γ -ABC: Outlier-Robust Approximate Bayesian Computation **Based on a Robust Divergence Estimator**

Masahiro Fujisawa

The University of Tokyo RIKEN AIP

fujisawa@ms.k.u-tokyo.ac.jp

Takeshi Teshima

The University of Tokyo RIKEN AIP

teshima@ms.k.u-tokyo.ac.jp

Issei Sato The University of Tokyo RIKEN AIP

sato@k.u-tokyo.ac.jp

Masashi Sugiyama

RIKEN AIP The University of Tokyo sugi@k.u-tokyo.ac.jp

Abstract

Approximate Bayesian computation (ABC) is a likelihood-free inference method that has been employed in various applications. However, ABC can be sensitive to outliers if a data discrepancy measure is chosen inappropriately. In this paper, we propose to use a nearest-neighbor-based γ -divergence estimator as a data discrepancy measure. We show that our estimator possesses a suitable theoretical robustness property called the redescending property. In addition, our estimator enjoys various desirable properties such as high flexibility, asymptotic unbiasedness, almost sure convergence, and linear-time computational complexity. Through experiments, we demonstrate that our method achieves significantly higher robustness than existing discrepancy measures.

Introduction 1

Approximate Bayesian computation (ABC) has been proposed as a "likelihood-free" inference scheme to approximately perform Bayesian inference when a complex model is used and it is impossible or difficult to compute its likelihood (see [53] for a general overview). Instead of investigating the explicit form of the likelihood function, ABC seeks parameters of a simulator-based model that can generate data that is close to the observed data under some discrepancy measure. ABC has been applied to many research fields, e.g., evolutionary biology [76], dynamic systems [83], economics [63], epidemiology [11]. aeronautics [18], and astronomy [15].

Rejection ABC [76, 65, 42], the basic ABC algorithm, proceeds as follows: (i) we draw an independent sam-

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ple of the parameter θ from some prior π , (ii) we simulate data $Y^m = \{Y_j\}_{1:m}$ for each value of θ , (iii) the parameter θ is discarded if the discrepancy $D(X^n, Y^m)$ between the observed data $X^n = \{X_i\}_{1:n}$ and the simulated data $Y^m = \{Y_j\}_{1:m}$ exceeds a tolerance threshold ϵ . The accepted θ is used in the subsequent inference as a sample from an approximation to the posterior distribution called the ABC posterior distribution. Many studies have been performed to enhance the computational efficiency of the rejection ABC scheme, e.g., applying Markov Chain Monte Carlo (MCMC) [54, 80] or sequential Monte Carlo (SMC) [72, 24, 57].

The core element of ABC is the data discrepancy measure $D(X^n, Y^m)$ and the accuracy of parameters from the ABC posterior distribution crucially depends on its choice. While many discrepancies for ABC have been proposed, such as the distance between summary statistics [12, 25, 80], the maximum mean discrepancy (MMD) [60], the Wasserstein distance [7], a Kullback-Leibler (KL) divergence estimator [42], and the classification accuracy discrepancy (CAD) [35], these are often not robust to severe contamination of data [68, 49, 74]. Recently, two outlier-robust discrepancies have been proposed: one is a robust discrepancy based on MMD [49], and the other is using a robust M-estimator, e.g., Huber's estimation function [68]. However, these methods do not possess an ideal robust property for an extreme outlier, called the redescending property [55]. In addition, the former method has the cubic time cost $\mathcal{O}((n+m)^3/Q^2)$, where Q is the number of blocks that divide the data. When ABC is applied to astronomy [47, 15], for example, we have to deal with noisy large-scale datasets, and the cubic time cost can be intractable. For the CAD, we may improve the robustness of the CAD by employing a robust classifier, such as robust LDA [20], robust FDA [40], or robust logistic regression [28]; however, its performance depends on the choice of the classifier, and its validity and robustness for heavy contamination data are not guaranteed in the ABC framework. Outside the ABC framework, recently, many robust inference schemes have been proposed, e.g., using robust divergences for parametric model inference [4, 29], Bayesian inference [45, 41, 58], variational

Table 1: Relationship between previous work and our work (OR: Outlier robustness, RP: Redescending property [55], AU: Asymptotically unbiasedness, ASC: Almost sure convergence, QA: ABC posterior analysis). In MONK [49], the number of blocks that divide the data is denoted by Q. The order of time costs for the q-Wasserstein distance is based on approximate optimization algorithms [21, 22]. The order of time costs for the CAD is based on logistic regression, where d is the dimension of the observed and synthesized data. The symbol $(n \vee m)$ denotes $\max\{n, m\}$.

Discrepancy measure	OR	RP	AU	ASC	QA	Time cost
MMD [60, 73]	-	-	-	-	-	$\mathcal{O}((n+m)^2)$
q-Wasserstein distance [7]	-	-	-	-	-	$\mathcal{O}((n+m)^2)$
CAD [35]	-	-	-	-	\checkmark	$\mathcal{O}((n+m)d)$
MONK BCD-Fast [49]	✓	-	-	-	-	$\mathcal{O}\!\left(rac{(n\!+\!m)^3}{Q^2} ight)$
KL-divergence estimator [61, 42]	-	-	\checkmark	\checkmark	\checkmark	$\mathcal{O}((n \vee m) \log(n \vee m))$
γ -divergence estimator (ours)	✓	\checkmark	\checkmark	\checkmark	\checkmark	$\mathcal{O}((n \lor m) \log(n \lor m))$

inference [30], and constructing Bayesian inference through a pseudo-likelihood via MMD [17]. Unfortunately, these methods cannot be used as a data discrepancy measure for ABC because these assume a tractable likelihood or parametric models. Therefore, there is no discrepancy measure that has both well-guaranteed robustness for an extreme outlier and reasonable time costs.

In this paper, we propose a novel outlier-robust and computationally-efficient discrepancy measure based on the γ -divergence [29]. Our discrepancy measure results in a robustness property of the ABC posterior called the redescending property [55], i.e., it automatically ignores extreme outliers in the observed data. Furthermore, we show that the γ -divergence estimation using a naive k-nearest neighbor density estimate has desirable asymptotic properties, which is not straightforward to prove unlike divergence estimators in f-divergence class, such as α -divergence estimator [64]. Table 1 summarizes the relations among our method and major existing discrepancy measures. Our contributions are as follows.

- We construct a non-parametric and robust divergence estimator based on the γ -divergence (Section 3.3).
- We show that our method theoretically enjoys the robustness and validity (Sections 3.4 and 4.2).
- · We show that our method has the asymptotic unbiasedness and the almost sure convergence property, which are mathematically much harder to show than those for the divergence estimators belonging to the *f*-divergence family (Section 4.1).
- Through experiments, we show that our estimator can significantly reduce the influence of the outliers even when the observed data have a large number of outliers (Section 5).

The rest of this paper is organized as follows. We summarize the ABC framework in Section 2. In Sections 3 and 4, we introduce the k-nearest neighborhood (k-NN) based density estimation, explain how to derive our divergence estimator based on k-NN, and conduct the theoretical analyses. Fi-

Algorithm 1 Rejection ABC Algorithm [76, 65]

Require: Observed data $\{X_i\}_{i=1}^n$, prior $\pi(\theta)$ on the parameter space Θ , tolerance threshold ϵ , data discrepancy measure D

- 1: Initialize: ϵ
- 2: **for** t = 1 to T **do**
- **repeat:** propose $\theta \sim \pi(\theta)$ and draw $Y_1 \ldots, Y_m \stackrel{\text{i.i.d.}}{\sim} p_\theta$ until: $D(X^n, Y^m) < \epsilon$
- Obtain $\theta^{(t)} = \theta$ 5:
- 6: end for
- 7: **return** $\{\theta^{(t)}\}_{t=1}^{T}$

nally, we show the experimental results and the conclusion in Sections 5 and 6.

Preliminaries

In this section, we give an overview of ABC. More detailed descriptions of the discrepancy measures which are often used in ABC can be found in Appendix E.

2.1 Approximate Bayesian Computation

We define $\mathcal{X} \subset \mathbb{R}^d$ as the data space and Θ as the parameter space. The model $\{p_{\theta}: \theta \in \Theta\}$ is a family of probability distributions on \mathcal{X} and has no explicit formula, but we assume that we can generate i.i.d. random samples from p_{θ} given the value of θ . The purpose of ABC is to seek the model parameter θ by comparing the observed data $X_1,\dots,X_n\stackrel{\text{i.i.d.}}{\sim} p_{\theta^*}$ and the synthetic data $Y_1, \ldots, Y_m \overset{\text{i.i.d.}}{\sim} p_{\theta}$, where $\theta^* \in \Theta$ is the true parameter. The criterion used to compare these datasets $X^n = \{X_1, \dots, X_n\}$ and $Y^m = \{Y_1, \dots, Y_m\}$ is the data discrepancy measure $D(X^n, Y^m)$ defined over $\mathcal{X}^n \times \mathcal{X}^m$.

A well known algorithm of ABC is the rejection ABC [76, 65, 42], which proceeds as follows: (i) we draw an independent sample of the parameter θ from some prior π , (ii) we simulate data $Y^m = \{Y_j\}_{1:m}$ for each value of θ , (iii) the parameter θ is discarded if the discrepancy $D(X^n, Y^m)$ between the observed data $X^n = \{X_i\}_{1:n}$ and the simulated data $Y^m = \{Y_j\}_{1:m}$ exceeds a tolerance threshold ϵ . The rejection ABC algorithm is shown in Algorithm 1. It enables us to obtain i.i.d. random samples $\{\theta^{(t)}\}_{t=1}^T$ from the ABC posterior distribution defined as follows.

Definition 1 (ABC posterior distribution). *Let* ϵ *be fixed. Then, the ABC posterior distribution is defined by*

$$\pi(\theta|X^n, D, \epsilon) \propto \int \pi(\theta) \mathbb{1}\{D(X^n, Y^m) < \epsilon\} p_{\theta}(Y^m) dY^m,$$
(1)

where $\pi(\theta)$ is a prior over the parameter space Θ , $\epsilon > 0$ is a tolerance threshold, and $p_{\theta}(Y^m) = \prod_{j=1}^m p_{\theta}(Y_j)$.

We only focus on the rejection ABC [76, 65, 42] throughout this paper. The main reason is two-fold: (i) to make a fair comparison and followed the experimental setting of the recent paper [42] proposing discrepancy measures for ABC, and (ii) to give theoretical guarantees to the ABC posterior explicitly, e.g., Theorem 1 and Corollary 1 in this paper. The rejection ABC is a reasonable choice for this purpose. While there are many sophisticated ABC algorithms, they are often extensions of the rejection ABC [54, 80, 72, 24, 57]; therefore, we can easily combine our development of the rejection ABC with these algorithms.

2.2 Model of Data Contamination

In this paper, we assume that the *observed* data are contaminated with outliers and focus on Huber's contamination-by-outlier case [38], where observed data are sampled i.i.d. from the following distribution:

$$(1 - \eta)G(x) + \eta H(x), \tag{2}$$

where G(x) is a distribution we are interested in, H(x) is an arbitrary contamination distribution, and $\eta \in [0, 1]$ is the proportion of contamination. If η is relatively high, e.g., $\eta = 0.2$, the observed data are highly contaminated by H.

Due to distribution contamination described above, severe bias occurs in parameter estimation. Many robust estimation methods have been proposed to reduce the estimation bias caused by outliers [38, 39, 82, 4]. However, these methods tend to exhibit undesirable behaviors both empirically and theoretically, for heavily contaminated data [29]. Furthermore, for non-parametric inference schemes such as ABC, many of such robust inference frameworks cannot be used because they normally assume that the likelihood is tractable. Although Lerasle et al. [49] and Ruli et al. [68] have proposed robust discrepancy measures that can be compatible with non-parametric inference, these methods also cannot deal with a heavy contamination and the former method has high time costs. To conduct a robust non-parametric inference for heavily contaminated data, it is necessary to construct an alternative discrepancy measure with both robustness for an extreme outlier and reasonable time costs.

3 γ -ABC and Its Robustness

In this section, we construct a *non-parametric* "likelihood-free" inference scheme based on the γ -divergence that has been used in robust parameter estimation from heavily contaminated data. In Section 3.1, we introduce the γ -divergence and explain why we choose a k-NN based density estimation to derive our estimator. Next, we overview a k-NN based density estimation in Section 3.2 and derive our estimator in Section 3.3. Finally, we guarantee the robustness of the ABC based on our estimator in Section 3.4.

3.1 γ -divergence and Its Estimation

To make a robust parameter estimation in the heavily contamination situation described in Section 2.2, Fujisawa and Eguchi [29] proposed the γ -divergence, which possesses strong robustness for heavily contaminated data.

Definition 2 (γ -divergence [29]). Let p and q be positive measurable functions from a measurable set $\mathcal{M}_0 \subseteq \mathbb{R}^d$ to \mathbb{R} . Let $\gamma > 0$. Then, the γ -divergence is defined as

$$D_{\gamma}(p||q) = \frac{1}{\gamma(1+\gamma)} \log \frac{\left(\int_{\mathcal{M}_0} p^{1+\gamma}(x) dx\right) \left(\int_{\mathcal{M}_0} q^{1+\gamma}(x) dx\right)^{\gamma}}{\left(\int_{\mathcal{M}_0} p(x) q^{\gamma}(x) dx\right)^{1+\gamma}}.$$

To combine the γ -divergence with ABC, we need to estimate Eq. (3) from observed and synthesized data. A potential approach we can consider to estimating Eq. (3) is extending f-divergence estimation frameworks, e.g., kernel density estimation (KDE) [37] and direct density ratio estimation methods such as KLIEP [75] or uLSIF [44]. However, the former method suffers from high time cost due to a kernel function and the necessity to select appropriate kernels and its parameters. Furthermore, the latter methods need to construct a model directly for a density ratio; therefore, it is hard to use this approach in the estimation of Eq. (3) since γ -divergence, which is not included in the f-divergence class, is not expressed as a functional of the density ratio.

For these reasons, we consider using a k-NN based density estimation to estimate γ -divergence. This approach has only one hyper-parameter, k. Furthermore, this approach does not depend on any additional models.

3.2 k-Nearest Neighbor based Density Estimation

Let X^n be an i.i.d. sample of size n from a probability distribution with density p, and Y^m be an i.i.d. sample of size m from q. Furthermore, we define $\rho_k(i)$ as the Euclidean distance between the i-th sample X_i of X^n and its k-th nearest neighbor (k-NN) among $X^n \setminus X_i$. Similarly, we define $\nu_k(i)$ as the Euclidean distance between the i-th sample X_i and its

k-NN among Y^m . Let $\mathcal{B}(x,R)$ be a closed ball with radius R around $x \in \mathbb{R}^d$. Finally, $\mathcal{V}(\mathcal{B}(x,R)) = \bar{c}R^d$ is defined as its volume, where \bar{c} is the volume of the d-dimensional unit ball.

Loftsgaarden and Quesenberry [51] constructed the density estimators of p and q at the i-th sample X_i via k-NN as follows:

$$\hat{p}_k(x_i) = \frac{k}{(n-1)\mathcal{V}(\mathcal{B}(x_i, \rho_k(i)))} = \frac{k}{(n-1)\bar{c}\rho_k^d(i)}, (4)$$

$$\hat{q}_k(x_i) = \frac{k}{m\mathcal{V}(\mathcal{B}(x_i, \nu_k(i)))} = \frac{k}{m\bar{c}\nu_{\nu}^d(i)}.$$
 (5)

These density estimators, Eqs. (4) and (5), are consistent estimators of the density only when the number of neighbors k goes to infinity as the sample size n goes to infinity. We use these estimators for constructing our robust divergence estimator. Hereafter, we fix the value of k and show that our divergence estimator still has desirable asymptotic properties, including consistency.

3.3 Robust Divergence Estimator on γ -divergence

Now we derive a *non-parametric* γ -divergence estimator based on k-NN density estimation. In ABC settings, outliers could be included in the observed data X^n . To reduce the influence of outliers, we rewrite the term $\int_{\mathcal{M}_0} q^{1+\gamma}(x) \mathrm{d}x$ in Eq. (3) to be k-NN estimatable from $\mathcal{M}' \subseteq \mathbb{R}^d$, where \mathcal{M}' is the support of q, i.e.,

$$\int_{\mathcal{M}'} q^{1+\gamma}(y) \mathrm{d}y.$$

We can use the same notion of Eq. (4) when we focus on the synthetic data Y^m ; therefore, the density estimation for q(y) based on k-NN can be written as

$$\hat{q}_k(y_j) = \frac{k}{(m-1)\mathcal{V}(\mathcal{B}(y_j, \bar{\rho}_k(j)))} = \frac{k}{(m-1)\bar{c}\bar{\rho}_k^d(j)},$$
(6)

where $\bar{\rho}_k(j)$ is the Euclidean distance between the j-th sample Y_j of Y^m and its k-NN among $Y^m \setminus Y_j$.

By plugging in the k-NN density estimator into Eqs. (4), (5), and (6), we derive the k-NN based γ -divergence estimator as

$$\widehat{D}_{\gamma}(X^{n}||Y^{m}) = \frac{1}{\gamma(1+\gamma)}$$

$$\times \left(\log \frac{\left(\frac{1}{n}\sum_{i=1}^{n} \left(\frac{\bar{c}}{k}\hat{p}_{k}(x_{i})\right)^{\gamma}\right) \left(\frac{1}{m}\sum_{j=1}^{m} \left(\frac{\bar{c}}{k}\hat{q}_{k}(y_{j})\right)^{\gamma}\right)^{\gamma}}{\left(\frac{1}{n}\sum_{i=1}^{n} \left(\frac{\bar{c}}{k}\hat{q}_{k}(x_{i})\right)^{\gamma}\right)^{1+\gamma}} \right).$$
(7)

The details of the derivation is in Appendix A.

The estimator in Eq. (7) involves 2n and 2m operations of nearest neighbor search. If we implement them by KD trees [5, 52], the time cost of finding $\widehat{D}_{\gamma}(X^n \| Y^m)$ is $\mathcal{O}((n \vee m)\log(n \vee m))$, where $(n \vee m) = \max\{n, m\}$, which is among the fastest (up to log factors) of the existing robust discrepancy approximators (see Table 1). Furthermore, this estimator fortunately enjoys ideal asymptotic properties: asymptotic unbiasedness and almost surely convergence under mild assumptions. We will show them in Section 4.1.

3.4 Robustness Property of γ -ABC against Outliers

Here, we investigate the behavior of the *sensitivity curve* (SC), which is a finite-sample analogue of the *influence function* (IF), both of which are used in quantifying the robustness of statistics [36, 30, 68]. We fix the observed data X^n and consider a contamination by an outlier X_0 . We define the contaminated data as $X_{[X_0]}^n := (X_0, X_1, \ldots, X_n)$. Then, the SC is defined as follows.

Definition 3 (Sensitivity curve [36, 2.1e]). Let $\gamma, \epsilon > 0$. Let us define the (population) pseudo-posterior as $\hat{\pi}(\theta|X^n) := \pi(\theta|X^n, \widehat{D}_{\gamma}, \epsilon)$. The sensitivity curve of $\hat{\pi}$ is defined as

$$SC_{n+1}^{\theta}(X_0) := (n+1) \left(\hat{\pi}(\theta|X_{[X_0]}^n) - \hat{\pi}(\theta|X^n) \right).$$

We consider SC instead of IF for two reasons: (i) we are interested in the pseudo-posterior distribution $\hat{\pi}(\theta|X^n)$ with respect to a finite sample X^n , and (ii) the IF of the quantities based on the considered divergence estimator may not be even defined (a detailed explanation is in Remark 2 in Appendix B.3).

Under this definition and some additional assumptions, we obtain the following theorem. Our analysis is a finite-sample analogue of what is called the *redescending property* [55] in the context of IF analysis.

Theorem 1 (Sensitivity curve analysis). Assume $k < \min\{n, m\}$. Also assume that $F_{\theta}(\epsilon) := \int \mathbb{1}\{\widehat{D}_{\gamma}(X^n\|Y^m) < \epsilon\}p_{\theta}(Y^m)\mathrm{d}Y^m$ is β -Lipschitz continuous for all $\theta \in \Theta$. Then, we have

$$\lim_{\|X_0\| \to \infty} \operatorname{SC}_{n+1}^{\theta}(X_0) \le -\frac{\beta \pi(\theta)}{\Lambda_n(1+\gamma)} \log\left(1 - \frac{1}{n^2}\right)^{n+1},$$

where $\Lambda_n := \int \pi(\theta') F_{\theta'}(\epsilon) d\theta'$. Furthermore, if $\lim_{n\to\infty} \Lambda_n$ exists and is non-zero, then the right-hand side of the above inequality converges to 0.

The proof is in Appendix B.2. Through Theorem 1, we can see that the influence of contamination is reduced when we have enough data, even if the magnitude of the outlier X_0 is very large. Intuitively, an estimator has the redescending property if its IF first ascends away from zero as outliers

become more pronounced, while the IF "redescends" towards zero as outliers become increasingly extreme. Since our analysis is a finite-sample analogue of the redescending property in the context of IF, this result implies the robustness of our method that an extreme outlier is automatically ignored.

3.5 Robustness on Estimation Error of Discrepancy

In Section 3.4, we showed the theoretical robustness of our method. Here, we experimentally investigate the robustness based on the estimation error of discrepancy. Figure 1 shows the discrepancy estimation error. In this figure, we show the errors between robust MMD and true MMD, and the KL- or γ -divergence estimator and true KL-divergence. We considered the 1-dimensional standard normal distribution $\mathcal{N}(0,1)$ and the contaminated 1-dimensional standard normal distribution $(1-\eta)\mathcal{N}(0,1)+\eta\mathcal{N}(10,1)$. Whereas the outliers negatively affect the KL divergence estimator [61], MONK-BCD [49] and our γ -divergence estimator are robust to an increase in the contamination rate η . Furthermore, if we choose the hyper-parameter γ properly, our discrepancy estimator achieves comparable accuracy to the KL-divergence estimator in the non-contaminated case.

4 Asymptotic Analysis on ABC

In this section, we elucidate essential asymptotic properties, such as asymptotic unbiasedness and almost sure convergence, for our divergence estimator defined by Eq. (7). Furthermore, we analyze an asymptotic behavior of the ABC posterior distributions built on our divergence estimator.

4.1 Theoretical Analysis for γ -divergence Estimator

To confirm the validity of the proposed estimator in Eq. (7), we show two properties: the asymptotic unbiasedness and the almost sure convergence.

We show the asymptotic unbiasedness by assuming that \mathcal{M} , i.e., the support of p, has the following mild regularity condition. These conditions are commonly used for investigating the asymptotic properties of divergence estimators, e.g., the α -divergence estimator in Poczos and Schneider [64].

Assumption 1 (Restrictions on the domain \mathcal{M} [64]). We assume

$$\inf_{0<\delta<1}\inf_{x\in\mathcal{M}}\frac{\mathcal{V}(\mathcal{B}(x,\delta)\cap\mathcal{M})}{\mathcal{V}(\mathcal{B}(x,\delta))}\coloneqq r_{\mathcal{M}}>0.$$

Assumption 1 states that the intersection of \mathcal{M} with an arbitrary small ball having the center in \mathcal{M} has a volume that cannot be arbitrarily small relative to the volume of the ball. It intuitively means that almost all points of \mathcal{M} are in its interior.

Furthermore, we define the following function:

$$H(x, p, \delta, \omega) := \sum_{j=0}^{k-1} \left(\frac{1}{j!}\right)^{\omega} \Gamma(\kappa + j\omega) \left(\frac{p(x) + \delta}{p(x) - \delta}\right)^{j\omega} \times (p(x) - \delta)^{-\gamma} ((1 - \delta)\omega)^{-\kappa - j\omega},$$
(8)

where $\Gamma(\cdot)$ is the gamma function defined as $\Gamma(z) = \int_0^\infty t^{z-1} \exp(-t) \mathrm{d}t$. Poczos and Schneider [64] used Assumption 1 to show a uniform variant of Lebesgue's lemma and to show that Definition 4 below is well-defined. The function in Eq. (8) appears in the upper bound of the moment for the ω -powered conditional distribution function (CDF) when Assumption 1 holds (see Theorem 37 in Poczos and Schneider [64]). In addition, we impose some reasonable assumptions, which are also assumed in Poczos and Schneider [64].

Definition 4 (Uniformly Lebesgue-approximable function [64]). Denote by $L_1(\mathcal{M})$ the set of Lebesgue integrable functions on \mathcal{M} and let $g \in L_1(\mathcal{M})$. The function g is uniformly Lebesgue approximable on \mathcal{M} if for any series $R_n \to 0$ and any $\delta > 0$, there exists $n_0 = n_0(\delta) \in \mathbb{Z}^+$ such that if $n > n_0$, then for almost all $x \in \mathcal{M}$,

$$g(x) - \delta < \frac{\int_{\mathcal{B}(x,R_n)\cap\mathcal{M}} g(t)dt}{\mathcal{V}(\mathcal{B}(x,R_n)\cap\mathcal{M})} < g(x) + \delta.$$
 (9)

Assumption 2 (Condition for p and q from Poczos and Schneider [64]). The positive functions p and q are bounded away from zero and uniformly Lebesgue approximable. Furthermore, the expectations of the l_2 -norm powered by κ over p and q are bounded, i.e.,

$$\int_{\mathcal{M}} \|x - y\|^{\kappa} p(y) dy < \infty, \quad \int_{\mathcal{M}} \|x - y\|^{\kappa} q(y) dy < \infty,$$

for almost all $x \in \mathcal{M}$. Furthermore, the following conditions hold:

$$\int \int_{\mathcal{M}^2} \|x - y\|^{\kappa} p(y) p(x) dy dx < \infty,$$
$$\int \int_{\mathcal{M}^2} \|x - y\|^{\kappa} q(y) p(x) dy dx < \infty.$$

Assumption 3 (Condition for powered CDF in \mathcal{M} [64]). The expectations of $H(x, p, \delta, 1)$ and $H(x, q, \delta, 1)$ are bounded as follows: $\exists \delta_0$ s.t. $\forall \delta \in (0, \delta_0)$,

$$\int_{\mathcal{M}} H(x, q, \delta, 1) p(x) dx < \infty, \int_{\mathcal{M}} H(x, p, \delta, 1) p(x) dx < \infty.$$

This assumption indicates that the expectations of the ω -powered CDFs of p and q are bounded, respectively. The expectations appear in the upper bound of the moment of the ω -powered CDFs.

Since our method has a term involving an expectation with respect to q, we set the following assumption that is almost the same as the condition for the support of p.

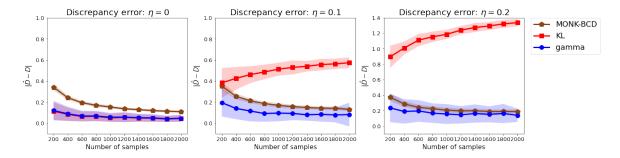


Figure 1: Experimental results for the absolute error of discrepancy. We compared the robustness of the discrepancy measure based on robust MMD (MONK-BCD) and divergence-based discrepancies (KL and ours). The mean \pm std. values of each error are plotted (solid lines are mean values and shaded areas represent the range of mean \pm std values). Lower values are better. The true discrepancy D was estimated by 10^4 Monte Carlo samples. We conducted experiments on each discrepancy for 100 times for various contamination rates ($\eta=0,0.1,0.2$) and sample sizes ($200,400,\ldots,2000$). We set the hyper-parameter candidates of our γ -divergence estimator as $\gamma=(0.1,0.2,0.25,0.4,0.5,0.6,0.75,0.9)$ and the one with the smallest mean score among them is displayed.

Assumption 4 (Extra condition for powered CDF in \mathcal{M}'). *The expectation of* $H(y, q, \delta, 1)$ *is bounded as*

$$\exists \delta_0 \text{ s.t. } \forall \delta \in (0, \delta_0), \ \int_{\mathcal{M}'} H(y, q, \delta, 1) q(y) dy < \infty.$$

This assumption means that the expectation of the ω -powered CDF with respect to q is bounded. The above expectation appears in the upper bound of the moment for the ω -powered CDFs. Under these assumptions, the following theorem holds.

Theorem 2 (Asymptotic unbiasedness). Let $0 < \gamma < k$ or $-k < \gamma < 0$. Suppose that Assumption 2 holds with $\kappa = \gamma$ and that Assumptions 3 and 4 hold. Also assume that q is bounded from above. Then, $\widehat{D}_{\gamma}(X^n \| Y^m)$ defined in Eq. (7) is asymptotically unbiased, i.e.,

$$\lim_{n,m\to\infty} \mathbb{E}\bigg[\widehat{D}_{\gamma}(X^n || Y^m)\bigg] = D_{\gamma}(p||q).$$

From this result, we can see that the asymptotic unbiasedness holds even if we set γ as $-k < \gamma < 0$ (see Theorems 8 and 9 in Appendix D.1).

Next, we establish the almost sure convergence of our estimator.

Theorem 3 (Almost sure convergence). Let $\gamma < k$. Suppose that Assumption 2 holds with $\kappa = \gamma$ and that Assumptions 3 and 4 hold. Also assume that p and q are bounded from above. Let k(n) denote the number of neighbors applied at sample size n such that $\lim_{n\to\infty} k(n) = \infty$, $\lim_{n\to\infty} n/k(n) = \infty$, $\lim_{m\to\infty} k(m) = \infty$ and $\lim_{m\to\infty} m/k(m) = \infty$. Then, our estimator converges almost surely to $D_{\gamma}(p||q)$, that is,

$$\widehat{D}_{\gamma}(X^n || Y^m) \stackrel{a.s.}{\to} D_{\gamma}(p || q).$$

The proofs for these theorems are in Appendices D.1 and D.2. Note that in the proofs of Theorems 2 and 3, we cannot reuse the known theoretical results for the divergence estimators in the f-divergence class [61, 64] and it required us to newly show several asymptotic properties specifically for γ -divergence estimation, which are given in Appendices C and D.

4.2 Asymptotic Property of ABC Posterior Distributions with γ -divergence Estimator

Now we analyze whether the ABC posterior based on our robust discrepancy measure can accurately estimate the parameter θ with small exact γ -divergence $D_{\gamma}(p_{\theta^*} || p_{\theta})$ asymptotically.

According to Theorem 1 in [42], the asymptotic ABC posterior is a restriction of the prior π to the region $\{\theta \in \Theta : D(p_{\theta^*} \| p_{\theta}) < \epsilon\}$ with appropriate scaling. Combining this with the almost sure convergence of $\widehat{D}_{\gamma}(X^n \| Y^m)$ established in Theorem 3, we can obtain the following corollary.

Corollary 1 (Asymptotic ABC posterior with γ -divergence estimator). Suppose that Assumptions 2-4 are satisfied with $\kappa = \gamma$. Let $n \to \infty$ and $m/n \to \alpha > 0$. Let $\pi(\theta|D_{\gamma}(p_{\theta^*}\|p_{\theta}) < \epsilon)$ be the posterior under $D_{\gamma}(p_{\theta^*}\|p_{\theta}) < \epsilon$. If $\widehat{D}_{\gamma}(X^n\|Y^m)$ is used as the data discrepancy measure in Algorithm 1, the ABC posterior distribution satisfies

$$\pi(\theta|X^n; \widehat{D}_{\gamma}, \epsilon) \to \pi(\theta|D_{\gamma}(p_{\theta^*}||p_{\theta}) < \epsilon),$$

almost surely, and therefore

$$\lim_{n,m\to\infty} \pi(\theta|X^n; \widehat{D}_{\gamma}, \epsilon) \propto \pi(\theta) \mathbb{1}\{D_{\gamma}(p_{\theta^*}||p_{\theta}) < \epsilon\},$$

almost surely.

Proof sketch. In the same way as Jiang et al. [42], we use Lévy's upward theorem (enabled by Theorem 3; see Theorem 4 in Appendix C) to $Z_n = \mathbb{1}\{\widehat{D}_{\gamma}(X^n\|Y^{\infty}) < \epsilon\}$ and apply the dominated convergence theorem [78] to complete the proof.

Corollary 1 shows that the ABC posterior based on our estimator converges to the maximum likelihood estimator minimizes the exact γ -divergence between the empirical distribution of p_{θ^*} and p_{θ} . Thus, ABC with our γ -divergence estimator asymptotically collects the θ with small γ -divergence.

5 Experiments

In this section, we report the performance of our estimator through five benchmark experiments of ABC. Here, we confirm that the ABC with our discrepancy measure has immunity against heavily contaminated data.

5.1 Settings

We set n=m following Jiang et al. [42] to prevent the resulting ABC posterior of the indirect method to be overprecise [25] and to avoid arbitrariness in the experiments. The tolerance threshold ϵ was adaptively initialized so that 0.5% of proposed parameters θ were accepted in each experiment by calculating each discrepancy measure 10^3 times. Furthermore, we artificially generated the n i.i.d. observed data from $G(X_i)$ and replaced them by some outliers from $\mathcal{N}(10,1)$, where $G(X_i)$ is an observed data distribution. In short, the contaminated data can be expressed as $(1-\eta)G(X_i)+\eta\mathcal{N}(10,1)$ in each dimension. In addition, we varied the contamination level η in $\{0,0.1,0.2\}$ to confirm the robustness. The hyper-parameter γ was selected from $\{0.1,0.2,0.25,0.4,0.5,0.6,0.75,0.9\}$ for our method.

We measured the accuracy by the simulation error based on the *energy distance*, which is a standard metric for distributions in statistics and has been used in the ABC literature, e.g., Kajihara et al. [43]. This allows us to directly compare the distributions between the non-contaminated observed data and the synthesized data simulated with the estimated parameter. We approximated the MAP estimator $\hat{\theta}_{\text{MAP}}$ of the ABC posterior by kernel density estimation with the Gaussian kernel with the bandwidth parameter $n^{-1/(d+4)}$, that is known as Scott's Rule [70].

From each of the 10 different models, we sampled the data and performed the ABC (Algorithm 1) with $T=10^5$. We repeated the procedure independently for 10 times, and reported the average results. The results with the standard errors are reported in Appendix G.2.6, and the results of the mean-squared error (MSE) between $\hat{\theta}_{\rm MAP}$ and the true parameter are also reported in Appendix G.

For our method, we conducted experiments independently

for several γ and displayed the one with the smallest mean score of the energy distance and the MSE among them. The full results are reported in Figures 6–10 and 13–17 in Appendix G. Furthermore, we compared the ABC posteriors of our method and that of the second-best method. These results are reported in Figures 18–22 in Appendix G.3.

5.2 Models and Results

Here, we summarize the model settings and the results of each experiment. The details of the baseline discrepancies and the model architectures are shown in Appendices E and E.

Gaussian Mixture Model (GM): The univariate Gaussian mixture model is the most basic benchmark setup in the ABC literature [81, 42]. We adopted a bivariate Gaussian mixture model with the true parameters $p^* = 0.3$, $\mu_0^* = (0.7, 0.7)$ and $\mu_1^* = (-0.7, -0.7)$, where p^* is the mixture weight and μ_0^* , μ_1^* are the means of the component distributions. The variances are fixed as $0.5I - 0.3I^{\top}$ and 0.25I, where I is the identity matrix of size (2, 2).

From the experimental results in Figure 2, we can see that our method achieves a better performance when the observed data are contaminated, whereas the other methods fail to give good scores. In addition, in terms of the MSE, our method outperforms the baseline methods (see Appendix G) under contamination. From the results in Figure 4, we can confirm that the ABC posterior with our method places high density around the ground-truth parameter, whereas the baseline method fails to do so.

M/G/1-queuing Model (MG1): Queuing models are an example of stochastic models which are easy to sample from but have intractable likelihoods [27]. The M/G/1-queuing model has been often used in the ABC literature [27, 42]. This model has three parameters: $\theta = (\theta_1, \theta_2, \theta_3)$. We adopted this model with the true parameter $\theta^* = (1, 5, 0.2)$.

From the experimental results in Figure 2, we can see that our method outperforms the other methods even if the data has no contamination. In addition, our method also achieves better performance in terms of the MSE scores than the baseline methods (see Appendix G). Figure 5 indicates that the ABC posterior with our method places high density around the ground-truth parameter, e.g., for θ_2 . On the other hand, the CAD via boosting places higher density around the wrong parameter than our method, e.g., for θ_3 .

Bivariate Beta Model (BB): The bivariate beta model can be used to model data sets exhibiting positive or negative correlation [2]. This model was originally proposed as a model with 8 parameters $\theta = (\theta_1, \dots, \theta_8)$ by Arnold and Ng [2], and Crackel and Flegal [19] later reconsidered its 5-parameter sub-model by restricting to $\theta_3, \theta_4, \theta_5 =$

Figure 2: Simulation error for the GM (left) and the MG1 model (right) experiments.

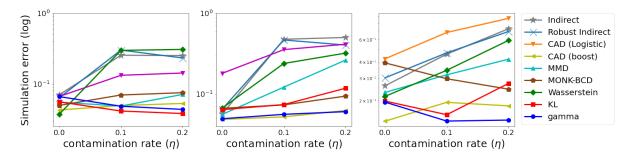


Figure 3: Simulation error for the BB (left), the MA2 (center), and the GK model (right) experiments.

0. Jiang et al. [42] used the 5-parameter models for ABC experiments and therefore we also adopted this with the true parameter $\theta^* = (3, 2.5, 2, 1.5, 1)$ as a benchmark model.

From the experimental results in Figure 3, the KL- and the γ -divergence based methods achieve better performances than those of the baseline methods when the observed data are heavily contaminated. The Wasserstein method achieves a better performance than the others when the data has no contamination; however, the performance becomes significantly worse when the contamination occurs. In addition, the CAD with boosting method achieves a better performance in terms of the MSE; however, the simulation error is worse than the KL- and the γ -divergence based methods (see Appendix G). Figure 5 shows that the ABC posterior with our method places higher density around the groundtruth parameter than the KL method. In addition, the KL method sometimes places high density around the wrong parameter, e.g., for θ_8 . However, in this experiment, the simulation error of the KL method is slightly better than that of our method. This indicates that carefully tuning the hyperparameter γ is important in our method.

Moving-average Model of Order 2 (MA2): The moving-average model is often used for modeling univariate time series. Marin et al. [53] used the moving-average model of order 2 as a benchmark model for ABC. We adopted this model with 10-length time series. For the unobserved noise distribution, we used Student's t-distribution with 5 degrees of freedom. We set the true parameter $\theta^* = (0.6, 0.2)$.

From the experimental results in Figure 3, our method and the CAD with boosting outperform the other methods. The CAD with boosting achieves comparable performance to our method even if the observed data are contaminated; however, in terms of the time cost, our method is better than that of this method because the gradient boosting has $\mathcal{O}(Kd(n+m)+(n+m)\log B)$ time cost, where K is the total number of trees and B is s the maximum number of rows in each block (see Chen and Guestrin [16]). In addition, in terms of the MSEs, our method achieves better performance when the observed data are heavily contaminated (see Appendix G). In Figure 4, we found that the ABC posterior with our method places high density around the ground-truth parameter. On the other hand, the CAD via boosting places higher density around the wrong parameter than our method.

Multivariate g-and-k **Distribution** (**GK**): The univariate g-and-k distribution is a generalization of the standard normal distribution with extra parameters: the *skewness* and the *kurtosis*. This distribution is known to have no analytical form of the density function, and the numerical evaluation of the likelihood function is costly [66]. Thus, it is a model for which ABC is specifically suited [27, 1]. Some studies [24, 50] also considered the multivariate g-and-k distribution. We adopted the multivariate model proposed by Drovandi and Pettitt [24] with the true parameters $A^* = 3$, $B^* = 1$, $g^* = 2$, $k^* = 0.5$ and $\rho^* = -0.3$, where A^*, B^*, g^*, k^* control the location, the scale, the skewness and the kurtosis, respectively.

From the experimental results in Figure 3, we can see that

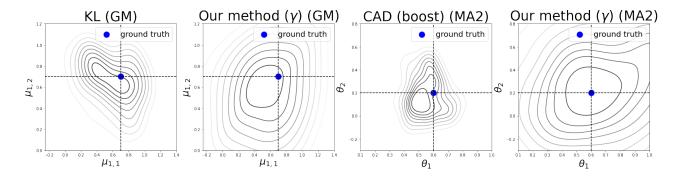


Figure 4: ABC posterior distributions of the GM and MA2 model experiments for $\eta = 0.2$ (excerpted).

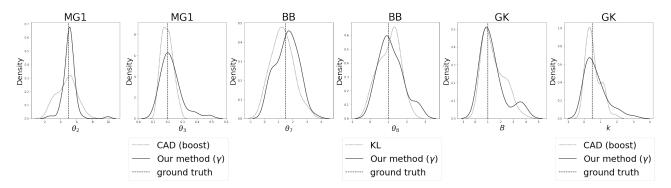


Figure 5: ABC posterior distributions of the MG1, BB, and GK model experiments for $\eta = 0.2$ (excerpted).

our method achieves better performance even if the observed data are contaminated, although the other baseline methods fail to give good scores. In addition, in terms of the MSE, our method outperforms the other baseline methods when the observed data have heavy contamination (see Appendix G). Figure 5 shows that the ABC posterior with our method places slightly higher density on the ground-truth parameter than that of the CAD via boosting.

6 Conclusion and Discussion

We have proposed a γ -divergence estimator and used it as a robust data discrepancy for ABC. We theoretically have guaranteed its robustness against outliers and its desirable asymptotic properties, i.e., the asymptotic unbiasedness and the almost sure convergence to the approximate posterior. In addition, we have shown the redescending property of the ABC posterior of our method, indicating the high robustness of our method against extreme outliers. Through the experiments on benchmark models, we empirically confirmed that our method is robust against heavy contamination by outliers.

Our work has two limitations: (i) our method can become statistically inefficient in high-dimensional cases (the curse of dimensionality) due to the k-NN based density estimation, and therefore (ii) its performance has only been confirmed in some low-dimensional cases. To overcome these

limitations, in the future, we will consider extending our method to a non-parametric estimation that can handle high dimensions and conduct experiments for more realistic high-dimensional cases. Furthermore, on the basis of our idea, we plan to develop outlier-robust methods for other ABC approaches, e.g., ABC without discrepancies [59, 32, 77].

It is worth mentioning that there have been several studies on general losses within Bayesian procedures [10, 46], and recent studies have connected the ideas of these studies with ABC [69]. Following these studies, it would be interesting to see whether our method stands in the framework of generalized approximate Bayesian inference under the condition of ABC with a general loss function [69].

In addition, research on the consistency and robustness of Bayesian estimation against model misspecification has attracted attention recently. For example, Cherief-Abdellatif and Alquier [17] has proposed Bayesian estimation based on a pseudo-likelihood by using MMD and has theoretically shown that it is effective in this problem setting. We also explore the potential of our method in the context of model misspecification.

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