K2-ABC: Approximate Bayesian Computation with Infinite Dimensional Summary Statistics via Kernel Embeddings

Mijung Park∗
Wittawat Jitkrittum∗
The Gatsby Unit, University College London, U.K.

Dino Sejdinovic
Department of Statistics & University College, University of Oxford, U.K.

Abstract

Complicated generative models often result in a situation where computing the likelihood of observed data is intractable, while simulating from the conditional density given a parameter value is relatively easy. Approximate Bayesian Computation (ABC) is a paradigm that enables simulation-based posterior inference in such cases by measuring the similarity between simulated and observed data in terms of a chosen set of summary statistics. However, there is no general rule to construct sufficient summary statistics for complex models. Insufficient summary statistics will “leak” information, which leads to ABC algorithms yielding samples from an incorrect (partial) posterior. In this paper, we propose a fully nonparametric ABC paradigm which circumvents the need for manually selecting summary statistics. Our approach, K2-ABC, uses maximum mean discrepancy (MMD) as a dissimilarity measure between the distributions over observed and simulated data. MMD is easily estimated as the squared difference between their empirical kernel embeddings. Experiments on a simulated scenario and a real-world biological problem illustrate the effectiveness of the proposed algorithm.

1. Introduction

ABC is an approximate Bayesian inference framework for models with intractable likelihoods. Originated in population genetics (Beaumont et al., 2002), ABC has been widely used in a broad range of scientific applications including ecology, cosmology, and bioinformatics (Ratmann et al., 2007; Bazin et al., 2010; Schafer & Freeman, 2012). The goal of ABC is to obtain an approximate posterior distribution over model parameters. These parameters usually correspond to interpretable inherent mechanisms in natural phenomena.

However, in many complex models of interest, exact posterior inference is doubly intractable since: (1) the likelihood function, the probability of observations $y^*$ for given model parameters $\theta$, is either expensive or impossible to evaluate; and (2) the marginal likelihood, which requires integrating out $\theta$ from the likelihood function, is also intractable.

M.P.∗ and W.J.∗ contributed equally to this work.
Even due to (1) alone, the posterior cannot be computed even up to a normalisation constant.

ABC resolves these intractabilities by approximating the likelihood function using simulated observations that are similar to the actual observations. Most ABC algorithms evaluate the similarity between the simulated and actual observations in terms of a pre-chosen set of summary statistics. Since the full dataset is represented in a lower-dimensional space of summary statistics, unless the selected summary statistic is sufficient, ABC results in inference on the partial posterior $p(\theta | s^*)$, rather than the desired full posterior $p(\theta | y^*)$. Therefore, selection of the summary statistic is a crucial step in ABC to avoid an unknown loss of information due to the use of insufficient summary statistics (Cam, 1964; Abril, 1994; Joyce & Marjoram, 2008; Aeschbacher et al., 2012).

In this light, we introduce a method that circumvents an explicit selection of summary statistics. Our method proceeds by applying a similarity measure to data themselves, via embeddings of the empirical data distributions into an infinite-dimensional (characteristic) reproducing kernel Hilbert space (RKHS). Such embedding captures all possible differences between data distributions, e.g., all the high-order moments that are necessary to describe the distributions: no information loss occurs in going from the posterior given data $p(\theta | y^*)$ to that given embeddings of data $p(\theta | \mu(y^*))$, regardless of the form of $p(y | \theta)$.

Embeddings of probability measures into RKHSs (Berlinet & Thomas-Agnan, 2004; Smola et al., 2007; Sriperumbudur et al., 2010) offer a flexible representation of probability measures and have been used in nonparametric hypothesis testing (Gretton et al., 2012), inference in graphical models (Song et al., 2013) and constructing proposals in adaptive MCMC (Sejdinovic et al., 2014). The key quantity arising from this framework is an easily computable notion of distance between probability measures, termed Maximum Mean Discrepancy (MMD). When the kernel used is characteristic (Sriperumbudur et al., 2011), embeddings of probability measures are injective, meaning that the MMD gives a metric on probability measures.

Here, we adopt MMD in the context of ABC as a nonparametric distance between empirical distributions of simulated and observed data using a characteristic kernel. Additionally, we apply another kernel function to MMD to obtain an effective measure of data similarities. For this reason, we refer to our method as double-kernel ABC, or $K^2$-ABC.

A dilemma that ABC practitioners typically face stems from the two sides: since it is unclear which set of summary statistics is sufficient for given data, adding as many relevant statistics as possible (up to the availability of computational resources) sounds like a safe bet. However, this ends up causing another problem. The acceptance rate or parameter weights of the ABC method become exponentially small as the dimension of the statistics increases due to the curse of dimensionality. Thus, one should balance the dimensionality of the summary statistic with its approximate sufficiency. Although the kernel embeddings in our approach imply that we take into account infinite-dimensional summary statistics, it is not affected by the curse of dimensionality since no explicit vector of statistics is formed in the process. Computing a distance in the feature space without forming an explicit feature vector is known as the kernel trick (Schölkopf & Smola, 2001). Our results (in Sec. 4) demonstrate that by choosing an appropriate similarity measure between infinite-dimensional summary statistics, an effective and robust ABC method can be obtained.

The rest of the paper is organised as follows. In Sec. 2, we overview classical approaches (rejection and soft ABC) as well as recent approaches (synthetic likelihood ABC and kernel ABC) to which we will compare our method in Sec. 4. In Sec. 3, we introduce our proposed algorithm. Experimental results are presented in Sec. 4.
2. Background

We start by introducing ABC and reviewing existing algorithms.

2.1. ABC

Consider a situation where it is possible to simulate a generative model and thus sample from the conditional density \( p(y|\theta) \), given a value \( \theta \in \Theta \) of parameters, while the computation of the likelihood \( p(y^*|\theta) \) for the observed data \( y^* \) is intractable. Neither exact posterior inference nor posterior sampling are possible in this case, as the posterior \( p(\theta|y^*) \propto p(y^*|\theta)p(\theta) \) for a prior \( p(\theta) \) cannot be computed up to a normalizing constant. ABC uses an approximation of the likelihood obtained from simulation. The simplest form of ABC is rejection ABC given in Algorithm 1.

In Algorithm 1, \( \epsilon > 0 \) is a similarity threshold, and \( \rho \) is a notion of distance, e.g., a premetric on domain \( \mathcal{Y} \) of observations. The result of ABC is an exact sample \( \{\theta_i\}_{i=1}^M \) from the approximate (wrong) posterior \( \tilde{p}_{\epsilon}(\theta|y^*) \propto \pi(\theta)p_{\epsilon}(y^*|\theta) \), where \( p_{\epsilon}(y^*|\theta) = \int_{B_\epsilon(y^*)} p(y|\theta)dy \) and \( B_\epsilon(y^*) = \{y : \rho(y, y^*) < \epsilon\} \). Choice of \( \rho \) is crucial for the design of an accurate ABC algorithm. Applying a distance directly on dataset \( y \) is often challenging, when the dataset consists of a large number of (possibly multivariate) observations. Thus, one resorts to first choosing a summary statistic \( s(y) \) and comparing them between the datasets, i.e., \( \rho(y, y') = \|s(y) - s(y')\| \). Since it is generally difficult to construct sufficient statistics for complex models, this will often “leak” information, e.g., if \( s(y) \) represents first few empirical moments of dataset \( y \). It is only when the summary statistic \( s \) is sufficient, that this approximation is consistent as \( \epsilon \to 0 \), i.e., that the ABC posterior \( \tilde{p}_{\epsilon}(\theta|y^*) \) will converge to the full posterior\(^3\). Otherwise, ABC operates on the partial posterior \( p(\theta|s(y^*)) \), rather than the full posterior \( p(\theta|y^*) \).

Another interpretation of the approximate likelihood \( \tilde{p}_{\epsilon}(\theta|y^*) \) is as the convolution of the true likelihood \( p(y|\theta) \) and the “similarity” kernel \( \kappa_{\epsilon}(y, y^*) = 1 (y \in B_\epsilon(y^*)) \). Being the indicator of the \( \epsilon \)-ball \( B_\epsilon(y^*) \) computed w.r.t. \( \rho \), this kernel imposes a hard-constraint leading to the rejection sampling. In fact, one can use any similarity kernel parametrised by \( \epsilon \) which approaches delta function \( \delta_{y^*} \) as \( \epsilon \to 0 \). A frequently used similarity kernel takes the form

\[
\kappa_{\epsilon}(y, y') = \exp\left(-\frac{\rho^2(y, y')}{\epsilon}\right), \quad q > 0. \tag{1}
\]

Such construction would result in a weighted sample \( \{y_j, \omega_j\}_{j=1}^M \), where \( \omega_j = \frac{\kappa_{\epsilon}(y_j, y^*)}{\sum_{i=1}^M \kappa_{\epsilon}(y_i, y^*)} \), which can be directly utilised in estimating posterior expectations. That is, for a test function \( f \), the expectation \( \int f(\theta)p(\theta|y^*)d\theta \) is estimated using:

\[
\hat{E}[f(\theta)] = \sum_{i=1}^M \omega_j f(\theta_j).
\]

This is an instance of a soft ABC, where parameter samples from the prior are weighted, rather than accepted or rejected. Variance in weights \( \omega_j \) can be reduced by sampling \( L_j \) datasets \( y_{(j)} \) given \( \theta_j \), for each parameter sample \( \theta_j \) and averaging their similarity to \( y^* \),

\[
w_j = \frac{1}{L_j} \sum_{i=1}^{L_j} \kappa_{\epsilon}(y_{(j)}^i, y^*) \frac{1}{\sum_{j=1}^M \frac{1}{L_j} \sum_{i=1}^{L_j} \kappa_{\epsilon}(y_{(j)}^i, y^*)}.
\]

In all experiments in Sec 4, we set \( L_j \) to 1 for simplicity.

\(^3\)Details on consistency of ABC schemes as well as their convergence properties are given in Barber et al. (2013).
2.2. Synthetic likelihood ABC (SL-ABC)

Introduced in Wood (2010), the synthetic likelihood ABC models simulated data in terms of their summary statistics and further assumes the summary statistics are multivariate normal distributed

\[ s \sim \mathcal{N}(\mu_\theta, \Sigma_\theta). \]

The mean and covariance are approximated from their empirical values, i.e., \( \hat{\mu}_\theta = \frac{1}{M} \sum_{i=1}^{M} s_i \) and \( \hat{\Sigma}_\theta = \frac{1}{M-1} \sum_{i=1}^{M} (s_i - \hat{\mu}_\theta)(s_i - \hat{\mu}_\theta)^T \), where the vector of summary statistics of the \( i \)th simulated dataset is denoted by \( s_i \). Using the following similarity kernel to measures the distance from the summary statistics of actual observations \( s^* \), \( \kappa_i(s^*, s) = \left| 2\pi \mathcal{F} \right|^{-\frac{1}{2}} \exp \left( -\frac{(s^*-s)^T (s^*-s)}{2\epsilon^2} \right) \), the resulting synthetic likelihood is given by

\[
p(s^*|\theta) = \int \kappa_i(s^*, s) \mathcal{N}(s|\hat{\mu}_\theta, \hat{\Sigma}_\theta) \, ds
= \mathcal{N}(s^*|\hat{\mu}_\theta, \hat{\Sigma}_\theta + \epsilon^2 I).
\]

Relying on the synthetic likelihood above, SL-ABC algorithm performs MCMC sampling based on Metropolis-Hastings accept/reject steps with the acceptance probability given by

\[
\alpha(\theta'|\theta) = \min \left[ 1, \frac{\pi(\theta')p(s^*|\theta')q(\theta|\theta')}{\pi(\theta)p(s^*|\theta)q(\theta'|\theta)} \right],
\]

where \( q(\theta|\theta') \) is a proposal distribution.

2.3. Kernel ABC (K-ABC)

The use of a positive definite kernel in ABC has been explored recently in Nakagome et al. (2013) (K-ABC) in the context of population genetics. In K-ABC, ABC is cast as a problem of estimating a conditional mean embedding operator mapping from summary statistics \( s(y) \) to corresponding parameters \( \theta \). The problem is equivalent to learning a regression function in the RKHSs of \( s(y) \) and \( \theta \) induced by their respective kernels (Grünewälder et al., 2012). The training set \( T \) needed for learning the regression function is generated by firstly sampling \( \{(y_i, \theta_i)\}_{i=1}^{M} \sim p(y|\theta)\pi(\theta) \) from which

\[
T := \{(s_i, \theta_i)\}_{i=1}^{M} \text{ by summarising each pseudo dataset } y_i \text{ into a summary statistic } s_i.
\]

In effect, given a summary statistic \( s^* \) corresponding to the observations \( y^* \), the learned regression function allows one to represent the embedding of the posterior distribution in the form of a weighted sum of \( \{k(\cdot, \theta_i)\}_{i=1}^{M} \) where \( k \) is a kernel associated with an RKHS \( \mathcal{H}_\theta \). In particular, if we assume that \( k \) is a linear kernel (as in Nakagome et al. (2013)), the posterior expectation of a function \( f \in \mathcal{H}_\theta \) is given by

\[
E[f(\theta)|s^*] \approx \sum_{i=1}^{M} w_i(s^*)f(\theta_i)
\]

\[
w_i(s^*) = \sum_{j=1}^{M} ((G + M\lambda I)^{-1})_{ij} k(s_j, s^*),
\]

where \( G_{ij} = g(s_i, s_j), g \) is a kernel on \( s \), and \( \lambda \) is a regularization parameter. The use of a kernel \( g \) on summary statistics \( s \) implicitly transforms \( s \) non-linearly, thereby increasing the representativeness of \( s \). Nevertheless, the need for summary statistics is not eliminated.

3. Proposed Method

We first overview Kernel MMD, a notion of distance between probability measures that is used in the proposed K2-ABC algorithm.

3.1. Kernel MMD

For a probability distribution \( F_x \) on a domain \( \mathcal{X} \), its kernel embedding is defined as \( \mu_{F_x} = \mathbb{E}_{X \sim F_x} k(\cdot, X) \) (Smola et al., 2007), an element of an RKHS \( \mathcal{H} \) associated with a positive definite kernel \( k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R} \). An embedding exists for any \( F_x \) whenever the kernel \( k \) is bounded, or if \( F_x \) satisfies a suitable moment condition w.r.t. an unbounded kernel \( k \) (Sejdinovic et al., 2013). For any two given probability measures \( F_x \) and \( F_y \), their maximum mean discrepancy (MMD) is simply the
Hilbert space distance between their embeddings:

\[
\text{MMD}^2(F_x, F_y) = \left\| \mu_{F_x} - \mu_{F_y} \right\|^2_{H^*} = E_X E_Y k(X, X') + E_Y E_Y k(Y, Y') - 2E_X E_Y k(X, Y),
\]

where \( X, X' \) \( i.i.d. \) \( F_x \) and \( Y, Y' \) \( i.i.d. \) \( F_y \). While simple kernels like polynomial of order \( r \) capture differences in first \( r \) moments of distributions, particularly interesting are kernels with a characteristic property\(^4\) (Sriperumbudur et al., 2011), for which the kernel embedding is injective and thus MMD defined by such kernels gives a metric on the space of probability distributions. Examples of such kernels include widely used kernels such as Gaussian RBF and Laplacian. Being written in terms of expectations of kernel functions allows straightforward estimation of MMD on the basis of samples: given \( \{ x^{(i)} \}^{n_x}_{i=1} \sim F_x \) \( \{ y^{(j)} \}^{n_y}_{j=1} \sim F_y \), an unbiased estimator is given by:

\[
\widehat{\text{MMD}}^2(F_x, F_y) = \frac{1}{n_x(n_x - 1)} \sum_{i=1}^{n_x} \sum_{j \neq i} k(x^{(i)}, x^{(j)}) + \frac{1}{n_y(n_y - 1)} \sum_{i=1}^{n_y} \sum_{j \neq i} k(y^{(i)}, y^{(j)}) - \frac{2}{n_x n_y} \sum_{i=1}^{n_x} \sum_{j=1}^{n_y} k(x^{(i)}, y^{(j)}).
\]

Further operations are possible on kernel embeddings - one can define a positive definite kernel on probability measures themselves using their representation in a Hilbert space, e.g.,

\[
\kappa_\epsilon(F_x, F_y) = \exp \left( -\frac{\text{MMD}^2(F_x, F_y)}{\epsilon} \right), \quad \epsilon > 0
\]

is an example of a kernel on probability measures (Christmann & Steinwart, 2010). This has recently lead to a thread of research tackling the problem of learning on distributions, e.g., (Szabó et al., 2014). These insights are essential to our contribution, as we employ such kernels on probability measures in the design of the K2-ABC algorithm which we describe next.

3.2. K2-ABC

The first component of K2-ABC is a nonparametric distance \( \rho \) between empirical data distributions. Given datasets \( y = \{ y^{(1)}, \ldots, y^{(n)} \} \) and \( y' = \{ y'^{(1)}, \ldots, y'^{(n)} \} \) consisting of \( n \) i.i.d. observations\(^5\), we use MMD to measure the distance between \( y, y' \):

\[
\rho^2(y, y') = \text{MMD}^2(F_y, F_{y'}) \text{, i.e., } \rho^2 \text{ is an unbiased estimate of } \text{MMD}^2 \text{ between probability distributions } F_y \text{ and } F_{y'} \text{ used to generate } y \text{ and } y'.
\]

This is almost the same as setting empirical kernel embedding \( s(y) = \mu_{F_y} = \sum_{j=1}^{n} k(\cdot, y^{(j)}) \) to be the summary statistic. However, in that case \( ||s(y) - s(y')||_H^2 = \text{MMD}^2(F_{x}, F_{y'}) \) would have been a biased estimate of the population \( \text{MMD}^2 \) (Gretton et al., 2012). Our choice of \( \rho \) is guaranteed to capture all possible differences (i.e., all moments) between \( F_y \) and \( F_{y'} \) whenever a characteristic kernel \( k \) is employed, i.e., we are operating on a full posterior and there is no loss of information due to the use of insufficient statistics.

Further, we introduce a second kernel into the ABC algorithm, the one that operates directly on probability measures, and compute the ABC posterior sample weights with

\[
\kappa_\epsilon(F_y, F_{y'}) = \exp \left( -\frac{\text{MMD}^2(F_y, F_{y'})}{\epsilon} \right)
\]

for a suitably chosen parameter \( \epsilon > 0 \). Now, the datasets are compared using the estimated similarity \( \kappa_\epsilon \) between their generating distributions. There are two sets of parameters in K2-ABC, parameters of kernel \( k \) (on original domain) and of kernel \( \kappa \) (on probability measures). The K2-ABC algorithm is summarised in Algorithm 2, and all of the ABC algorithms discussed are qualitatively compared in Table. 1.

\(^4\)A related notion of universality is often employed.

\(^5\)The i.i.d. assumption can be relaxed in practice, as we demonstrate in Sec. 4 on time series data.
We compare three ABC algorithms: K2-ABC, rejection ABC, and soft ABC. Here, soft ABC refers to an ABC algorithm which uses a similarity kernel in Eq. 1 with $q = 2$ and $\rho(y, y') = \|s(y) - s(y')\|_2$. For K2-ABC, a Gaussian kernel defined as

$$k(a, b) = \exp\left(-\frac{\|a - b\|_2^2}{2\gamma^2}\right)$$  \hspace{1cm} (3)

is used where $\gamma$ is set to median($\|y^*(i) - y^*(j)\|_{i,j}$) (Schölkopf & Smola, 2001). We test different values of $\epsilon$ on a coarse grid, and report the estimated $E[\theta|y^*]$ which is closest to $\theta^*$ as measured with a Euclidean distance.

The results are shown in Fig. 1 where the top row shows the estimated $E[\theta|y^*]$ from each method, associated with the best $\epsilon$ as reported in the third row. The second row of Fig. 1, from left to right, shows $y^*$ and 400 realizations of $y$ drawn from $p(y|E[\theta|y^*])$ obtained from the three algorithms. In all cases, the mean and variance of the drawn realizations match that of $y^*$. However, since the first two moments are insufficient to characterise $p(y|\theta^*)$, there exists other $\theta'$ that can give rise to the same $s(y')$, which yields inaccurate posterior means shown in the top row. In contrast, K2-ABC taking into account infinite-dimensional sufficient statistic correctly estimates the posterior mean.

### 4.1. Toy Problem

We start by illustrating how the choice of summary statistics can significantly affect the inference result, especially when the summary statistics are not sufficient. We consider a symmetric Dirichlet prior and a likelihood $p(y|\theta)$ given by a mixture of uniform distributions as follows

$$\begin{align*}
\pi(\theta) &= \text{Dirichlet}(\theta; 1), \\
p(y|\theta) &= \sum_{i=1}^{5} \theta_i \text{Uniform}(y; [i-1, i]). \hspace{1cm} (2)
\end{align*}$$

The model parameters $\theta$ are a vector of mixing proportions. The goal is to estimate $E[\theta|y^*]$ where $y^*$ is generated with true parameter $\theta^* = [0.25, 0.04, 0.33, 0.04, 0.34]^\top$ (see Fig. 1A). The summary statistics are chosen to be empirical mean and variance as often used in practice i.e., $s(y) = (E[y], V[y])^\top$.

We compare three ABC algorithms: K2-ABC, rejection ABC, and soft ABC. Here, soft ABC refers to an ABC algorithm which uses a similarity kernel in Eq. 1 with $q = 2$ and $\rho(y, y') = \|s(y) - s(y')\|_2$. For K2-ABC, a Gaussian kernel defined as

$$k(a, b) = \exp\left(-\frac{\|a - b\|_2^2}{2\gamma^2}\right)$$  \hspace{1cm} (3)

is used where $\gamma$ is set to median($\|y^*(i) - y^*(j)\|_{i,j}$) (Schölkopf & Smola, 2001). We test different values of $\epsilon$ on a coarse grid, and report the estimated $E[\theta|y^*]$ which is closest to $\theta^*$ as measured with a Euclidean distance.

The results are shown in Fig. 1 where the top row shows the estimated $E[\theta|y^*]$ from each method, associated with the best $\epsilon$ as reported in the third row. The second row of Fig. 1, from left to right, shows $y^*$ and 400 realizations of $y$ drawn from $p(y|E[\theta|y^*])$ obtained from the three algorithms. In all cases, the mean and variance of the drawn realizations match that of $y^*$. However, since the first two moments are insufficient to characterise $p(y|\theta^*)$, there exists other $\theta'$ that can give rise to the same $s(y')$, which yields inaccurate posterior means shown in the top row. In contrast, K2-ABC taking into account infinite-dimensional sufficient statistic correctly estimates the posterior mean.

### 4.2. Ecological Dynamic Systems

As an example of statistical inference for ecological dynamic systems, we use observations on adult blowfly populations over time introduced in Wood (2010). The population dynamics are modelled by
K2-ABC: Approximate Bayesian Computation with Kernel Embeddings

![Figure 1](image)

**Figure 1.** A possible scenario for ABC algorithms to fail due to insufficient summary statistics. A: Using the 5-dimensional true parameters (top), 400 observations (bottom) are sampled from the mixture of uniform distributions in Eq. 2. B (top): Estimated posterior mean of parameters from each method. We drew 1000 parameters from the Dirichlet prior and 400 simulated datapoints given each parameter. In rejection and soft ABC algorithms, we used empirical mean and variance of observations as summary statistics to determine similarity between simulated and observed data. B (middle): Histograms of 400 simulated datapoints given estimated posterior means by each method. Though the mean and variance of simulated data from rejection and soft ABC match that of the observed data, the shapes of the empirical distributions notably differ. B (bottom): Euclidean distance between true and estimated posterior mean of parameters as a function of $\epsilon$. We varied the $\epsilon$ values to find the optimal range in terms of the Euclidean distance. The magnitude of $\epsilon$ is algorithm-specific and not comparable across methods.

A discretised differential equation:

$$N_{t+1} = P N_{t-\tau} \exp \left( \frac{-N_{t-\tau}}{N_0} \right) e_t + N_t \exp(-\delta e_t),$$

where an observation at time $t + 1$ is denoted by $N_{t+1}$ which is determined by time-lagged observations $N_t$ and $N_{t-\tau}$ as well as Gamma distributed noise realisations $e_t \sim \text{Gam}(\frac{1}{\sigma_d^2}, \sigma_d^2)$ and $e_t \sim \text{Gam}(\frac{1}{\sigma_p^2}, \sigma_p^2)$. Here, the parameters are $\theta = \{P, N_0, \sigma_d, \sigma_p, \tau, \delta\}$. We put broad Gaussian priors on log of parameters as shown in Fig. 2A. Note that the time series data given the parameters drawn from the priors vary drastically (see Fig. 2B), and therefore inference with those data is very challenging as noted in (Meeds & Welling, 2014).

The observation (black trace in Fig. 2B) is a time-series of length $T = 180$, where each point in time indicates how many flies survive at each time under food limitation. For SL-ABC and K-ABC, we adopted the 10 summary statistics used in Meeds & Welling (2014): the log of the mean of all 25% quantiles of $\{N_t/1000\}_{t=1}^T$ (four statistics), the mean of 25% quantiles of the first-order differences of $\{N_t/1000\}_{t=1}^T$ (four statistics), and the maximal peaks of smoothed $\{N_t\}_{t=1}^T$, with two different thresholds (two statistics).

For setting $\epsilon$ and kernel parameters, we split the data into two sets: training (75\% of 180 datapoints) and test (the rest) sets. Using the training data, we ran each ABC algorithm given each value of $\epsilon$ and kernel parameters defined on a coarse grid, then, computed test error\(^6\) to choose the optimal values of $\epsilon$ and kernel parameters in terms of the minimum pre-

\[^6\text{We used Euclidean distance between the histogram (with 10 bins) of test data and that of predictions made by each method. We chose the difference in histogram rather than in the realisation of } y \text{ itself, to avoid the error due to the time shift in } y.\]
K2-ABC: Approximate Bayesian Computation with Kernel Embeddings

Figure 2. Blowfly data. A (top): Histograms of 10,000 samples for four parameters \{log P, log \(N_0\), log \(\sigma_p\), log \(\tau\)\} drawn from the prior. A (middle/bottom): Histogram of samples from the posteriors obtained by K2-ABC / SL-ABC (acceptance rate: 0.2, burn-in: 5000 iterations), respectively. In both cases, the posteriors over parameters are concentrated around their means (black bar). The posterior means of \(P\) and \(\tau\) obtained from K2-ABC are close to those obtained from SL-ABC, while there is noticeable difference in the means of \(N_0\) and \(\sigma_p\). Note that we were not able to show the same histogram for K-ABC since the posterior obtained by K-ABC is improper. B (top): Three realisations of \(y\) given three different parameters drawn from the prior. Small changes in \(\theta\) drastically change \(y\). B (middle to bottom): Simulated data using inferred parameters (posterior means) shown in A. Our method (in red) produces the most similar dynamic trajectory to the actual observation (in black) among all the methods.

5. Conclusion

In this paper, we investigated the feasibility of using MMD as a discrepancy measure of samples from two distributions in the context of ABC. Via embeddings of empirical data distributions into an RKHS, we effectively take into account infinitely many features that are sufficient to explain the statistic of observed data.

When tested on both simulated and real-world data, K2-ABC outperforms other methods in terms of Euclidean distance between the chosen 10 summary statistics of \(y^*\) and \(y\) given the posterior mean of parameters, although both SL-ABC and K-ABC explicitly operate on the summary statistic in the comparison while K2-ABC does not.
datasets, our approach obtained more accurate posteriors, compared to other methods that rely on hand-crafted summary statistics. It is our hope that our kernel-based ABC method can save scientists from the laborious procedure of manually choosing summary statistics for ABC, freeing more time for solving more interesting inference problems.

Possible extensions of K2-ABC include (1) an MCMC algorithm with an accept/reject step for more selectively choosing posterior samples; (2) adaptive algorithms to reduce computational costs such as SMC-ABC that adaptively updates the prior where the parameter samples are drawn (Del Moral et al., 2012) and GPS-ABC that adds a memory in the MCMC algorithm to save useful samples and re-use them (Meeds & Welling, 2014).

Acknowledgments

We thank Edward Meeds for sharing his Python implementation of synthetic likelihood ABC algorithm. We thank Shuhei Mano for clarification on K-ABC implementation and Arthur Gretton for useful inputs. We also thank Thomas Desautels, Zoltán Szabó, and Vincent Adam for their valuable comments on the manuscript. This project was supported by the Gatsby Charitable Foundation.

References

Abril, J. C. On the concept of approximate sufficiency. Pakistan Journal of Statistics, 10:171–177, 1994.

Aeschbacher, S., Beaumont, M. A., and Futschik, A. A Novel Approach for Choosing Summary Statistics in Approximate Bayesian Computation. Genetics, 192(3):1027–1047, 2012.

Barber, S., Voss, J., and Webster, M. The Rate of Convergence for Approximate Bayesian Computation. ArXiv e-prints:1311.2038, 2013.

Bazin, E., Dawson, K. J., and Beaumont, M. A. Likelihood-free inference of population structure and local adaptation in a bayesian hierarchical model. Genetics, 185(2):587–602, 06 2010.

Beaumont, M. A., Zhang, W., and Balding, D. J. Approximate Bayesian Computation in Population Genetics. Genetics, 162(4):2025–2035, 2002.

Berlianc, A. and Thomas-Agnan, C. Reproducing Kernel Hilbert Spaces in Probability and Statistics. Kluwer, 2004.

Cam, L. Le. Sufficiency and approximate sufficiency. Ann. Math. Statist., 35(4):1419–1455, 12 1964.

Christmann, A. and Steinwart, I. Universal kernels on non-standard input spaces. In NIPS, pp. 406–414, 2010.

Del Moral, P., Doucet, A., and Jasra, A. An adaptive sequential monte carlo method for approximate bayesian computation. Statistics and Computing, 22(5):1009–1020, 2012. ISSN 0960-3174.

Gretton, A., Borgwardt, K., Rasch, M., Schölkopf, B., and Smola, A. A kernel two-sample test. J. Mach. Learn. Res., 13:723–773, 2012.

Grünewälder, S., Lever, G., Gretton, A., Baldassarre, L., Patterson, S., and Pontil, M. Conditional mean embeddings as regressors. In Proceedings of the 29th International Conference on Machine Learning, ICML, 2012.

Joyce, P. and Marjoram, P. Approximately sufficient statistics and bayesian computation. Statistical Applications in Genetics and Molecular Biology, 7(1):1544–6115, 2008.

Meeds, E. and Welling, M. Gps-abc: Gaussian process surrogate approximate bayesian computation. In Uncertainty in Artificial Intelligence, volume 30, pp. 593–601, 2014.

Nakagome, S., Fukumizu, K., and Mano, S. Kernel approximate bayesian computation in population genetic inferences. Statistical Applications in Genetics and Molecular Biology, 12(6):667–678, 2013.

Ratmann, O., Jørgensen, O., Hinkley, T., Stumpf, M., Richardson, S., and Wiuf, C. Using
likelihood-free inference to compare evolutionary dynamics of the protein networks of H. pylori and P. falciparum. *PLoS Computational Biology*, 3(11):e230, 11 2007.

Robert, C. P., Cornuet, J., Marin, J., and Pillai, N. S. Lack of confidence in approximate Bayesian computation model choice. *Proceedings of the National Academy of Sciences*, 108 (37):15112–15117, 2011.

Schafer, C. M. and Freeman, P. E. Likelihood-free inference in cosmology: Potential for the estimation of luminosity functions. In *Statistical Challenges in Modern Astronomy V*, Lecture Notes in Statistics, pp. 3–19. Springer New York, 2012. ISBN 978-1-4614-3519-8.

Schölkopf, B. and Smola, A. J. *Learning with Kernels: Support Vector Machines, Regularization, Optimization, and Beyond*. MIT Press, Cambridge, MA, USA, 2001. ISBN 0262194759.

Sejdinovic, D., Sriperumbudur, B., Gretton, A., and Fukumizu, K. Equivalence of distance-based and RKHS-based statistics in hypothesis testing. *Ann. Statist.*, 41(5):2263–2291, 2013.

Sejdinovic, D., Strathmann, H., Lomeli, M.G., Andrieu, C., and Gretton, A. Kernel Adaptive Metropolis-Hastings. In *International Conference of Machine Learning*, 2014.

Smola, A., Gretton, A., Song, L., and Schölkopf, B. A hilbert space embedding for distributions. In *Algorithmic Learning Theory*, number 4754 in Lecture Notes in Computer Science, pp. 13–31. Springer Berlin Heidelberg, 2007.

Song, L., Fukumizu, K., and Gretton, A. Kernel embeddings of conditional distributions: A unified kernel framework for nonparametric inference in graphical models. *IEEE Signal Process. Mag.*, 30 (4):98–111, 2013.

Sriperumbudur, B., Gretton, A., Fukumizu, K., Lanckriet, G., and Schölkopf, B. Hilbert space embeddings and metrics on probability measures. *J. Mach. Learn. Res.*, 11:1517–1561, 2010.

Sriperumbudur, B., Fukumizu, K., and Lanckriet, G. Universality, characteristic kernels and RKHS embedding of measures. *J. Mach. Learn. Res.*, 12:2389–2410, 2011.

Szabó, Z., Gretton, A., Póczos, B., and Sriperumbudur, B. Two-stage Sampled Learning Theory on Distributions. *ArXiv e-prints:1402.1754*, February 2014.

Wood, S. N. Statistical inference for noisy nonlinear ecological dynamic systems. *Nature*, 466(7310):1102–1104, 08 2010.