An experimental study on Synthetic Tabular Data Evaluation

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(Abstract) In this paper, we present the findings of our investigation into various methodologies for measuring the similarity of synthetic data generated from real data samples. Our focus is on cases where the synthetic data has a significantly larger number of samples than the real data, which presents a unique challenge in terms of evaluating the reliability of the generated data. We evaluate commonly used global metrics from the literature and introduce a novel approach based on topological data analysis. This approach has several advantages for addressing the complexity of high-dimensional synthetic data with a greatly increased sample size. It allows for the study of geometric properties without considering quantitative distance function values, and focuses on the concept of “closeness” between points. We also propose an approach using Eigen vectors to evaluate the level of noise in synthetic data and assess the similarity to the original data.

Key words: tabular data, synthetic data, Low Sample Size (HDLSS), global statistical tests, topological data analysis.

1. TABULAR SYNTHETIC DATA

Because of considerations such as privacy constraints, bias in some algorithms’ training, and improving existing data quality, the use of generative models to build synthetic data is becoming more widespread. In this article, we will look at a specific application of generative models to synthetic tabular data generation: generating synthetic data with much more samples than the real data. The existing literature does not explicitly address this issue, instead refers to the generation and evaluation of synthetic data, presuming that increasing the quantity of samples is not the primary goal (Benaim et al., 2020; Cheng et al., 2019; Eno & Thompson, 2008; Goncalves et al., 2020; Hou et al., 2022; Karras et al., 2018; Rashid & Louis, 2019).

Tabular data is one of the most prevalent data sources in data analysis. This data is widely used in applications such as academics, business management, and any other case where a spreadsheet is used to collect data from multiple variables in tables. These tables use to have a small number of samples (rows) and, in most of the cases, several columns or variables. This data is known as HDLSS (High Dimension, Low Sample Size) (Hall et al., 2005). But the use of HDLSS with machine learning algorithms is frequently questioned since the sample size is considered insufficient for producing reliable conclusions. Many users of these tables would like to gain insights into the data and even make predictions. The generation of synthetic data from tabular data is well studied in the literature. However, there are no references to the specific challenge that we propose: generating synthetic data from small-sized samples.

2. GLOBAL DATA METRICS

In this work, we will explore some of the most important global data metrics identified in the literature (Benaim et al., 2020; Borgwardt et al., 2006; Chundawat et al., 2022; Eno & Thompson, 2008; Goncalves et al., 2020; Goodfellow, 2014; Rosenbaum & Rubin, 1983; Snoke et al., 2018; Snoke & Slavković, 2018; Sutherland et al., 2016, 2017; Theis et al., 2016; Woo et al., 2009a, 2009b; Xu et al., 2018). We will not consider two-sample statistical tests to be valid metrics since they do not capture the interdependencies and patterns between the multiple independent variables. Confirming the hypothesis that synthetic and original data samples represent the same underlying metrics since they do not prove that a synthetic dataset can replace the original when used with a machine learning algorithm to make predictions or gather insights. Global metrics captures not only the underlaying probability distribution of all variables. They also capture relationships between them.

In this section we are going to describe two global metrics: propensity score and cluster analysis measure. This metrics consider

Definition 2.1 Let $\mathcal{X}$ be a sub spaces of $\mathbb{R}^m$ with the same metric $k$. Let $\text{Prob}(\mathcal{X})$ denote the spaces of probability measures defined on $\mathcal{X}$. $\mathbb{P}_d$ is the probability distribution of original data and $\mathbb{P}_s$ the distribution of synthetic data, where $\mathbb{P}_d \mathbb{P}_s \in \text{Prob}(\mathcal{X})$. This methods are not based in finding
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elementary distances and divergences between the two distributions \( \mathbb{P}_d, \mathbb{P}_s \in \text{Prob}(\mathcal{X}) \) as it happens with other methods as Total Variation (TV) distance or the Kullback-Leibler (KL) divergence (Arjovsky et al., 2017), that can be defined as and

\[
d : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}^+
\]

satisfying

\[
d(\mathbb{P}_d, \mathbb{P}_s) \geq 0
\]

and

\[
d(\mathbb{P}_d, \mathbb{P}_s) = 0 \quad \text{if and only if} \quad \mathbb{P}_d = \mathbb{P}_s
\]

For this reason, these methods (propensity score and cluster analysis measure) can’t be considered “distances” neither “divergences”.

2.1 Propensity score

The propensity score is the conditional probability of assignment to a particular treatment given a vector of observed covariates (Rosenbaum & Rubin, 1983). If to samples has similar distributions of covariates, their propensity scores distributions tends to be the same. This equivalence is valid for univariate and multivariate distributions. This model proposes a method for assessing data quality (Woo et al., 2009b). For its calculations, the steps will be the following: we combine the original and synthetic data sets, assigning a variable with a value of one to all synthetic data instances and a value of zero to all original data instances. The probability of each case occurring in both the synthetic and original data sets is then computed (the propensity score) using a classification algorithm. Then, we examine the propensity score probability distributions in both, the original and synthetic data. When both distributions are similar, the validity, and so its utility, of the data should be relatively high.

Definition 2.1.1 To calculate the propensity score we can use a classification algorithm like the logistic regression where the predicted probability for each instance will be the values of the propensity score. Snoke et al., 2018 proposed the following definition:

\[
p^{\text{MSE}} = \frac{1}{N} \sum_{i=1}^{N} (\hat{p}_i - 0.5)^2
\]

where \( N \) is the number of samples, \( p_i \) the predicted probabilities and \( p^{\text{MSE}} \) is the mean-squared error of the logistic regression-predicted probabilities.

Cluster analysis measure uses a supervised machine learning classification algorithm to validate the likelihood of a data instance belonging to an original or synthetic sample. Note that this method follows a similar rationale than the discriminator network in a Generative Adversarial Network or GAN originally proposed by Goodfellow et al., 2014. In GAN’s, the discriminator network is trained to maximize the probability of assigning the correct label to both training examples and samples from generator network’s train. Propensity score also quantifies the probability of assigning the correct label to a combined dataset including both original and synthetic samples.

2.2 Cluster analysis measure

Cluster analysis measure (Woo et al., 2009b) also uses a supervised machine learning technique but it looks for similarities in the data using distances.

Definition 2.2.1 If we divide a dataset \( \mathcal{X} \) in two parts of size \( \mathcal{L} \) and \( \mathcal{L}' \) it's expected that the percentage of observations in \( \mathcal{L} \) is given by

\[
\frac{N_L}{N_L + N_{L'}} = c
\]

To proceed, we also combine the original and synthetic data sets, assigning a variable with a value of one to all synthetic data instances and a value of zero to all original data instances. Then we perform a cluster analysis choosing a fixed number of clusters \( \mathcal{C} \) and calculate the following:
\[ U_c = \frac{1}{c} \sum_{i=1}^{c} w_i \left[ \frac{n_{iD}}{n_i} - c \right]^2 \quad (2) \]

where \( n_i \) is the number of observations in the \( i \)-th cluster, \( n_{iD} \) is the number of observations from the original data in the \( i \)-th cluster, \( w_i \) is the weight assigned to \( i \)-th cluster. Large values of \( U_c \) means that points in the original and synthetic data spaces are too separated to fall in the same cluster. In this case we can “infer” that both probability distribution \( \mathbb{P}_d, \mathbb{P}_s \) are different.

Because both methods rely on a supervised-learning algorithm to identify original and synthetic samples, they cannot be considered hypothesis testing methods. Instead, both compute the likelihood that a sample belongs to each class.

### 2.3 Maximum Mean Discrepancy

Maximum Mean Discrepancy (MMD) is a non-parametric hypothesis testing statistic for comparing samples from two probability distributions (Gretton et al., 2006, 2009). However, it has been proved that the rate of convergence of MMD estimators to population size is independent of the underlying dimension of the data (Gretton et al., 2012; Ramdas et al., 2015). The use of test statistics based on quantities defined in reproducing kernel Hilbert spaces (RKHSs) is an approach that has gained a lot of popularity over the past few years. In parallel to this approach, the replacement of Euclidean norms for methods based on pairwise distances between points also have become popular (Lyons, 2013), with the advantage that performs better with high dimensions.

**Definition 2.3.1** Given \( m \) samples \( x_1 \ldots x_m \) drawn from a distribution \( P \) from subspace \( \mathcal{X} \), where \( \mathcal{X} \subseteq \mathbb{R}^d \), and \( n \) samples \( y_1 \ldots y_n \) drawn from a distribution \( Q \) from subspace \( \mathcal{Y} \), where \( \mathcal{Y} \subseteq \mathbb{R}^d \) (Lyons, 2013; Ramdas et al., 2015).

Let \( k : \mathcal{X} \times \mathcal{X} \to \mathbb{R} \) and \( k \in \mathcal{H} \), be a positive-definite kernel corresponding to RKHS \( \mathcal{H}_k \) with inner product \( \langle \cdot, \cdot \rangle_k \). Let \( k \) correspond to feature maps at \( x \) denoted by \( \phi_x \in \mathcal{H}_k \), satisfying

\[ \phi_x(x) = \langle \phi_x, \phi'_x \rangle = k(x, x') \]

The mean embedding of \( P \) is \( \mu_p := \mathbb{E}_x \sim p \phi_x \). The Maximum Mean Discrepancy (MMD) is defined

\[ \text{MMD}^2(P, Q) := \| \mu_p - \mu_q \|^2 \quad (3) \]

\( \text{MMD}^2 \) satisfy the conditions \( \text{MMD}^2(P, Q) \geq 0 \), and \( \text{MMD}^2(P, Q) = 0 \) if \( P = Q \). One of the most common kernels is Gaussian rbf. The function rbf kernels computes the radial basis function (RBF) kernel between two vectors. This kernel is defined as

\[ k(x, x') = \exp(-\gamma \| x - x' \|^2) \]

Small \( \gamma \) values defines a Gaussian function with a large variance.

The advantage of this method is the use of kernel methods for clustering. Kernel defines similarities between observations, hence providing all the information needed to assess the quality of a clustering.

### 3. TOPOLOGICAL DATA ANALYSIS

Topological data analysis or TDA is a collection of methods that provides qualitative data analysis (Carlsson, 2009). The mathematical field of topology is concerned with the study of qualitative geometric information. In order to gain knowledge from high-dimensional data sets, the connectivity of the data, or how a data space’s connected elements are organized, TDA has become an essential tool. The benefits of using data connectivity were emphasized by Carlsson, 2009.
“Topology studies geometric properties in a way which is much less sensitive to the actual choice of metrics than straightforward geometric methods, which involve sensitive geometric properties such as curvature.”

One of the most practical benefits of replacing distances with connectivity information is definitely found in high-dimensional spaces. The data in high-dimensional spaces is sparse and tends to concentrate close to a certain region. In these regions, the connectivity between the points becomes more substantial than their distance (Beyer et al., 1998). The choice of a distance metric is generally not straightforward in high-dimensional data applications, and the idea for similarity calculation is very heuristic (Aggarwal et al., 2001).

### 3.1 Homology and Persistence diagrams

Homology is an algebraic invariant that counts the topological attributes of a space (Carlsson et al., 2004). The collection of these components is a qualitative invariant of the space. Spaces are path-connected in a specific way, and this property is preserved under continuous deformations. We can differentiate between two spaces with a mathematical formulation of these properties. Among these properties, line-connections are considered level-zero connectivity information and loops level-one connectivity information.

**Definition 3.1.1** For any topological space \( X \), abelian group \( X \), and integer \( k \geq 0 \), there is assigned a group \( H_k(X, A) \).

**Definition 3.1.2** Filtered complex: Let \( X \) denote a metric space, with metric \( d \). Then the Vietoris-Rips complex for \( X \), attached to the parameter \( \varepsilon \), denoted by \( VR(X, \varepsilon) \), will be the simplicial complex whose vertex set is \( X \), and where \( x_0, x_1, \ldots, x_k \) spans a \( k \)-simplex if and only if \( d(x_i, x_j) \leq \varepsilon \) for all \( 0 \leq i, j \leq k \).

A simplicial complex is an expression of the space as a union of points, intervals, triangles, and higher dimensional analogues (Carlsson, 2009). Topological spaces can be approximated using simplicial complexes.

**Definition 3.1.3** Betti numbers: For any field \( F \), \( H_k(X, F) \) will be a vector space over \( F \). Its dimension, if it is finite dimensional, will be written as \( \beta_k(X, F) \), and will be referred to as the \( k \)-th Betti number with coefficients in \( F \). The \( k \)-th Betti number corresponds to an informal notion of the number of independent \( k \)-dimensional surfaces. If two spaces are homotopy equivalent, then all their Betti numbers are equal (Carlsson, 2009).

![Figure 1. The Rips complex on a point cloud VR(X, ε). a) A set of point cloud data X; b) Vietoris-Rips complex for X, VR(X, ε); c) Persistence simplicial complex as union of points, intervals, triangles, and higher dimensional analogues; d) Betti numbers \( \beta_0 \) and \( \beta_1 \) for \( H_0 \) and \( H_1 \).](image-url)
**Definition 3.1.4** The $k$-th persistent homology of the filtration $X$ is the sequence

$$PH_k(X, F): H_k(X_0, F) \rightarrow H_k(X_1, F) \rightarrow H_k(X_k, F)$$

of vector spaces and induced linear transformations (Barnes et al. 2021). If each $H_k(X_j, F)$ is finite dimensional and $\beta_k^{j,\ell}(X_k, F)$ denotes the rank of the linear transformation $H_k(X_j, F) \rightarrow H_k(X_k, F)$ induced by the inclusion $X_j \subset X_k$, $j \leq \ell$, the persistence diagram of $PH_k(X, F)$ denoted $dgm(X, F)$, is the collection of pairs $(j, \ell)$ with nonzero multiplicity.

**Definition 3.1.5** A barcode is a finite set of intervals that are bounded below (Carlsson et al., 2004). Barcodes represent the space at various scales. They are a family of intervals with endpoints in $\mathbb{R}^+$ derived from homology vector spaces $\{H_i(\text{VR}(X, \varepsilon))\}$ $\varepsilon > 0$. Each such interval can be considered as a point in the set $D = \{(x, y) \in \mathbb{R}^2 | x \leq y\}$.

Let $Y$ denote the collection of all possible barcodes. We need to define a quasi-metric $D(S_1, S_2)$ on all pairs of barcodes $(S_1, S_2)$, with $(S_1, S_2) \in Y$.

### 3.2 Comparison of persistence diagrams

#### 3.2.1 Distances between persistence diagrams

Topological spaces or shapes can be approximated by simplicial complexes, an expression of the space as a union of points, intervals, triangles, and higher dimensional analogues. We say that two shapes are similar if both have the same topological signature. The maximum difference between the distance functions of two shapes is equal to the Hausdorff distance between the shapes (Cohen-Steiner et al., 2005).

**Definition 3.2.1** The Hausdorff distance and the Bottleneck distance between $X$ and $Y$ are

$$d_H(X, Y) = \max\{\sup_x \inf_y \|x - y\|_{\infty}, \sup_y \inf_x \|y - x\|_{\infty}\} \quad (4)$$

$$d_B(X, Y) = \inf_{\gamma} \sup_x \|x - \gamma(x)\|_{\infty} \quad (5)$$

The bottleneck distance is based on a bijection between the points in a diagram and is bounded from below by the Hausdorff distance (Cohen-Steiner et al., 2005). Given two persistence diagrams $X, Y$

if $d_H(X, Y) < \varepsilon$ then $d_B(X, Y) < \varepsilon$.

#### 3.2.2 Empirical distribution tests

While the homology of $X$ captures information about the global topology of the metric space, the probability space structure plays no role at all (Blumberg et al., 2014). This leads us to a fundamental limitation when we want to use hypothesis testing and confidence intervals to compare different topological invariants. We want to determine if we can reject the hypothesis that two empirical distributions on barcode space $Y$ (definition 3.1.5) came from the same underlying distribution, and with transformations will be needed. As the majority of asymptotic results on non-parametric tests for distribution comparison work only for distributions on $\mathbb{R}$, so the first transformation will be to map data from barcode space $Y \rightarrow \mathbb{R}$.

**Definition 3.2.1** (Blumberg et al., 2014) Let $(X, \partial X, \mu_x)$ be a compact metric measure space and $k, n \in \mathbb{N}$. Let $\{z_1, z_2, ..., z_i\}$ a sequence of randomly drawn samples from $(X, \partial X, \mu_x)$. $z_i$ is a metric measure space using the subspace metric and the empirical measure. Then $\phi^0_k(z_i)$ converges in probability to $\phi^0_k(X, \partial X, \mu_x)$. For any $\varepsilon > 0$

$$\lim_{n \rightarrow \infty} p |\phi^0_k(z_i) - \phi^0_k(X, \partial X, \mu_x) > \varepsilon| = 0$$
Definition 3.2.2 (Blumberg et al., 2014) Y denote the collection of all possible barcodes. We can define a distance distribution \( D \) on \( \mathbb{R} \) to be the distribution on \( \mathbb{R} \) induced by applying \( d_S(\cdot, \cdot) \) to pairs \((S_1, S_2)\) drawn from \( \phi^n_k(X, \partial^1_\mathbb{R}, \mu_x) \).

Definition 3.2.2 (Blumberg et al., 2014) Let \( S \) be a barcode, \( S \in Y \). \( D_S \) will be the distribution induced by applying \( d_S(S, \cdot) \). Since \( D \) and \( D_S \) are continuous with respect to the Gromov-Prohorov metric, \( D_S \) converge in probability to \( D \).

So can directly compare distributions on barcode spaces \( D \in \mathbb{R} \) (Definition 3.2.2) using hypothesis testing. One application of these projections is the use of the two-sample Kolmogorov-Smirnov statistic (Massey, 1951). This test statistic offers a method of assessing whether two empirical distributions observed were drawn from the same underlying distribution. The most important strength of this statistic is that, for distributions on \( \mathbb{R} \), the test statistic’s p-values are asymptotically independent of the underlying distribution provided. An alternative to Kolmogorov-Smirnov test statistic is the Mann-Whitney U test (McKnight & Najab, 2010) which is also known as the Wilcoxon rank sum test and is used to find differences between two groups on a single, ordinal variable with no specific distribution. Finally, another suitable method for testing the independence of two barcodes distribution could be the Chi-square test of independence of variables in a contingency table (Lin et al., 2015; Virtanen et al., 2020).

4. SINGULAR VALUE DECOMPOSITION

Singular Value Decomposition or SVD is one of the most important and well-known linear algebra tools and is commonly used in dimensionality reduction. The Singular Value Decomposition of a matrix \( A_{mn} \) can be defined as the factorization of \( A_{mn} \) as \( A_{mn} = U_{mn}S_{mn}V_{mn}^T \). The columns of \( U \) and \( V \) are orthonormal eigenvectors of \( AA^T \). \( S \) is a diagonal matrix containing the square roots of eigenvalues from \( U \) or \( V \).

The diagonal matrix \( S \) elements are nonnegative numbers known as singular values, and its number is equal to the rank of \( A \), say \( k \). Furthermore, \( U \) and \( V \) have exactly \( k \) columns, which are referred to as the left and right singular vectors, respectively (Baker, 2005). Another important use of singular values is dimensionality reduction. Suppose we have a matrix \( A_{mn} \) with \( n \) columns that has some linear relations. Then we say that data lies in a \( k \)-subspace of \( \mathbb{R}^m \) where \( k < m \).

An intuitive explanation about SVD is that singular vectors “encode” meaningful concepts about data represented in \( A \) (Bradley, 2020). We can think of diagonal matrix \( S \) as providing a “bridge” between information about the rows of \( U \) (data samples) and information about the columns of \( V \) (data columns). \( S \) could then indicate the amount of “interaction” between the information stored by \( U \) and \( V \), and intervene in how those interactions contribute to the information represented by the original matrix \( A \). This amount of “interaction” can be understood as a quantitative measure of patterns available in data. Working with this intuition could be very useful when we compare original data with synthetically generated data. Both original and synthetic data matrices \( A, A' \) should have the same low rank \( k \) as long as synthetic data has to keep the existing relations between the \( m \) columns in the original data matrix. Therefore singular vectors \( S, S' \) should encode similar information even when they are matrices of different shape \( S_{mn}, S'_{m'n} \) where \( m' \gg m \). Han et al., 2021 have recently proposed a metric called Variance concentration that answer the following question: ¿What’s the data variance percentage concentrated on the direction of the first singular value?.

Definition 4.1 Given a dataset \( X \) with \( n \) observations and \( m \) variables: \( X \in \mathbb{R}^{n \times m} \), its variance concentration ratio (VCR) is defined as

\[
VCR(X) = \frac{s_1}{\Sigma_{i=1}^{\min(n,m)} s_i}
\]

where \( s \) are the singular vectors of the matrix \( S \). This ratio ranges from 0 to 1 (or 0 to 100%). When \( VCR = 1 \) means that \( USV = U_{1s}S_{1s}V_{1s}^T \). VCR measures if matrix \( A \) is closer to a rank-1 matrix than \( A' \). Low-rank approximation can be seen as a way to recover the “original” (the “ideal” matrix without noise) low-rank matrix.
**Definition 4.2** For evaluating the difference of a synthetic generated dataset we should consider the following inequality

\[
VCR(X_{\text{synthetic}}) \geq VCR(X_{\text{data}})
\]

First singular vector in synthetic dataset should encode similar information than the vector from the original data but not less (and presumably shouldn't offer more either). If \(VCR\) in synthetic data is lower than \(VCR\) in original data, it would mean that the synthetic data has lost some valuable information about the dependence of data variables as well as the relationships between data samples (rows) and data columns (variables).

\(VCR\) can also be used to evaluate the explainability of manifold learning in terms of DLPs (degree of locality preservation) on high-dimensional data (Han et al., 2022). A low-dimensional dataset, for example, would have a high \(VCR\) value, whereas a high-dimensional one would have a small one. In manifold learning a dataset with a high \(VCR\) is more likely to induce more entries from the local data geometry of a point \(x\) to repeat in the equivalent local data geometry of the embedding point of \(x\). Thus \(VCR\) can be used to evaluate if the local geometry of points in high dimensional data is preserved in its corresponding manifold.

**Definition 4.3** The isometry assumption (Donoho & Grimes, 2003). Given two points \(x, y \in \mathbb{R}^m\), the geodesic distance \(g\) satisfies

\[
g(x, y) = |\theta_x - \theta_y|, \text{ where } \forall x \leftrightarrow \theta_x, y \leftrightarrow \theta_y
\]

where \(\theta_x\) and \(\theta_y\) are vectors with some control parameters underlying \(x, y\), and \(|\cdot|\) denotes the Euclidean distance in \(\mathbb{R}^m\).

**Definition 4.4** Given two points \(x, y \in \mathbb{R}^n\) and a manifold \(f_d: X \rightarrow X'\) map where \(X \in \mathbb{R}^n\) and its embedding space \(X' \in \mathbb{R}^l\), with \(n > l\). The probability of that expected pairwise embedding distance and expected pairwise distance in the input space are approximately equal is defined as (Han et al., 2022)

\[
p\left(\frac{\|f_d(x) - f_d(y)\|}{\|x - y\|} \approx 1\right) = \frac{N}{n^2}
\]

where \(\|\cdot\|\) is a distance metric with \(L\) norm, \(N\) is \(th\)-total size of the largest neighborhoods keeping the locally isometric relationship, and \(n\) the number of variables of \(X\). In our experiments the total size of the largest neighborhoods keeping the locally isometric relationship can grow as we generate a larger number of new samples. But dimensionality \(n\) keeps constant and \(N_{X'} \geq N_X\), thus \(p\) has to be the same (or higher) in the synthetic dataset. If \(N\) is lower in the synthetic dataset, the local isometric geometry will not be kept, meaning that synthetic data does not preserve the complete structure or the original data.

**Definition 4.5** Let \(\mathcal{F}\) an arbitrary distribution with \(n\) points an dimensionality \(d\). We define \(D_{min_d}^k\) as the nearest distance of \(n\) points to the origin using the distance metric \(L_k\), and \(D_{max_d}^k\) as the farthest distance of \(n\) points to the origin using the distance metric \(L_k\). Then (Beyer et al., 1998)

\[
\lim_{d \to \infty} \mathbb{E}\left[\frac{D_{max_d}^k - D_{min_d}^k}{d^{k-2}}\right] = (n - 1) \cdot C_k
\]

where \(C_k\) is some constant dependent on \(k\).

For infinite dimensions, the distances \(D_{min_d}^k\) and \(D_{max_d}^k\) will converge to a constant value \(C_k\). For the Euclidean distance metric \((k = 2)\) the expression is bounded by \((C_k, (n - 1) \cdot C_k)\). The difference between max and min difference is independent on the dimension of the dataset and depends only of the number of samples. Then, the largest neighborhoods keeping the locally isometric relationship in Definition 4 will be dependent on the number of samples (and independent on the data dimensionality).
Corollary 4: Given a dataset $X$ with $n$ observations and $m$ variables $X \in \mathbb{R}^{n \times m}$ and a synthetically generated dataset $X'$ with $l$ observations and $m$ variables, $X' \in \mathbb{R}^{l \times m}$ where $l > n$ and $x', y' \in X'$ and $x, y \in X$. If

$$p \left\{ \frac{E \| f_d(x') - f_d(y') \|}{E \| x' - y' \|} \approx 1 \right\} \geq p \left\{ \frac{E \| f_d(x) - f_d(y) \|}{E \| x - y \|} \approx 1 \right\}$$

then we expect that

$$VCR(X') \geq VCR(X)$$

5. EXPERIMENTAL WORK

5.1 Datasets use in experiments

We have created two Low Sample Size or HDLSS datasets for our experimental work. The first dataset is call e-scooter and is a dataset for marketing analysis. It shows the relation between e-scooters price and some features. The data has a similar number of variables and observations, $n = 11$ observations and $m = 9$ variables. Data has both continuous and categorical variables. The second dataset is called SOFC (for solid oxide fuel cell) and include several features to model de cell’s output voltage. This dataset has $n = 30$ observations and $m = 13$ variables. This dataset contains only numerical variables. The SOFC modelling has been calculated according (Lakshmi & Geethanjali, 2013) and will have variables are directly correlated.

5.2 Results of the experimental work

We have generated a the synthetic datasets using the python open source library nbsynthetic that with a non-conditional generative Wassertein Generative Adversarial Network (Arjovsky et al., 2017). For the first experiment we have created synthetic dataset with $50 \times n$ observations (it means a total of 550 samples in the e-scooter dataset and 1500 in the SOFC dataset).

![Figure 2. Visual comparison of some features relations in original and synthetic data. SOFC dataset (left) and e-scooter dataset (right)](image)

In Figure 2 we can see a visual comparison of some features relations in the original and synthetic data. We see the original dataset has a significant lower number of points than synthetic data. Table 1 shows results the global data metrics used to compare both datasets.

| TABLE 1. Global metrics comparison |
|-----------------------------------|
| **SOFC** | **e-scooter** |
| Propensity score  | 0.08 | 0.11 |
| Cluster analysis measure  | -0.59 | 1.18 |
| MMD (Maximum Mean Discrepancy)  | 0.0340 | 0.0927 |

In the case of the propensity score and the MMD it’s values can range $(0, +\infty)$. Large values of Cluster analysis measure indicate disparities in the cluster memberships, which in turn suggest differences in the original and the synthetic data. Negative values suggest a high similarity between both datasets.
We observe higher similarity between original and synthetic data in the SOFC dataset according the propensity score and the MMD metrics. But, in both cases, all values tends to zero (but the cluster analysis measure), indicating that for both datasets, original and synthetic data is very similar.

We also wanted to evaluate the influence of the number of synthetic generated samples in the metrics. We have conducted four different experiments where we have created $5 \times n$, $10 \times n$, $20 \times n$ and $50 \times n$ synthetic samples for each dataset (remember that $n$ is the original number of samples in the dataset). Results can be seen in tables 2 and 3.

### TABLE 2. Metrics comparison for SOFC dataset with different number of samples

|                      | $5 \times n$ | $10 \times n$ | $20 \times n$ | $50 \times n$ |
|----------------------|--------------|---------------|---------------|---------------|
| Propensity score     | 0.03         | 0.02          | 0.05          | 0.08          |
| Cluster analysis measure | 0.37       | -0.38         | -0.57         | 43.59         |
| MMD (Maximum Mean Discrepancy) | 0.040    | 0.0367        | 0.0350        | 0.034         |
| Bottleneck distance  | 31.45        | 16.31         | 11.06         | 16.59         |
| Hausdorff distance   | 31.45        | 17.78         | 16.68         | 18.46         |
| Kolmogorov-Smirnov (p-value) | 0.4175 | 0.4175        | 0.4175        | 0.0524        |
| Mann-Whitney U test (p-value) | 0.6193 | 0.2687        | 0.4917        | 0.0351        |
| Chi-square test (p-value) | 0.1848 | 0.4454        | 0.4454        | 0.377         |
| Variance concentration (original) | 0.9788 | 0.9788        | 0.9788        | 0.9788        |
| Variance concentration (synthetic) | 0.9421 | 0.9475        | 0.9118        | 0.9492        |

Significance level $\alpha = 0.05$.

In these tables we have also included the test values obtained from the analysis of the topological signatures of data together with the global data metrics. Table 2 shows the results of evaluation the SOFC dataset. For topological data analysis of data we have computed the Haussdorff and the Bottleneck distances together with the statistical tests described in section 3.2.2.

Despite the global metrics could indicate that both, original SOFC data and synthetic data are very similar, the stational tests performed on topological signatures show that null hypothesis ($H_0$ - both distributions comes from the same sample can’t be rejected. Thus we could conclude that both persistence diagrams underlying distributions are not coming from the same sample distribution. This evidence is valid but for the case of generating a dataset with $50 \times n$ samples, where, surprisingly, we observe that null hypothesis can be rejected in Mann-Whitney U test. This there is a contradiction in the conclusions from using global metrics and analyzing topological attributes of data. For the other side, experiments generating different sample-size synthetic data shows that global metrics are stable but the cluster analysis measure. Also in the case of the data topology analysis we can think of similar conclusions but the rarity mentioned with the Mann-Whitney U test applied to the largest generated synthetic dataset. Given the random nature of both the method used to generate synthetic data and some tests, it is normal that the values obtained may vary within reasonable limits.

The results shown in Table 3 result from the e-scotter dataset analysis. We can validate some coherence between the results obtained with global metrics and the statistical test with topological signatures. Both groups of tests show that original and synthetic data are very similar, regardless of the number of generated samples. In this case, we can use the two approaches to formalize the same conclusion: Both the global metrics similarity test and the hypothesis test performed on topological data features illustrate that synthetic and original data samples are very similar.

### TABLE 3. Metrics comparison for e-scotter dataset with different number of samples

|                      | $5 \times n$ | $10 \times n$ | $20 \times n$ | $50 \times n$ |
|----------------------|--------------|---------------|---------------|---------------|
| Propensity score     | 0.1091       | 0.021         | 0.023         | 0.11          |
| Cluster analysis measure | -0.14     | -0.28         | -0.15         | 1.18          |
| MMD (Maximum Mean Discrepancy) | 0.1091   | 0.100         | -0.095        | 0.0927        |
| Bottleneck distance  | 725.51       | 725.51        | 725.53        | 725.53        |
| Hausdorff distance   | 1180.19      | 1117.86       | 976.28        | 1110.3        |
| Kolmogorov-Smirnov (p-value) | 0.0021 | 0.0002        | 0.0002        | 0.0002        |
| Mann-Whitney U test (p-value) | 0.0018 | 0.0002        | 0.0007        | 0.0002        |
| Chi-square test (p-value) | 0.0075  | 0.0186        | 0.0671        | 0.0103        |
| Variance concentration (original) | 0.9810 | 0.9810        | 0.9810        | 0.9810        |
| Variance concentration (synthetic) | 0.9785 | 0.9792        | 0.9820        | 0.9830        |

Significance level $\alpha = 0.05$.

In the case of SOFC model, we can see that Bottleneck and Hausdorff distances are very close, $d_H(X,Y)_{\text{synthetic}} \approx d_W(X,Y)_{\text{synthetic}}$ meanwhile in e-scotter data, both distances are clearly different. But in both cases the inequality presented in Definition 3.2.2 (Chazal et al., 2014) is valid.
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To dive into the reasons why SOFC dataset presents this deviation from the global metrics and the topological signature statistical tests conclusions, we have to look at the Variance concentration ratio VCR. The analysis of Variance concentration ratios of both datasets confirm the results obtained by the statical tests performed on topological signatures. In the case of SOFC data, the inequality $VCR_{synthetic} < VCR_{original}$ does not follow the definition 4.2. With e-scoter data, $VCR_{synthetic} \geq VCR_{original}$. It means that synthetically generated data from SOFC dataset has indeed an important amount of points that can be considered as noise. To check this observation, we have created a random synthetic dataset with the same number of samples than in synthetically generated data, and with equal limits (table 4).

| TABLE 4. Comparison of random data with synthetically generated data in SOFC dataset |
|---------------------------------|
|                                | 5 $\times$ n | 10 $\times$ n | 20 $\times$ n | 50 $\times$ n |
| $VCR_{original}$              | 0.9788         | 0.9788         | 0.9788         | 0.9788         |
| $VCR_{synthetic}$             | 0.9421         | 0.9475         | 0.9118         | 0.9492         |
| $VCR_{random}$                | 0.9347         | 0.9332         | 0.9328         | 0.9330         |

In Table 4 we show that the variance concentration ratio of synthetically generated data in SOFC data is more close to the random generated data than to original data. It proves that synthetic data is populated with a large number of samples that can be considered as random noise. An approach to validate the presence of a significant amount of noise in the synthetic data samples is by directly observing the representation of its persistence diagrams.

In Figure 3 we show the persistence diagrams of synthetic datasets for SOFC data with different number of samples. In homology dimension $H_0$ (links) we can see that all diagrams looks very similar (blue colored points). All points are concentrated with the exception of one or two than has an small separation of the main group. This can be interpreted as a “small cluster” of points a bit far from the main body of points forming a topological compact group. But in homology dimension $H_1$ (loops) we can see differences between the representations (red colored points). All points lying on the diagonal or very close can be considered as noise. Only distant points represent “real” data loops. We observe that in all cases the number of points close to the diagonal is very significative, and increasing with the number of data samples. Confidently the Figure 3 d) is the one that has a lower proportion of “noise” points. It can be certainly counterintuitive to think that when we generate a large number of samples we are generating less noise.

Figure 3. Persistence diagrams for dimensions $H_0$ and $H_1$ of synthetic generated datasets for SOFC data.

a) $5 \times n$, b) $10 \times n$, c) $20 \times n$ and d) $50 \times n$ samples
When we compare with the plots of persistence diagrams for synthetic data generated from e-scotter dataset (Figure 4) we discover important differences. When we generate a small number of samples points in homology dimension $H_1$ lies in the diagonal, therefore can be considered as noise. But there are only two points, thus we can consider them irrelevant for the analysis. In the large sample synthetic data there are also points lying in the diagonal, but with less proportion than what we have seen in diagrams from Figure 3. There is a high concentration of points near the diagonal that represent the highest proportion of points in $H_1$ and aren’t noise.

Another interesting observation arising from Figure 4 is that points in homology dimension $H_0$ are more sparse than observed in SOFC data’s diagrams (Figure 3). It indicates the presence of some clusters in path-connected components $H_0$ - green marked in Figure 4 a) - .This evidence is closely related with the conclusions obtained from the synthetic data evaluation. Global metrics, hypothesis test in topological signatures and variance concentration ratios prove that both e-scotter original and synthetic data are similar.

![Persistence diagrams for dimensions $H_0$ and $H_1$ of synthetic generated datasets for e-scotter data.](image)

The presence of these clusters as topological properties proves the existence of patterns in the data, which is certainly useful when efficiently generating synthetic data. Not all data sets can be used to generate synthetic data efficiently. Topological data analysis can also be used as a practical tool prior to applying generative models to predict if the data set may be coherently augmented.

6. CONCLUSIONS

In this article, we discussed the challenge of generating synthetic tabular data from data sets with a small number of samples and the need for accurate and robust metrics to evaluate the similarity between generated and synthetic data. We studied a selection of commonly used global metrics from the literature and developed a new method based on topological data analysis. Our experiments with different datasets proved that metrics produced from topological data analysis are more reliable than common global metrics. We also introduced a novel approach based on data eigenvalues, showing that this is more robust than existing global metrics and helps validate the results obtained through topological data analysis.

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