
A DENSITY RATIO FRAMEWORK FOR EVALUATING THE UTILITY OF SYNTHETIC DATA

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ABSTRACT

Synthetic data generation is a promising technique to facilitate the use of sensitive data while mitigating the risk of privacy breaches. However, for synthetic data to be useful in downstream analysis tasks, it needs to be of sufficient quality. Various methods have been proposed to measure the utility of synthetic data, but their results are often incomplete or even misleading. In this paper, we propose to use the density ratio estimation framework to improve quality evaluation for synthetic data, and thereby improve the quality of synthesized datasets. We show how this framework relates to and builds on existing measures, yielding global and local utility measures that are informative and easy to interpret. The proposed methodology employs automatic, non-parametric model selection for the density ratio, and thus requires little to no manual model specification. Through simulations, we find that density ratio estimation yields more accurate estimates of global utility than established procedures. A real-world data application demonstrates how the density ratio can guide refinements of synthesis models and can be used to improve downstream analyses. We conclude that density ratio estimation is a valuable tool in synthetic data generation workflows and make the methodology available through the open source R-package `densityratio`.

Keywords synthetic data, utility, density ratio, privacy, disclosure limitation • synthetic data, utility, density ratio, privacy, disclosure limitation

1 Introduction

Openly accessible research data accelerates scientific progress tremendously. Open data allows third-party researchers to answer research questions with already collected data, freeing up resources that would otherwise be devoted to data collection ([Ramachandran, Bugbee, and Murphy 2021](#)). Sharing data in combination with code allows others to validate research findings and build upon the work ([Obels et al. 2020](#); [Crosas et al. 2015](#)). Students can benefit from open data, as it fosters education with realistic data ([Atenas, Havemann, and Priego 2015](#)), as well as the general public, through stimulating citizen science projects ([Newman et al. 2012](#)). However, making data openly available is often (rightfully) hampered by official legislation, like the General Data Protection Regulation (GDPR; [European Parliament and Council of the European Union 2016](#)), and general privacy concerns. In the worst case, sharing data may cause harm to individuals or organizations, which may withhold these entities from participating in future research. These privacy constraints have been named among the biggest hurdles in the advancement of computational social science ([Lazer et al. 2009](#)), and among top reasons for companies to not share their data with researchers ([Future of Privacy Forum 2017](#)).

Multiple approaches exist to balance the benefits of open data with potential privacy risks. Traditionally, data providers employed a suite of different disclosure limitation techniques before sharing the data, such as top-coding, record-swapping or adding noise (e.g., [Hundepool et al. 2012](#); [Willenborg and De Waal 2001](#)). More recently, synthetic data has gained traction as a means to disseminate private data ([Abowd, Stinson, and Benedetto 2006](#); [Hawala 2008](#); [Drechsler 2012](#); [van de Wiel et al. 2023](#); [Obermeyer et al. 2019](#); [Zettler et al. 2021](#)), although the conceptual framework traces back to the previous century ([Little 1993](#); [Rubin 1993](#)). Simply put, the idea of synthetic data is to replace some, or all, of the observed values in a data set by synthetic values that are generated from some model (e.g., [Drechsler 2011](#)). If only some values are replaced, disclosure risks can be reduced because the sensitive or identifying values do not correspond to their true values anymore. If all values are replaced, there is also no one-to-one mapping between the original and the synthetic data, further reducing the disclosure risk. However, an increase in privacy typically comes at the cost of a decrease in utility. As more of the data is altered, the quality of the released data becomes more sensitive to the suitability of the generative model. Regardless of the approach to disclosure limitation, if the technique used to generate or alter the data does not align with the intricacies of the problem at hand, the utility of the released data will be further reduced than necessary.

Given that all disclosure limitation techniques reduce the utility of the data, the challenge that arises is how to determine whether the released data still has acceptable utility. Alternatively, one might consider different disclosure limitation techniques that all satisfy the defined privacy restrictions, and employ the one which yields data with the highest utility. That is, given a set of methods that all meet the privacy restrictions, one may aim to maximize the utility of the released data. Both strategies require a reliable and encompassing measure of data utility that allows to evaluate the quality of the released data, and that allows to compare different disclosure limitation techniques and/or synthesis models in terms of utility. Moreover, adequate utility measures often guide the synthesis process, by providing detailed feedback

on important discrepancies between the original and synthetic data. Lastly, good utility measures help the data user in determining what the synthetic data can and cannot be used for.

In the synthetic data field, three classes of utility measures have been distinguished (see [Drechsler and Haensch 2023](#) for a thorough review): fit-for-purpose measures, analysis-specific utility measures and global utility measures. Fit-for-purpose measures are often the first step in assessing the quality of the synthetic data. These typically involve comparing the univariate distributions of the observed and synthetic data (for example using visualization techniques or goodness-of-fit measures). Although these measures provide an initial impression of the quality of the synthesis models used, this picture is by definition limited, because only one or two variables are assessed at the same time. Hence, complex relationships between variables will always be out of scope. Such relationships may be captured by analysis-specific utility measures, which quantify whether analyses on synthetic data provide results that are comparable to results from the same analysis performed on the observed data. These measures can, for example, evaluate how similar the coefficients of a regression model are (e.g., using the confidence interval overlap; [Karr et al. 2006](#)), or whether prediction models trained on the synthetic and observed data perform comparably in terms of evaluation metrics. However, analysis-specific utility generally does not carry over: high specific utility for one analysis does not at all imply high utility for another analysis. Since data providers typically do not know which analyses will be performed with the synthetic data, it is impossible to provide analysis-specific utility measures for all potentially relevant analyses (see also [Drechsler 2022](#)).

Global utility measures may overcome the shortcomings of the previous approaches, as they evaluate the discrepancy between the entire multivariate distribution of the observed and synthetic data. As such, global utility measures yields the most promising class of utility measures, because if the observed and synthetic data have similar (multivariate) distributions, all potential analyses should yield similar results. Global utility can be evaluated using some divergence measure, such as the Kullback-Leibler divergence ([Karr et al. 2006](#)), or by evaluating whether the observed and synthetic data are distinguishable using a classification model (a technique called $pMSE$; [Woo et al. 2009](#); [Snoke et al. 2018](#)). However, a common critique of global utility measures is that they tend to be too general ([Drechsler 2022](#)). That is, analyses on a synthetic data set that is overall quite similar to the observed data (i.e., has high global utility), may still yield results that are far from the results obtained from the real data. Also, commonly used methods for estimating the $pMSE$, as logistic regression and classification and regression trees, tend to become less reliable as the dimensionality of the data increases, and are vulnerable to model misspecification ([Drechsler 2022](#)). Lastly, the output of global utility measures can be hard to interpret, and say little about the regions in which the synthetic data do not resemble the true data accurately enough.

To overcome the issues related to traditional global utility measures, we propose to use the density ratio estimation framework ([Sugiyama, Suzuki, and Kanamori 2012a](#)) as a way of evaluating utility. Intuitively, if two data sets have similar multivariate distributions, the density ratio should be close to one over the range of the data. If the distributions of the observed and synthetic data are very different, the density ratio should be far from one at those regions where the distributions differ. As density estimation is known to be a difficult problem, the density ratio estimation framework

provides techniques to directly estimate the density ratio, rather than the two separate densities, in a non-parametric way (Sugiyama, Suzuki, and Kanamori 2012a). These non-parametric estimation techniques come with automatic model specification, which mitigates the issue of model specification. This functionality is implemented in the R-package `densityratio` (Volker 2023). Importantly, the density ratio is estimated over the entire range of the data, which provides measures of utility at every (possible) point in the data space. This point-specific quantification of utility turns out to be a useful side-product, as it allows to reweigh analyses on synthetic data when further improving the utility directly is not possible.

In the remainder of the article, we introduce the density ratio framework and the associated estimation techniques, and connect the framework to traditional utility measures as the $pMSE$ and the Kullback-Leibler divergence. We then present simulations to demonstrate the performance of density ratio estimation in stylized settings and compare it to traditional utility measures. Subsequently, we apply density ratio estimation in a case study where we evaluate the utility of multiple synthetic versions of the U.S. Current Population Survey. We conclude with a discussion of the results, highlight the strengths and weaknesses of the density ratio framework, and provide recommendations for future research.

2 Background

Over the years, many methods have been introduced to generate synthetic data, all with the aim of providing a suitable balance between privacy and utility. These methods can be relatively simple, such as a sequence of generalized linear models (e.g., Reiter 2004), or as complex as deep learning models with thousands of parameters (e.g., Xu et al. 2019), with many options in between. However, the complexity of the generation process is not necessarily a good indicator of the quality of the synthetic data. That is, relatively simple methods could still capture the most important aspects of the data that complex methods fail to capture (and vice versa). Hence, data providers typically do not know which synthesis method will provide the highest utility a priori, and might compare multiple synthesis strategies to determine which data set will be released. Good global utility measures can help in this process, by allowing to quantify the quality of the candidate synthetic data sets.¹ Moreover, such global utility measures may guide the synthesis process itself, if they provide sufficiently specific information about the degree of misfit of the synthetic data. In the upcoming section, we provide an overview of existing global utility measures, and introduce the density ratio framework as an encompassing approach to evaluating global utility.

2.1 Existing global utility measures

Global utility measures typically attempt to quantify the distributional similarity between the observed and synthetic data samples. The intuition is that two data sets are realizations from the same underlying distribution, the data sets can be used for the same purposes, and analyses on the two data sets should yield similar results. One way to evaluate

¹We focus on global utility measures, because in many situations the data provider does not know which analysis will be performed with the synthetic data. If the data provider knows for which purposes the data will be used, analysis-specific utility measures may be more informative.

distributional similarity is by assessing whether a classification model can tell samples from the two distributions apart (see [Kim et al. 2021](#), who formalize the connection between classification accuracy and two-sample testing). Hence, if a classification model can distinguish between the observed and synthetic data with high accuracy, the distributional similarity is low, and so is the global utility. If a classifier cannot distinguish between the observed and synthetic data, one would conclude that the global utility is high. The propensity score mean-squared error ($pMSE$), introduced by Woo et al. (2009) and further developed in Snoke et al. (2018), formalizes this intuition. Let I_i denote an indicator variable that equals 1 if observation i ($i \in 1, \dots, N$, $N = n_{\text{obs}} + n_{\text{syn}}$) belongs to the synthetic data, and 0 otherwise. We then train a classifier that outputs the predicted probability of observation i being a synthetic record $\hat{\pi}_i$ based on the observation's scores on the variables (this can be the set of all variables, but also a subset). From these, we can calculate the utility statistic

$$pMSE = \frac{1}{N} \sum_{i=1}^N \left(\hat{\pi}_i - \frac{n_{\text{syn}}}{N} \right)^2, \quad (1)$$

which ought to be smaller when the synthetic data is more like the observed data. Crucially, the $pMSE$ depends on the classification model used and increases in the flexibility of the classification model, making it prone to overfitting and hard to interpret. To combat these issues, Snoke et al. (2018) suggests to compare the $pMSE$ -value with its expected value under the null hypothesis that the observed and synthetic data are indistinguishable. Provided that the classification model is a logistic regression model with k parameters (including the intercept), Snoke et al. (2018) show that the expected $pMSE$ is given by

$$\mathbb{E}[pMSE] = \left(\frac{k-1}{N} \right) \left(\frac{n_{\text{obs}}}{N} \right)^2 \left(\frac{n_{\text{syn}}}{N} \right).$$

For other classification models, the expectation can be approximated through a resampling procedure. Accordingly, the $pMSE$ -ratio is given by

$$pMSE\text{-ratio} = \frac{pMSE}{\mathbb{E}[pMSE]}.$$

Apart from the $pMSE$, several other measures can be constructed from the estimated propensity scores, such as the percentage of records correctly predicted ([Gillian M. Raab, Nowok, and Dibben 2021](#)) or the Kolmogorov-Smirnov statistic ([Bowen, Liu, and Su 2021](#)), both which are strongly correlated with the $pMSE$ ([Gillian M. Raab, Nowok, and Dibben 2021](#)).

Due to its intuitive nature, multiple studies advice the use of the $pMSE$ as a promising technique to evaluate the quality of synthetic data (e.g., [Gillian M. Raab, Nowok, and Dibben 2017](#); [Gillian M. Raab, Nowok, and Dibben 2021](#); [Hu and Bowen 2024](#)). Yet, it is not free of criticism. The usefulness of the $pMSE$ hinges on choosing a model that can capture the important intricacies of the observed data. Drechsler (2022) illustrated that the utility score is highly dependent on the model used to estimate the propensity scores, and that clear improvements in synthesis models are not necessarily picked up in the $pMSE$. Moreover, selecting an appropriate propensity score model may be difficult, as the challenges associated with model selection, such as the bias-variance trade-off, typically apply.

Another way to formalize distributional similarity is through the Kullback-Leibler (KL) divergence, as proposed in Karr et al. (2006). The KL-divergence measures the relative entropy from the probability distribution of the observed data $p_{\text{obs}}(\mathbf{x})$ to the probability distribution of the synthetic data $p_{\text{syn}}(\mathbf{x})$ (with $\mathbf{x} \in \mathbb{R}^d$), and is defined as²

$$D_{\text{KL}}(p_{\text{obs}}||p_{\text{syn}}) = \int p_{\text{obs}}(\mathbf{x}) \log \frac{p_{\text{obs}}(\mathbf{x})}{p_{\text{syn}}(\mathbf{x})} d\mathbf{x}. \quad (2)$$

Karr et al. (2006) argue that the KL-divergence can be computed by approximating the integral using density estimators \hat{p}_{obs} and \hat{p}_{syn} . An implementation of this approach for divergence estimation has been described in Wang, Kulkarni, and Verdu (2009), where the densities are estimated using nearest-neighbor density estimation. Another approach posed by Karr et al. (2006) is to assume multivariate normality for both p_{syn} and p_{obs} , and calculate the KL-divergence in closed form from the sample means and covariance matrices. Although all these approaches are easy to implement, they have their limitations. Density estimation is challenging in high-dimensional settings, and assuming multivariate normality might be too restrictive. We show in later sections that the KL-divergence naturally fits into the density ratio estimation framework.

2.2 Density ratio estimation

The density ratio estimation framework was originally developed in the machine learning community for the comparison of two probability distributions (for an overview, see Sugiyama, Suzuki, and Kanamori 2012a). The framework has been shown to be applicable to prediction (Sugiyama et al. 2010; Sugiyama 2010), outlier detection (Hido et al. 2008), change-point detection in time-series (Liu et al. 2013), importance weighting under domain adaptation (i.e., sample selection bias; Kanamori, Hido, and Sugiyama 2009), and two-sample homogeneity tests (Sugiyama, Suzuki, et al. 2011). The general idea of density ratio estimation is depicted in Figure 1, and boils down to comparing two distributions by modelling the density ratio $r(\mathbf{x})$. In our case, we define $r(\mathbf{x})$ as the ratio between the probability distributions of the numerator samples, taken from the observed data distribution, $p_{\text{obs}}(\mathbf{x})$, and the denominator samples, taken from the synthetic data distribution, $p_{\text{syn}}(\mathbf{x})$, such that

$$r(\mathbf{x}) = \frac{p_{\text{obs}}(\mathbf{x})}{p_{\text{syn}}(\mathbf{x})}. \quad (3)$$

This specification has the intuitive interpretation that in locations where the density ratio takes values larger than 1, too few synthetic observations are generated in that region. Conversely, in locations where the density ratio takes values smaller than one, too many synthetic observations are generated in that region (see Figure 1). We put $p_{\text{obs}}(\mathbf{x})$ in the numerator such that it plays the role of the actual distribution, while $p_{\text{syn}}(\mathbf{x})$ serves as the approximating distribution (we briefly come back to this in the next section). A straightforward approach to estimating $r(\mathbf{x})$ from samples of $p_{\text{obs}}(\mathbf{x})$ and $p_{\text{syn}}(\mathbf{x})$ would be to estimate the observed and synthetic data density separately, for example using kernel density estimation (e.g., see Scott 1992 for an overview), and subsequently compute the ratio of these estimated densities.

²In contrast to Karr et al. (2006), we define the KL-divergence as the relative entropy of p_{obs} with respect to p_{syn} , such that it is consistent with our later formulations.

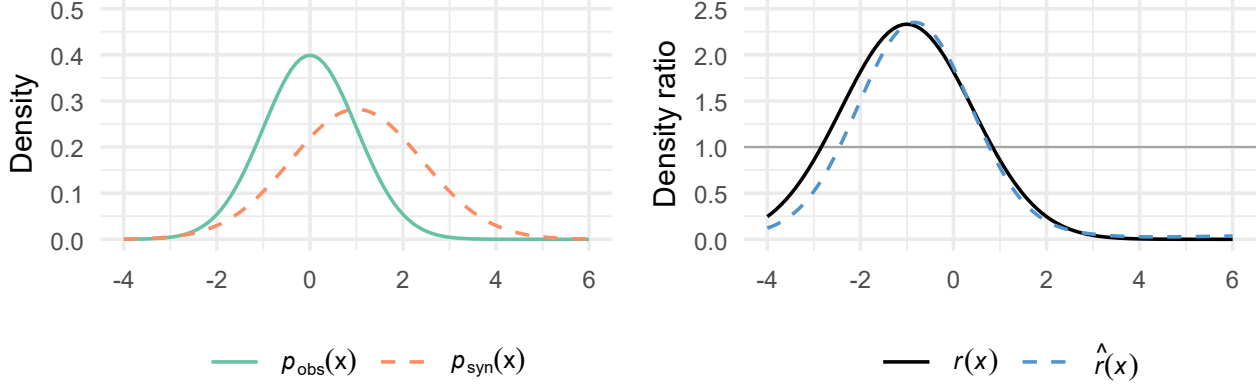


Figure 1: Example of the true and estimated density ratio of two normal distributions with different means and variances (i.e., $p_{\text{syn}}(\mathbf{x}) = N(0, 1)$ and $p_{\text{obs}}(\mathbf{x}) = N(1, 2)$). The function $r(\mathbf{x}) = p_{\text{obs}}(\mathbf{x})/p_{\text{syn}}(\mathbf{x})$ denotes the true density ratio, the function $\hat{r}(\mathbf{x})$ denotes an estimate of the density ratio based on $n_{\text{syn}} = n_{\text{obs}} = 200$ samples from each distribution obtained with unconstrained Least-Squares Importance Fitting (uLSIF). Note that the density ratio is itself not a proper density.

However, density estimation is one of the hardest tasks in statistical learning, unavoidably leading to estimation errors for both densities, especially in high dimensions (Sugiyama, Suzuki, and Kanamori 2012a). When subsequently taking the ratio of the estimated densities, estimation errors tend to be magnified. Direct density ratio estimation avoids this issue by specifying and estimating a model directly for the ratio without first estimating the separate densities. Extensive simulations on a wide variety of tasks showed that this approach typically outperforms density ratio estimation through kernel density estimation for each distribution separately, especially when the dimensionality of the data increases (e.g., Kanamori, Suzuki, and Sugiyama 2012b; Hido et al. 2008; Kanamori, Hido, and Sugiyama 2009).

2.2.1 Estimating the density ratio

Over the past years, several methods for direct density ratio estimation have been developed. A large class of these methods attempt to directly minimize the error between the true density ratio $r(\mathbf{x})$ and a density ratio model $\hat{r}(\mathbf{x})$. Following this approach, we define a loss function $\mathcal{L}(r(\mathbf{x}), \hat{r}(\mathbf{x}))$ that measures the discrepancy between the true and estimated density ratio. To give an example, consider the following loss based on the squared error

$$\begin{aligned} \mathcal{L}_S^*(r(\mathbf{x}), \hat{r}(\mathbf{x})) &= \frac{1}{2} \int (\hat{r}(\mathbf{x}) - r(\mathbf{x}))^2 p_{\text{syn}}(\mathbf{x}) d\mathbf{x} \\ &= \frac{1}{2} \int \hat{r}(\mathbf{x})^2 p_{\text{syn}}(\mathbf{x}) d\mathbf{x} - \int \hat{r}(\mathbf{x}) r(\mathbf{x}) p_{\text{syn}}(\mathbf{x}) d\mathbf{x} + \frac{1}{2} \int r(\mathbf{x})^2 p_{\text{syn}}(\mathbf{x}) d\mathbf{x}. \end{aligned} \quad (4)$$

The second term can be rewritten, because the denominator in $r(\mathbf{x})$ cancels with $p_{\text{syn}}(\mathbf{x})$, while the third term is a constant with respect to the parameters in the density ratio model and can thus be ignored. Hence, we are left with the following loss function to minimize

$$\mathcal{L}_S(r(\mathbf{x}), \hat{r}(\mathbf{x})) = \frac{1}{2} \int \hat{r}(\mathbf{x})^2 p_{\text{syn}}(\mathbf{x}) d\mathbf{x} - \int \hat{r}(\mathbf{x}) p_{\text{obs}}(\mathbf{x}) d\mathbf{x}, \quad (5)$$

which is termed least squares importance fitting (LSIF) by Kanamori, Hido, and Sugiyama (2009).

This approach can be straightforwardly generalized to a wide class of loss functions that fall under the family of Bregman divergences (see Sugiyama, Suzuki, and Kanamori 2012b; Mohamed and Lakshminarayanan 2017). Then, a general class of losses is encompassed by the expression

$$\mathcal{L}_f^*(r(\mathbf{x}), \hat{r}(\mathbf{x})) = \int \left(f(r(\mathbf{x})) - f(\hat{r}(\mathbf{x})) - f'(\hat{r}(\mathbf{x}))(r(\mathbf{x}) - \hat{r}(\mathbf{x})) \right) p_{\text{syn}}(\mathbf{x}) d\mathbf{x}, \quad (6)$$

where f is a differentiable and strictly convex function with derivative f' . Then, ignoring the terms independent of $\hat{r}(\mathbf{x})$ and noting that $r(\mathbf{x})p_{\text{syn}}(\mathbf{x}) = p_{\text{obs}}(\mathbf{x})$, we obtain the following objective

$$\mathcal{L}_f(r(\mathbf{x}), \hat{r}(\mathbf{x})) = \int \left(f'(\hat{r}(\mathbf{x}))\hat{r}(\mathbf{x}) - f(\hat{r}(\mathbf{x})) \right) p_{\text{syn}}(\mathbf{x}) d\mathbf{x} - \int f'(\hat{r}(\mathbf{x})) p_{\text{obs}}(\mathbf{x}) d\mathbf{x}. \quad (7)$$

Minimizing this loss over $\hat{r}(\mathbf{x})$ for different functions f yields different estimators for the density ratio, that focus on different regions of the density ratio.³ Specifically, some estimators place more emphasis on accurately modelling the regions in which the true density ratio is large, but less emphasis on accurately estimating the density ratio in regions where it takes small values, and vice versa (see Sugiyama, Suzuki, and Kanamori 2012b; Menon and Ong 2016). Importantly, Sugiyama, Suzuki, and Kanamori (2012b) show that the Bregman divergence minimization approach to density ratio estimation is equivalent to estimating an f -divergence (Ali and Silvey 1966) of the observed data distribution from the synthetic data distribution. Hence, when estimating the density ratio, one implicitly estimates the divergence between the observed and synthetic data distributions.

After defining a loss function, we need a model for the density ratio function $\hat{r}(\mathbf{x})$. There are many possibilities to specify this model, but a common choice is to use a linear model for the density ratio (e.g., Huang et al. 2006; Kanamori, Hido, and Sugiyama 2009; Izbicki, Lee, and Schafer 2014; Gruber et al. 2024). That is, we define the density ratio model as

$$\hat{r}(\mathbf{x}) = \varphi(\mathbf{x})\theta, \quad (8)$$

where $\varphi(\mathbf{x})$ is a basis function vector (optionally including an intercept term), that transforms the data from a p -dimensional to a b -dimensional space, and θ is a b -dimensional parameter vector. Although the model is linear in its parameters, the density ratio itself is typically a non-linear function of the data due to the basis functions. The parameter vector θ is estimated to minimize the discrepancy with the true density ratio using the loss function $\mathcal{L}(r(\mathbf{x}), \hat{r}(\mathbf{x}))$ in Equation 7. Potentially, the loss function can be extended with a regularization term (e.g., a L_1 or L_2 norm on the parameters of the model), to decrease the flexibility of the density ratio. Parameter estimation can be carried out using standard optimization techniques (see Appendix A for a brief demonstration in R).

Also for the basis functions, several specifications are possible, ranging from an identity function (Qin 1998) to normalizing flows (Choi, Liao, and Ermon 2021) or neural networks (Tiao 2018; Uehara et al. 2016). A commonly used basis function in the density ratio literature is the Gaussian kernel function (e.g., Huang et al. 2006; Sugiyama et al. 2007; Kanamori, Hido, and Sugiyama 2009; Liu et al. 2013; Gruber et al. 2024). The Gaussian kernel function is

³It is easy to see that using $f(x) = \frac{1}{2}(x - 1)^2$ turns the Bregman divergence (Equation 6) into the squared error (Equation 4).

defined as

$$\varphi(\mathbf{x}) = \mathcal{K}(\mathbf{x}, c_j) = \exp\left(-\frac{\|\mathbf{x} - c_j\|^2}{2\sigma^2}\right),$$

where c_j ($j \in 1, \dots, b$) denotes the centers of the Gaussian kernel functions, and σ controls the kernel width (i.e., it defines over which distance differences between the observations and the centers are considered relevant; for more information on kernel functions, see, e.g., [Murphy 2022](#)). The appropriate width of the kernel and the optimal value of the regularization parameter can be determined using cross-validation. The centers are typically sampled from the data (in our case, both the observed and synthetic data).

After defining the model and the loss function, the density ratio can be estimated. The `densityratio` package in R ([Volker 2023](#)) provides an implementation of commonly used loss functions with a Gaussian kernel basis function. The package comes with an easy-to-use interface, automatic cross-validation of hyperparameters and builds on C++ for fast computation (see Appendix A for a brief demonstration). The density ratio estimation framework thus equips researchers with a measure of utility which is accurate, fast to compute and does not require user specification of the model.

2.2.2 Evaluating data utility with the density ratio

Having estimated the density ratio, we can evaluate both global and local utility of the synthetic data. Like other global utility measures, the density ratio can be used to construct a single discrepancy measure that quantifies the degree of misfit of the synthetic data. The density ratio can be used to directly calculate some f -divergence between the observed and synthetic data distributions, which serves as a measure of utility for the synthetic data. Although this divergence statistic is difficult to interpret in an absolute sense, it can be used as a relative measure of the quality of the synthetic data. That is, for different synthetic data sets, we can calculate the divergence to the observed data, and compare these values to determine which synthetic data set is most similar to the observed data. More formally, the f -divergence can be used in a hypothesis test to determine whether the synthetic data is generated from the same distribution as the observed data. The corresponding p -value can be calculated by comparing the observed divergence measure to the null distribution of divergence measures obtained using random permutations of the observed and synthetic data (see, for example, [Sugiyama, Suzuki, et al. 2011](#); [Wornowizki and Fried 2016](#); [Kanamori, Suzuki, and Sugiyama 2012a](#)).

An appealing characteristic of the density ratio framework is that it also readily allows for evaluating local utility. As said, the estimated density ratio shows in which regions the synthetic data diverges from the observed data. By inspecting which observations have a high, or small, estimated density ratio, we can identify the regions in which the synthetic data is most different from the observed data. Visual inspection can aid this process, for example by plotting the estimated density ratio against variables or pairs of variables in the data. On an even finer scale, the density ratio can be used to identify individual observations that are far from what can be expected on the basis of the observed data. This information could identify flaws in the synthetic data model, or could be used directly to remove such observations from the synthetic data. An additional advantage of the density ratio lies in the fact that for every synthetic observation, the predicted density ratio value can be regarded as an importance weight. Releasing

the predicted density ratio values for each synthetic observation allows data users to reweigh analyses on the synthetic data. We illustrate these features in Section 4.

A final advantage of the density ratio estimation framework lies in its flexibility. The combination of a non-parametric kernel-based model with automatic cross-validation for hyperparameter selection (e.g., kernel and regularization parameters) allows for flexible estimation of the density ratio. This flexibility reduces the burden on the user in terms of model specification when evaluating the utility of the synthetic data. All functionality described above, including visualization, divergence estimation (and testing), extracting importance weights and automatic cross-validation for hyperparameter selection, is readily available in the `densityratio` R-package (Volker 2023). The package provides fast and efficient algorithms for density ratio estimation, and uses default implementations that work across a wide range of data distributions, which will be shown in the upcoming simulations.

3 Numerical illustrations: Simulation studies

To evaluate the performance of density ratio estimation and compare it to existing methods, we conduct a series of simulation studies (all code is available on GitHub⁴). First, we illustrate the approach in a univariate simulation, after which we evaluate the performance of the approach in a multivariate setting, varying the distributions, number of variables and sample sizes. To perform density ratio estimation, we use unconstrained Least-Squares Importance Fitting (uLSIF; Kanamori, Hido, and Sugiyama 2009) as implemented in the `densityratio` package in R (Volker 2023), because it is fast and has been shown to perform well in a variety of settings (e.g., Kanamori, Hido, and Sugiyama 2009; Li et al. 2010; Kanamori, Suzuki, and Sugiyama 2012b). We compare the performance of uLSIF to the performance of state-of-the-art software implementations of the $pMSE$ (Nowok, Raab, and Dibben 2016) and Kullback-Leibler divergence estimation through k -nearest neighbor density estimation (Hartung 2024). Note that Kullback-Leibler divergence estimation through k -nearest neighbor density estimation implicitly performs direct density ratio estimation, and the procedure can be regarded as a special case of density ratio estimation (see Appendix B).

3.1 Univariate illustrations

We first illustrate the behavior of density ratio estimation in a univariate setting, which simplifies visualization of the estimated density ratios. Specifically, we consider four settings in which we generate the real data from a distribution, and generate synthetic data from an approximating Gaussian distribution with the same mean and variance as the true data generating mechanism. The real data is generated from (1) a Laplace distribution, (2) a log-normal distribution, (3) a location-scale t -distribution and (4) a normal distribution (see Figure 2). Subsequently, we approximate the true data generating mechanism using a Gaussian model with the same mean and variance as the original data. This setting is similar to situations commonly encountered in the synthetic data field, in the sense that the true data generating mechanism is unknown and needs to be approximated using a simpler approximating model. The exact specifications of the data generating mechanisms are as follows:

⁴<https://github.com/thomvolker/dr-utility>

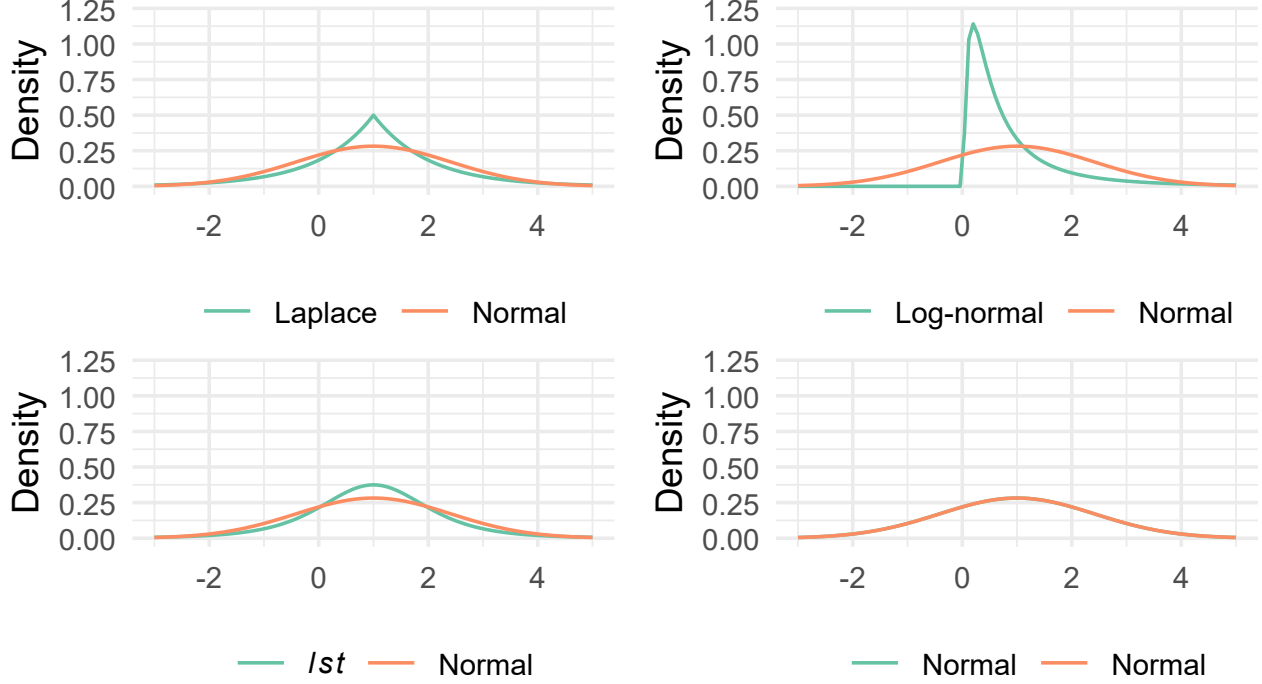


Figure 2: True and synthetic data densities for the four simulations with Laplace, Log-normal, location-scale t - and Normal densities. All data-generating mechanisms have the same mean $\mu = 1$ and variance $\sigma^2 = 2$. Note that the true and synthetic data density in the bottom right panel are completely overlapping.

1. Laplace distribution with location parameter $\mu = 1$ and scale parameter $b = 1$.
2. Log-normal distribution with log-mean parameter $\mu_{\log} = \log\{1/\sqrt{3}\}$ and log-variance parameter $\sigma_{\log}^2 = \log 3$.
3. Location-scale t -distribution with location parameter $\mu = 1$, scale parameter $\tau^2 = 1$ and degrees of freedom $\nu = 4$.
4. Normal distribution with mean $\mu = 1$ and variance $\sigma^2 = 2$.

These data generating mechanisms are chosen such that they all have the same population mean $\mu = 1$ and variance $\sigma^2 = 2$. The approximating Gaussian distribution has mean $\mu = 1$ and variance $\sigma^2 = 2$. Hence, the synthetic data has the same population mean and variance, but differs in higher-order moments, except in the fourth scenario, where it is equal to true data generating mechanism. In all scenarios, we generate 1000 data sets with $n_{\text{obs}} = 250$ observations from the true data generating mechanism, and $n_{\text{syn}} = 250$ synthetic observations from the approximating Gaussian model. The density ratio model is estimated using uLSIF with the default Gaussian kernel and L_2 -penalty on the parameter vector θ . Both the kernel bandwidth and the regularization parameter are selected using cross-validation, using the default settings in the `densityratio` package.

Figure 3 shows that the estimated density ratios (the blue lines) follow the general trend of the true density ratio (the solid black line) for each data-generating mechanism. Especially in the center of each panel, approximately between -2 and 4 , the average density ratio (the dashed black line) closely matches the true density ratio. Moreover, all estimated density ratios model the peak in the center of each panel, where the true data generating distribution

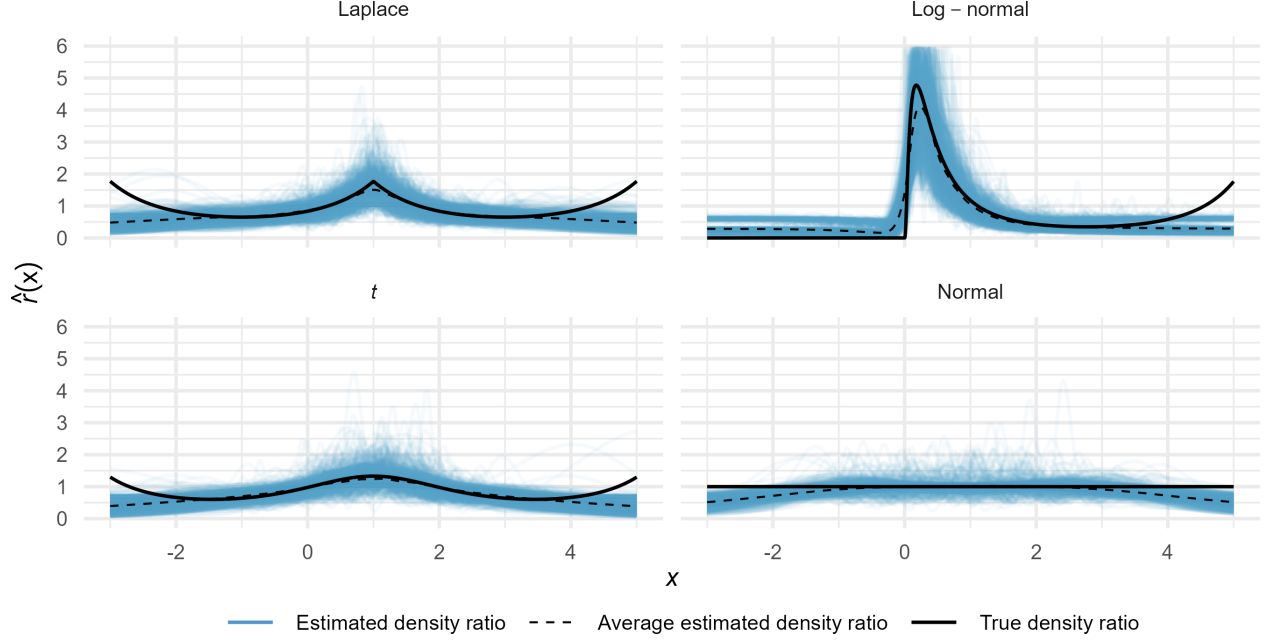


Figure 3: Estimated density ratios by unconstrained least-squares importance fitting in four univariate examples: A Laplace distribution, a log-normal distribution, a location-scale t -distribution and a normal distribution, all approximated by a normal distribution with the same mean and variance as the sample from the true distribution. Note that the mass of the synthetic data distribution in the tails (smaller than -2 or greater than 4) is smaller than 0.034 .

has more mass than the synthetic data distribution (except the bottom right panel, where the true and synthetic data distributions are the same). When moving from the middle to the sides, where the synthetic data distribution has more mass than the true data generating distributions, the estimated density ratios still follow the true density ratios, in the sense that they are typically smaller than 1. In the tails of the distribution, where the synthetic data distribution has almost no mass ($P(x \leq -2) = P(x \geq 4) \approx 0.017$), estimating the density ratio becomes difficult, leading to estimated density ratios that diverge from the true density ratios. In these regions, the kernel function yields low values for most observations, which, combined with the L_2 -penalty on the density ratio parameters, yields a downward bias for the estimated density ratio.

When assessing the panels individually, the following observations can be made. In the top-left panel, showing the estimated density ratio of the Laplace-distributed samples over the synthetic Gaussian-distributed samples, the peak in the center is well approximated. Yet, the discontinuity in the peak of the Laplace distribution cannot be captured by a Gaussian kernel, which by definition models the density ratio as a smooth function. The same can be said about the log-normal distribution, where the cut-off at 0 is not captured exactly. Moreover, this panel clearly shows the shrinkage due to the regularization parameter. When there are no samples in one of the two distributions, the regularization has relatively more influence and shrinks the density ratio parameters towards zero. Accordingly, the estimated density ratio is shrunk towards the estimated intercept parameter. The same behavior can be seen in the bottom-left panel, showing the estimated density ratios of location-scale t -distribution over the Gaussian samples. In the centre of the distributions, the density ratio is well approximated, but the density ratio is consistently underestimated in the tails of

the distribution. Lastly, it can be seen that, although the estimated density ratios follow the general trends of the true density ratios, there is also some variability around the true values, yielding rather wiggly lines in some simulations.

Finally, we briefly compare the performance of uLSIF to k -nearest neighbor density ratio estimation, which is implicitly used in Kullback-Leibler divergence estimation through k -nearest neighbor density estimation (see Appendix B for details). We set the number of neighbors to $k = 15 \approx \sqrt{n}$ (as suggested by Loftsgaarden and Quesenberry 1965). Figure A2 shows that the estimated density ratios by uLSIF are less variable than the estimated density ratios by k -nearest neighbor density ratio estimation. Moreover, the estimated density ratios by k -nearest neighbor density ratio estimation have similar bias in the tails of the distribution, where data is scarce. We conclude that uLSIF is able to provide more accurate estimates of the density ratio if there are enough samples in the regions of interest.

3.2 Multivariate simulations

To further investigate the performance of density ratio estimation, we conducted a simulation study in a multivariate setting to compare against existing global utility measures. The goal of these simulations is to evaluate whether density ratio estimation is able to capture improvements in the synthetic data model, and is able to reflect these improvements in the utility statistics. In what follows, we describe the data-generating mechanism, the synthetic data models, the utility measures used to evaluate the quality of the synthetic data models and the results of the simulations.

3.2.1 True data-generating mechanism

We generate the real data according to three data-generating mechanisms, consisting of $D \in \{5, 25, 50\}$ variables. When $D = 5$, the first four variables are multivariate normally distributed. These normally distributed variables have mean $\mu_d = 0$, variance $\sigma_{d,d}^2 = 1$ and covariance $\sigma_{d,d'}^2 = 0.5$, for $d = 1, \dots, D - 1$. The fifth variable is non-linearly related to the first variable, such that $X_5 \sim \mathcal{N}(X_1^2, \hat{\text{Var}}(X_1^2))$. When $D = 25$ or $D = 50$, the first 20 and 45 variables are distributed normally, again with zero mean, unit variance and covariance $\sigma_{d,d'}^2 = 0.5$ for $d = 1, \dots, D - 5$. The last five variables have a non-linear relationship with the first five variables, defined as $X_{D-5+j} \sim \mathcal{N}(X_j^{j+1}, \hat{\text{Var}}(X_j^j))$, for $j = 1, \dots, 5$. Hence, the first variable with a non-linear relationship is obtained by raising the first variable to the power 2, the second is obtained by raising the second variable to the power 3, and so on, with an additional variance term that scales with the variability due to raising terms to a higher power. For each number of variables, we generate 1000 data sets, with three different numbers of observations ($n \in \{100, 1000, 2000\}$).

3.2.2 Synthetic data generation

We generate synthetic data via three mechanisms, each incrementally closer to the true data generating mechanism. The first synthetic data model is a multivariate normal distribution with mean and variance estimated from the real data, but neither covariances nor non-linear relationships are taken into account. The second synthetic data model is a multivariate normal distribution with means, variances and covariances estimated from the real data, but without the non-linear relationships. The final, and correctly specified, synthetic data model estimates the means, variances,

Table 1: Proportion of simulations in which the true synthetic data model order is captured by the utility measure. The column PE refers to the Pearson divergence estimated using uLSIF, KL_1 and $KL_{\sqrt{n}}$ refer to the Kullback-Leibler divergence estimated using k -nearest neighbor density ratio estimation with respectively $k = 1$ and $k = \sqrt{n}$, and $pMSE_{\text{CART}}$ and $pMSE_{\text{logit}}$ refer to the $pMSE$ -ratio estimated using a CART model and a logistic regression model, respectively.

n	D	PE	KL_1	$KL_{\sqrt{n}}$	$pMSE_{\text{CART}}$	$pMSE_{\text{logit}}$
100	5	0.583	0.844	0.904	0.369	0.188
100	25	0.450	0.838	0.933	0.364	0.250
100	50	0.363	0.673	0.786	0.348	0.352
1000	5	1.000	1.000	1.000	0.887	0.173
1000	25	1.000	1.000	1.000	0.893	0.242
1000	50	0.995	1.000	1.000	0.846	0.316
2000	5	1.000	1.000	1.000	0.885	0.173
2000	25	1.000	1.000	1.000	0.822	0.247
2000	50	1.000	1.000	1.000	0.788	0.324

covariances and non-linear parameters from the data. Each synthetic data set has the same number of observations as the observed data.

3.2.3 Utility measures

The goal of the simulation study is to evaluate whether the global utility measures are able to detect the improvements in the synthesis models. To this end, we use three different utility measures, and two different specifications of each measure. First, we use uLSIF with automatic hyperparameter selection through cross-validation (the default in the `densityratio`-package). We summarize the estimated utility of the synthetic data into a single number using the Pearson divergence (PE ; [Sugiyama, Suzuki, et al. 2011](#)). Additionally, we use the Kullback-Leibler divergence based on k -nearest neighbor density ratio estimation as implemented in the R-package `kldest` ([Hartung 2024](#)), varying the number of neighbors between $k = 1$ (the default in the software) and $k = \sqrt{n}$ (as advocated by [Loftsgaarden and Quesenberry 1965](#)). Finally, we use the $pMSE$ -ratio, based on a CART model using the default settings in `synthpop` ([Nowok, Raab, and Dibben 2016](#)) and a logistic regression model without interactions, as not all combinations of number of variables and samples allow to include interactions in the model.

3.2.4 Results

Table 1 shows the proportion of simulations in which the utility measures correctly order the synthetic data sets in terms of quality of the synthesis model. That is, the first synthesis model, using only the means and variances of each variable, should have the lowest utility (highest divergence or $pMSE$ -ratio), followed by the second synthesis model, using the correct means, variances and covariances but not the non-linear relationships, and the third, correctly specified synthesis model should obtain the highest utility score. Table 1 shows that the KL -divergence based on $k = \sqrt{n}$ neighbors correctly ranks the synthetic data sets most often, followed by the KL -divergence based on $k = 1$ neighbors and the uLSIF model. Unless the sample size is small, these approaches correctly rank the synthetic data sets in almost all instances. Both the KL -divergence and the density ratio based Pearson divergence clearly outperform the

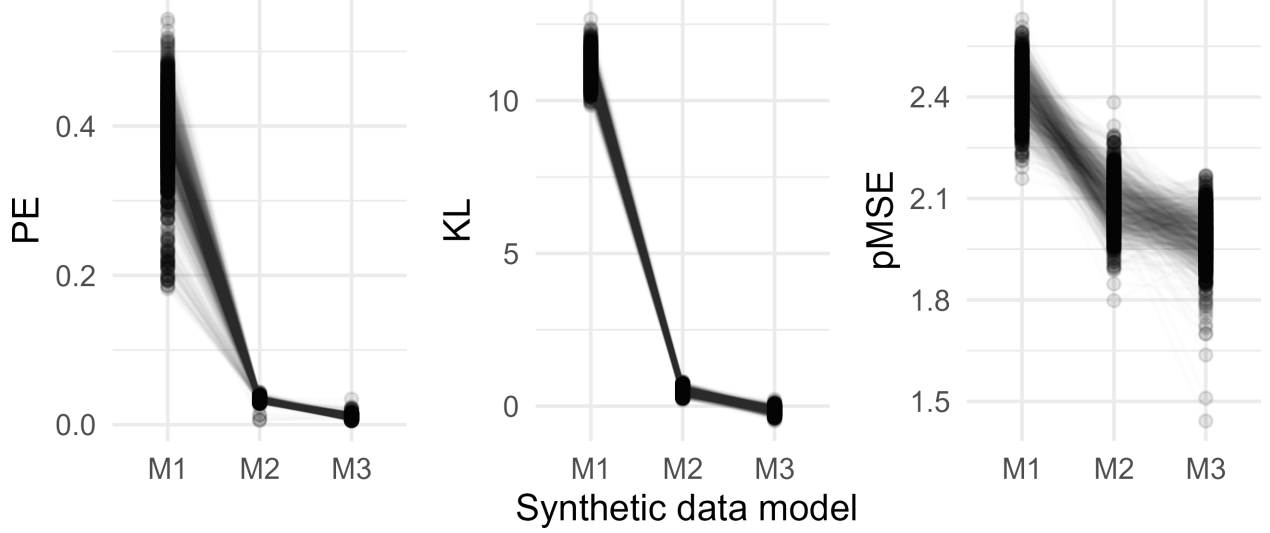


Figure 4: Utility measures for $n = 1000$ and $D = 25$ for PE , $KL_{\sqrt{n}}$ and $pMSE_{\text{cart}}$ for 1000 simulations of the three synthetic data models.

common $pMSE$. Additionally, Table 1 shows that the performance of all utility measures improves with the sample size, and decreases when the dimensionality of the data increases. The only exception to the latter trend is the logistic regression based $pMSE$ -ratio model, which consistently improves with the dimensionality of the data).

To zoom in on the behavior of the three methods, we visualize the results of uLSIF, the KL -divergence based on $k = \sqrt{n}$ neighbors, and the $pMSE$ -ratio based on a CART model for $n = 1000$ and $D = 50$ in Figure 4. For PE and $KL_{\sqrt{n}}$, the improvements in the synthesis model are consistently picked up by the utility measures, whereas for $pMSE_{\text{cart}}$, the estimated changes in utility are much more variable across the simulations. Additionally, the figures show that the improvement in utility due to modelling the covariances rather than only the means and variances is much larger than the improvement due to also modelling the non-linear relationships. That is, the increase in utility is much more pronounced when moving from the first to the second synthetic data set than moving from the second to the third synthetic data set.

These results have a remarkable implication for the evaluation of synthetic data generation methods. When the aim is to rank candidate synthetic data sets using a global utility statistic, using a rather flexible model seems advisable. In Section 3.1 and Appendix B, we showed that the k -nearest neighbor density ratio estimate is substantially more variable than the uLSIF-based estimate, but when the aim is to quantify the utility of the synthetic data, this variability does not seem to be problematic. Rather, these simulations seem to suggest that a more flexible model is better able to detect discrepancies between the observed and synthetic data. Obtaining a stable and accurate estimate of the density ratio (or, by analogy, of the propensity scores in the $pMSE$) does not seem to be required when one is solely interested in globally ranking different synthetic data sets. However, local information on the misfit of the synthetic data is valuable in itself, which we illustrate in the next section.

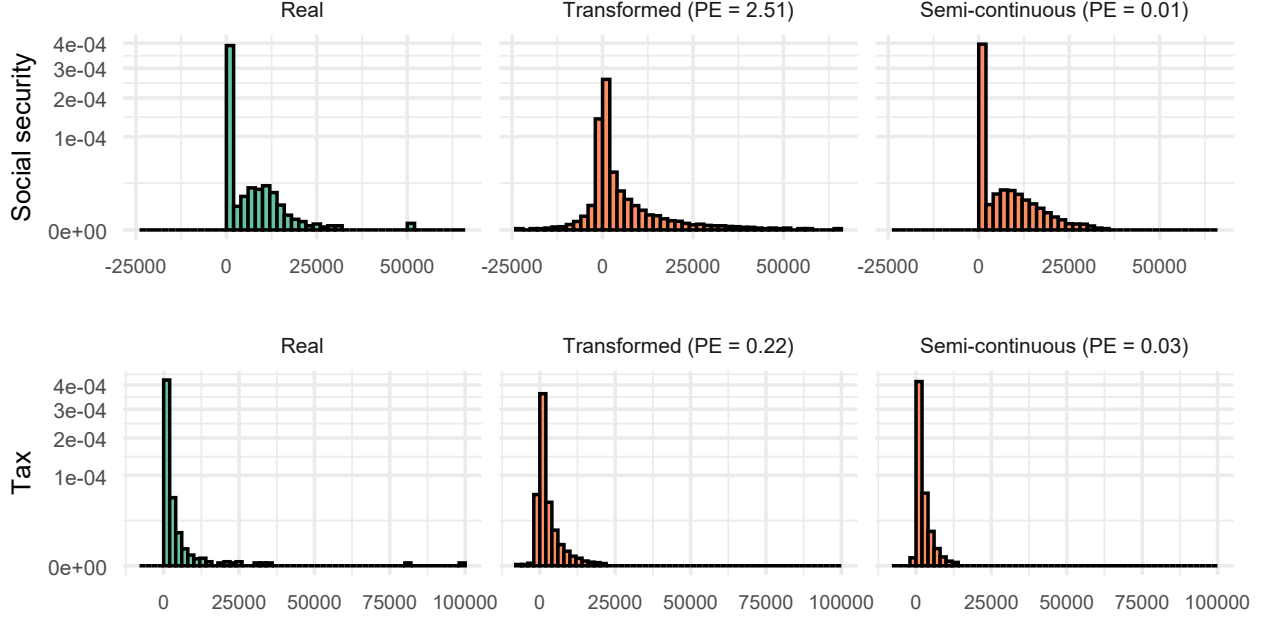


Figure 5: Real and synthetic data distributions for the variables household property taxes and social security benefits (social security) for the transformed and semi-continuous synthesis strategy. The panel titles display the estimated Pearson divergence for each variable between the observed and synthetic data, estimated using a density ratio model for each variable separately. Note that the y-axis is displayed on a square-root scale to enhance visibility.

4 Application: Synthetic data generation for the U.S. Current Population Survey

To further illustrate the use of density ratio estimation for synthetic data utility using the March 2000 U.S. Current Population Survey (CPS). The data contains the continuous variables age, household income, household property taxes and social security payments, and the categorical variables sex, race, marital status and education level measured on $n_{\text{obs}} = 5000$ individuals. We compare two different synthesis strategies that increasingly tailor toward the data at hand (using the R-package `synthpop`; Nowok, Raab, and Dibben 2016). Note that all continuous variables except age are substantially skewed. Moreover, the variables household property taxes and social security payments have a point-mass at zero (see the first column in Figure 5). To account for the skewness, we transform the continuous variables to cubic root scale ($f(x) = |x|^{1/3} \cdot \text{sign}(x)$). Accordingly, the first modelling strategies applies a linear regression model on the transformed continuous variables. The categorical variables are modelled using (multinomial) logistic regression models. The second modelling strategy extends the first strategy by applying a semi-continuous model to the transformed variables household property taxes and social security payments. Here, the point mass is modelled first using a logistic regression model, after which the non-zero values are synthesized using a linear regression model. All other variables are modelled according to the first strategy. We generate $m = 5$ synthetic data sets for both strategies, each with $n_{\text{syn}} = 5000$ observations, and evaluate their utility using unconstrained least-squares importance fitting. We emphasize that throughout the illustration, we use the same default settings as in the previous sections.

4.1 Evaluating global utility using density ratio estimation

Figure 5 displays the distributions of the variables social security payments (Social security) and household property taxes (Tax) for the real data and the synthetic data according to the transformed and semi-continuous modelling strategies. The figure shows that the semi-continuous modelling strategy fits the observed data better than the transformed modelling strategy, as it better captures the point mass and does not yield an excessive number of negative values. Note that there are only minor differences for the other variables, as there are no differences in synthesis methods. When evaluating the global utility of the two synthetic data sets, the improvement in synthesis models is reflected in the Pearson divergence. That is, the transformed modelling strategy has a higher average estimated Pearson divergence ($\bar{P}E_{\text{transformed}} = 0.090$, range = $[0.084, 0.100]$) than the semi-continuous modelling strategy ($\bar{P}E_{\text{semi-continuous}} = 0.050$, range = $[0.047, 0.053]$). Although the difference may seem small in an absolute sense, it is substantial in a relative sense. Additionally, the variability in estimated Pearson divergences for each synthesis strategy is much smaller than the difference between the two strategies. Finally, we remark that when estimating the density ratio on the level of the individual variables, the semi-continuous modelling strategy obtains substantially lower Pearson divergences than the transformed modelling strategy see the panel titles in Figure 5. Hence, we conclude that the Pearson divergence serves as an adequate measure of synthetic data utility.

4.2 Density ratios as local utility estimates

Besides quantifying the global utility of synthetic data, the density ratio also provides local information about the utility of synthetic data. First, the estimated density ratio can provide an intuition about which variables are not modelled adequately. That is, by plotting the estimated density ratio against each variable or pairs of variables, one can identify variables for which there is a clear pattern in the density ratio values. Figure 6 shows the estimated density ratio values (on a log-scale) for the variables social security payments and household property taxes for the first synthetic data set under both synthesis strategies. First, the figure shows that the spread in density ratio values is substantially larger for the transformed modelling strategy than for the semi-continuous modelling strategy. Second, the estimated density ratios indicate that the transformed modelling strategy misses the point mass at zero for social security, but generated too many values slightly larger than zero. Moreover, figure shows that the transformed modelling strategy yielded too little mass at the values around 10000, as indicated by the spike in density ratio values around 10000. Plotting the density ratio against household property taxes is less insightful, as the difference in marginal distributions is relatively small. For the semi-continuous modelling strategy, there is some spread in density ratio values, but there is no clear pattern, and the synthetic and observed data points are mostly overlapping. Hence, marginally, the density ratio values do not reveal a substantial misfit of the semi-continuous strategy.

Additionally, we note that in the tails of the distribution, the estimated density ratios are regularized, such that the high values for tax in the observed data do not yield extremely high density ratio values. From a utility perspective, this might be undesirable, as misfit in the tails of the distribution might go by unnoticed. However, from a privacy perspective, this regularization is beneficial, as it prevents the density ratio from becoming very large around the

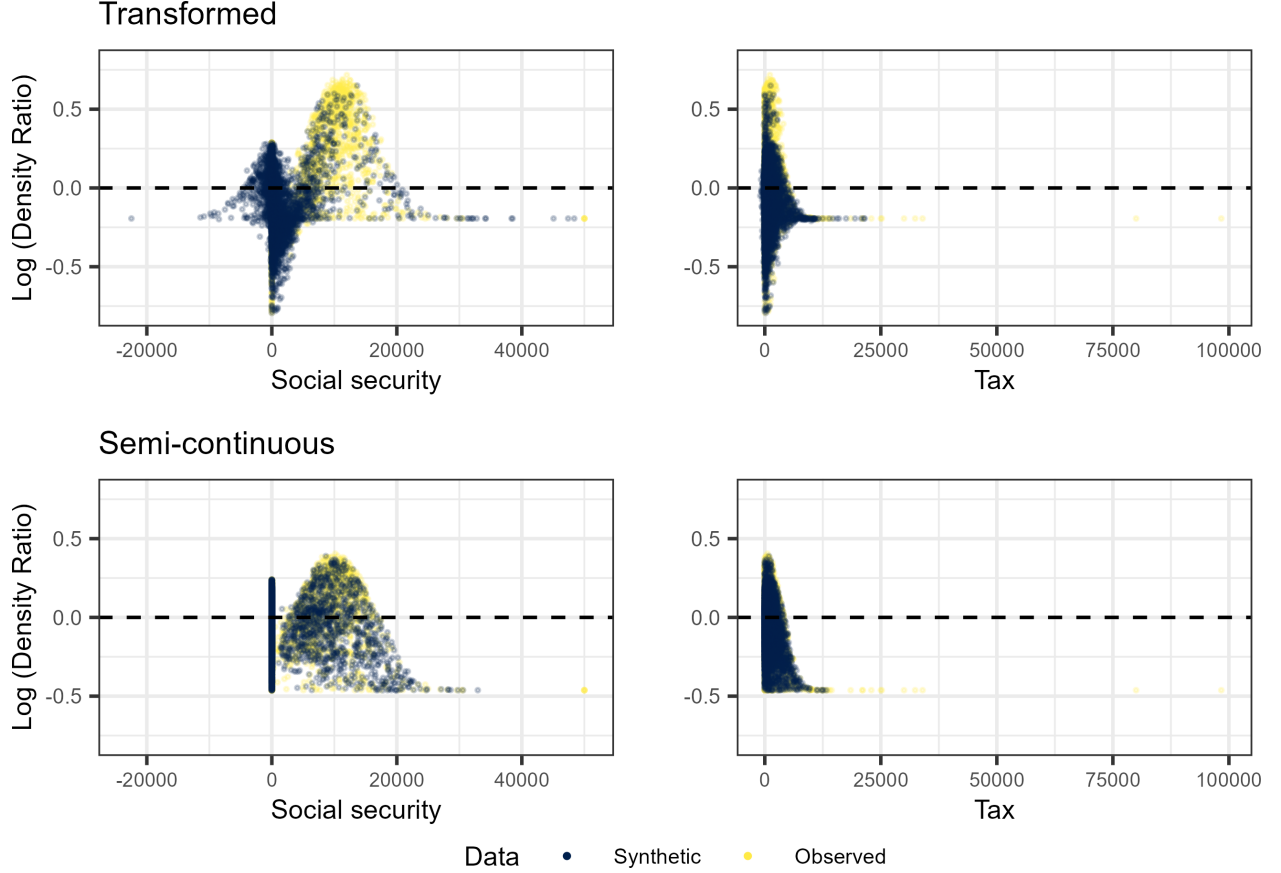


Figure 6: Estimated density ratios (on log-scale) for the first synthetic data set under the two synthesis strategies plotted against the variables social security payments (Social security) and household property taxes (Tax) for the observed and synthetic data. Note that the density ratios are estimated using a single model for the entire data set.

location of outlying observed data points, potentially revealing the location of these points. The regularization thus ensures that the density ratio is not overly sensitive to individual observations.

Finally, we illustrate another use of the density ratio as a local utility measure, namely, using the density ratio as importance weights in downstream analysis tasks. In this case, we consider the synthetic data as a sample that suffers from selection bias, and we use the estimated density ratio as importance weights to correct for this bias when making inferences. Using importance weighting after density ratio estimation, it is possible to obtain consistent estimates of the population parameters (Kanamori, Hido, and Sugiyama 2009; Kanamori, Suzuki, and Sugiyama 2012b), even when the synthesis method is not consistent. Consider the case that we deem our semi-continuous synthetic data model sufficient from both a privacy and utility perspective. Perhaps using more complex synthesis models would yield higher utility, but at the cost of a higher disclosure risk. To further improve the utility of the semi-continuous synthetic data, we can release the estimated density ratio values, such that a third-party can use these values as importance weights in their analysis. Releasing these weights obviously adds to the disclosure risk as more information about the observed data is provided. However, the density ratio values might be less disclosive than synthetic data generated with a more

Table 2: Linear regression coefficients for the observed data, synthetic data and reweighted synthetic data using the density ratio as importance weights. Boldface text indicates which coefficient has smaller absolute bias relative to the observed data.

Variable	Observed	Synthetic	Reweighted
Intercept	10.297	10.192	10.195
Age	-0.003	-0.005	-0.004
Education: High school	0.283	0.415	0.385
Education: Associate or Bachelor’s degree	0.593	0.782	0.731
Education: Master’s degree or higher	1.016	1.135	1.080
Marital: Separated	-0.500	-0.434	-0.437
Marital: Widowed	-0.467	-0.471	-0.450
Marital: Single	-0.491	-0.592	-0.565
Marital: Widowed or divorced	-0.549	-0.518	-0.508
Race: Non-white	-0.090	-0.109	-0.111
Sex: Female	-0.117	-0.134	-0.126
log(Tax + 1)	0.067	0.071	0.066
log(Social security + 1)	-0.026	-0.009	-0.017

complex synthesis model. Although this is no formal guarantee, the regularization in the density ratio model limits the influence each observation has on the density ratio values. We return to this issue in the discussion.

To demonstrate the idea, we fit a linear regression model predicting the logarithm of household income using all predictors in the data set (i.e., age, household property taxes, social security payments, sex, race, marital status and education level) on the observed data and the semi-continuous synthetic data. Subsequently, we estimate the model on the semi-continuous synthetic data using the estimated density ratio values as importance weights. Table 2 shows the coefficients of these regression models averaged over the $m = 5$ synthetic datasets, where boldface text denotes the coefficient with smallest absolute bias compared to the estimate obtained from the observed data. The table shows that although the synthetic regression coefficients are quite close to the observed data coefficients, the reweighed coefficients further improve the accuracy. Especially for the continuous predictors, age, household property taxes and social security payments, using the density ratio weights improves the estimates. Averaging the absolute normalized bias over all coefficients and all synthetic data sets yields an improvement from approximately $\text{avg}(|\beta_{\text{obs}} - \beta_{\text{syn}}|/SE_{\text{obs}}) = 1.98$ to $\text{avg}(|\beta_{\text{obs}} - \beta_{\text{syn-adj}}|/SE_{\text{obs}}) = 1.41$ after reweighing. Hence, besides providing a measure of global utility, the estimated density ratio can be used to further improve the utility of the synthetic data.

5 Discussion and conclusion

High quality utility measures are essential when creating synthetic data for use in downstream tasks. These measures provide an insight into the quality of the synthetic data, and can be used to guide the synthesis process, fostering higher quality synthetic data. In this paper, we provided a framework for evaluating synthetic data utility through density ratio estimation. Our simulations and illustration show that the density estimation framework can be used in a wide variety of settings, and yields more accurate results than established procedures for evaluating synthetic data utility under a variety of synthetic data models and sample sizes, all using the same default hyperparameter specifications. Moreover, we showed that the estimated density ratio, besides providing a global utility measure, serves as a measure of local

utility, and can even be used directly to further improve specific utility of the synthetic data. We have made these methods openly available through the `densityratio` package in R (Volker 2023).

Throughout the paper, we have contrasted the density ratio framework with existing utility measures as the $pMSE$ and the Kullback-Leibler divergence. Both measures can be considered special cases of the density ratio framework. The Kullback-Leibler divergence explicitly contains the density ratio in its definition, and Appendix B describes how the k -nearest neighbor approach to KL -divergence estimation gives rise to a direct estimate of the density ratio. The $pMSE$ can also be seen as a special case of the density ratio framework, by noting that the predicted probabilities are easily transformed into density ratios (see Sugiyama, Suzuki, and Kanamori 2012a). In fact, Menon and Ong (2016) show that density ratio estimation is equivalent to class probability estimation (as performed in the $pMSE$), in the sense that minimizing a class probability estimation loss is equivalent to minimizing a Bregman divergence to the true density ratio function. These connections raise the question which model class, and which loss function, is most appropriate when the goal is to evaluate the utility of synthetic data.

While we leave a formal evaluation of this question to future work, we can provide some intuitions. First, utility measures ought to be robust, in the sense that they should not be too sensitive to extreme values in the observed data, as this may pose a privacy risk. That is, extreme cases typically bear higher disclosure risk as they do not blend into the crowd (Gehrke et al. 2012). If the utility measure is too sensitive to these extreme cases, small discrepancies that serve to protect privacy may seem to reflect low quality synthetic data. Sugiyama, Suzuki, and Kanamori (2012b) showed that uLSIF is relatively robust to outliers compared to density ratio estimation using the KL -loss, but the robustness can further be improved by using different loss functions (such as Basu’s power divergence; Basu et al. 1998). Second, utility measures should work well in a wide-variety of settings, so users do not need to fine-tune utility measures and focus on the problem at hand. To this end, non-parametric methods may be preferred over parametric methods, as they do not hinge upon an appropriate model specification. Although correctly specified parametric models are more efficient in a statistical sense, they are less reliable when the model is misspecified (Sugiyama, Suzuki, and Kanamori 2012a). Throughout the paper, we have shown that uLSIF serves as a suitable compromise between flexibility and robustness, although the KL -divergence using k -nearest neighbor density ratio estimation may be more sensitive to discrepancies between the observed and synthetic data.

By viewing synthetic data utility through the lens of density ratio estimation, several appealing properties are obtained. First, the density ratio perspective encompasses global and local utility in a single framework. The estimated density ratio gives rise to global utility measures, but also allows for the identification of variables that have not been modelled adequately. Additionally, the estimated density ratio can be used directly to improve the utility of the synthetic data, by reweighing the synthetic data to better match the observed data. These findings are supported by other research showing that synthetic data utility can be improved by importance weighting (Ghalebikesabi et al. 2022). The proposed framework provide a flexible class of models that are easily implemented through the `densityratio` package (Volker 2023), that tailor to a wide variety of settings. Moreover, several extensions are available to deal with high-dimensional data, enabling the evaluation of the quality of synthetic data with many variables, such as spectral density

ratio estimation (Izbicki, Lee, and Schafer 2014) and least-squares heterodistributional subspace search (Sugiyama, Yamada, et al. 2011), both implemented in the `densityratio` package. Finally, the framework can be used directly to create synthetic data, as the density ratio can serve the role of discriminator in generative models (Uehara et al. 2016).

Despite the appealing characteristics of density ratio estimation, several open questions remain. Kernel methods, as typically employed in density ratio estimation, can be sensitive to the choice of kernel, and the use of a Gaussian kernel may not be appropriate in any situation. Categorical variables, for instance, are not straightforwardly incorporated in the current set-up. To deal with this issue, we created dummy variables for each category in our illustration, which seemed to provide reasonable results. However, other solutions (i.e., different kernels or distance measures) may lead to improvements. Additionally, our results showed that the current approach to regularization is not ideal, as the density ratio estimates are shrunk towards an estimated intercept. However, when the intercept deviates from one, the numerator or denominator density are up or downweighted. Rather, one would like to shrink the density ratio estimates towards one, as this is more in line with the interpretation that there is no information to estimate the density ratio. Finally, releasing information from the density ratio may pose an additional privacy risk, as it leaks additional information about the original data. Presumably, solely releasing a global utility measure, such as the Pearson divergence, will yield only additional risk. Releasing the density ratio values themselves may, however, pose unacceptable privacy risks, especially when the density ratio model is sensitive to extreme cases. Privatizing density ratio estimation presents an interesting avenue for future research.

Despite these open questions, we have shown that already in its current form, density ratio estimation provides a flexible and informative framework for evaluating synthetic data utility. Due to its in-built model selection, it requires little specification on behalf of the user and works well in a wide variety of settings. The framework can be readily incorporated into synthetic data workflows using the `densityratio` package.

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A Density ratio estimation in R

To perform density ratio estimation in R, we can use the `densityratio` package, which includes model fitting functions for multiple popular loss functions. Additionally, we can complement the package with standard optimization routines in R. Here, we show an example of both approaches.

We generate two small toy datasets, x and y , that serve as numerator and denominator data, respectively. Moreover, we set x as the centers in the Gaussian kernel, and we pre-define the kernel bandwidth to be $\sigma = 1$ and fix the regularization parameter to $\lambda = 0.5$. Note that we do not perform cross-validation for hyperparameter selection to enhance illustrational clarity. Subsequently, we fit a density ratio model using the `ulsif()` function from the `densityratio` package.

```
library(densityratio)

set.seed(123)

x <- rnorm(250) |> as.matrix()
y <- rnorm(250, 1, sqrt(2)) |> as.matrix()

fit_dr <- ulsif(x, y, centers = x, scale = NULL, sigma = 1, lambda = 0.5)
rhat_dr <- predict(fit_dr)
```

We can obtain the same solution using standard optimization techniques. In order to do this, we first need to define the kernel matrices for the numerator and denominator data, and define a loss function that can be used in optimization. We then use the `optim()` function to minimize the loss function. Recall that we use a linear model for the density ratio, as per Equation 8, we use a Gaussian kernel as basis function, and we use the least-squares loss of Equation 5.

```
Dx <- distance(x, x, TRUE)
Dy <- distance(y, x, TRUE)

Kx <- kernel_gaussian(Dx, sigma = 1)
Ky <- kernel_gaussian(Dy, sigma = 1)

loss <- function(alpha, Kx, Ky) {
  mean((Ky %*% alpha - 1) * Ky %*% alpha - (Ky %*% alpha - 1)^2 / 2) -
  mean(Kx %*% alpha - 1) +
  0.5/2 * sum(alpha^2) # ridge penalty
}

alpha <- runif(ncol(Kx))
fit_optim <- optim(alpha, loss, Kx = Kx, Ky = Ky,
  method = "BFGS",
  control = list(maxit = 10000))

rhat_optim <- Kx %*% fit_optim$par
```

Subsequently, we can show that both procedures yield equivalent results (see Figure A1). Moreover, the sum of squared difference between the estimated density ratio parameters equals $6.5e-11$, and the sum of squared difference between the predicted density ratios equals $1.75e-08$.

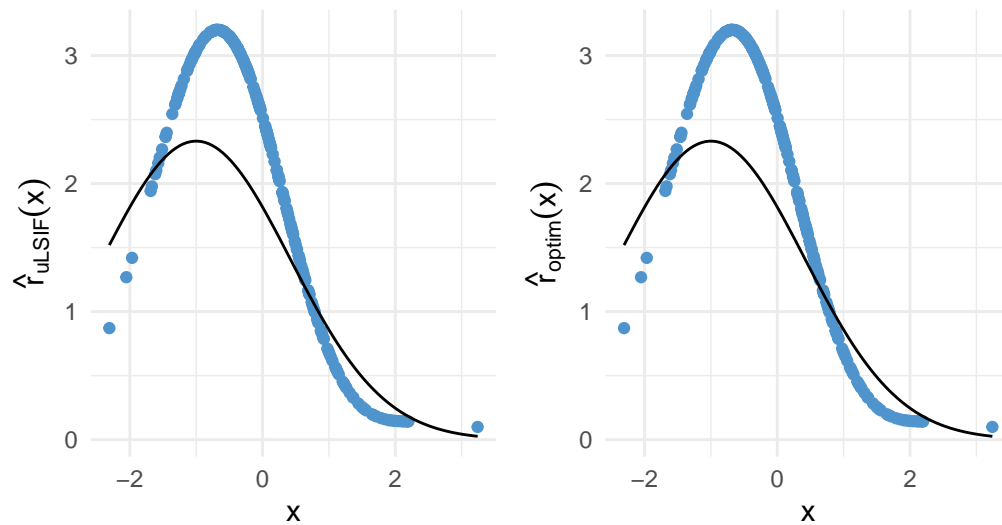


Figure A1: Density ratio estimation using `ulsif()` from the `densityratio`-package and using standard optimization in R.

If we were to perform cross-validation for hyperparameter selection, we could run the `ulsif()`-function without specifying the `sigma` and `lambda` arguments. The function then performs a grid search over a predefined range of hyperparameters. Moreover, it is possible to supply a vector of `sigma` and `lambda` values to `ulsif()`, after which cross-validation is automatically performed.

```
fit <- ulsif(x, y, centers = x, scale = NULL)
fit
```

Call:

```
ulsif(df_numerator = x, df_denominator = y, scale = NULL, centers = x)
```

Kernel Information:

Kernel type: Gaussian with L2 norm distances

Number of kernels: 250

sigma: num [1:10] 0.0601 0.177 0.2971 0.4228 0.5583 ...

Regularization parameter (lambda): num [1:20] 1000 483.3 233.6 112.9 54.6 ...

Optimal sigma: 0.7045195

Optimal lambda: 1.43845

Optimal kernel weights (loocv): num [1:251] 0.03123 0.03174 0.02443 0.00876 0.01296 ...

The model output shows the optimal `sigma` parameter out of a vector containing ten values, and the optimal `lambda` parameter out of a vector containing twenty values. The package also includes density ratio estimation techniques, such as `klipe()`, `kmm()`, `spectral()`, `lhss()` and `naive()`, that all work in a similar fashion. Additionally, the package contains generic functions to `predict()` with, `plot()`, or `summarize` (e.g., `summary()`) the fitted models. Moreover, computationally intensive code is implemented in C++ through Rcpp ([Eddelbuettel 2013](#)) and most func-

tions allow for parallel computation through the `openmp`-backend in C++. The interested reader is referred to the package documentation (Volker 2023) for additional information.

B k -Nearest neighbor density ratio estimation

We note that density ratio estimation through k -nearest neighbor density estimation can also be considered a direct approach to density ratio estimation. Using k -nearest neighbors, an estimate of the density can be obtained by

$$\hat{p}_{\text{obs}}(\mathbf{x}_i) = \frac{k}{n-1} \cdot \frac{\Gamma(d/2+1)}{\pi^{d/2} B_k^d(\mathbf{x}_i^{(\text{obs})})},$$

where d denotes the dimensionality of the input data, $\Gamma(d/2+1)/\pi^{d/2}$ is a normalizing constant, and $B_k^d(\mathbf{x}_i^{(\text{obs})})$ denotes the Euclidean distance of each observation in $\mathbf{x}^{(\text{obs})}$ to its k -th nearest neighbor in $\mathbf{x}^{(\text{obs})}$ raised to the power d (see, e.g., Wang, Kulkarni, and Verdu 2009;). Applying the same procedure for the denominator data (i.e., the synthetic data), we can estimate the density ratio as

$$\begin{aligned} \hat{r}(\mathbf{x}_i) &= \frac{\hat{p}_{\text{obs}}(\mathbf{x}_i)}{\hat{p}_{\text{syn}}(\mathbf{x}_i)} \\ &= \frac{\frac{k}{n-1} \cdot \frac{\Gamma(d/2+1)}{\pi^{d/2} B_k^d(\mathbf{x}_i^{(\text{obs})})}}{\frac{k}{m} \cdot \frac{\Gamma(d/2+1)}{\pi^{d/2} B_k^d(\mathbf{x}_i^{(\text{syn})})}} \\ &= \frac{m}{n-1} \cdot \frac{B_k^d(\mathbf{x}_i^{(\text{syn})})}{B_k^d(\mathbf{x}_i^{(\text{obs})})}, \end{aligned}$$

where m denotes the number of observations in the synthetic data, and $B_k^d(\mathbf{x}_i^{(\text{syn})})$ denotes the Euclidean distance of each observation in $\mathbf{x}^{(\text{obs})}$ to its k -th nearest neighbor in $\mathbf{x}^{(\text{syn})}$ raised to the power d . Accordingly, a direct estimate of the density ratio can be obtained as

$$\hat{r}(\mathbf{x}) = \text{diag}\{\tilde{B}_k^d(\mathbf{x}^{(\text{obs})})\}^{-1} \tilde{B}_k^d(\mathbf{x}^{(\text{syn})}),$$

where $\tilde{B}_k^d(\mathbf{x}^{(\text{obs})})$ and $\tilde{B}_k^d(\mathbf{x}^{(\text{syn})})$ denote the vectors with distances of each observation in $\mathbf{x}^{(\text{obs})}$ to their k -th nearest neighbor in $\mathbf{x}^{(\text{obs})}$ and $\mathbf{x}^{(\text{syn})}$ raised to the power d , multiplied by the respective sample sizes.

Applying this estimate of the density ratio to the simulated data from the univariate simulations, and setting $k = 15 \approx \sqrt{n}$, as suggested by the authors who introduced k -nearest neighbor density estimation (Loftsgaarden and Quesenberry 1965), we can compare the performance of the k -nearest neighbor density ratio estimation to the density ratio estimation through uLSIF.

It can be seen that the k -nearest neighbor density ratio estimation performs well on average (the green lines in Figure A2), especially in the center of the distribution. However, it suffers from a similar bias in regions where the number of observations is low (as the density ratio is typically underestimated in the tails). Moreover, k -nearest neighbor den-

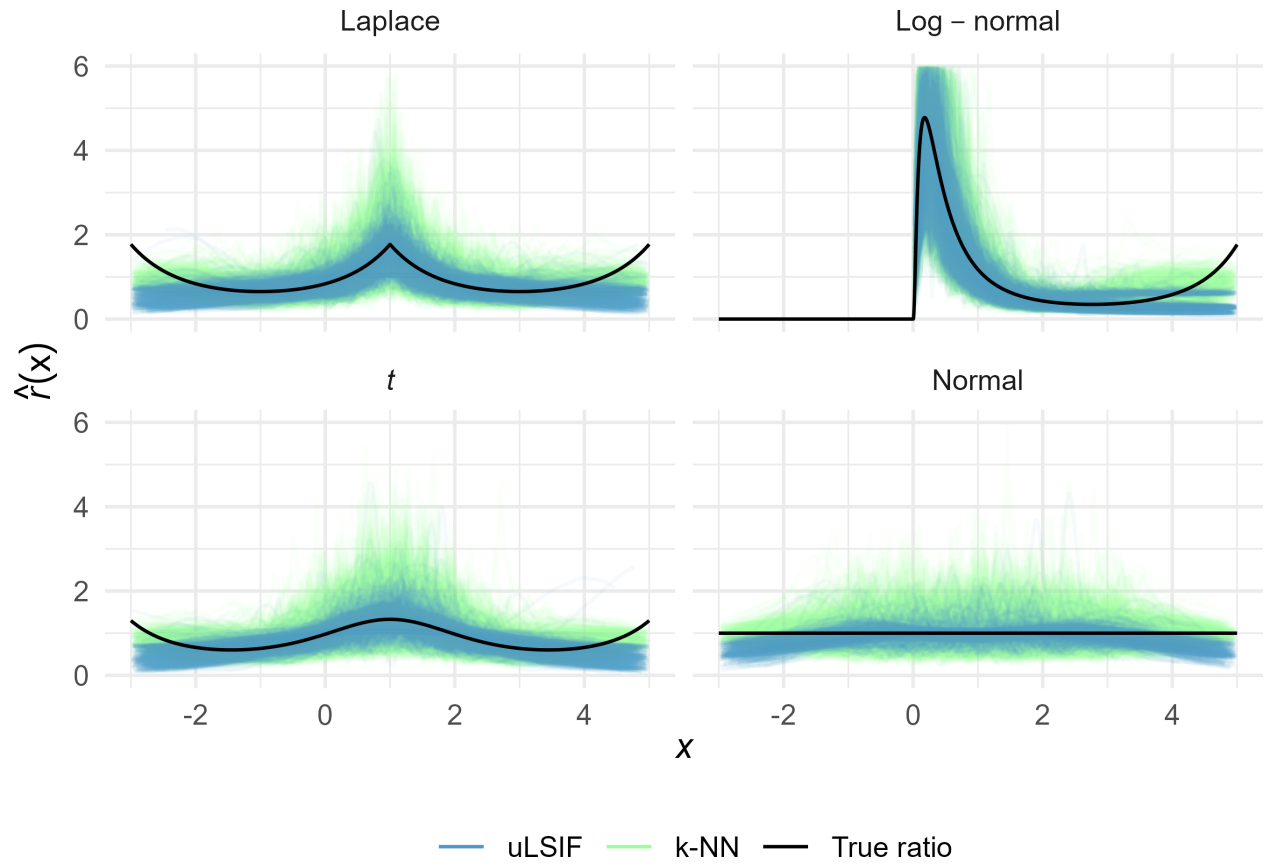


Figure A2: Density ratio estimation through k -nearest neighbor density ratio estimation ($k = 15$) and uLSIF.

sity ratio estimation has much higher variance than density ratio estimation through uLSIF, as can be seen by the fact that the green lines cover a much wider band than the blue lines.