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ASSESSING THE UTILITY OF SYNTHETIC DATA: A DENSITY RATIO PERSPECTIVE

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Abstract

High quality synthetic data can be a solution to overcome disclosure risks that arise when disseminating research data to the public. However, for inferential purposes, the usefulness of the synthetic data largely depends on whether the synthetic data model approximates the distribution of the observed data close enough. Often, multiple candidate models are considered and improvements are made iteratively. Evaluating the utility of the synthetic data after the model building steps is a crucial but complicated endeavor, and although many methods exist, their results may tell an incomplete story. We propose to evaluate the utility of synthetic data using density ratio estimation techniques, which allows to embed both general and specific utility measures into a common framework. Using techniques from the density ratio estimation field, we show how an interpretable global utility measure can be obtained from the ratio of the observed and synthetic data densities that can even be used to express the utility of individual (synthetic) data points. Applying these techniques on (an approximation to the) posterior distributions of parameters gives rise to analysis-specific utility measures. Using empirical examples, we show that framing utility from a density ratio perspective improves on existing global utility measures. Lastly, we implemented the procedure along with existing utility measures in an R-package.

Introduction

In recent years, the academic interest in synthetic data has exploded. Synthetic data is increasingly being used as a solution to overcome privacy and confidentiality issues that are inherently linked to the dissemination of research data. National statistical institutes and other government agencies have started to disseminate synthetic data to the public while restricting access to the original data to protect sensitive information (e.g., [Abowd, Stinson, and Benedetto 2006](#); [Hawala 2008](#); [Drechsler 2012](#)). At the same time, researchers start to share a synthetic version of their research data to comply with open science standards (e.g., [Wiel et al. 2023](#); [Obermeyer et al. 2019](#); [Zettler et al. 2021](#)). Rather than sharing the original research data, a synthetic surrogate is shared to facilitate reviewing the data processing and analysis pipeline. Additionally, synthetic data is increasingly being used for training machine learning models ([Nikolenko 2021](#)). On a lower level, synthetic data can be used in model testing pipelines (before access to the real data is provided), for data exploration (misschien YOUTH citeren all), and for educational purposes.

In short, the general idea of synthetic data is to substitute values from the collected data with synthetic values that are generated from a model. In this way, it is possible to generate an entirely new synthetic data set [commonly referred to as the *fully* synthetic data approach; [Rubin \(1993\)](#)], but one could also replace only those values that would yield a high risk of disclosure when released [called *partially* synthetic data; [Little \(1993\)](#)]. Both approaches essentially attempt to build a model that incorporates as much of the information in the real data as possible. The models used to generate synthetic data were originally closely related to methods used for multiple imputation of missing data, such as fully conditional specification ([Volker and Vink 2021](#)) or sequential regression ([Nowok, Raab, and Dibben 2016](#)). Recently, significant improvements in generative modelling in combination with work on formal privacy guarantees sparked the development of a great deal of novel methods in the computer science community (e.g., [Patki, Wedge, and Veeramachaneni 2016](#); [Xu et al. 2019](#)). Through these developments, the quality of synthetic data improved significantly, and while the notion of using fake data for research purposes was originally regarded as laughable, it is nowadays increasingly being used in practice.

The main challenge when generating synthetic data is to adequately balance the privacy leakage with the utility (i.e., quality) of the synthetic data. On the upper limit of this privacy-utility trade-off, the synthesis model is so good (or, rather, bad), that the real data is exactly reproduced, resulting in the same privacy loss as when disseminating the real data. In statistical terms, the synthesis model is overparameterized to such an extent that there are no degrees of freedom left, and there is thus no randomness involved in the generation of the synthetic values. On the lower limit of the trade-off, synthetic values are generated without borrowing any information from the real data. For example, we could place the value 0 or a random draw from a standard normal distribution for every record and every variable, such that the synthetic data contains only noise. A synthesis model usually sits somewhere between these two extremes, and contains some information from the real data, which implies that the synthetic data resembles the real data to some extent, yielding more than zero utility, but also some disclosure risk. The data provider typically wants to know what privacy loss is incurred by disseminating the synthetic data, while the user wants to know whether any analysis can be reliably performed. At the same time, knowledge about the utility can help the data provider to improve the quality of the synthesis model. Hence, the synthetic data provider is left with the complicated task of qualifying where on this continuum the synthetic data is located.

Based on this privacy-utility trade-off, it seems obvious that any attempt of data synthesis results in the loss of information. Accordingly, the utility of the synthetic data will always be lower than the utility of the real data. The questions that naturally arise are how much information is sacrificed, and how much the synthetic data deviates from the observed data. In the synthetic data literature, three classes of utility measures have been distinguished (for a thorough review of these measures, see [Drechsler and Haensch 2023](#)): fit-for-purpose measures, analysis-specific utility measures and global utility measures. Fit-for-purpose measures are typically the first step in assessing the quality of the synthetic data. They typically involve comparing the univariate distributions of the observed and synthetic data (for example using visualization techniques or goodness-of-fit measures). Although very useful to get an initial impression of the quality of the data synthesis models used, this picture is by definition limited, because only one or two variables variables are assessed at the same time. Hence, complex relationships between variables will always be out of scope. Global utility measures build up on the fit-for-purpose measures, by comparing the distribution of the synthetic data with the distribution of the observed data in a more general way. This can be done using some distance measure [e.g., the Kullback-Leibler divergence; see [Karr et al. \(2006\)](#)], but also by estimating how well a prediction model can distinguish between the observed and synthetic data, and using the predicted probabilities [propensity scores; [Rosenbaum and Rubin \(1983\)](#)] as a measure of discrepancy [e.g., the propensity score mean squared error, $pMSE$; [Woo et al. \(2009\)](#); [Snoke et al. \(2018\)](#)]. While global utility measures paint a rather complete picture, that is, over the entire range of the data, they tend to be too general. That is, global utility measures can be so

broad that important discrepancies between the real and synthetic data can be missed, and an a synthetic data set with high global utility might still yield analyses with results that are far from the results from real data analyses (see Drechsler 2022). Lastly, the analysis-specific utility measures quantify to what extent analyses performed on the synthetic data align with the same analyses on the observed data. These measures can evaluate to what degree the coefficients of a regression model are similar [e.g., using the confidence interval overlap; Karr et al. (2006)], but also to what extent prediction models trained on the synthetic and observed data are perform similarly in terms of evaluation metrics. However, also these measures have important shortcomings. Analysis-specific utility generally does not carry over, even not to closely related analyses: 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 (for a more thorough discussion, see Drechsler 2022).

From the other perspective on the privacy-utility trade-off, that is, the privacy-side, several promising advances have been made with respect to building formal privacy guarantees into the data generation mechanism through differential privacy (CITE DWORK; CITE DP-SYNTHESIS METHOD). In addition to these privacy-by-design mechanisms, some measures exist to quantify privacy loss of synthetic data after generation. However, the practical applicability of these measures depends on whether the data is fully or partially synthetic, and especially in case of the former, the practical applicability of these measures is often limited (for an extensive discussion of these issues, see Drechsler and Haensch 2023). More research on measures to evaluate disclosure risks in synthetic is thus certainly needed, but the current paper focuses on utility measures for synthetic data.

Specifically, we illustrate a group of methods under the umbrella of density ratio estimation (for a thorough evaluation of work done in this area, see Sugiyama, Suzuki, and Kanamori 2012a) for assessing synthetic data utility that incorporates fit-for-purpose, global and analysis-specific utility measures. In short, the framework of density ratio estimation attempts to compare the multivariate distributions of two data sets (e.g., two different samples or groups) by directly estimation the ratio of their densities. The idea is that if two data sets are drawn from the same data-generating mechanism, their densities should be similar, and the ratio of their densities should thus be close to one at all possible points in the multivariate space. This approach easily extends from univariate to bivariate and multivariate densities. As such, it bridges the gap between fit-for-purpose and global utility measures. Moreover, a density ratio can also be estimated for the posterior distributions of parameters, and thus also incorporates specific utility measures. The only requirement of density ratio estimation is that there are samples (e.g., observations, samples from a posterior) from the observed and synthetic data (or parameter) distributions, or that these distributions can be approximated, for example with a (multivariate) normal distribution. It is not required to assume some parametric distribution, but in cases where no samples are available, it can help to simplify the process of estimation the density ratio. Note that density ratio estimation deliberately does not entail estimating the densities of the observed and synthetic data separately, and taking their ratio. Estimating the probability distribution of a data set is one of the hardest challenges in statistics, unavoidably resulting in estimation errors. When performing this task for two data sets, and subsequently taking the ratio, may magnify the estimation errors, resulting in a poorer estimate of the density ratio than necessary when directly estimating the density ratio.

In what follows, we describe the density ratio estimation framework, summarizing some of the work done in this area. We will briefly relate the method to existing utility measures, and describe how existing utility measures either fall under the umbrella of density ratio estimation, or are related to those. Subsequently, we will illustrate how the method can be used in practice by providing multiple examples. Lastly, we will discuss shortcomings of the method and relate these to avenues for future work.

Density ratio estimation

The framework of density ratio estimation 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 for 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 [or, in statistical terms, sample selection bias; Kanamori, Hido, and Sugiyama (2009)], and, importantly, two-sample homogeneity tests (Sugiyama et al. 2011). Regardless of the exact goal, the idea is to compare two distributions by estimating the density ratio $r(\mathbf{x})$ between the probability distributions of the numerator samples, which we take to be the synthetic data samples, $p_{syn}(\mathbf{x})$, and the denominator samples, which we take to be the observed data samples, $p_{obs}(\mathbf{x})$. A naive approach would

be to estimate the observed and synthetic data density separately, for example using kernel density estimation [REF], and subsequently compute the ratio from these estimated densities. However, density estimation is one of the hardest tasks in statistical learning, and is prone to estimation errors that would affect both estimated densities. When subsequently taking the ratio of the estimated densities, the estimation errors might be magnified, and the validity of the resulting density ratio might be lower than strictly necessary. In fact, extensive simulations on a wide variety of tasks showed that directly estimating the density ratio typically outperforms naive kernel density estimation, especially when the dimensionality of the data increases (e.g., [Kanamori, Suzuki, and Sugiyama 2012](#); [Hido et al. 2008](#); [Kanamori, Hido, and Sugiyama 2009](#)).

Over the past years, several methods for direct density ratio estimation have been developed, that typically employ some divergence measure to estimate the distance from the density ratio model to the true density ratio function. To keep the discussion general, we focus here on a class of methods that employ the *Bregman* divergence to quantify this distance (for a thorough review and technical discussion, see [Sugiyama, Suzuki, and Kanamori 2012b](#)). In some sense, this framework bears some resemblance to model selection using information criteria (e.g., Akaike's information criterion), where the distance from a statistical model to the true data-generating mechanism is estimated (e.g., by relying on an estimate of the Kullback-Leibler divergence). In fact, the Kullback-Leibler divergence is a special case of the more general class of Bregman divergences, and one of the density ratio estimation techniques (the Kullback-Leibler importance estimation procedure; [Sugiyama et al. 2008](#)) relies on the Kullback-Leibler divergence to estimate the density ratio function. Other special cases of the Bregman divergence include the Euclidean distance and the Mahalanobis distance.

HIER PLAATJE TOEVOEGEN VAN DENSITY RATIO ESTIMATION

[[COMMENT: TO BE FAIR, IM NOT SO SURE HERE ABOUT ALL TECHNICALITIES IN THE UPCOMING SECTION. PERHAPS IT'S BETTER TO LEAVE THESE OUT, AND JUST DISCUSS THE GENERAL IDEA WITHOUT GOING INTO THE DETAILS. I'M STILL SEEKING A BIT ABOUT THE RIGHT TRADE-OFF BETWEEN TECHNICAL AND NON-TECHNICAL STUFF]]

Formally, for a strictly convex and continuously-differentiable function f , the Bregman divergence measures the distance from the value of f at point t and the value of the first-order Taylor expansion of f at point \hat{t} , such that

$$\text{BR}'_f(t, \hat{t}) = f(t) - f(\hat{t}) - \partial f(\hat{t})(t - \hat{t}),$$

with $\langle \cdot, \cdot \rangle$ denoting the inner product, and ∂f denoting the derivative of f . Let the true density ratio function of the synthetic data samples over the observed data samples be defined as

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

Approximating the true density ratio function $r(\mathbf{x})$ with the density ratio model $\hat{r}(\mathbf{x})$, the Bregman divergence is expressed as

$$\text{BR}'_f(r, \hat{r}) = \int p_{\text{obs}}(\mathbf{x}) \left(f(r(\mathbf{x})) - f(\hat{r}(\mathbf{x})) - \partial f(\hat{r}(\mathbf{x}))(r(\mathbf{x}) - \hat{r}(\mathbf{x})) \right) d\mathbf{x}.$$

Accordingly, the true Bregman divergence can be approximated empirically by

$$\hat{\text{BR}}_f(\hat{r}) = \frac{1}{n_{\text{obs}}} \sum_{i=1}^{n_{\text{obs}}} \partial f(\hat{r}(\mathbf{x}_i^{\text{obs}})) \hat{r}(\mathbf{x}_i^{\text{obs}}) - \frac{1}{n_{\text{obs}}} \sum_{i=1}^{n_{\text{obs}}} f(\hat{r}(\mathbf{x}_i^{\text{obs}})) - \frac{1}{n_{\text{syn}}} \sum_{i'=1}^{n_{\text{syn}}} \partial f(\hat{r}(\mathbf{x}_{i'}^{\text{syn}})),$$

where n_{obs} and n_{syn} denote the sample size of the observed and synthetic data, respectively (for a more elaborate explanation, see Chapter 7 in [Sugiyama, Suzuki, and Kanamori 2012a](#)). Accordingly, the following minimization criterion can be defined:

$$\min_{\hat{r}} \hat{\text{BR}}_f(\hat{r}).$$

Note that how to minimize this function is dependent on the function f .

By choosing the function f in different ways, we can formulate the optimization problem such that it agrees with several density ratio estimation procedures. For the sake of brevity, we only show how to formulate the optimization problem such that it corresponds with one specific density ratio estimation technique, called least-squares importance fitting (LSIF; [Kanamori, Hido, and Sugiyama 2009](#)), which has favorable theoretical properties. However, multiple other density ratio estimation techniques can also be formulated in terms of a member of the Bregman divergence family (for a more extensive discussion, see [Sugiyama, Suzuki, and Kanamori 2012b](#)). If the function f is specified as

$$f(\hat{t}) = \frac{1}{2}(\hat{t} - 1)^2,$$

the Bregman divergence can be reformulated as the squared distance

$$\begin{aligned}\text{BR}'_f(t, \hat{t}) &= f(t) - f(\hat{t}) - \partial f(\hat{t})(t - \hat{t}) \\ &\equiv \frac{1}{2}(t - \hat{t})^2 = \text{SQ}'.\end{aligned}$$

Expressing the squared distance between the true density ratio and the density ratio model yields

$$\text{SQ}'(\hat{r}) = \frac{1}{2} \int (\hat{r}(\mathbf{x}) - r(\mathbf{x}))^2 p_{obs}(\mathbf{x}) d\mathbf{x}.$$

Now, dropping $r(\mathbf{x})^2$ which is constant with respect to the data, and rewriting $2\hat{r}(\mathbf{x})r(\mathbf{x})$ as $2\hat{r}(\mathbf{x})p_{syn}(\mathbf{x})/p_{obs}(\mathbf{x})$ yields

$$\text{SQ}'(\hat{r}) = \frac{1}{2} \int \hat{r}(\mathbf{x})^2 p_{obs}(\mathbf{x}) d\mathbf{x} - \int r(\mathbf{x}) p_{syn}(\mathbf{x}) d\mathbf{x}.$$

Consequently, Kanamori, Hido, and Sugiyama (2009) show how the integrals can be approximated with empirical averages,

$$\hat{\text{SQ}}(\hat{r}) = \frac{1}{2n_{obs}} \sum_{i=1}^{n_{obs}} \hat{r}(\mathbf{x}_i^{obs})^2 - \frac{1}{n_{syn}} \sum_{i'=1}^{n_{syn}} \hat{r}(\mathbf{x}_i^{syn}),$$

after which this criterion can be minimized.

To actually minimize this criterion, we need a density ratio model. For least-squares importance fitting, Kanamori, Hido, and Sugiyama (2009) define the following model

$$\hat{r}(\mathbf{x}) = \sum_{\ell=1}^b \theta_\ell \psi_\ell(\mathbf{x}) = \boldsymbol{\psi}(\mathbf{x})' \boldsymbol{\theta},$$

with $\boldsymbol{\psi}(\mathbf{x})$ a non-negative basis function vector and $\boldsymbol{\theta}$ the vector with parameter estimates. Rewriting the estimated squared error in accordance with this density ratio model yields

$$\hat{\text{SQ}}(\boldsymbol{\theta}) = \frac{1}{2n_{obs}} \boldsymbol{\theta}' \boldsymbol{\psi}(\mathbf{x}^{obs})' \boldsymbol{\psi}(\mathbf{x}^{obs}) \boldsymbol{\theta} - \frac{1}{n_{syn}} \boldsymbol{\psi}(\mathbf{x})' \mathbf{1}_{n_{syn}} + \lambda \boldsymbol{\theta}' \boldsymbol{\theta},$$

where the last term is added for regularization purposes. The solution to this optimization problem can be obtained analytically by solving

$$\hat{\boldsymbol{\theta}} = \left(\frac{1}{n_{obs}} \boldsymbol{\psi}(\mathbf{x})' \boldsymbol{\psi}(\mathbf{x}) + \lambda \mathbf{I}_b \right)^{-1} \frac{1}{n_{syn}} \boldsymbol{\psi}(\mathbf{x})' \mathbf{1}_{n_{syn}}.$$

Note that this procedure is called unconstrained least-squares importance fitting, because the solution is unconstrained, potentially resulting in negative density ratio values. This can be accounted for by either setting negative density ratio values to 0, or by using a convex quadratic program to solve the optimization problem (using an ℓ_1 regularizer instead of an ℓ_2 regularizer). The regularization parameter λ , as well potential parameters of the basis functions, can be optimized using cross-validation, by computing the out-of-sample squared error (see Kanamori, Hido, and Sugiyama 2009).

Hier nog iets zeggen over dat een gaussian kernel een goede keus is voor basis function, omdat deze goede properties heeft.

Nog toevoegen dat een statistische test gebaseerd op permutaties gedaan kan worden.

Illustrations of density ratio estimation as a utility measure

Deze tekst moet nog aangepast worden, maar wilde eerst graag weten of de voorbeelden oke zijn. Ik wil ook nog een voorbeeld toevoegen met een lognormale verdelingen die benaderd wordt door een normaalverdeling, maar ik ben nog even bezig met uitzoeken hoe ik dan de variantie en het gemiddelde gelijk krijg (omdat de verwachting van een lognormaalverdeelde variabele een functie is het gemiddelde en de standaarddeviatie op de logschaal). Een alternatief kan ook zijn om iets met een zero-inflated (en dus bimodal) model te doen, omdat dit dan zou voortborduren op de presentatie van Jorg Drechsler bij PSD.

Verder wil ik ook nog graag een multivariaat voorbeeld toevoegen, maar ik twijfel nog een beetje over de context (misschien iets met aflopende correlaties, zoals Snoke et al. in hun pmse paper doen), maar het kan ook iets met subspaces of dimension reduction zijn (maar vraag me af of het dan niet teveel wordt).

En ik wil graag aan de voorbeelden zoals ze nu zijn nog graag een permutatie-test statistiek toevoegen, zodat we een beetje kunnen classificeren hoe goed de methode het doet. Als dat erbij zit, zitten we denk ik wel aan tien pagina's [VRAAG AAN PP: IS DEZE LIMIET INCLUSIEF OF EXCLUSIEF VOORBLAD EN REFERENTIES?]. Ook over specific-utility moeten we het dan misschien nog eventjes hebben, want het lijkt me wat veel om dat hier ook nog als voorbeeld in te gooien, dus misschien alleen in de discussie kort bespreken. Laten we het hier maandag over hebben!

In the upcoming section, we display how density ratio performs in some typical examples. In the synthetic data field, it is easily happens that some complicated data distribution is approximated by a simpler one. For example, when the real data distribution follows a Laplace distribution, it is quite plausible that this data is approximated by some normal distribution. Similarly, it can very well be that data that is distributed according to a t -distribution with, say, three degrees of freedom (and thus with relatively fat tails), is approximated by a normal distribution.

```
library(purrr)
library(densityratio)
library(ggplot2)

set.seed(123)

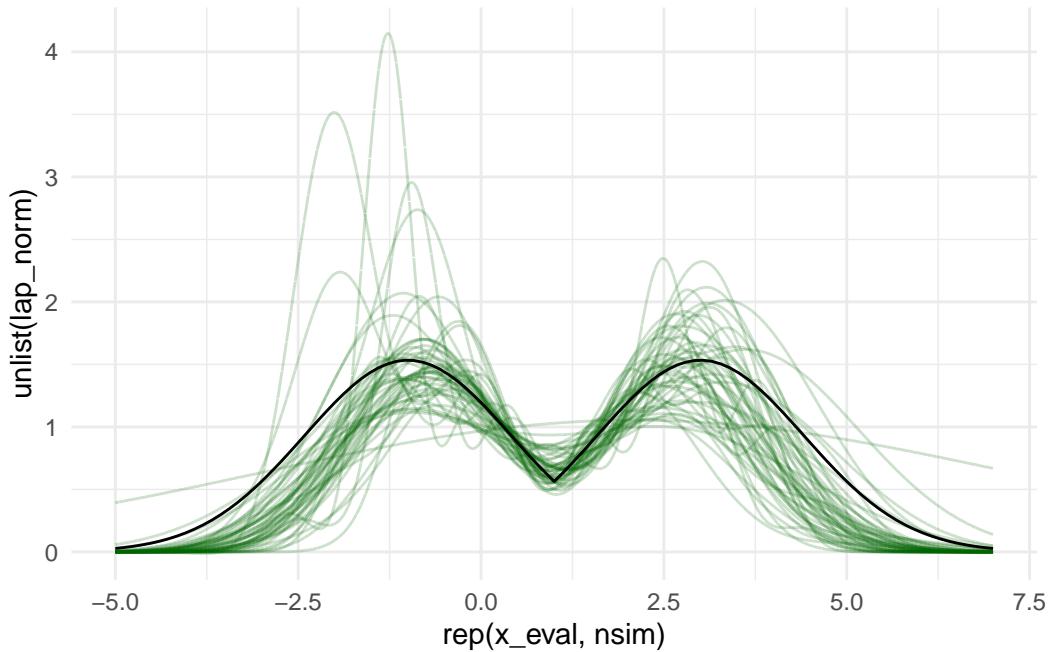
nsim <- 50
n <- 500
mu <- 1
sd <- sqrt(2)

x_eval <- seq(-5, 7, length.out = 10000) |> matrix()

dlaplace <- function(x, mu = 0, sd = 1) exp(-abs(x-mu)/(sd / sqrt(2))) / (2*(sd / sqrt(2)))
rlaplace <- function(n, mu = 0, sd = 1) {
  p <- runif(n)
  b <- sd / sqrt(2)
  mu - b * sign(p - 0.5) * log(1 - 2*abs(p - 0.5))
}
dratio <- function(x, mu_norm = 0, mu_laplace = 0, sd_norm = 1, sd_laplace = 1) {
  dnorm(x, mu_norm, sd_norm) / dlaplace(x, mu_norm, sd_norm)
}

lap_norm <- map(1:nsim, function(x) {
  normal <- rnorm(n, mu, sd)
  laplace <- rlaplace(n, mu, sd)
  ratio <- ulsif(normal, laplace, ncenters = 100, nsigma = 10, nlambda = 10, progressbar = FALSE)
  predict(ratio, newdata = x_eval)
})

ggplot() +
  geom_line(mapping = aes(x = rep(x_eval, nsim),
                          y = unlist(lap_norm),
                          group = rep(1:nrow(x_eval), each = nsim) |> factor()),
            alpha = 0.2, col = "darkgreen") +
  stat_function(fun = dratio,
                args = list(mu_norm = mu, mu_laplace = mu, sd_norm = sd, sd_laplace = sd)) +
  theme_minimal()
```



```

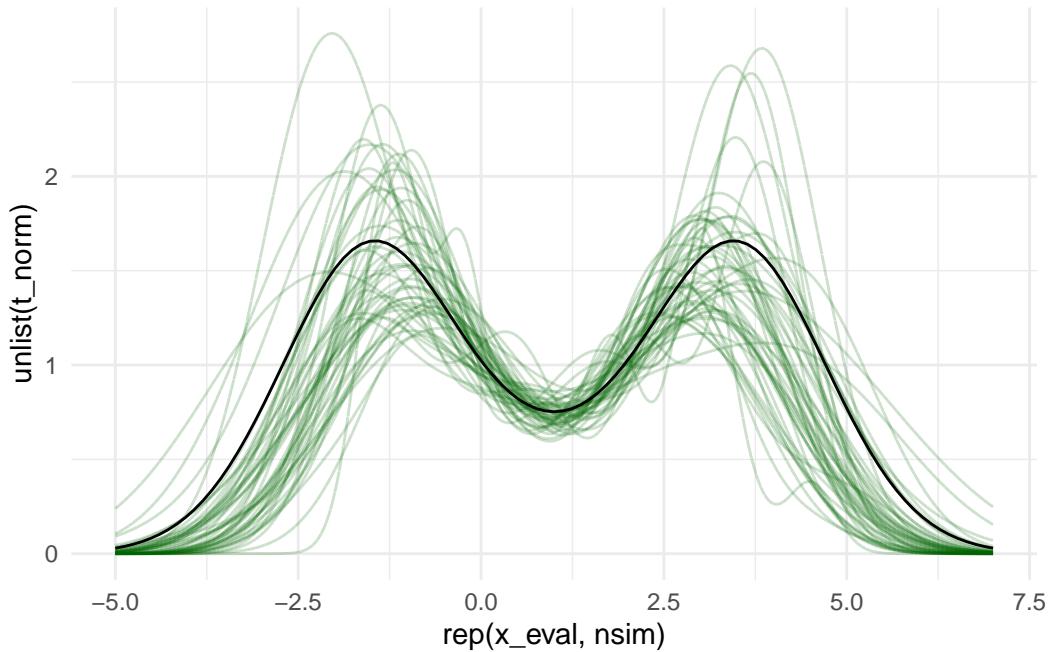
mean_rlnorm <- log(log(exp(1) / sqrt(1 + 2 / exp(2 * 1))))
sd_rlnorm <- sqrt(log(1 + 2 / exp(2 * 1)))

dratio_norm_t <- function(x, mu = 0, df = 4) {
  dnorm(x - mu, 0, sqrt(df / (df-2))) / dt(x - mu, df)
}

t_norm <- map(1:nsim, function(x) {
  normal <- rnorm(n, 1, sqrt(2))
  t <- rt(n, 4) + 1
  ratio <- ulsif(normal, t, ncenters = 100, nsigma = 10, nlambda = 10, progressbar = FALSE)
  predict(ratio, newdata = x_eval)
})

ggplot() +
  geom_line(mapping = aes(x = rep(x_eval, nsim),
                          y = unlist(t_norm),
                          group = rep(1:nrow(x_eval), each = nsim) |> factor(),
                          alpha = 0.2, col = "darkgreen") +
    stat_function(fun = dratio_norm_t,
                 args = list(mu = 1, df = 4)) +
    theme_minimal())

```

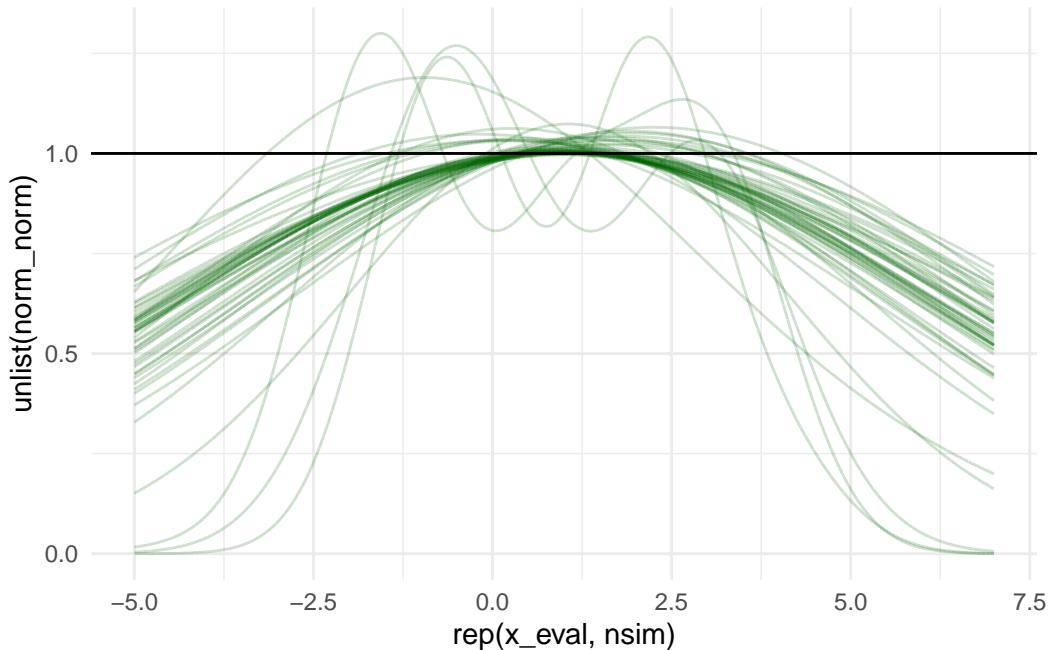


```

norm_norm <- map(1:nsim, function(x) {
  normal1 <- rnorm(n, 1, sqrt(2))
  normal2 <- rnorm(n, 1, sqrt(2))
  ratio <- ulsif(normal1, normal2, ncenters = 100, nsigma = 10, nlambd = 10, progressbar = FALSE)
  predict(ratio, newdata = x_eval)
})

ggplot() +
  geom_line(mapping = aes(x = rep(x_eval, nsim),
                          y = unlist(norm_norm),
                          group = rep(1:nrow(x_eval), each = nsim) |> factor()),
            alpha = 0.2, col = "darkgreen") +
  geom_abline(intercept = 1, slope = 0) +
  theme_minimal()

```



```
# multivariate normal versus multivariate normal
#
# multivariate normal versus something else
```

Discussion

Number of centers

Model selection

Dealing with categorical variables

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