because \( \Delta_{\theta} \) in Eq. A.27 is obviously non-negative, the amount of probability mass of the Gaussian density on the negative values of \( \Delta_{\theta} \) will typically be very small. Finally, while the analysis of this section and our empirical investigations shown in Fig. A.1 support the Gaussian assumption, for a particular problem at hand and as in all Bayesian modelling, the goodness of the model fit should be assessed.

**B Additional details on implementation and experiments**

**B.1 Implementation details**

We present additional implementation details of our inference algorithm. When \( p > 2 \), we used the adaptive MCMC method by Haario et al. (2006) to sample from the GP model-based estimates of the ABC posterior and from the instrumental densities needed for the IS approximation of EIV and EIMAD acquisition functions. Adaptive MCMC was also used for the IS approximation needed for ABC posterior uncertainty quantification. In all of these cases, we run multiple chains initialised at the point with highest log-density value computed over the current points in \( D_t \). The first half of each chain was always neglected as burn-in and the chains were then combined and thinned. In 2D, equivalent grid-based numerical computations were used instead.

When sampling from the model-based estimates of the ABC posterior (Eq. 12 and 14), the samples were thinned to the size of \( 10^4 \) and kernel density estimation was used to estimate the (marginal) densities from the resulting samples. For the grid-based numerical computations in 2D, we used \( 100 \times 100 \) equidistant grid.

To evaluate EIV and EIMAD acquisition functions, we first sampled from the instrumental density which is the current loss surface interpreted as a pdf as mentioned in Section 3.2. These samples were thinned to the size of

\[ = \arg \max_{\theta^* \in \Theta} \{ s_i(\theta^*) \Phi^{-1}(\alpha) - m_i(\theta^*) \} \]  
(A.25)

\[ = \arg \min_{\theta^* \in \Theta} \{ m_i(\theta^*) - \Phi^{-1}(\alpha) s_i(\theta^*) \}. \]  
(A.26)

Comparison of Eq. A.26 and the LCB acquisition function \( LCB(\theta^*) = m_i(\theta^*) - \beta_i s_i(\theta^*) \) shows immediately that these coincide if \( \beta_i = \Phi^{-1}(\alpha) \) i.e. if \( \alpha = \Phi(\beta_i) \).

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\(^5\)This assumption is also made in the synthetic likelihood method (Wood, 2010).
Figure A.1: Empirical distributions of the discrepancy of the three real-world problems used in this paper at their true parameter values. The histogram shows the discrepancy values corresponding to 500 simulations and the red line shows corresponding Gaussian densities. The discrepancy for the Lorenz and g-and-k model model is formed as a Mahalanobis distance (see Section B.3 for additional details). It is seen that the Gaussian assumption is reasonable.

500 points used for computing the importance weights. In 2D, 50 × 50 grid-based computations were used instead. The same instrumental density and thus the same set of importance samples was used for greedily optimising each point in the batch although it is also possible to use different instrumental densities. The global optimisation of the acquisition functions was performed by first using random search (with 1000 points in 2D and 2000 in 3D and 4D) to roughly locate good regions and then improving the best 10 points found this way by initialising gradient-based algorithm at these points. The best point evaluated was taken as the optimal solution. While many other optimisation approaches are possible, our method already produced good results.

We used the following settings for the uncertainty quantification of the ABC posterior in Section 4: In 2D the integrals over $\Theta$ were computed numerically in a 80 × 80 grid, i.e. we used $\bar{n} = 80$ producing 6400 grid points. For $p > 2$, we used the adaptive MCMC with 15 chains each with length 20000. The chains were finally combined and thinned to $\bar{n} = 7500$ representative points for computing the importance weights. We used $s = 2000$ GP sample paths. Marginal densities for e.g. Fig. C.5 were computed from the resulting weighted sample sets using weighted kernel density estimation.

### B.2 Computation times for optimising the acquisition functions

Computational cost of evaluating the acquisition functions in Section 3 depends on various factors. We here report computation times\(^6\) of our MATLAB implementation for obtaining the next evaluations when the simulation budget is $t = 810$ in 2D (Multimodal toy model) and $t = 820$ in 4D (g-and-k model). We report the computation times at both the first and the last iteration. These show the minimum and maximum costs, respectively.

In 2D, where grid-based numerical computations were used, sequential MAXV required 0.3 - 1.5s and its batch version 5 - 35s for constructing the whole batch of size $b = 5$. In 4D, the computation times roughly doubled. In 2D, sequential EIV required 2.5 - 13s and its batch version 18 - 80s for the whole batch of size $b = 5$. In 4D, these times were 9 - 80s and 27 - 250s, respectively. The computation time of EIV scales faster than linearly for $b$ in 4D because we sample only once from the instrumental density and re-use the same importance weights for selecting all points in the current batch. In 2D, this scaling was roughly linear.

The difference in computation times between MAXMAD and MAXV, as well as between EIMAD and EIV, was small. This is because the computation costs are dominated by the GP-based computations and evaluations of the Owen’s T function needed for both. Finally, we emphasise that while the GP computations and the optimisation of the acquisition function are not particularly cheap, the simulation times for realistic models typically dominate the total cost. The reported computation times can be also reduced by more efficient implementation. However, if running the simulation model is very fast (e.g. less than a fraction of a second), standard ABC methods should be preferred even if they require substantially more simulations.

\(^6\)We used \texttt{fmincon} in MATLAB. Finite differences were used to approximate gradients for simplicity but analytical gradient computations could be also used to improve optimisation.

\(^7\)These times were obtained on a standard laptop with Intel Core i5 2.3GHz CPU and 8Gb RAM.
**B.3 Additional details on experiments**

We describe additional details of the experimental set-up. Fig. B.1 visualises the four synthetically constructed 2D posteriors used in Section 6.1. These examples were taken from Järvenpää et al. (2019a) where further details can be found.

![Synthetic 2D posterior densities used in the experiments of Section 6.1.](image)

Figure B.1: Synthetic 2D posterior densities used in the experiments of Section 6.1.

We used ABC-MCMC to obtain the ground truth ABC posterior. The algorithm was initialised with the true value or, in the case of the bacterial infections model, using a point estimate from earlier studies (Numminen et al., 2013). The proposal density for ABC-MCMC was hand-tuned. For Lorenz model we used 8 chains with length $3 \cdot 10^6$ and for g-and-k model 8 chains with length $10^7$ samples. For bacterial infections model we used 20 chains with length $7.5 \cdot 10^4$ samples. The chains were finally combined and thinned to $10^4$ samples to represent the ground truth ABC posterior.

Mahalanobis distance as in Eq. A.27 was used as the discrepancy for Lorenz and g-and-k models. The simulation model was run 500 times to estimate the covariance matrix of the summary statistics at the true parameter and the matrix $W$ was chosen to be the inverse of the covariance matrix. Of course, such discrepancy is unavailable in practice because the true parameter is unknown and the computational budget limited. However, as the main goal of this paper is to approximate any given ABC posterior with a limited simulation budget, we chose our target ABC posterior this way. For this reason we also fixed $\varepsilon$ to small predefined value for each test problem. Investigating whether one could adaptively adjust the discrepancy in our Bayesian ABC framework (and without a high number of replicates at each proposed point as is required e.g. in the synthetic likelihood method (Wood, 2010)) is left as a topic for future work.

Gutmann and Corander (2016) defined a discrepancy for the bacterial infections model by summing four $L^1$-distances computed between certain individual summaries. For details, see example 7 in Gutmann and Corander (2016). We used the same discrepancy except that we further took square root of their discrepancy function. We obtained a similar ABC posterior as the original article (Numminen et al., 2013) where ABC-PMC algorithm and slightly different approach for comparing the data sets were used.

**C Additional results and illustrations**

We show additional results and illustrations of the experiments in Section 6. Fig. C.1 and C.2 show the evaluation locations and the resulting estimates of the ABC posteriors after 100 iterations corresponding to 110 simulations for two synthetic 2D models of Section 6.1.

Fig. C.3 and C.4 show typical estimated ABC posterior densities of the Lorenz and bacterial infections models of Section 6.2, respectively. These results are shown to demonstrate the accuracy obtainable with very limited simulations. These particular results were obtained with the sequential EIV method using 600 iterations corresponding to 610 simulations (Lorenz model) or 620 simulations (bacterial infections model).

Fig. C.5 illustrates the ABC posterior uncertainty quantification for the bacterial infections model. Fig. C.6 shows the evolution of the uncertainty of the ABC posterior expectations over 600 iterations. Sequential EIV method was used and one typical case is shown. The results suggest that while the ABC posterior is well estimated at the last iteration, there is some uncertainty left about its exact shape. Similar observations were also done with g-and-k model of the next section (results not shown). The true value is not always contained in the 95% CI which is likely because the uncertainty in the GP hyperparameters is ignored for simplicity and because the GP is reasonable but imperfect model for the discrepancy.
Figure C.1: Multimodal test problem. The first row shows the sequential methods and the second row the corresponding greedy batch methods. The blue diamonds show the 10 initial points and the black dots 100 additional points selected using each acquisition function (the last two batches in the second row are however highlighted by red plus-signs and crosses). The TV value in the title shows the total variation distance between the true and estimated ABC posteriors for each particular case.

Figure C.2: Banana test problem. See the caption of Fig. C.1 for description.

Although we used quadratic GP mean function to encode the prior assumption of unimodal posterior, we observed that the uncertainty of the ABC posterior near the boundaries of the parameter space during the early iterations can be high leading to multimodality. Such cases can be difficult for the MCMC as it can fail to locate all the modes or sample sufficiently from them. For this reason, the uncertainty quantification based on the proposed IS approach needs to be interpreted cautiously. More elaborate sampling techniques might be useful as
D Additional experiments: g-and-k model

We present the g-and-k distribution and our additional experiments with this benchmark model. The g-and-k model is a probability distribution defined via its quantile function

\[
Q(\Phi^{-1}(q); \theta) = a + b \left( 1 + c \frac{1 - \exp(-g\Phi^{-1}(q))}{1 + \exp(-g\Phi^{-1}(q))} \right) (1 + (\Phi^{-1}(q))^2)^k \Phi^{-1}(q),
\]

where \(a, b, c, g \text{ and } k\) are unknown parameters, \(q \in [0, 1]\) is a quantile and \(\Phi^{-1}\) denotes the quantile function of the standard normal distribution. There is no analytical formula for the likelihood but sampling from it is straightforward (Price et al., 2018). We fix \(c = 0.8\) as is common in literature and estimate the parameters \(\theta = (a, b, g, k)\) from \(10^4\) samples generated using \(\theta = (3, 1, 2, 0.5)\) as the true parameter value. We use independent uniform priors \(a \sim \mathcal{U}([2, 4]), b \sim \mathcal{U}([0, 3]), g \sim \mathcal{U}([1, 4]), k \sim \mathcal{U}([0, 2])\). We consider the four summary statistics defined via an auxiliary model as suggested by Price et al. (2018) and use them to form a Mahalanobis discrepancy function as already described in Section B.3. Although the discrepancy is formed only from four summary statistics, we observed that it is very close to Gaussian near the true parameter value, see Fig. A.1.

The results for the g-and-k model are shown in Fig. D.1 and Fig. D.2. The conclusions from the results resemble those of the Lorenz and bacterial infections models in that the proposed batch techniques produce substantial improvements over the corresponding sequential ones. However, the overall approximation errors are slightly larger than for the bacterial model presumably due to more noticeable model misspecification (the
Figure C.5: Uncertainty quantification for the ABC posterior marginals of the bacterial infections model at the 100th iteration corresponding $t = 120$ simulations (top row) and at the last iteration corresponding $t = 620$ simulations (bottom row). Red line shows the true ABC posterior, blue line shows the estimate based on Eq. 12 and the black lines show some sampled ABC marginal posteriors that (approximately) represent the uncertainty due to the limited number of simulations $t$.

Figure C.6: Evolution of the uncertainty of the ABC posterior expectations of the bacterial infections model over 600 iterations corresponding $t = 620$ simulations for one typical run of the inference algorithm. This is as Fig. 4(b-c) except that iteration is here not on the log-scale.

The variance of the discrepancy is only approximately constant near the true value) and the higher dimensionality of the parameter space. Interestingly, in this problem the heuristic MAXV method eventually produces the most accurate approximations. However, EIV, producing more conservative estimates, works more reliably if large batch sizes are used.
Figure D.1: Results for the g-and-k model. All proposed methods tested with two batch sizes.

Figure D.2: Results for the g-and-k model. Further analysis for two methods, MAXV and EIV, with varying batch sizes.