NEURAL APPROXIMATE SUFFICIENT STATISTICS FOR IMPLICIT MODELS

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ABSTRACT

We consider the fundamental problem of how to automatically construct summary statistics for implicit generative models where the evaluation of likelihood function is intractable but sampling / simulating data from the model is possible. The idea is to frame the task of constructing sufficient statistics as learning mutual information maximizing representation of the data. This representation is computed by a deep neural network trained by a joint statistic-posterior learning strategy. We apply our approach to both traditional approximate Bayesian computation (ABC) and recent neural likelihood approaches, boosting their performance on a range of tasks.

1 INTRODUCTION

Many data generating processes can be well-described by a parametric statistical model that can be easily simulated forward but does not possess an analytical likelihood function. These models are called implicit generative models (Diggle & Gratton, 1984) or simulator-based models (Lintusaari et al., 2017) and are widely used in science and engineering domains, including physics (Sjöstrand et al., 2008), genetics (Järvenpää et al., 2018), computer graphics (Mansinghka et al., 2013), finance (Bansal & Yaron, 2004), cosmology (Weyant et al., 2013), ecology (Wood, 2010) and epidemiology (Chinazzi et al., 2020). For example, the number of infected/healthy people in an outbreak could be well modelled by stochastic differential equations (SDE) simulated by Euler-Maruyama discretization but the likelihood function of a SDE is generally non-analytical. Directly inferring the parameters of these implicit models is often difficult or even impossible.

The techniques coined as *likelihood-free inference* open us a door for performing Bayesian inference in such circumstances. Likelihood-free inference needs to evaluate neither the likelihood function nor its derivatives. Rather, it only requires the ability to sample (*i.e.* simulate) data from the model. Early approaches in approximate Bayesian computation (ABC) perform likelihood-free inference by repeatedly simulating data from the model, and pick a small subset of the simulated data close to the observed data to build the posterior (Pritchard et al., 1999; Marjoram et al., 2003; Beaumont et al., 2009; Sisson et al., 2007). Recent advances make use of flexible neural density estimators to approximate either the intractable likelihood (Papamakarios et al., 2019) or directly the posterior (Papamakarios & Murray, 2016; Lueckmann et al., 2017; Greenberg et al., 2019).

Despite the algorithmic differences, a shared ingredient in likelihood-free inference methods is the choice of summary statistics. Well-chosen summary statistics have been proven crucial for the performance of likelihood-free inference methods (Blum et al., 2013; Fearnhead & Prangle, 2012; Sisson et al., 2018). Unfortunately, in practice it is often difficult to determine low-dimensional and informative summary statistic without domain knowledge from experts. In this work, we propose a novel deep neural network-based approach for automatic construction of summary statistics. Neural networks have been previously applied to learning summary statistics for likelihood-free inference (Jiang et al., 2017; Dinev & Gutmann, 2018; Alsing et al., 2018; Brehmer et al., 2020). Our approach is unique in that our learned statistics directly target at *global sufficiency*. The main idea is to exploit the link between statistical sufficiency and information theory, and to formulate the task of learning sufficient statistic as the task of learning information-maximizing representation of data. We achieve this with recent neural mutual information estimators (Belghazi et al., 2018; Hjelm et al., 2018). Importantly, such neural sufficient statistic could be learned jointly with the posterior, resulting in fast learning where the two could refine each other iteratively. To sum up, our main contributions are:

- We propose a new neural approach to automatically extract compact, *near-sufficient* statistics from raw data. The approach removes the need for carefully handcrafted design of summary statistics;
- With the proposed statistics, we develop two new likelihood-free inference methods namely SMC-ABC+ and SNL+. Experiments on tasks with various types of data demonstrate their effectiveness.

2 BACKGROUND

Likelihood-free inference. LFI considers the task of Bayesian inference where the likelihood function of the model is intractable but simulating (sampling) data from the model is possible:

$$\pi(\boldsymbol{\theta}|\mathbf{x}_o) \propto \pi(\boldsymbol{\theta}) \underbrace{p(\mathbf{x}_o|\boldsymbol{\theta})}_{?} \tag{1}$$

where $\mathbf{x}_o$ is the observed data, $\pi(\boldsymbol{\theta})$ is the prior over the model parameters $\boldsymbol{\theta}$, $p(\mathbf{x}_o|\boldsymbol{\theta})$ is the (possibly) non-analytical likelihood function and $\pi(\boldsymbol{\theta}|\mathbf{x}_o)$ is the posterior over $\boldsymbol{\theta}$. We assume while we do not have access to the exact likelihood, we could still sample (simulate) data from the model with a simulator: $\mathbf{x} \sim p(\mathbf{x}|\boldsymbol{\theta})$. The task is then to infer $\pi(\boldsymbol{\theta}|\mathbf{x}_o)$ given $\mathbf{x}_o$ and the sampled data: $\mathcal{D} = \{\boldsymbol{\theta}_i, \mathbf{x}_i\}_{i=1}^n$ where $\boldsymbol{\theta}_i \sim p(\boldsymbol{\theta}), \mathbf{x}_i \sim p(\mathbf{x}|\boldsymbol{\theta}_i)$. Note that $p(\boldsymbol{\theta})$ is not necessarily the prior $\pi(\boldsymbol{\theta})$.

Curse of dimensionality. Different likelihood-free inference algorithms might learn $\pi(\boldsymbol{\theta}|\mathbf{x}_o)$ in different ways, nevertheless most of existing methods suffer from the curse of dimensionality. For example, traditional ABC methods use a small subset of $\mathcal{D}$ closest to $\mathbf{x}_o$ under some metric to build the posterior (Pritchard et al., 1999; Marjoram et al., 2003; Beaumont et al., 2009; Sisson et al., 2007), however in high-dimensional space measuring the distance sensibly is notoriously hard (Sorzano et al., 2014; Xie et al., 2017). On the other hand, recent advances (Papamakarios et al., 2019; Lueckmann et al., 2017; Papamakarios & Murray, 2016; Greenberg et al., 2019) utilize neural density estimators (NDE) to model the intractable likelihood or the posterior. Unfortunately, modeling high-dimensional distributions with NDE accurately is also known to be very difficult (Oord et al., 2016; Rippel & Adams, 2013; Oord et al., 2017), especially when the available training (simulated) data is scarce.

Our interest here is not to design a new inference algorithm, but to find a low-dimensional statistic $\mathbf{s} = s(\mathbf{x})$ that is (Bayesian) sufficient:

$$\pi(\boldsymbol{\theta}|\mathbf{x}_o) \approx \pi(\boldsymbol{\theta}|\mathbf{s}_o) \propto \pi(\boldsymbol{\theta}) p(\mathbf{s}_o|\boldsymbol{\theta}), \tag{2}$$

where $s : \mathcal{X} \to \mathcal{S}$ is a deterministic function also learned from $\mathcal{D}$. We conjecture that the learning of $s(\cdot)$ might be an easier task than direct density estimation. The resultant statistic $\mathbf{s}$ could then be applied to a wide range of likelihood-free inference algorithms as we will elaborate in Section 3.2.

3 METHODOLOGY

3.1 NEURAL SUFFICIENT STATISTICS

Our new deep neural network-based approach for automatic construction of (near-)sufficient statistics is based on the infomax principle, as illustrated by the following proposition :

Proposition 1. *Let $\boldsymbol{\theta} \sim p(\boldsymbol{\theta})$, $\mathbf{x} \sim p(\mathbf{x}|\boldsymbol{\theta})$, and $s : \mathcal{X} \to \mathcal{S}$ be a deterministic function. Then $\mathbf{s} = s(\mathbf{x})$ is a sufficient statistic for $p(\mathbf{x}|\boldsymbol{\theta})$ if and only if*

$$s = \underset{S:\mathcal{X}\to\mathcal{S}}{\arg\max} \;\; I(\boldsymbol{\theta}; S(X)),$$

where S is deterministic mapping and $I(\cdot,\cdot)$ is the mutual information between random variables.

Proof. We defer the complete proof to the Appendix. This proposition is a variant of Theorem 8 in (Shamir et al., 2008) with an adaption to likelihood-free inference scenario. □

This important result suggests that we could find the sufficient statistic $s(\mathbf{x})$ for a likelihood function $p(\mathbf{x}|\boldsymbol{\theta})$ by maximizing the mutual information (MI) $I(\boldsymbol{\theta}; S) = KL[p(\boldsymbol{\theta}, S) \| p(\boldsymbol{\theta})p(S)]$ between $\boldsymbol{\theta}$ and S. Moreover, as our interest is in maximizing MI rather than knowing its precise value, we can maximize a non-KL surrogate, which has been proven to yield better performance (Hjelm et al., 2018; Ozair et al., 2019; Wen et al., 2020). To this end, we utilize the Jensen-Shannon divergence (JSD)

surrogate (Hjelm et al., 2018), a distribution-free, non-KL MI estimator. This estimator was shown to be much less sensitive to sample size (Hjelm et al., 2018). More specifically, it estimates MI as:

$$\hat{I}^{\text{JSD}}(\boldsymbol{\theta}; S) = \sup_{T:\Theta\times\mathcal{S}\to\mathbb{R}} \mathbb{E}_{p(\boldsymbol{\theta},\mathbf{s})}\left[-\operatorname{sp}(-T(\boldsymbol{\theta},\mathbf{s}))\right] - \mathbb{E}_{p(\boldsymbol{\theta})p(\mathbf{s})}\left[\operatorname{sp}(T(\boldsymbol{\theta},\mathbf{s}))\right], \tag{3}$$

where $\operatorname{sp}(t) = \log(1+\exp(t))$ is the softplus function. With this estimator, we set up the following objective for learning the sufficient statistics, which simultaneously estimates and maximizes the MI:

$$\mathcal{L}(S,T) = \mathbb{E}_{p(\boldsymbol{\theta},\mathbf{x})}\left[-\operatorname{sp}\left(-T(\boldsymbol{\theta}; S(\mathbf{x}))\right)\right] - \mathbb{E}_{p(\boldsymbol{\theta})p(\mathbf{x})}\left[\operatorname{sp}\left(T(\boldsymbol{\theta}; S(\mathbf{x}))\right)\right], \tag{4}$$

where the two deterministic mappings S and T are parameterized by two neural networks.

With considerable training samples and powerful neural networks S and T, we could obtain near-sufficient statistic with $s = \arg\max_S \max_T \mathcal{L}(S,T)$. The statistic $\mathbf{s}$ of data $\mathbf{x}$ is then given by

$$\mathbf{s} = s(\mathbf{x}). \tag{5}$$

In the above construction, we have not specified the form of the networks S and T. For T, we choose it to be a split architecture:

$$T(\boldsymbol{\theta}; S(\mathbf{x})) = T'(H(\boldsymbol{\theta}); S(\mathbf{x})), \tag{6}$$

where $T'(\cdot,\cdot), H(\cdot)$ are both MLPs. For S, any prior knowledge about the data $\mathbf{x}$ could in principle be incorporated into its design. For example, for sequential data we can realize S as a LSTM network (Gers et al., 1999), and for exchangeable data we can realize S as a exchangeable neural network (Chan et al., 2018). Here we simply adopt a fully-connected architecture for S, and leave the problem-specific design of S as future work. Therefore we separately learn representations for $\mathbf{x}$ and $\boldsymbol{\theta}$ before processing them together. This could be seen as that we incorporate the inductive bias into the design of the networks that $\mathbf{x}$ and $\boldsymbol{\theta}$ should *not* interact with each other directly, based on their true relationship, (for example, consider the exponential family: $L(\boldsymbol{\theta}; \mathbf{x}) \propto \exp(H(\boldsymbol{\theta})^\top S(\mathbf{x}))$).

We are left with the problem of how to select d, the dimensionality of the sufficient statistics. The Pitman-Koopman-Darmois theorem tells us that sufficient statistics with fixed dimensionality only exists for exponential family, so one might better determine d in a data-driven way. To do this, we can in principle set d to be as low as possible while preserving enough information about $\boldsymbol{\theta}$:

$$d = \min\{d' : \hat{I}(s_{d'}(X), \boldsymbol{\theta}) \geq \lambda \hat{I}(s_{d^*}(X), \boldsymbol{\theta})\} \tag{7}$$

where $s_{d'}$ is the statistic with dimensionality d', d^* is the dimensionality that achieves the highest MI and $\lambda \in (0,1)$ quantifies how much information we are to preserve in the learnt statistics. Due to space limit we do not pursue this idea further in this paper and leave its verification to future work.

Furthermore, we have the following proposition comparing our method to the existing *posterior-mean-as-statistic* approaches (Fearnhead & Prangle, 2012; Jiang et al., 2017).

Proposition 2. *Let $\boldsymbol{\theta} \sim p(\boldsymbol{\theta})$ and $\mathbf{x} \sim p(\mathbf{x}|\boldsymbol{\theta})$. Let $s(\cdot)$ be the maximizer of the following objective:*

$$s = \arg\min_{S:\mathcal{X}\to\mathcal{S}} \ \mathbb{E}_{p(\boldsymbol{\theta},\mathbf{x})}[\|S(\mathbf{x}) - \boldsymbol{\theta}\|_2^2],$$

then $\mathbf{s} = s(\mathbf{x})$ is generally not a maximizer of $I(S(\mathbf{x}), \boldsymbol{\theta})$ and hence it is not a sufficient statistic.

Proof. We defer the proof to the Appendix. □

This proposition tells us that unlike our method, the existing posterior-mean-as-statistic approaches widely used in likelihood-free inference community loose information about the posterior, and it is only optimal for predicting the posterior mean (Fearnhead & Prangle, 2012; Jiang et al., 2017). Nonetheless which method to use depends on the task e.g. full posterior estimate vs. point estimate).

3.2 Dynamic statistic-posterior learning

The above neural sufficient statistic could, in principle, be learned via a pilot run before the inference starts, as typically done in the work by Drovandi et al. (2011); Fearnhead & Prangle (2012); Jiang et al. (2017). Such a strategy requires extra simulation cost, and the learned statistic is kept fixed during inference. We propose a dynamic learning strategy below to overcome these limitations.

Our idea is to *jointly learn the statistic and the posterior in multiple rounds*. More concretely, at round r, we use the current statistic $s(\cdot)$ to build the r-th estimate to the posterior: $q_r(\boldsymbol{\theta}|\mathbf{s}_o) \approx \pi(\boldsymbol{\theta}|\mathbf{x}_o)$,

Algorithm 1 SMC-ABC+

Input: prior $\pi(\boldsymbol{\theta})$, observed data $\mathbf{x}_o$
Output: estimated posterior $\hat{\pi}(\boldsymbol{\theta}|\mathbf{x}^o)$
Initialization: $\mathcal{D} = \varnothing, p_1(\boldsymbol{\theta}) = \pi(\boldsymbol{\theta})$
for j in 1 to r **do**
  repeat
    sample $\boldsymbol{\theta}^{(i)} \sim p_j(\boldsymbol{\theta})$;
    simulate $\mathbf{x}^{(i)} \sim p(\mathbf{x}|\boldsymbol{\theta}_i)$;
  until n samples
  $\mathcal{D} \leftarrow \mathcal{D} \cup \{\boldsymbol{\theta}_i, \mathbf{x}_i\}_{i=1}^n$
  fit statistic net $s(\cdot)$ with $\mathcal{D}$ by equation 4 ;
  sort $\mathcal{D}$ according to $\|s(\mathbf{x}_i) - s(\mathbf{x}_o)\|$;
  fit $p(\boldsymbol{\theta}|\mathbf{s}_o)$ with the top m $\boldsymbol{\theta}$s in $\mathcal{D}$;
  $q_j(\boldsymbol{\theta}|\mathbf{s}_o) \propto \pi(\boldsymbol{\theta}) / \sum_j p_j(\boldsymbol{\theta}) \cdot p(\boldsymbol{\theta}|\mathbf{s}_o)$;
  $p_{j+1}(\boldsymbol{\theta}) \leftarrow q_j(\boldsymbol{\theta}|\mathbf{s}_o)$;
end for
return $\hat{\pi}(\boldsymbol{\theta}|\mathbf{x}_o) = q_r(\boldsymbol{\theta}|\mathbf{s}_o)$

Algorithm 2 SNL+

Input: prior $\pi(\boldsymbol{\theta})$, observed data $\mathbf{x}_o$
Output: estimated posterior $\hat{\pi}(\boldsymbol{\theta}|\mathbf{x}^o)$
Initialization: $\mathcal{D} = \varnothing, p_1(\boldsymbol{\theta}) = \pi(\boldsymbol{\theta})$
for j in 1 to r **do**
  repeat
    sample $\boldsymbol{\theta}^{(i)} \sim p_j(\boldsymbol{\theta})$;
    simulate $\mathbf{x}^{(i)} \sim p(\mathbf{x}|\boldsymbol{\theta}_i)$;
  until n samples
  $\mathcal{D} \leftarrow \mathcal{D} \cup \{\boldsymbol{\theta}_i, \mathbf{x}_i\}_{i=1}^n$
  fit statistic net $s(\cdot)$ with $\mathcal{D}$ by equation 4;
  convert $\mathcal{D}$ with the learned/selected $s(\cdot)$;
  fit $q(\mathbf{s}|\boldsymbol{\theta})$ with converted $\mathcal{D}$ by equation 10;
  $q_j(\boldsymbol{\theta}|\mathbf{s}_o) \propto \pi(\boldsymbol{\theta}) \cdot q(\mathbf{s}_o|\boldsymbol{\theta})$;
  $p_{j+1}(\boldsymbol{\theta}) \leftarrow q_j(\boldsymbol{\theta}|\mathbf{s}_o)$;
end for
return $\hat{\pi}(\boldsymbol{\theta}|\mathbf{x}_o) = q_r(\boldsymbol{\theta}|\mathbf{s}_o)$

whereas at round r+1, this estimate is used as the new proposal distribution to simulate data: $p_{r+1}(\boldsymbol{\theta}) \leftarrow q_r(\boldsymbol{\theta}|\mathbf{s}_o), \boldsymbol{\theta}_i \sim p_{r+1}(\boldsymbol{\theta}), \mathbf{x}_i \sim p(\mathbf{x}|\boldsymbol{\theta}_i)$. We then re-learn $s(\cdot)$ and $q(\cdot)$ with all the data up to the new round. In this process, $s(\cdot)$ and $q(\cdot)$ refine each other: a good $s(\cdot)$ helps to learn $q(\cdot)$ more accurately, whereas an improved $q(\cdot)$ as a better proposal in turn helps to learn $s(\cdot)$ more efficiently.

In practice, any likelihood-free inference algorithm that learns the posterior sequentially naturally fits well within the above joint statistic-posterior learning framework. Here we study two such instances:

Sequential Monte Carlo ABC (SMC-ABC) (Beaumont et al., 2009). This classical algorithm learns the posterior in a non-parametric way within multiple rounds. Here, we consider a variant of it to better make use of the above neural sufficient statistic, and to re-use all previous simulated data. The new SMC-ABC algorithm estimates the posterior $q_r(\boldsymbol{\theta}|\mathbf{s}_o)$ at the r-th round as follows. We first sort data in $\mathcal{D} = \{\mathbf{x}_i, \boldsymbol{\theta}_i\}_{i=1}^{nr}$ according to the distances $\|s(\mathbf{x}_i) - s(\mathbf{x}_o)\|$. We then pick the top-$m$ $\boldsymbol{\theta}$s whose corresponding distances are the smallest. The picked $\boldsymbol{\theta}$s then follow $\boldsymbol{\theta} \sim p(\boldsymbol{\theta} \mid \mathbf{s}_o)$ as below:

$$p(\boldsymbol{\theta} \mid \mathbf{s}_o) \propto \sum_{j=1}^{r} p_j(\boldsymbol{\theta}) \cdot \Pr(\|\mathbf{s} - \mathbf{s}_o\| < \epsilon \mid \boldsymbol{\theta}), \tag{8}$$

where the threshold ϵ is implicitly defined by the ratio $\frac{m}{nr}$ (which automatically goes to zero as $r \to \infty$). We then fit $p(\boldsymbol{\theta}|\mathbf{s}_o)$ with the collected $\boldsymbol{\theta}$s by a flexible parametric model (e.g. a Gaussian copula), with which we can obtain the r-th estimate to the posterior by importance (re-)weighting:

$$q_r(\boldsymbol{\theta} \mid \mathbf{s}_o) \propto \pi(\boldsymbol{\theta}) / \sum_{j=1}^{r} p_j(\boldsymbol{\theta}) \cdot p(\boldsymbol{\theta} \mid \mathbf{s}_o). \tag{9}$$

The whole procedure of the new inference algorithm, SMC-ABC+, is summarized in Algorithm 1.

Sequential Neural Likelihood (SNL) (Papamakarios et al., 2019). This recent algorithm learns the posterior in a parametric way, also in multiple rounds. The original SNL method approximates the likelihood function $p(\mathbf{x}|\boldsymbol{\theta})$ by a conditional neural density estimator $q(\mathbf{x}|\boldsymbol{\theta})$, which could be difficult to learn if the dimensionality of $\mathbf{x}$ is high. Here, we alleviate such difficulty with our neural statistic. The new SNL algorithm estimates the posterior $q_r(\boldsymbol{\theta}|\mathbf{s}_o)$ at the r-th round as follows. At round r, where we have nr simulated data $\mathcal{D} = \{\boldsymbol{\theta}_i, \mathbf{x}_i\}_{i=1}^{nr}$, we fit a neural density estimator $q(\mathbf{s}|\boldsymbol{\theta})$ as:

$$q(\mathbf{s} \mid \boldsymbol{\theta}) = \arg\max_{Q} \sum_{i=1}^{nr} \log Q(s(\mathbf{x}_i) \mid \boldsymbol{\theta}_i), \tag{10}$$

where $s(\cdot)$ is the current statistic network. With nr being moderately large, this would yield us $q(\mathbf{s}|\boldsymbol{\theta}) \approx p(\mathbf{s}|\boldsymbol{\theta})$. We then obtain the r-th estimate of the posterior by Bayes rule:

$$q_r(\boldsymbol{\theta} \mid \mathbf{s}^o) \propto \pi(\boldsymbol{\theta}) \cdot q(\mathbf{s}^o \mid \boldsymbol{\theta}). \tag{11}$$

The whole procedure of this new SNL algorithm, denoted as SNL+, is summarized in Algorithm 2.

4 RELATED WORKS

Approximate Bayesian computation. ABC denotes techniques for likelihood-free inference which work by repeatedly simulating data from the model and picking those data similar to the observed data to estimate the posterior (Sisson et al., 2018). Naive ABC performs simulation with the prior, whereas advanced variants like MCMC-ABC (Marjoram et al., 2003; Meeds et al., 2015) and SMC-ABC (Beaumont et al., 2009; Sisson et al., 2007) perform simulation with informed proposals. To measure the similarity to the observed data sensibly, it is often wise to use low-dimensional summary statistic rather than the raw data in ABC. Here we develop a way to learn compact sufficient statistic for ABC.

Neural density estimator-based inference. Apart from ABC, a recent line of research uses a conditional neural density estimator to (sequentially) learn the intractable likelihood (e.g SNL Papamakarios et al. (2019); Lueckmann et al. (2019)) or directly the posterior (e.g SNPE Papamakarios & Murray (2016); Lueckmann et al. (2017); Greenberg et al. (2019)). Likelihood-targeting approaches has the advantage that they could readily make use of any proposal distribution in sequential learning, but rely on low-dimensional, well-chosen summary statistic. Posterior-targeting methods on the contrary need no design of summary statistic, but they require non-trivial efforts to facilitate sequential learning. Our approach (e.g SNL+) could be seen as taking the advantages from both worlds.

Automatic construction of summary statistics. A set of works have been proposed to automatically construct low-dimensional summary statistics. Two lines of them are most related to our approach. The first line (Fearnhead & Prangle, 2012) and its variants (Jiang et al., 2017; Chan et al., 2018; Wiqvist et al., 2019; Dinev & Gutmann, 2018) train a neural network to predict the posterior mean and use this prediction as the summary statistic. These mean-as-statistic approaches, as analyzed previously in Proposition 2, indeed do not guarantee sufficiency. Rather than taking the predicted mean, the works (Alsing et al., 2018; Brehmer et al., 2020) take the score function $\nabla_{\boldsymbol{\theta}} \log p(\mathbf{x}|\boldsymbol{\theta})|_{\boldsymbol{\theta}=\boldsymbol{\theta}^*}$ around some fiducial parameter $\boldsymbol{\theta}^*$ as the summary statistic. However, these score-as-statistic approaches are only *locally* sufficient around $\boldsymbol{\theta}^*$, and it requires to first identify $\boldsymbol{\theta}^*$ which could itself be difficult. Our approach differs from all these methods as it is *globally* sufficient for all $\boldsymbol{\theta}$.

MI and ratio estimation. It has been shown in the literature that many variational MI estimators $I(X;Y)$ also estimate the ratio $p(X,Y)/p(X)p(Y)$ up to a constant (Nowozin et al., 2016; Nguyen et al., 2010). Therefore our MI-based statistic learning method is closely related to ratio estimation approaches like (Cranmer et al., 2015; Thomas et al., 2016; Hermans et al., 2019). The differences are 1) we estimate the ratio in the low-dimensional space rather than in the original space by a particular network architecture, based on a novel sufficient statistics perspective; 2) we decouple the task of statistic learning from the task of density estimation, which grants us the privilege to use any infomax representation learning methods even if they are ratio-free, e.g. Ozair et al. (2019); Wen et al. (2020).

5 EXPERIMENTS

5.1 SETUP

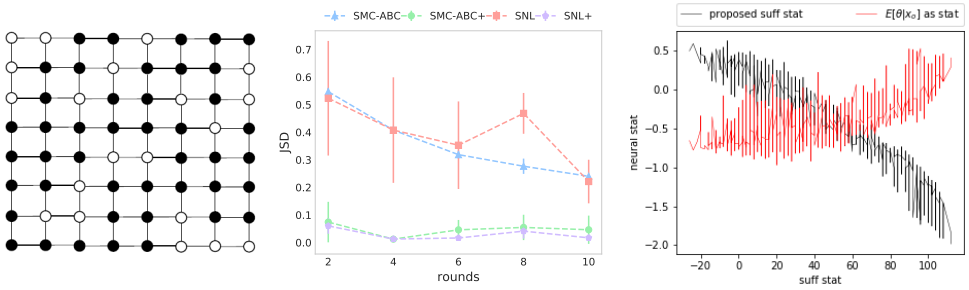
Baselines. We apply the proposed statistic to two aforementioned likelihood-free inference methods: (i) SMC-ABC (Beaumont et al., 2009) (the slightly modified version) and (ii) SNL (Papamakarios et al., 2019). We compare the performance of the algorithms augmented with our neural statistic (dubbed as SMC-ABC+ and SNL+) to their original versions as well as the versions based on expert-designed statistics (details presented later; we call the corresponding methods SMC-ABC' and SNL'). We also compare to the sequential neural posterior estimate (SNPE) method [1] which needs no statistic design, as well as the sequential ratio estimate (SRE) method (Hermans et al., 2019) which is closely related to our MI-based method[2]. All methods are run for 10 rounds with 1,000 simulations each.

Evaluation metric. To assess the quality of the estimated posterior, we compare the Jensen-Shannon divergence (JSD) between the approximate posterior Q and the true posterior P in each method:

$$\text{JSD}(P,Q) = \frac{1}{2}\text{KL}[P\|(Q+P)/2] + \frac{1}{2}\text{KL}[Q\|(Q+P)/2]$$

[1] More specifically, the version B. We select to compare with SNPE-B (Lueckmann et al., 2017) rather than the more recent SNPE-C (Greenberg et al., 2019) due to its similarity to SRE shown in (Durkan et al., 2020).

[2] For fair comparison, we control that the neural network in SRE has the similar number of parameters/same number of layers as in our method. See the Appendix for more details about the settings of the neural networks.



(a) (b) (c)

Figure 1: **Ising model**. (a) The 64D observed data $\mathbf{x}_o \in \{-1, 1\}^{64}$. (b) The JSD between the true and the learned posteriors. (c) The relationship between the learned statistics and the sufficient statistic.

SMC'	SMC+	SNL'	SNL+	SRE	SNPE
0.008 ± 0.006	0.046 ± 0.051	0.007 ± 0.002	0.017 ± 0.011	0.083 ± 0.029	0.058 ± 0.039

Table 1: **Ising model**. The JSD between the learned and true posterior with 10,000 simulations. Here SMC' and SNL' utilize the ground-truth sufficient statistics guided by human prior knowledge.

For the problems we consider in the experiments, the true posterior P is either analytically available, or could be accurately approximated by a standard rejection ABC algorithm (Pritchard et al., 1999) with known low-dimensional sufficient statistic (e.g $s(\mathbf{x}) \in \mathbb{Z}$) and extensive simulations (e.g 10^6).

5.2 Results

We demonstrate the effectiveness of our method in three cases: (a) an Ising model; (b) a Gaussian copula model; (c) an Ornstein-Uhlenbeck process. The Ising model does not have an analytical likelihood but the posterior can be approximated accurately by rejection ABC due to the existence of low-dimensional, discrete sufficient statistic. The last two models have analytical likelihoods and hence analytical posteriors. These models cover the cases of graph data, i.i.d data and sequence data.[3]

Ising model. The first model we consider is a mathematical model in statistical physics that describes the states of atomic spins on a 8×8 lattice (see Figure 1(a)). Each spin has two states described by a discrete random variable $x_i \in \{-1, +1\}$, and is only allowed to interact with its neighbour. Given parameters $\boldsymbol{\theta} = \{\theta_1, \theta_2\}$, the probability density function of the Ising model is:

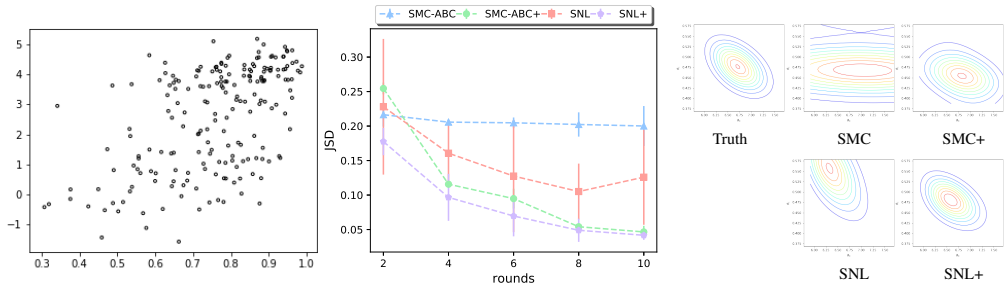
$$p(\mathbf{x}|\boldsymbol{\theta}) \propto e^{-H(\mathbf{x};\boldsymbol{\theta})},$$

$$H(\mathbf{x};\boldsymbol{\theta}) = -\theta_1 \sum_{\langle i,j \rangle} x_i x_j - \theta_2 \sum_i x_i.$$

where $\langle i, j \rangle$ denotes that spin i and spin j are neighbours. H is also called the Hamiltonian of the model. Here, the likelihood function of this model is not analytical due to the intractable normalizing constant $Z(\boldsymbol{\theta}) = \sum_{\mathbf{x} \in \{-1,1\}^{m \cdot m}} e^{-H(\mathbf{x};\boldsymbol{\theta})}$. However, sampling from the model by MCMC is possible. Note that the sufficient statistic is known for this model: $s^*(\mathbf{x}) = \{\sum_{\langle i,j \rangle} x_i x_j, \sum_i x_i\}$. The true posterior in this model can easily be approximated by a rejection ABC algorithm run with this low-dimensional sufficient statistic and extensive simulations. Here, we assume that θ_2 is known, and the task is to infer the posterior of θ_1 under an uniform prior $\theta_1 \sim \mathcal{U}(0, 1.5)$ (in this case the sufficient statistic becomes only 1D: $s^*(\mathbf{x}) = \sum_{\langle i,j \rangle} x_i x_j$). The true parameters are $\boldsymbol{\theta}^* = \{0.3, 0.1\}$.

In Figure 1(c), we investigate whether the proposed statistic could achieve sufficiency. Ideally, if the learned statistic s in our method does recover the true sufficient statistic s^* well, the relationship between s and s^* should be nearly monotonic (note that both s and s^* here are 1D). To verify this,

[3] We chose to conduct experiments on these models rather than common tasks like M/G/1 and Lotka-Volterra since they lack a known true likelihood, making it hard to verify the sufficiency of the proposed statistics.



(a) (b) (c)

Figure 2: **Gaussian copula**. (a) The observed data $\mathbf{x}_o$ in this problem, which is comprised of a population of 200 i.i.d samples. (b) The JSD between the true/learned posteriors. (c) The contours.

SMC'	SMC+	SNL'	SNL+	SRE	SNPE
0.183 ± 0.014	0.047 ± 0.009	0.054 ± 0.016	0.042 ± 0.006	0.052 ± 0.032	0.037 ± 0.018

Table 2: **Gaussian copula**. The JSD between the learned and true posterior with 10,000 simulations. Here SMC' and SNL' utilize the hand-crafted summary statistics guided by human prior knowledge.

we plot the relationship between s^* and s. We see from the figure that s learned in our method does increase monotonically with s^* approximately, suggesting that s recovers $\mathbf{s}^*$ reasonably well. As comparison, the statistic learned in the widely-used posterior-mean-as-statistic approach only has weak dependence on the true sufficient statistic; it is nearly indistinguishable for different s^*. In other words, it loses sufficiency. The result also verifies our previous theoretical result in Proposition 2.

Figure 1(b) further shows the JSD between the true and learned posterior for different methods across the rounds (the vertical lines indicates standard errors, each JSD is obtained by calculating the average of 3 independent runs. The results shown in the below experiments have the same setup). It can be seen from the figure that for this model, likelihood-free inference methods augmented with the proposed statistic (SMC-ABC+, SNL+) outperform their original counterparts (SMC-ABC, SNL) by a large margin. In Table 1, we further compare our statistic with the expert designed statistic, from which one can see their close performance (here the expert statistic is taken as the true sufficient statistic $\mathbf{s}^*$). We also see that our method also seems to outperform SRE which directly estimates the ratio $t(\mathbf{x}, \boldsymbol{\theta}) = p(\mathbf{x}, \boldsymbol{\theta})/p(\mathbf{x})p(\boldsymbol{\theta}) \propto L(\boldsymbol{\theta}; \mathbf{x})$ in high-dimensional space (note that the true likelihood is actually of the form $L(\boldsymbol{\theta}; \mathbf{x}) = \exp(\boldsymbol{\theta} s^*(\mathbf{x}))/Z(\boldsymbol{\theta})$) as well as SNPE (version B). The reason why SNPE(-B) does not perform more satisfactorily might be due to the fact that it relies on importance weights to facilitate sequential learning, which induces high variance that makes its training unstable.

Gaussian copula. The second model we consider is a 2D Gaussian copula model (Chen & Gutmann, 2019). Data $\mathbf{x}$ in this model can be seen as generated from the latent variable $\mathbf{z}$ as follows:

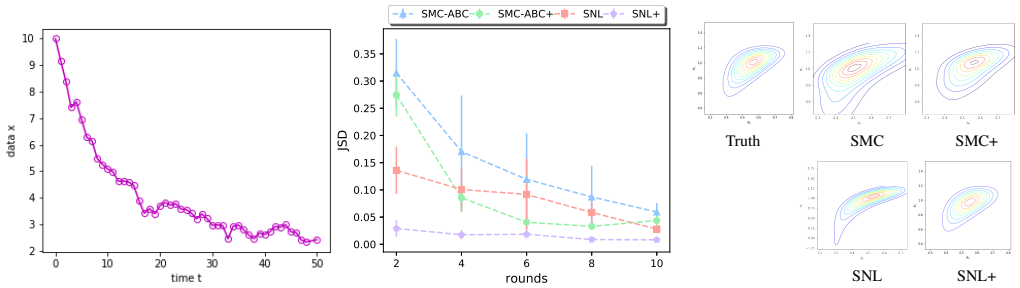
$$\mathbf{z} \sim \mathcal{N}\Big(\mathbf{z}; \mathbf{0}, \begin{bmatrix} 1, & \theta_3 \\ \theta_3, & 1 \end{bmatrix}\Big),$$

$$x_1 = F_1^{-1}(\Phi(z_1); \theta_1), \quad x_2 = F_2^{-1}(\Phi(z_2); \theta_2),$$

$$f_1(x_1; \theta_1) = \text{Beta}(x_1; \theta_1, 2), \quad f_2(x_2; \theta_2) = \theta_2 \mathcal{N}(x_2; 1, 1) + (1 - \theta_2)\mathcal{N}(x_2; 4, 1/4).$$

where $\Phi(\cdot)$, $F_1(x_1; \theta_1)$, $F_2(x_2; \theta_2)$ are the cumulative distribution function (CDF) of standard normal distribution, the CDF of $f_1(x_1; \theta_1)$ and the CDF of $f_2(x_2; \theta_2)$ respectively. We assume that a total number of 200 samples are i.i.d drawn from this model, yielding a population $\mathbf{X} = \{\mathbf{x}_i\}_{i=1}^{200}$ that serves as our observed data. Note that the likelihood of this model can be computed analytically by the law of variable transformation. To perform inference, we compute a rudimentary statistic to describe $\mathbf{X}$, namely (a) the 20-equally spaced quantiles of the marginal distributions of $\mathbf{X}$ and (b) the correlation between the latent variables z_1, z_2 in $\mathbf{X}$, resulting in a statistic of dimensionality 41. An uniform prior is set: $\theta_1 \sim \mathcal{U}(0.5, 12.5), \theta_2 \sim \mathcal{U}(0, 1), \theta_3 \sim \mathcal{U}(0.4, 0.8)$ and $\boldsymbol{\theta}^* = \{6, 0.5, 0.6\}$.

In Figure 2(b), we demonstrate the power of our neural sufficient statistic learning method on the Gaussian copula problem. Overall, we see that the proposed method improves the accuracy of



(a) (b) (c)

Figure 3: **OU process**. (a) The observed time-series data $\mathbf{x}_o = \{x_t\}_{t=1}^{50}$. (b) The JSD between the true and the learned posteriors. (c) The contours of the true posterior and the learned posteriors.

SMC'	SMC+	SNL'	SNL+	SRE	SNPE
0.040 ± 0.006	0.044 ± 0.018	0.004 ± 0.001	0.009 ± 0.002	0.022 ± 0.013	0.019 ± 0.009

Table 3: **OU process**. The JSD between the learned and the true posterior with 10,000 simulations. Here SMC' and SNL' utilize the hand-crafted summary statistics guided by human prior knowledge.

existing likelihood-free inference methods, as well as their robustness (see e.g the reduced variability in SNL+. The high variability in SNL may be due to the lack of training data required to learn the 41-dimensional likelihood function well). This is also confirmed by the contours plots in Figure 2(c). In Table 2 we further compare the proposed statistic with the expert-designed low-dimension statistic (here the expert statistic is taken to be the 5-equally spaced marginal quantiles + the correlations between z_1, z_2), from which we see that our proposed statistic achieves a better performance. For this model, our method seems to perform slightly worse than SNPE (possibly due to the imperfect infomax learning on this problem), but the gap there is indeed very small (≤ 0.005 JSD). We conjecture that more reliable infomax learning methods might help to resolve this issue.

Ornstein-Uhlenbeck process. The last model we consider is a discretized stochastic differential equation (SDE). Data $\mathbf{x} = \{x_t\}_{t=1}^{D}$ in this model is sequentially generated as:

$$x_{t+1} = x_t + \Delta x_t,$$
$$\Delta x_t = \theta_1(\exp(\theta_2) - x_t)\Delta t + 0.5\epsilon, \quad \epsilon \sim \mathcal{N}(\epsilon; 0, \Delta t).$$

where $D = 50$, $\Delta t = 0.2$ and $x_0 = 10$. This model is Markovian, and has an analytical likelihood. It has a wide applications in financial mathematics and physical sciences. Here, the parameters of interest are $\boldsymbol{\theta} = \{\theta_1, \theta_2\}$, and a uniform prior is placed on these parameters: $\theta_1 \sim \mathcal{U}(0, 1), \theta_1 \sim \mathcal{U}(-2.0, 2.0)$. The true parameters are set to be $\boldsymbol{\theta}^* = \{0.5, 1.0\}$.

Figure 3(b) compares the JSD of each method against the simulation cost. Again, we find that the proposed neural sufficient statistics greatly improves the performance of both SMC-ABC and SNL. In Table 3, we compare our statistics to expert statistic (here the expert statistics are taken as the mean, standard error and autocorrelation with lag 1, 2, 3 of the time series). It can be seen that our statistics are comparable to the expert statistics. Our method also seems to outperform SRE and SNPE.

6 Conclusion

We propose a new deep learning-based approach for automatically constructing low-dimensional sufficient statistics in likelihood-free inference. The obtained neural approximate sufficient statistics can be applied to both traditional ABC-based and recent NDE-based methods. The main hypothesis of the approach is that learning such sufficient statistic via the infomax principle might be easier than estimating the density itself. We verify this hypothesis by experiments on various tasks with graphs, i.i.d and sequence data. Our method establishes a link between representation learning and likelihood-free inference communities. For future works, we can consider other infomax representation learning approaches, as well as ways to automatically determine the dimensionality of the sufficient statistics.

REFERENCES

Justin Alsing, Benjamin Wandelt, and Stephen Feeney. Massive optimal data compression and density estimation for scalable, likelihood-free inference in cosmology. *Monthly Notices of the Royal Astronomical Society*, 477(3):2874–2885, 2018.

Ravi Bansal and Amir Yaron. Risks for the long run: A potential resolution of asset pricing puzzles. *The journal of Finance*, 59(4):1481–1509, 2004.

Mark A Beaumont, Jean-Marie Cornuet, Jean-Michel Marin, and Christian P Robert. Adaptive approximate Bayesian computation. *Biometrika*, 96(4):983–990, 2009.

Mohamed Ishmael Belghazi, Aristide Baratin, Sai Rajeswar, Sherjil Ozair, Yoshua Bengio, Aaron Courville, and R Devon Hjelm. Mine: mutual information neural estimation. *arXiv preprint arXiv:1801.04062*, 2018.

Michael GB Blum, Maria Antonieta Nunes, Dennis Prangle, Scott A Sisson, et al. A comparative review of dimension reduction methods in approximate bayesian computation. *Statistical Science*, 28(2):189–208, 2013.

Johann Brehmer, Gilles Louppe, Juan Pavez, and Kyle Cranmer. Mining gold from implicit models to improve likelihood-free inference. *Proceedings of the National Academy of Sciences*, 117(10): 5242–5249, 2020.

Jeffrey Chan, Valerio Perrone, Jeffrey Spence, Paul Jenkins, Sara Mathieson, and Yun Song. A likelihood-free inference framework for population genetic data using exchangeable neural networks. In *Advances in Neural Information Processing Systems*, pp. 8594–8605, 2018.

Yanzhi Chen and Michael U Gutmann. Adaptive gaussian copula abc, 2019.

Matteo Chinazzi, Jessica T Davis, Marco Ajelli, Corrado Gioannini, Maria Litvinova, Stefano Merler, Ana Pastore y Piontti, Kunpeng Mu, Luca Rossi, Kaiyuan Sun, et al. The effect of travel restrictions on the spread of the 2019 novel coronavirus (covid-19) outbreak. *Science*, 368(6489):395–400, 2020.

Tm Cover, Ja Thomas, and J Wiley. *Elements of information theory.* Tsinghua University Pres, 2003.

Kyle Cranmer, Juan Pavez, and Gilles Louppe. Approximating likelihood ratios with calibrated discriminative classifiers. *arXiv preprint arXiv:1506.02169*, 2015.

Peter J Diggle and Richard J Gratton. Monte Carlo methods of inference for implicit statistical models. *Journal of the Royal Statistical Society. Series B*, pp. 193–227, 1984.

Traiko Dinev and Michael U Gutmann. Dynamic likelihood-free inference via ratio estimation (dire). *arXiv preprint arXiv:1810.09899*, 2018.

Christopher C Drovandi, Anthony N Pettitt, and Malcolm J Faddy. Approximate Bayesian computation using indirect inference. *Journal of the Royal Statistical Society: Series C (Applied Statistics)*, 60(3):317–337, 2011.

Conor Durkan, Iain Murray, and George Papamakarios. On contrastive learning for likelihood-free inference. *arXiv preprint arXiv:2002.03712*, 2020.

Paul Fearnhead and Dennis Prangle. Constructing summary statistics for approximate Bayesian computation: semi-automatic approximate Bayesian computation. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 74(3):419–474, 2012.

Felix A Gers, Jürgen Schmidhuber, and Fred Cummins. Learning to forget: Continual prediction with lstm. 1999.

David Greenberg, Marcel Nonnenmacher, and Jakob Macke. Automatic posterior transformation for likelihood-free inference. In *International Conference on Machine Learning*, pp. 2404–2414, 2019.

Arthur Gretton, Karsten M Borgwardt, Malte J Rasch, Bernhard Schölkopf, and Alexander Smola. A kernel two-sample test. *The Journal of Machine Learning Research*, 13(1):723–773, 2012.

Joeri Hermans, Volodimir Begy, and Gilles Louppe. Likelihood-free mcmc with amortized approximate ratio estimators. *arXiv preprint arXiv:1903.04057*, 2019.

R Devon Hjelm, Alex Fedorov, Samuel Lavoie-Marchildon, Karan Grewal, Phil Bachman, Adam Trischler, and Yoshua Bengio. Learning deep representations by mutual information estimation and maximization. *arXiv preprint arXiv:1808.06670*, 2018.

M. Järvenpää, M.U. Gutmann, A. Vehtari, and P. Marttinen. Gaussian process modeling in approximate Bayesian computation to estimate horizontal gene transfer in bacteria. *Annals of Applied Statistics*, 2018.

Bai Jiang, Tung-yu Wu, Charles Zheng, and Wing H Wong. Learning summary statistic for approximate bayesian computation via deep neural network. *Statistica Sinica*, pp. 1595–1618, 2017.

Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*, 2014.

J. Lintusaari, M.U. Gutmann, R. Dutta, S. Kaski, and J. Corander. Fundamentals and recent developments in approximate Bayesian computation. *Systematic Biology*, 66(1):e66–e82, January 2017.

Jan-Matthis Lueckmann, Pedro J Goncalves, Giacomo Bassetto, Kaan Öcal, Marcel Nonnenmacher, and Jakob H Macke. Flexible statistical inference for mechanistic models of neural dynamics. In *Advances in Neural Information Processing Systems*, pp. 1289–1299, 2017.

Jan-Matthis Lueckmann, Giacomo Bassetto, Theofanis Karaletsos, and Jakob H Macke. Likelihood-free inference with emulator networks. In *Symposium on Advances in Approximate Bayesian Inference*, pp. 32–53, 2019.

Vikash K Mansinghka, Tejas D Kulkarni, Yura N Perov, and Josh Tenenbaum. Approximate bayesian image interpretation using generative probabilistic graphics programs. In *Advances in Neural Information Processing Systems*, pp. 1520–1528, 2013.

Paul Marjoram, John Molitor, Vincent Plagnol, and Simon Tavaré. Markov chain Monte Carlo without likelihoods. *Proceedings of the National Academy of Sciences*, 100(26):15324–15328, 2003.

Edward Meeds, Robert Leenders, and Max Welling. Hamiltonian abc. In *Proceedings of the Thirty-First Conference on Uncertainty in Artificial Intelligence*, pp. 582–591, 2015.

XuanLong Nguyen, Martin J. Wainwright, and Michael I. Jordan. Estimating divergence functionals and the likelihood ratio by convex risk minimization. *IEEE Transactions on Information Theory*, 56(11):5847–5861, Nov 2010. ISSN 1557-9654. doi: 10.1109/tit.2010.2068870. URL `http://dx.doi.org/10.1109/TIT.2010.2068870`.

Sebastian Nowozin, Botond Cseke, and Ryota Tomioka. f-gan: Training generative neural samplers using variational divergence minimization. In *Advances in neural information processing systems*, pp. 271–279, 2016.

Aaron Van Den Oord, Nal Kalchbrenner, and Koray Kavukcuoglu. Pixel recurrent neural networks. 2016.

Aaron van den Oord, Yazhe Li, Igor Babuschkin, Karen Simonyan, Oriol Vinyals, Koray Kavukcuoglu, George van den Driessche, Edward Lockhart, Luis C Cobo, Florian Stimberg, et al. Parallel wavenet: Fast high-fidelity speech synthesis. *arXiv preprint arXiv:1711.10433*, 2017.

Sherjil Ozair, Corey Lynch, Yoshua Bengio, Aaron Van den Oord, Sergey Levine, and Pierre Sermanet. Wasserstein dependency measure for representation learning. In *Advances in Neural Information Processing Systems*, pp. 15604–15614, 2019.

George Papamakarios and Iain Murray. Fast ε-free inference of simulation models with bayesian conditional density estimation. In *Advances in Neural Information Processing Systems*, pp. 1028–1036, 2016.

George Papamakarios, Theo Pavlakou, and Iain Murray. Masked autoregressive flow for density estimation. In *Advances in Neural Information Processing Systems*, pp. 2338–2347, 2017.

George Papamakarios, David Sterratt, and Iain Murray. Sequential neural likelihood: Fast likelihood-free inference with autoregressive flows. In *AISTATS*, pp. 837–848, 2019.

Jonathan K Pritchard, Mark T Seielstad, Anna Perez-Lezaun, and Marcus W Feldman. Population growth of human y chromosomes: a study of y chromosome microsatellites. *Molecular biology and evolution*, 16(12):1791–1798, 1999.

Oren Rippel and Ryan Prescott Adams. High-dimensional probability estimation with deep density models, 2013.

Ohad Shamir, Sivan Sabato, and Naftali Tishby. Learning and generalization with the information bottleneck. 2008.

S.A. Sisson, Y Fan, and M.A. Beaumont. *Handbook of Approximate Bayesian Computation.*, chapter Overview of Approximate Bayesian Computation. Chapman and Hall/CRC Press, 2018.

Scott A Sisson, Yanan Fan, and Mark M Tanaka. Sequential Monte Carlo without likelihoods. *Proceedings of the National Academy of Sciences*, 104(6):1760–1765, 2007.

Torbjörn Sjöstrand, Stephen Mrenna, and Peter Skands. A brief introduction to pythia 8.1. *Computer Physics Communications*, 178(11):852–867, 2008.

Carlos Oscar Sánchez Sorzano, Javier Vargas, and A Pascual Montano. A survey of dimensionality reduction techniques. *arXiv preprint arXiv:1403.2877*, 2014.

Owen Thomas, Ritabrata Dutta, Jukka Corander, Samuel Kaski, and Michael U Gutmann. Likelihood-free inference by ratio estimation. *arXiv preprint arXiv:1611.10242*, 2016.

Liangjian Wen, Yiji Zhou, Lirong He, Mingyuan Zhou, and Zenglin Xu. Mutual information gradient estimation for representation learning. *arXiv preprint arXiv:2005.01123*, 2020.

Anja Weyant, Chad Schafer, and W Michael Wood-Vasey. Likelihood-free cosmological inference with type ia supernovae: approximate Bayesian computation for a complete treatment of uncertainty. *The Astrophysical Journal*, 764(2), 2013.

Samuel Wiqvist, Pierre-Alexandre Mattei, Umberto Picchini, and Jes Frellsen. Partially exchangeable networks and architectures for learning summary statistics in approximate bayesian computation. In *International Conference on Machine Learning*, pp. 6798–6807, 2019.

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

Haozhe Xie, Jie Li, and Hanqing Xue. A survey of dimensionality reduction techniques based on random projection. *arXiv preprint arXiv:1706.04371*, 2017.

A THEORETICAL PROOFS

A.1 PROOF OF PROPOSITION 1

Proof. Firstly, assume $s(\cdot)$ is a sufficient statistic. By the definition of sufficient statistic we know $p(\mathbf{x}|\boldsymbol{\theta}) = p(\mathbf{x}|\mathbf{s})p(\mathbf{s}|\boldsymbol{\theta})$. Then we have the Markov chain $\boldsymbol{\theta} \to \mathbf{s} \to X$ for the data generating process. On the other hand, since $\mathbf{x} \sim p(\mathbf{x}|\boldsymbol{\theta})$ and S is a deterministic function we have the Markov chain $\boldsymbol{\theta} \to X \to S$. By data processing inequality we have $I(\boldsymbol{\theta}; s(X)) \leq I(\boldsymbol{\theta}; X)$ for the first chain and $I(\boldsymbol{\theta}; X) \leq I(\boldsymbol{\theta}; s(X))$ for the second chain. This implies that $I(\boldsymbol{\theta}; X) = I(\boldsymbol{\theta}; s(X))$ i.e s is the maximizer of $I(\boldsymbol{\theta}; S(X))$. For the other direction, since $I(\boldsymbol{\theta}; s(X)) = \max_{S:\mathcal{X}\to\mathcal{S}} \; I(\boldsymbol{\theta}; S(X))$, we have $I(\boldsymbol{\theta}; s(X)) = I(\boldsymbol{\theta}; X)$. Note that $\boldsymbol{\theta} \to X \to s$ is a Markov chain, from Theorem 2.8.1 of Cover et al. (2003) we can get $\boldsymbol{\theta}$ and $\mathcal{X}$ is conditionally independent given s. This results in that s is sufficient. □

A.2 PROOF OF PROPOSITION 2

Proof. We can rewrite the above objective as $\mathbb{E}_{p(\boldsymbol{\theta},\mathbf{x})}[\|S(\mathbf{x}) - \boldsymbol{\theta}\|_2^2] = \int p(\boldsymbol{\theta}, \mathbf{x}) \log e^{\|S(\mathbf{x})-\boldsymbol{\theta}\|_2^2} d\mathbf{x} d\boldsymbol{\theta}$. On the other hand we have $I(\boldsymbol{\theta}, S(\mathbf{x})) = \int p(\boldsymbol{\theta}, \mathbf{x}) \log p(S(\mathbf{x})|\boldsymbol{\theta})/p(S(\mathbf{x})) d\mathbf{x} d\boldsymbol{\theta}$. By comparing them it is easy to see that they are generally not equivalent except for very rare case (e.g Gaussian). □

B MORE EXPERIMENTAL DETAILS AND RESULTS

B.1 DETAILED EXPERIMENTAL SETTINGS

Neural networks settings. For the statistic network S in our method, we adopt a D-100-100-d fully-connected architecture with D being the dimensionality of input data and d the dimensionality of the statistic. For the network H used to extract the representation of $\boldsymbol{\theta}$, we adopt a D-100-100-K fully-connected architecture with K being the dimensionality of the model parameter. For the critic network, we adopt a $(d + K)$-100-1 fully connected architecture with K being the dimensionality of $\boldsymbol{\theta}$. ReLU is adopted as the non-linearity in all networks. For SRE, which is closely related to our method, we use a $(D + K)$-144-144-100-1 architecture. This architecture has a similar complexity as our networks. All these neural networks are trained with Adam (Kingma & Ba, 2014) with a learning rate of 1×10^{-3} and a batch size of 100. No weight decay is applied.

For the neural density estimator in SNL/SNPE, which is realized by a Masked Autoregressive Flow (MAF) (Papamakarios et al., 2017), we adopt 5 autoregressive layers, each of which has two hidden layers with 50 tanh units. This is the same settings as in SNL. The MAF are trained with Adam with a learning rate of 5×10^{-4} and a batch size of 500 and a slight weight decay ($1e^{-5}$).

For all networks, we take 20% of the data for validation, and stop training if the validation error does not improve after 100 epochs. We take the snapshot with the best validation error as the result.

Sampling from the approximate posterior. For fair comparison, we adopt simple rejection sampling for all LFI methods (ABC, SNL, SNPE, SRE) when sampling from the learnt posterior, so that each LFI algorithm only differs in the way they learn the posterior.

Dimensionality of the learned statistic. For the JSD/contour plots presented in the experiment part in the main text, we use $d = \lfloor D/5 \rfloor, \lfloor D/5 \rfloor, \lfloor D/10 \rfloor$ for the Ising model problem, Gaussian copula problem and OP process problem respectively (remark that D is the dimensionality of the raw data).

Training of statistic network. Remark that the statistic network $S(\cdot)$ is trained with the following objective together with the scoring network $T(\cdot)$:

$$\text{maximize}_{S,T} \;\; \mathcal{L}(S,T) = \mathbb{E}_{p(\boldsymbol{\theta},\mathbf{x})}\left[-\operatorname{sp}\left(-T(\boldsymbol{\theta}; S(\mathbf{x}))\right)\right] - \mathbb{E}_{p(\boldsymbol{\theta})p(\mathbf{x})}\left[\operatorname{sp}\left(T(\boldsymbol{\theta}; S(\mathbf{x}))\right)\right]$$

the mini-batch approximation to this objective is:

$$\mathcal{L}(S,T) \approx \frac{1}{n}\sum_{i}^{n}\left[-\operatorname{sp}\left(-T(\boldsymbol{\theta}_i; S(\mathbf{x}_i))\right)\right] - \frac{1}{m}\frac{1}{n}\sum_{j}^{m}\sum_{i}^{n}\left[\operatorname{sp}\left(T(\boldsymbol{\theta}_{j_i}; S(\mathbf{x}_i))\right)\right]$$

where $\{j_1, j_2, ..., j_n\}$ is the j-th random permutation of the indexes $\{1, 2, ..., n\}$ and the pair $(\boldsymbol{\theta}_i, \mathbf{x}_i)$ are randomly picked from the data $\mathcal{D} = \{\boldsymbol{\theta}_i, \mathbf{x}_i\}_{i=1}^N$. Here we simply set $m = 200$ and $n = 100$.

JSD calculation between true posterior and approximate posterior. The calculation of the Jensen-Shannon divergence between true posterior P and approximate posterior Q namely $\text{JSD}(P,Q) = \frac{1}{2}\text{KL}[P\|(P+Q)/2] + \frac{1}{2}\text{KL}[Q\|(P+Q)/2]$ is done numerically by a Riemann sum over 30^K equally spaced grid points with K being the dimensionality of $\boldsymbol{\theta}$. The region of these grid points is jointly defined by the min and max values of 500 samples drawn from P and Q. When we are only equipped with samples of the true posterior (e.g the Ising model problem), we estimate P by KDE (remark that for the Ising model the posterior is 1D).

B.2 Additional experimental results

Comparison of different MI estimators

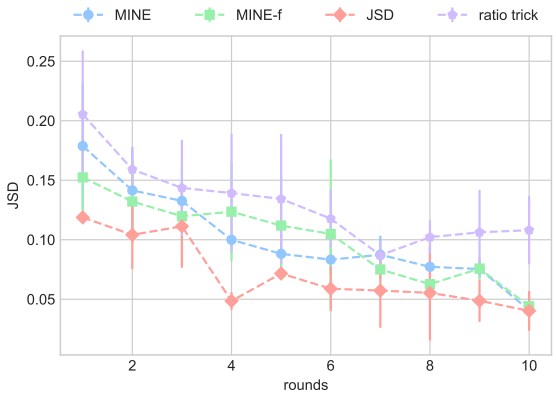


Figure 4: Comparison for different mutual information estimators.

We conduct empirical study on a 10-round Gaussian copula task with four different mutual information estimators: MINE (Belghazi et al., 2018), MINE-f (Belghazi et al., 2018), Jensen-Shannon divergence (JSD) estimators (Hjelm et al., 2018), and classical ratio trick method (Hermans et al., 2019; Thomas et al., 2016). The results are averaged over 3 independent runs. We use the JSD between the true posterior and approximate posterior as in the main text as the metric. From Figure 4 we see the JSD estimator achieves the best performance, and as such we adopt it as the MI estimator in our method.

Results under MMD metric. For reference, we also conduct experiments with MMD (Gretton et al., 2012) discrepancy on Gaussian copula and OU process with different reruns as a reference. Our proposed methods achieve consistent performance under JSD metric (we remind the reader here that the result by JSD should be more reliable since it directly compares two analytical densities). The results are averaged over 3 independent runs.

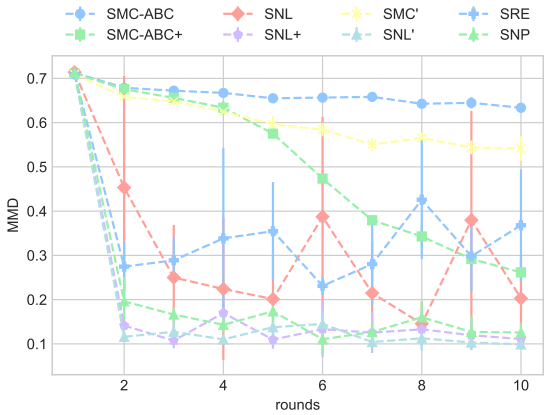


Figure 5: results on GC model.

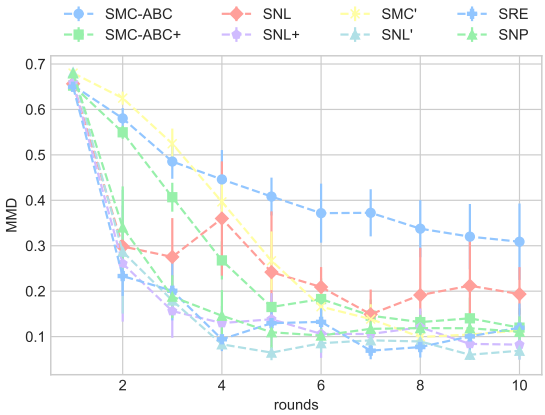


Figure 6: results on OU process.

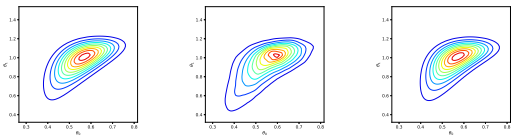
On directly extracting the posterior from the MI network. As mentioned in the main text, it has been shown that the optimal critic $t(\boldsymbol{\theta}, \mathbf{s})$ in f-divergence-based MI estimator $I(\boldsymbol{\theta}, \mathbf{s})$ indeed corresponds to the density ratio up to a constant: $p(\boldsymbol{\theta}, \mathbf{s})/p(\boldsymbol{\theta})p(\mathbf{s})$. In JSD-based MI estimator, which we used to learn the sufficient statistics, we can extract the ratio as

$$p(\boldsymbol{\theta}, \mathbf{s})/p(\boldsymbol{\theta})p(\mathbf{s}) = e^{t(\boldsymbol{\theta}, \mathbf{s})}$$

with which we can recover the (sufficient statistics-based) posterior estimate as:

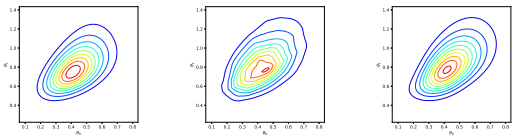
$$\pi(\boldsymbol{\theta}|\mathbf{s}_o) \propto \pi(\boldsymbol{\theta})L(\boldsymbol{\theta}; \mathbf{s}_o) \propto \pi(\boldsymbol{\theta})e^{t(\boldsymbol{\theta}, \mathbf{s}_o)}, \quad \forall \mathbf{s}_o$$

So one might wonder how the posterior estimated in this strategy is compared to the strategy mentioned in the main text (namely re-fitting a neural density estimator $q(\mathbf{s}|\boldsymbol{\theta})$ on $\mathbf{s}$). The figures below show the results.



truth extract from T NDE refit

Figure 7: OU process.



truth extract from T NDE refit

Figure 8: Wrapped Gaussian.

We discover that the posteriors returned by NDE refit seem to be more accurate than the one directly extracted from the critic T. Here, the JSD in the two problems are (0.000, 0.014, 0.004) and (0.000, 0.010, 0.004) respectively (the OU process is the same as in the main text. The wrapped Gaussian model is one where the data is generated as $\mathbf{x} \sim \mathcal{N}(\mathbf{x}, \tanh(\boldsymbol{\theta}), \mathbf{I})$. All results are obtained with 10,000 simulations). More specifically, we discover that the NDE posteriors tends to be smoother and hence closer to a realistic pdf. We conjecture that this might due to two reasons:

- In NDE refit, the density is guaranteed to be a valid pdf during the learning procedure. This might be a good inductive bias that helps to learn the density better. The density extracted from the ratio on the contrary is not guaranteed to be a valid one, so it is less realistic;
- It is also possible that even if the whole statistics + critic networks does not estimate the density perfectly, the statistics network itself might still do a good job in learning the sufficient statistics. This opinion was also appreciated in previous works (see e.g Cranmer et al. (2015)).

Nonetheless we feel more exploration is required to draw a conclusion. We leave it to future work.

Contrastive learning v.s. MLE. In the experiment in the main text, we discover that our method does not always achieve the best performance: SNPE-B performs better on the Gaussian copula problem than our method. Here we would like to investigate why this happens.

Upon a closer look, we discover that SRE, which is closely related to our method, is also outperformed by SNPE-B on the Gaussian copula problem. Remark that both SRE and our method uses contrastive learning rather than MLE. Since both of these two contrastive learning methods are outperformed by the MLE-based SNPE-B, it makes us suspect the reason is due to imperfect contrastive learning. To verify this, we further conduct experiments for SNPE-C, which shares the same loss function with SRE but with a different parameterization to the density ratio (SRE: fully-connected network; SNPE-C: NDE-based parameterization. This NDE is the same as in SNL). The result is as follows:

Ising model				Gaussian copula				OU process			
SRE	SNPE-B	SNPE-C	SNL+	SRE	SNPE-B	SNPE-C	SNL+	SRE	SNPE-B	SNPE-C	SNL+
0.083	0.058	0.030	0.017	0.052	0.037	0.047	0.042	0.022	0.018	0.016	0.009

Table 4: Commparing the the JSD of contrastive learning-based methods (SRE, SNPE-C, SNL+) and MLE-based method (SNPE-B) on the three models considered in the experiments in the main text.

Surprisingly, we find that like SRE and SNL+, SNPE-C also perform less satisfactorily than SNPE-B on the Gaussian copula problem. This suggests that contrastive learning might be less preferable than MLE on this problem, which might also explain the less satisfactory performance of our method.