Evaluating Synthetically Generated Data from Small Sample Sizes: An Experimental Study

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ABSTRACT

This work proposes a method to evaluate the similarity between low-sample tabular data and synthetically generated data with a larger number of samples than the original. The technique is known to as data augmentation. However, significance values derived from non-parametric tests are questionable when the sample size is limited. Our approach uses a combination of geometry, topology, and robust statistics for hypothesis testing to evaluate the "validity" of generated data. We additionally contrast the findings with prominent global metric practices described in the literature for large sample size data.

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

1. Generating 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 paper, we will address the specific problem of generate synthetic tabular data with a larger number of 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 enaim 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. In most of the cases this data is considered as "small data". 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.

The use of low sample data with machine learning algorithms is frequently questioned since the sample size is considered insufficient for producing reliable conclusions. Most machine learning applications involve fitting a probability distribution over a vector of observations. When the number of observation is small, algorithms tends to overfit to the training examples. In this context, the problem arises when users of these tables wants to gain insights into the data and even be able to make predictions using machine learning.

Furthermore, most non-parametric tests used to validate these models also relies in the use of a sufficiently large number of observations. As a result, users of low sample tabular data do not have access to these technologies. For the experiments in this work we have use the python open source library nbsynthetic that uses a non-conditional Wassertein-GAN that will be introduced in the next section. This library is specifically designed for low sample synthetic data generation and augmentation.

1.1 Generative Adversarial Nets (GANs)

Low sample data has the particularity of setting less constrains to generalization process in NN. Deep Neural Networks (DNN) are designed to ingest a large number of input samples with large amount of training parameters in order to improve the accuracy of a given task (Elman, 1993). A common generalization method Maximum likelihood estimation. MLE works by maximizing the probability of the observed data according to the model. When Goodfellow et al., 2014 proposed the generative adversarial nets, the idea of regularization was not based on MLE. Instead he proposed a method derived from Noise-contrastive estimation or NSE. NSE uses an arbitrary, fixed "noise" distribution for the generator p_g instead of real input distribution. This is done by defining a parametric family of densities p_θ where the objective is to minimize the distance between the density p_θ and input data p_r (that can be done by minimizing the Jensen-Shannon divergence) varying the parameter θ. The goal of GAN proposed method is to learn a distribution that represents the source of synthetically generated data, where the distribution of a discriminator D, a binary classifier, p_c that tries to Figure out whether

a particular sample was selected from training data or from a "generator" distribution, p_g, is parameterized directly.

In summary, GAN's minimizes a convex divergence in space defined by a parametric family of densities what proves its asymptotic consistency (Goodfellow, 2014), it is, when model has enough ability to reproduce real data distribution, the objective achieves the unique global optimum when model distribution matches real data distribution.

The Wassertein GAN we are going to use in this paper is based on the fact that Wasserstein distance or Earth mover distance, $W(p_r, p_\theta)$ may have better qualities on comparing probability distributions than, for example, the Jensen-Shannon divergence (Arjovsky et al., 2017).

1.2 The GAN convergence problem

The question of training GAN with low sample data have already been studied by several authors (Chaudhari et al., 2020; Liu et al., 2019). Even if we want to increase the amount of synthetic samples compared to the original data, generating synthetic data from original samples is a relatively simple task. GANs, as other nets, struggle to capture the underlying structure of the data with low sample training data, and specially with fewer samples than dimensions. The discriminator attempts to identify samples from the training data or generator distribution, and while it initially converges, it may drift apart due to overfitting if there is not enough data. The generator may also be unable to reach a stable state with limited data, resulting in a lack of convergence and inadequate weight/bias adjustments.

Furthermore, it may be difficult to split the data into training, test, and validation sets when dealing with small datasets, making it difficult to assess the model bias.

One question arises at this point: witch is the minimum number of samples needed to perform augmentation with GAN's? Central limit theorem (CLT) is a general indicator for any inference problem. The rule of thumb of minim sample size of 30 can be a guiding indicator. However, in practical applications, we want to create synthetically augmented data because we have a small number of samples (usually less than 30) that aren't suitable for using with standard supervised machine learning algorithms. Theoretically, ANNs has the same sample size limitations than other algorithms. In fact, some authors argue than ANNs need even more training samples than other ML algorithms if one wants to evaluate model performance in terms of Log-Likelihood-based measures. General consensus is that algorithms need, as a rule of thumb, at least 10 samples per each data dimension. In general, the more complex the data generating process is, the more observations will be needed for the ANN to reliably represent training data's underlying distribution. But GANs training rely on the interaction of two algorithms (adversarial learning). Both the generator and the discriminator are modeled as deep neural networks and are separately parametrized for gradient descent learning. But GAN training is done using gradient-based learning where two models are competing against each other (Mazumdar et al., 2020). The process converges quickly to a local Nash equilibrium, which is a point where neither player has an advantage. This process happens at a linear rate, meaning it converges rapidly. As a conclusion we could

say that GAN training shouldn't have the limitation of maximum likelihood estimation (MLE), where central limit theorem directly applies. This does not mean training GANs is a less complex task, in fact it's much more complicated than MLE.

In Figure 1, we can see the results of an experiment where we have trained two different datasets with a Wassertein GAN. We have used two datasets: a low sample –9 rows and 8 columns – and a larger one – 1055 rows and – 42 columns. Figure's left side shows that, with low sample data, after approximately 15 steps, generator stops learning a data representation, and from this point onwards, the discriminator fails to converge and becomes unstable. On Figure's right side – larger sample data- , we see that the discriminator is able to successfully converge during the entire training process. Intuitively, we can explain this behavior for the low sample training data as the generator quickly learning a representation of the underlying distribution of the input data. We could argue that this representation can't be very accurate but our experiments show that the distribution learn is very close to the real one. The discriminator then has to determine whether a given input was drawn from the training data or from the generator output. However, seems that at a given point, the discriminator appears to make this "classification" randomly. This behavior have already been predicted by Goodfellow, 2014 .
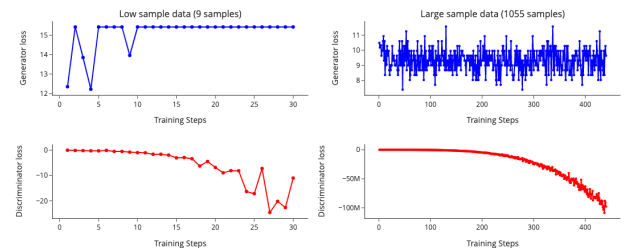

Figure 1. Model convergence comparison using a wGAN for low and large sample training data. Wassertein GAN model trained with batch size $m = 10$, $n_{Critic} = 1$, clipping parameter, $c = 0.01$, $\propto = 10^{-5}$, and RMSprop optimizer. Left plot: datasets with 9 samples. Right plot: dataset with 1055 samples.

As we already mentioned, despite this instability, generator G will learn an approximate distribution from training data, and discriminator will learn to predict data class quite accurately. Also, if we perform univariate test for comparing original and synthetic variable distributions we will see that both are drawn from the same probability distribution. But we think that this is not enough. The key will be to validate if patterns in this synthetic generated data will be useful for using this data with other machine learning algorithms. The main goal of our research is to Figure out how to do it.

2. Global data metrics

In this paper, 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; Q. Xu et al., 2018). We will not consider univariate two-sample and bivariate statistical tests.

Confirming the hypothesis that synthetic and original data samples represent the same underlying distribution for each variable does 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, on the other hand, capture not only the underlying distribution of all variables, they also observe their relationships. In this section we are going to describe and use three well known global metrics: Propensity score, Cluster analysis measure and Maximum Mean Discrepancy.

Definition 2.1 Let X be a sub-space of $\mathbb{R}^m$ with the same metric k. Let Prob(X) denote the spaces of probability measures defined on X. p_d is the probability distribution of original data and p_s the distribution of synthetic data, where $p_d, p_s \in Prob(X)$.

This methods are not based in finding elementary distances and divergences between the two distributions p_d, p_s as it happens with other methods as Total Variation distance, TV, or the Kullback-Leibler KL divergence (Arjovsky et al., 2017). KL divergence belongs to the family of f-divergences also known as Ali-Silvey distances (Nowozin et al., 2016). These distances can be defined as $d : X \times X \longrightarrow \mathbb{R}^+$, satisfying non-negativity assumption, $d(p_d, p_s) \geq 0$, and uniqueness $d(p_d, p_s) = 0$, if and only if $p_d = p_s$. As TV distance measures the maximal difference between the assignments of probabilities of two distributions, X can be considered as a metric space with distance TV, written as d_X. Meanwhile, Kullback-Leibler divergence KL is not a metric measure because it is not symmetric and does not satisfy the triangle inequality

$$KL(p(x)||q(x)) \neq KL(q(x)||p(x))$$

2.1 Propensity score

This model has become a common method for assessing data quality (Woo et al., 2009). Propensity score and cluster analysis measure can't be considered neither distances or divergences in the sense described above. The propensity score is defined as 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 both univariate and multivariate distributions. 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 samples and a value of zero to all original data samples. The probability of each case occurring in both, the synthetic and original data sets, is then computed (it's called the propensity score) using a classification algorithm. Then, we examine the propensity score probability distributions in both, the original and synthetic data.

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:

$$pMSE = \frac{1}{N} \sum_{i=1}^{N} (\widehat{p_i} - 0.5)^2$$

where N is the number of samples, p_i the predicted probabilities and pMSE is the mean-squared error of the logistic regression-predicted probabilities.

2.2 Cluster analysis measure

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. Cluster analysis measure (Woo et al., 2009) also uses a supervised machine learning technique, but it looks for similarities in the data using distances like Euclidean distance. This method but seems not applicable when comparing very high dimensionality datasets because of concentration of distances phenomena mentioned earlier (Beyer et al., 1998).

Definition 2.2.1 If we divide a dataset X in two parts of size $\mathcal{L}$ and $\mathcal{L}'$, the percentage of observations in $\mathcal{L}$ is given by

$$c = \frac{N_{\mathcal{L}}}{N_{\mathcal{L}} + N_{\mathcal{L}'}}$$

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:

$$U_c = \frac{1}{\mathcal{C}} \sum_{i=1}^{c} w_i \left[\frac{n_{iD}}{n_i} - c\right]^2$$

where n_i is the number of observations in the $i\text{-}th$ cluster, n_{iD} is the number of observations from the original data in the $i\text{-}th$ cluster, w_i is the weight assigned to $i\text{-}th$ 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 p_d, 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

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. Maximum Mean Discrepancy (MMD) is a non-parametric hypothesis testing statistic for comparing samples from two probability distributions (Gretton et al., 2006,

2009). MMD uses a kernel to define the similarities between probability distributions. 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

$$k(x, x') = exp(-\gamma \parallel x - x' \parallel^2)$$

Small **γ** values defines a Gaussian function with a large variance. The advantage of this method is the use of a kernel that defines similarities between observations. Maximum Mean Discrepancy is defined according the following expression:

$$MMD^2(p, q) := \parallel \mu_p - \mu_q \parallel^2$$

MMD^2 satisfy the non-negativity and uniqueness assumptions discussed in section 2 for other distances: $MMD^2(p, q) \geq 0$, and $MMD^2(p, q) = 0$, if $p = q$.

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 with the following statement:

> "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 where two known phenomena (concentration of distances and nearest neighbor search) limits our ability to "measure" how close distributions are in high dimensionality data spaces. In these spaces, as the number of dimensions gets close to infinity, the ratio of the distance between the furthest point to another one and the closest one becomes close to zero. This is known as the concentration phenomena. In these situation the connectivity between points becomes more substantial than their distance. For example, to find both discrete and continuous variables in tabular data is a common fact. A discrete variable in a high dimensional space represents a classification problem where data naturally falls into discrete classes or clusters. Distance between these clusters becomes negligible as dimensionality increases, making the search of a given point unstable (Beyer et al., 1998). It is implicitly assumed that stability of nearest neighbors search and concentration are related phenomena. The rationale is in a sense that a distance measure that is highly concentrated brings very little relevant discriminative information, thus the search for nearest neighbors is unstable.

Lastly, 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 summarize the topological information about the data space in the notion of a persistence module. Persistence homology is a mathematical formalism which allow us to infer topological information from a sample of a geometric object. We can compare two data spaces with a mathematical formulation of these properties as line-connections (level-zero connectivity information), loops(level-one connectivity information) and so on.

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 ε, denoted by $VR(X, \varepsilon)$, will be the simplicial complex whose vertex set is X, and where $x_0, x_1, ..., x_k$ 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 simplicical complexes.
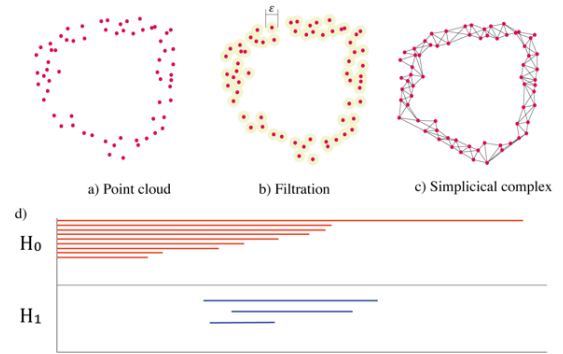

Figure 2. The Rips complex on a point cloud $VR(X, \varepsilon)$. a) A set of point cloud data X b) Vietoris-Rips complex for X, $VR(X, \varepsilon)$ c) ℝ- persistence simplicical complex as union of points, intervals, triangles, and higher dimensional analogues d) Betti numbers β_0 and β_1 for H_0 and H_1.

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).

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 $H_k(X_j,F) \rightarrow H_k(X_\ell,F)$ induced by the inclusion $X_j \subset X_\ell$, $j \leq \ell$, the persistence diagram of $PH_k(X,F)$ denoted $dgmn(X,F)$, is the collection of pairs (j,ℓ) 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 $\{H_i(VR(X,\varepsilon))\}_{\varepsilon \geq 0}$. 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   Stability of persistence diagrams

Persistence diagrams are stable with respect to perturbations of the input filtration. This is known as the stability theorem (Cohen-Steiner et al., 2005) .

3.2.1   Distances between persistence diagrams

To form a metric space over the collection of all persistent diagrams we need a metric. Let X be a topological space and $d : X \times X \rightarrow [0,\infty]$ such that:

-    for all $x \in X, d(x,x) = 0$, - uniqueness
-    for all $x,y \in X, d(x,y) = (y,x)$,
-    for all $x,y,z \in X, d(x,z) \leq d(x,y) + d(y,z)$ - triangle inequality

For any topological space $\mathcal{X}$ be a sub-space of $\mathbb{R}^m$, we represent a metric space as (X,d) for each $d : X \times X \rightarrow \mathbb{R}^+$.

Definition 3.2.1 The Hausdorff distance and the Bottleneck distance between X and Y are defined as

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

The bottleneck distance is based on a bijection between the points in a diagram.

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

Distances d_B and d_B satisfies the triangle inequality and therefore are distances. Both satisfies

$$X = Y \text{ then } d_B = d_H = 0, \text{ and}$$
$$X \subseteq Y \text{ then } d_B = d_H = 0$$

As a conclusion from the stability theorem of $Cohen-Steiner$ et al., 2005, if two spaces or sets $X,Y \subset \mathbb{R}^n$ are Hausdorff close, then their barcodes are Bottleneck close. Given two persistence diagrams X,Y

$$\text{if } d_H(X,Y) < \varepsilon, \text{ then } d_B(X,Y) < \varepsilon$$

Since the bottleneck distance satisfies one more constraint, then Bottleneck distance is bounded below by the Hausdorff distance ($Cohen-Steiner$ et al., 2005):

$$d_H(X,Y) \leq d_B(X,Y)$$

Definition 3.2.2   A continuous function between two topological spaces X and Y, abelian groups X, Y, induces linear maps between the homology groups. For an integer $k \geq 0$, we have

$$f_k: H_k(X) \rightarrow H_k(Y)$$

where H_k denotes the kth singular homology group (definition 3.1.1).

Definition 3.2.3 Bottleneck stability: Let X be a triangulable space with continuous tame functions, $f, g: X \rightarrow \mathbb{R}$. Then the persistence diagram satisfy $d_B(D(f), D(g)) \leq \|f-g\|_\infty$.

This definition shows that persistence diagrams are stable under some perturbations of small amplitude. Intuitively Bottleneck distance between two persistence diagrams can be seen as a measure of the cost of finding a correspondence between their points. Higher distance would mean that this cost is also higher, meaning that both diagrams does not match.

3.2.2   Empirical distribution tests on barcodes

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 $\mathbb{R}$, therefore 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, ∂_X, μ_x) be a compact metric measure space *and* $k, n \in \mathbb{N}$. Let $\{z_1, z_2 \ldots, z_i\}$ a sequence of randomly drawn samples from (X, ∂_X, μ_x). z_i is a metric measure space using the subspace metric and the empirical measure. Then $\phi_k^n(z_i)$ converges in probability to $\phi_k^n(X, \partial_X, \mu_x)$. For any $\varepsilon > 0$

$$\lim_{n \rightarrow \infty} p\ |\phi_k^n(z_i) - \phi_k^n(X, \partial_X, \mu_x) > \varepsilon| = 0$$

Definition 3.2.2 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 $d_S(-,-)$ to pairs (S_1, S_2), drawn from $\phi_k^n(X, \partial_X, \mu_x)^{\otimes 2}$ (Blumberg et al., 2014)

Definition 3.2.3 Let S be a barcode, $S \in Y$. D_S will be the distribution induced by applying $d_S(S, -)$. Since D and D_S are continuous with respect to the Gromov-Prohorovmetric, D_S converge in probability to D (Blumberg et al., 2014).

Therefore we 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, L, 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.   Experimental work

4.1   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 simulation has been created according (T. Lakshmi & Geethanjali, 2013).

4.2   Experimental results

In our research, we have used a special set of datasets with sample sizes equal to or less than the number of features. The two first datasets are e-scotter and SOFC (Table 1). Data E-scotter is an artificially generated low sample dataset designed for marketing analytics. SOFC dataset implements a simple solid oxide fuel cell battery modeling as described in T. V. V. S. Lakshmi et al., 2013. We have generated synthetic samples from original data with an augmentation rate of $10 \times n$ (where n is the number of samples in original data). It means a total of 110 samples in the e-scotter dataset and 300 in the SOFC dataset.

In Figure 2 we can see a visual representation of features "Price" and "Market share" in original and synthetic data for e-scotter dataset. The original dataset plots show a significantly fewer number of points compared to the synthetic data plot. It becomes evident how challenging it is to compare the two narratives. Even so, we can see than original data points are represented in synthetic data plot as well. Table 1 shows results the global data metrics used to compare both datasets. Propensity score values can range $(0, +\infty)$ and 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 cluster analysis 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, specially, according maximum mean discrepancy that is much lower than here than in e-scotter dataset. But, in both cases, these values are very close to zero (but the cluster analysis measure), indicating that both synthetic and real datasets are very similar. If we rely only in the propensity score metric we could argue than SOFC generated data is closer to original than e-scotter generated data, as indicate in MMD metric. This is one of the reason why validating synthetic data with global metrics or with univariate tests is not a straight forward process. In order to arrive at a conclusion, we will need to make use of a number of different metrics to finally arrive to a conclusion.

Table 1: Global metrics comparison for SOFC and e-scorter

	Dataset→	SOFC	e-scotter
Number of rows		30	11
Number of columns		13	9
Ratio rows/columns		2.3	1.2
	Global Metrics		
Propensity score* pMSE		0.020	0.021
Cluster analysis measure*, c		-0.38	-0.28
MMD (Maximum Mean Discrepancy) *		0.0367	0.100

* Number of synthetically generated samples = $10 \times n$
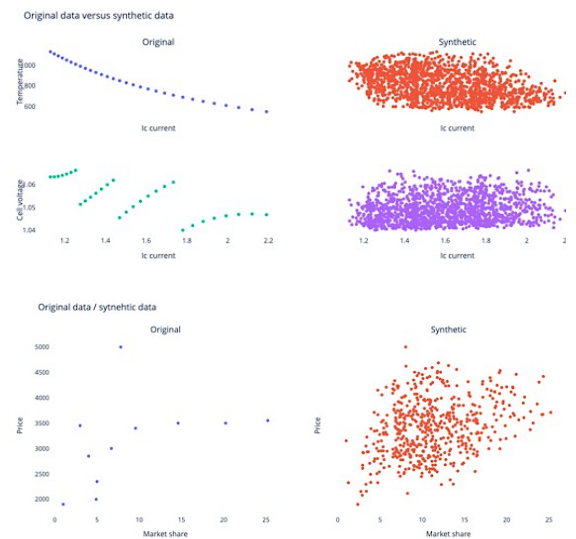*n: Number of data samples*

Figure 7. Visual comparison of some features relations in original and synthetic data. for SOFC dataset (upper section) and e-scooter dataset (lower section).

In our proposed method, we have used univariate non-parametric statistical tests to evaluate the topological signatures of original and synthetic data. We first computed the persistence barcodes distributions of the original and synthetic data, before applying the univariate non-parametric statistical tests. We also computed the Bottleneck distance between the original and synthetic data persistence diagrams   to measure the similarity between both datasets. Tables 2 and 3 present the results of comparing global metrics, Bottleneck distance, and non-parametric statistical tests.

We have first computed the persistence barcodes distributions of original and synthetic data and then apply univariate non parametric statistical tests. For these tests we are only using the H_0 dimension. We have also computed the Bottlenek distance between original and synthetic data persistence diagrams. Tables 2 and 3 shows the results of comparing global metrics, distances (Bottleneck) and non-parametric statistical tests.

Table 2. Metrics comparison for SOFC dataset with different number of samples. 30 rows/13 columns

Augmentation rate →	$5 \times n$	$10 \times n$	$20 \times n$	$50 \times n$
Propensity score* pMSE	0.03	0.02	0.05	0.08
Cluster analysis measure*, c	0.37	-0.38	-0.57	-0.59
MMD (Maximum Mean Discrepancy) *	0.040	0.0367	0.0350	0.034
Bottleneck distance, d_B	31.45	16.31	11.06	16.59
Kolmogorov-Smirnov (p-value)^c	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

* Test performed in homology group H_0
* Significance level $\alpha = 0.05$
n: Number of data samples

Global metrics analysis indicate that original and synthetic data are very similar in both datasets, as evidenced by the low propensity score and Maxim Mean Discrepancy values for all studied cases. However, in SOFC dataset, when using a high augmentation rate, the propensity score is much higher than the same score obtained for lower augmentation rates. This observation leads us to conclude that a synthetic dataset with a high augmentation rate could contain a significant number of samples that are noise.

In tables 2 and 3 we can see that in SOFC dataset, non-parametric statistical test reveals that original and synthetic were drawn from the same distribution at the 95% confidence level, but for the case of the highest augmentation rate ($\times 50$). In the case of e-scotter dataset these tests evidences the opposite result: all p-values but one are lower than the significance level, indicating that both spaces were not drawn from the same distribution at the 95% confidence level. In the case of e-scotter data, tests results does not change with the augmentation rate. Concerning the augmentation rate, we can see a significant difference in SOFC dataset when we augment data 50 times versus lower rates. This difference could suggest that a high augmentation rate is generating an important amount of noise samples. This difference is not seen in e-scotter dataset. It could indicate that rate is not important itself but number of new generated

samples is. With a rate of 50, in SOFC dataset we have generated 1500 synthetic samples and in e-scotter 450.

In addition to the datasets used in the first experiment, we have also tested two additional low sample size data sets: Balls (de Silva et al., 2020) and USA elections (MIT Election Data and Science Lab, 2021). In table 4 we show the results obtained with all datasets (SOFC, e-scotter, Balls, USA elections). We have used in the experiment an augmentation rate of 10 for all synthetic generated data.

Table 3. Metrics comparison for e-scotter dataset with different number of samples. 11 rows/9 columns

Augmentation rate →	$5 \times n$	$10 \times n$	$20 \times n$	$50 \times n$
Propensity score* pMSE	0.1091	0.021	0.023	0.11
Cluster analysis measure*, c	-0.14	-0.28	-0.15	1.18
MMD (Maximum Mean Discrepancy) *	0.1091	0.100	0.095	0.0927
Bottleneck distance, d_B	725.53	725.53	725.53	725.53
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) *	0.00725	0.0186	0.0671	0.0103

* Test performed in homology group H_0
* Significance level $\alpha = 0.05$
n: Number of data samples

Table 4. Metrics comparison several Low Sample Size datasets

Dataset→	SOFC	e-scotter	Balls	USA elections
Number of rows original	30	11	9	9
Number of columns	13	9	7	56
Ratio rows/columns original	2.3	1.2	1.3	0.16
Global Metrics				
Propensity score, pMSE	0.0367	0.100	0.0356	0.0507
Cluster analysis measure, c	-0.38	-0.28	1.33	-0.25
MMD (Maximum Mean Discrepancy)	0.020	0.021	0.1222	0.1229
Topological data analysis				
Bottleneck distance, d_B	16.31	725.53	297000	6.07
Kolmogorov-Smirnov (p-value) *	0.4175	0.0002	0.0002	0.0123
Mann-Whitney U test (p-value) *	0.2687	0.0002	0.0004	0.0055
Chi-square test (p-value) *	0.4454	0.0186	0.0246	0.0478

* Test performed in homology group H_0
* Significance level $\alpha = 0.05$
n: Number of data samples

Table 4 illustrates that there is no direct correlation between the global metrics and non-parametric statistical tests in topological signatures. For example, the propensity score metric for datasets is very close to zero, indicating that original and synthetic data is very similar. The MMD metric but shows significant differences among them. Values from SOFC and e-scooter datasets are close to zero, and lower than MMD values obtained from Balls and USA datasets. However, when comparing non parametric statistical tests, only in the case of the SOFC dataset, we can conclude that original and synthetic data were drawn from the same distribution at the 95% confidence level. We evaluated the Bottleneck distance to measure how similar persistence diagrams are. Results showed that for low distances there

aren't significant differences in the distributions of persistence barcodes, but in the case of USA elections dataset.

5. Discussion

In this paper, we discussed the challenge of generating synthetic tabular data from original data with a small number of samples, and the need for accurate and robust assessment methods to evaluate its validity. We propose a method for combining topology and robust statistics for hypothesis testing to assess data similarity. Analyzing data topology is important because it helps us better understand the structure and properties of data, including how it is organized, connected, and corelated. For this reason, preserving topological signatures is of great importance in the generation of synthetic tabular data. Our method applies persistent homology to find data descriptors and adapts them to the settings of hypothesis testing and confidence intervals. We have found that our method leads to different conclusions than common global metrics methods when deciding if synthetically generated data is similar to original data. Global metrics like propensity score or cluster analysis measure but has a limitation on the low number of samples in original data because rely on supervised methods. Our method has also this limitation as it uses as well non parametric methods to valuate this similarity (persistence diagrams and barcodes sets). We have used the Bottleneck distance as an additional straightforward similarity measure to validate the conclusions from our method. The results of this validation show that this distance is independent of sample size and suggests a positive correlation with non-parametric methods used to compare bar codes. This paper should be completed by validating both, our method and the global metrics used, with additional tests like the visual comparison of data, and the use of machine learning algorithms with domain adaptation. Reader can find a visual comparison for the Balls dataset in the appendix 2 of this paper.

6. References

Aggarwal, C. C., Hinneburg, A., & Keim, D. A. (2001). On the surprising behavior of distance metrics in high dimensional space. Lecture Notes in Computer Science (Including Subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics), 1973, 420–434. https://doi.org/10.1007/3-540-44503-X_27/COVER

Arjovsky, M., Chintala, S., & Bottou, L. (2017). Wasserstein Generative Adversarial Networks. International Conference on Machine Learning., 214–223.

Barnes, D., Polanco, L., & Perea, J. A. (2021). A Comparative Study of Machine Learning Methods for Persistence Diagrams. Frontiers in Artificial Intelligence, 4, 91. https://doi.org/10.3389/FRAI.2021.681174/BIBTEX

Benaim, A. R., Almog, R., Gorelik, Y., Hochberg, I., Nassar, L., Mashiach, T., Khamaisi, M., Lurie, Y., Azzam, Z. S., Khoury, J., Kurnik, D., & Beyar, R. (2020). Analyzing Medical Research Results Based on Synthetic Data and Their Relation to Real Data Results: Systematic Comparison From Five Observational Studies. JMIR Med Inform 2020;8(2):E16492 Https://Medinform.Jmir.Org/2020/2/E16492, 8(2), e16492. https://doi.org/10.2196/16492

Beyer, K., Goldstein, J., Ramakrishnan, R., & Shaft, U. (1998). When is "nearest neighbor" meaningful? Lecture Notes in Computer

Science (Including Subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics), 1540, 217–235. https://doi.org/10.1007/3-540-49257-7_15/COVER

Blumberg, A. J., Gal, I., Mandell, M. A., & Pancia, M. (2014). Robust Statistics, Hypothesis Testing, and Confidence Intervals for Persistent Homology on Metric Measure Spaces. Foundations of Computational Mathematics 2014 14:4, 14(4), 745–789. https://doi.org/10.1007/S10208-014-9201-4

Borgwardt, K. M., Gretton, A., Rasch, M. J., Kriegel, H.-P., Schö Lkopf, B., & Smola, A. J. (2006). Integrating structured biological data by Kernel Maximum Mean Discrepancy. Bioinformatics, 22(14), 49–57. https://doi.org/10.1093/bioinformatics/btl242

Carlsson, G. (2009). Topology and data. Bull. Amer. Math. Soc., 46(2), 255–308. https://www.ams.org/journals/bull/2009-46-02/S0273-0979-09-01249-X/

Carlsson, G., Zomorodian, A., Collins, A., & Guibas, L. (2004). Persistence barcodes for shapes. ACM International Conference Proceeding Series, 71, 124–135. https://doi.org/10.1145/1057432.1057449

Chaudhari, P., Agrawal, H., & Kotecha, K. (2020). Data augmentation using MG-GAN for improved cancer classification on gene expression data. Soft Computing, 24(15), 11381–11391. https://doi.org/10.1007/S00500-019-04602-2/METRICS

Chundawat, V. S., Tarun, A. K., Mandal, M., Lahoti, M., & Narang, P. (2022). TabSynDex: A Universal Metric for Robust Evaluation of Synthetic Tabular Data. ArXiv.Org. http://arxiv.org/abs/2207.05295

Cohen-Steiner, D., Edelsbrunner, H., & Harer, J. (2005). Stability of persistence diagrams. Proceedings of the Annual Symposium on Computational Geometry, 263–271. https://doi.org/10.1145/1064092.1064133

de Silva, B. M., Higdon, D. M., Brunton, S. L., & Kutz, J. N. (2020). Discovery of Physics From Data: Universal Laws and Discrepancies. Frontiers in Artificial Intelligence, 3, 25. https://doi.org/10.3389/FRAI.2020.00025/BIBTEX

Elman, J. L. (1993). Learning and development in neural networks: the importance of starting small. Cognition, 48(1), 71–99. https://doi.org/10.1016/0010-0277(93)90058-4

Eno, J., & Thompson, C. W. (2008). Generating synthetic data to match data mining patterns. IEEE Internet Computing, 12(3), 78–82. https://doi.org/10.1109/MIC.2008.55

Feng, R., Zhao, D., Learning, Z. Z.-C. on M., & 2021, undefined. (2021). Understanding noise injection in gans. International Conference on Machine Learning, 3284–3293. https://proceedings.mlr.press/v139/feng21g.html

Goncalves, A., Ray, P., Soper, B., Stevens, J., Coyle, L., & Sales, A. P. (2020). Generation and evaluation of synthetic patient data. BMC Medical Research Methodology, 20(1), 1–40. https://doi.org/10.1186/S12874-020-00977-1/TABLES/17

Goodfellow, I. J. (2014). ON DISTINGUISHABILITY CRITERIA FOR ESTIMATING GENERATIVE MODELS. ArXiv Preprint.

Goodfellow, I. J., Pouget-Abadie, J., Mirza, M., Xu, B., Warde-Farley, D., Ozair, S., Courville, A., & Bengio, Y. (2014). Generative Adversarial Nets. Advances in Neural Information Processing Systems, 27. http://www.github.com/goodfeli/adversarial

Gretton, A., Borgwardt, K. M., Rasch, M., Schölkopf, B., & Smola, A. J. (2006). A kernel method for the two-sample-problem. Advances in Neural Information Processing Systems, 19. https://proceedings.neurips.cc/paper/2006/hash/e9fb2eda3d9c55a0d89c98d6c54b5b3e-Abstract.html

Gretton, A., Fukumizu, K., Harchaoui, Z., & Sriperumbudur, B. K. (2009). A Fast, Consistent Kernel Two-Sample Test. Advances in Neural Information Processing Systems, 22.

Lakshmi, T., & Geethanjali, P. (2013). Mathematical modelling of solid oxide fuel cell using Matlab/Simulink. In IEEE (Ed.), 2013 Annual International Conference on Emerging Research Areas and 2013 International Conference on Microelectronics, Communications and Renewable Energy (pp. 1–5). https://ieeexplore.ieee.org/abstract/document/6576016/

Lakshmi, T. V. V. S., Geethanjali, P., & Krishna Prasad, S. (2013). Mathematical modelling of solid oxide fuel cell using

Matlab/Simulink. 2013 Annual International Conference on Emerging Research Areas and 2013 International Conference on Microelectronics, Communications and Renewable Energy. https://doi.org/10.1109/AICERA-ICMICR.2013.6576016

Lin, J. J., Chang, C. H., & Pal, N. (2015). A Revisit to Contingency Table and Tests of Independence: Bootstrap is Preferred to Chi-Square Approximations as Well as Fisher's Exact Test. Journal of Biopharmaceutical Statistics, 25(3), 438–458. https://doi.org/10.1080/10543406.2014.920851

Liu, Y., Zhou, Y., Liu, X., Dong, F., Wang, C., & Wang, Z. (2019). Wasserstein GAN-Based Small-Sample Augmentation for New-Generation Artificial Intelligence: A Case Study of Cancer-Staging Data in Biology. Engineering, 5(1), 156–163. https://doi.org/10.1016/J.ENG.2018.11.018

Massey, F. J. (1951). The Kolmogorov-Smirnov Test for Goodness of Fit. Journal of the American Statistical Association, 46(253), 68–78. https://doi.org/10.1080/01621459.1951.10500769

Mazumdar, E., Ratliff, L. J., & Sastry, S. S. (2020). On Gradient-Based Learning in Continuous Games. SIAM Journal on Mathematics of Data Science, 2(1), 103–131. https://doi.org/10.1137/18M1231298

McKnight, P. E., & Najab, J. (2010). Mann-Whitney U Test. The Corsini Encyclopedia of Psychology, 1–1. https://doi.org/10.1002/9780470479216.CORPSY0524

MIT Election Data and Science Lab. (2021). U.S. President 1976–2020. In Harvard Dataverse (Vol. 6). Harvard Dataverse. https://doi.org/10.7910/DVN/42MVDX

Nowozin, S., Cseke, B., & Tomioka, R. (2016). f-gan: Training generative neural samplers using variational divergence minimization. Advances in Neural Information Processing Systems, 29. https://proceedings.neurips.cc/paper/2016/hash/cedebb6e872f539bef8c3f919874e9d7-Abstract.html

Rosenbaum, P. R., & Rubin, D. B. (1983). The central role of the propensity score in observational studies for causal effects. Biometrika, 70(1), 41–55. https://doi.org/10.1093/BIOMET/70.1.41

Salimans, T., Goodfellow, I., Zaremba, W., Cheung, V., Radford, A., & Chen, X. (2016). Improved techniques for training GANs. Advances in Neural Information Processing Systems, 2234–2242.

Snoke, J., Raab, G. M., Nowok, B., Dibben, C., & Slavkovic, A. (2018). General and specific utility measures for synthetic data. Journal of the Royal Statistical Society. Series A: Statistics in Society, 181(3), 663–688. https://doi.org/10.1111/RSSA.12358

Snoke, J., & Slavković, A. (2018). pMSE mechanism: Differentially private synthetic data with maximal distributional similarity. Lecture Notes in Computer Science (Including Subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics), 11126 LNCS, 138–159. https://doi.org/10.1007/978-3-319-99771-1_10/FIGURES/4

Sutherland, D. J., Tung, H.-Y., Strathmann, H., De, S., Ramdas, A., Smola, A., & Gretton, A. (2016). GENERATIVE MODELS AND MODEL CRITICISM VIA OPTIMIZED MAXIMUM MEAN DISCREPANCY. ArXiv Preprint ArXiv:1611.04488.

Sutherland, D. J., Tung, H.-Y., Strathmann, H., De, S., Ramdas, A., Smola, A., & Gretton, A. (2017). GENERATIVE MODELS AND MODEL CRITICISM VIA OPTIMIZED MAXIMUM MEAN DISCREPANCY. ICLR 2017.

Theis, L., van den Oord, A., & Bethge, M. (2016). A NOTE ON THE EVALUATION OF GENERATIVE MODELS. International Conference on Learning Representations.

Virtanen, P., Gommers, R., Oliphant, T. E., Haberland, M., Reddy, T., Cournapeau, D., Burovski, E., Peterson, P., Weckesser, W., Bright, J., van der Walt, S. J., Brett, M., Wilson, J., Jarrod Millman, K., Mayorov, N., J Nelson, A. R., Jones, E., Kern, R., Larson, E., … van Mulbregt, P. (2020). SciPy 1.0: fundamental algorithms for scientific computing in Python. Nature Methods, 17, 261–272. https://doi.org/10.1038/s41592-019-0686-2

Woo, M.-J., Reiter, J. P., Oganian, A., & Karr, A. F. (2009a). Global Measures of Data Utility for Microdata Masked for Disclosure Limitation. Journal of Privacy and Confidentiality, 1(1), 111–124. https://doi.org/10.29012/jpc.v1i1.568

Woo, M.-J., Reiter, J. P., Oganian, A., & Karr, A. F. (2009b). Global Measures of Data Utility for Microdata Masked for Disclosure Limitation. Journal of Privacy and Confidentiality, 1(1), 111–124. https://doi.org/10.29012/jpc.v1i1.568

Xu, L., Skoularidou, M., Cuesta-Infante, A., & Veeramachaneni, K. (2019). Modeling Tabular data using Conditional GAN. Advances in Neural Information Processing Systems, 32. https://github.com/DAI-Lab/CTGAN

Xu, Q., Huang, G., Yuan, Y., Guo, C., Sun, Y., Wu, F., & Weinberger, K. Q. (2018). An empirical study on evaluation metrics of generative adversarial networks. ArXiv Preprint. https://github.com/xuqiantong/GAN-Metrics

Appendix 1

As described in section 1, for our experiments we have use nbsynthetic, a python open source library. This library uses a wGAN specially designed for generating and augmenting low sample input data. As we have already seen, training a GAN with low sample input data is unstable because of network regularization failures. GAN are unstable by definition even with large sample input data. Issues like model collapse have already been described in literature (Arjovsky et al., 2017b; Feng et al., 2021; Goodfellow et al., 2014; Salimans et al., 2016; L. Xu et al., 2019) . Let's recall that regularization in GANs uses a methods similar to Noise-contrastive estimation or NCE, where a fixed "noise" distribution is used for generator G, p_g. This is done by defining a parametric family of densities p_θ. The goal is to minimize the distance between the density p_θ and input data p_r varying the parameter θ. Discriminator net D, will behave as a binary classifier, p_c trying to Figure out whether a particular sample was selected from training data or from a "generator" distribution, p_g, is parameterized directly. This method is driven by the following value function

$$V\big(p_c, p_g\big) = \ \mathbb{E}_{x \sim p_d} \ log \ p_c(y = 1 \mid x) + \mathbb{E}_{x \sim p_g} \ log \ p_g(y = 0 \mid x)$$

GAN learning use a optimization algorithm to maximize V by learning in the generator. Each learning step in a GAN pair $V\big(p_c, p_g\big)$ consists of decreasing an expectation of a function of samples from the generator. To reach the equilibrium point p_g, it takes successive steps partially minimizing $V\big(p_c, p_g\big)$ using the current value of p_c at each step. Given θ as a parameter of p_g, we will have the following expression.

$$\frac{\partial}{\partial \theta} \mathbb{E}_{x \sim p_g} \ log \ p_g(y = 0 \mid x)$$

Wassertein GAN

In our research we have used Wassertein GAN. wGAN transforms the distance function between p_r, p_θ in a continuous function using Earth mover distance. It is supposed that $W(p_r, p_\theta)$ has better qualities on comparing p_r, p_θ than Jensen-Shannon divergence under some considerations (Arjovsky et al., 2017).

Definition 1.1.1 (Theorem 1 in Arjovsky et al., 2017) Let p_r be a fixed distribution over X. Let Z be a random variable over another space Z. Let p_θ denote the distribution of $g_\theta(Z)$ where

$$g: (z, \theta) \in Z \ \times \mathbb{R}^d \to g_\theta(z) \in X$$

Then,
   - If g is continuous in θ, then the Wasserstein distance $W(p_r, p_\theta)$ is also continuous.
   - If g is locally Lipschitz and satisfies regularity assumption 1, then $W(p_r, p_\theta)$ is continuous everywhere, and differentiable almost everywhere.
   - Statements 1-2 are false for the Jensen-Shannon divergence $JS(p_r, p_\theta)$ and all the Kullback-Leibler divergence $KL(p_r, p_\theta)$.

Arjovsky et al., 2017 indicates that Wasserstein distance's gradient over parameter θ can be calculated according the following expression:

$$\nabla_\theta W(p_r, p_\theta) = \ -\mathbb{E}_{z \sim p_{(z)}} \big[\nabla_\theta f(g_\theta(z))\big]$$

Another possible approach to avoid this regularization problem is to use a network architecture with significantly lower number of parameters to train. It can be achieved reducing the number of hidden layers. Figure 2 show the comparison of the same wGAN used before but removing a hidden layer. Regularization is clearly improved when using two hidden layers instead of three.

Limitations of training GAN's with small sample tabular data

We have already seen some limitations during training GAN with small sample tabular data. We can resume them as follows:

- **GAN's instability**
GANs are by definition unstable. This is the reason why we have chosen wGAN due it's, theoretically , better convergence capabilities.
- **Regularization**
Low sample training data shows significant regularization problems. A possible approach to avoid this problem is to use a network architecture with the lowest number of parameters to train. It can be achieved reducing the number of hidden layers. Figure 1 Appendix 1 show the results of training two low sample dataset with a wGAN with only one hidden layer. We can see the difference

in stability when we train data with 9 samples and with 30 samples. As number of samples grows, discriminator loss becomes more stable, even not being stable at all. In this Figure 1 Appendix 1, we can see a behavior that has been already noted by Goodfellow, 2014. Generator need few steps for learning the underlaying distribution of data as it isn't a difficult task at all. From this moment on, discriminator starts to classify p_c, p_g arbitrarily, an so the optimizer may fail to find the global optimum.
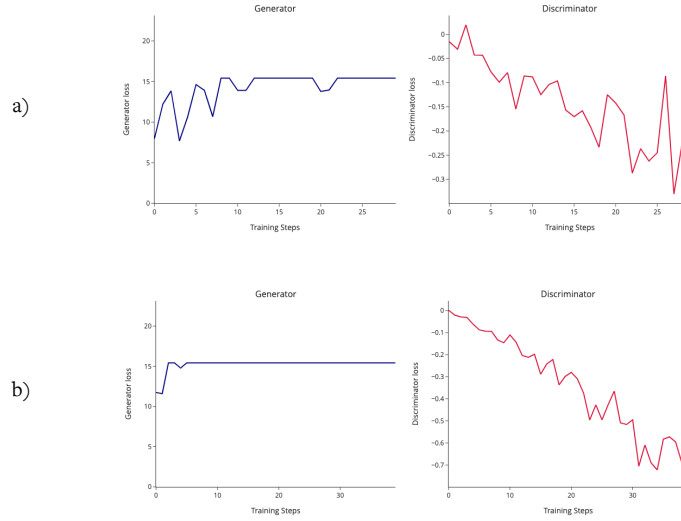

Figure 1 Appendix 1. wGAN model convergence for low sample training data . a) dataset "Balls" with n=9; b) dataset SOFC with n=30, where n is the number of samples. Both datasets are described in section 4.2. wGAN model trained with batch size $m = 10$, $n_{Critic} = 1$, $\propto = 10^{-5}$, clipping parameter c = 0.01, and RMSprop as optimizer. Left plot: generator loss. Right plot: discriminator loss.

- **Discrete variables**

GAN's sampling of discrete data features leads to instability because gradients can't be backpropagated to generator. One possible solution is to encode categorical variables in $g_\theta(z)$ as continuous features. The generator will create a random continuous distribution in the same interval than real data. The shape of this continuous distribution is a configuration parameter and can be neither a continuous uniform distribution $X' \sim U(min, max)$ or a continuous normal distribution $X' \sim N(\mu, \sigma)$. After training, GAN will have learnt an approximate of original data distribution in the form of a continuous distribution, $X_{syn} \sim U(\mu', \sigma')$ where $\mu \approx \mu'$ and $\sigma' \approx \sigma$. Then we have to discretize this distribution using the parameters from the real data distribution. One of the most common methods to this transformation is to force the probability mass function or pdf of X', $f_{X'}(x)$, retain the form of the probability density function (pdf) of X, $f_X(x)$, and that support of X' is set from full range of X. It can be written as follows:

$$f_{X'}(x) = f_X(x)$$

$$R_{X'} = \{x \in \mathbb{R}: f_X(x) > 0\}$$

After this transformations we will have

$$X_{syn} \sim U\{min, max\} \approx X_{or} \sim U\{min, max\}$$

Appendix 2

Visual comparison of balls dataset

This dataset collects the results of an experiment in which nine spherical balls of different diameters (Radius and Surface area) and weights (Density and Mass) are dropped from the same height and the time it took each ball to fall to the ground is measured (Land time). The balls may or may not have a rough surface (binary feature "Smooth"). The objective of the experiment is to relate the fall time of the balls with the rest of the variables from a machine learning algorithm. The synthetic dataset has augmented from nine samples in the original dataset to ninety samples (augmentation rate of 10). Synthetic data has been generated using the open source python's library nbsynthetic as described in the paper. We have chosen this dataset for this comparison because results shown in table 4 reveals differences between our method and the global metrics assessment.

In the Figure 1 Appendix 2 we can see a direct representation of all features from the Balls dataset. x-axis represents the same feature in all plots, Land time.
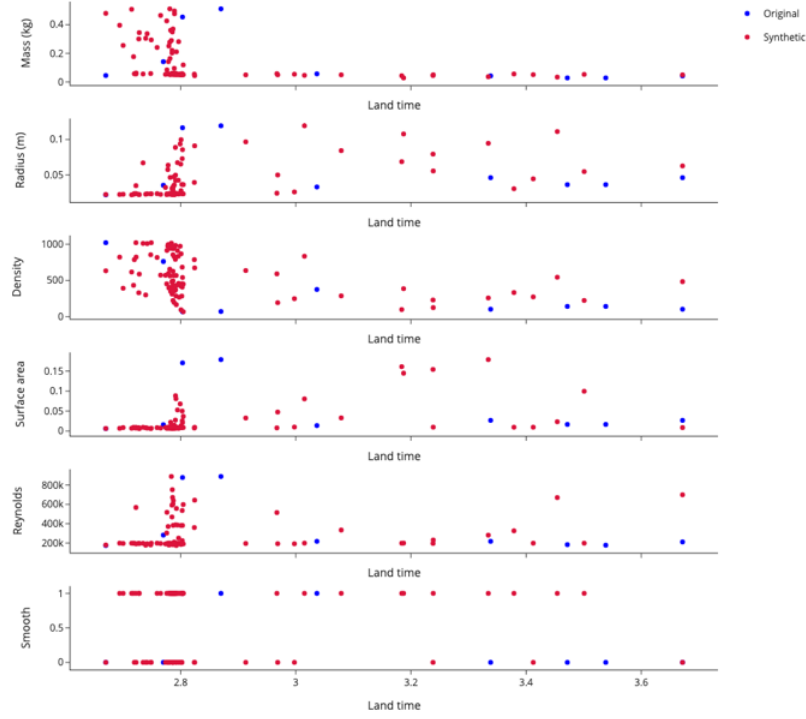

Figure 1 - **Appendix 2** : Plot of all variables in dataset represented versus "Land time"
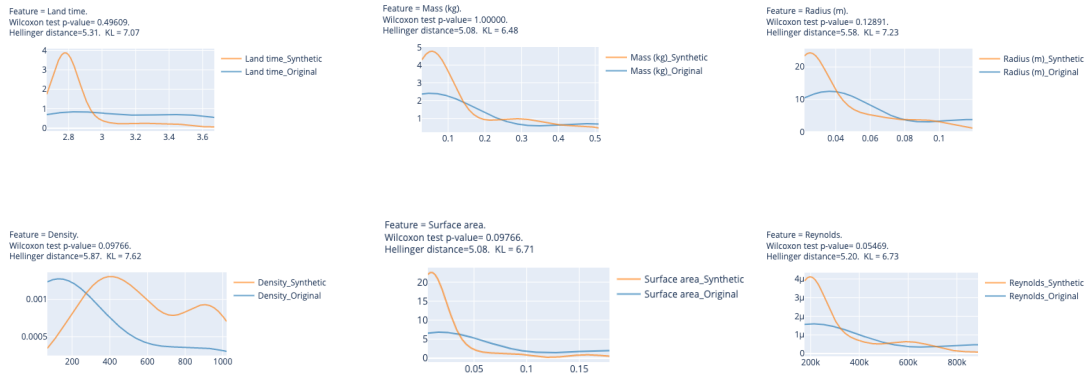

Figure 2 – **Appendix 2** : Comparison of original and synthetic probability distribution of features in dataset

In the Figure 2 – Appendix 2 we can see the probability distributions comparison of both datasets (real and synthetic) together with the results from some univariate statistical tests and the distance between them (Hellinger distance and KL divergence). Finally, Figure 3 – Appendix 2 shows the absolute difference between the linear correlation coefficient between the continuous features.
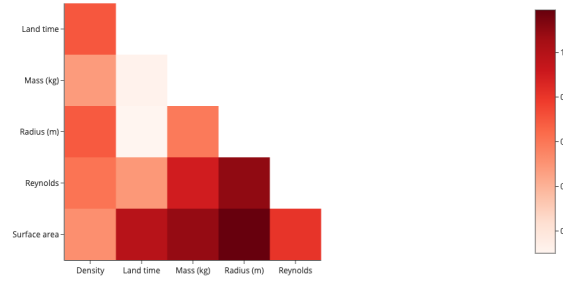
Figure 3 - **Appendix 2** : Difference between linear correlation coefficients of features in real and synthetic data.

Univariate test of Wilcoxon in Figure 2 – Appendix 2 evidences that probability distribution from both datasets comes from the same we can see that probability distributions were drawn from the same distribution at the 95% confidence level. The Wilcoxon rank-sum test or as Mann–Whitney U test, is a non-parametric hypothesis test used to check whether or not two independent samples correspond to the same distribution. It has the advantage over for example the two-sample t-test that does not require the data normality assumption. We have also calculated the Hellinger distance and the KL divergence as disparity measures. Hellinger distances are low (around 5) and so is KL divergence (between 6.48 and 7.62) indicating that both distributions are very close or, in terms of dataset comparison, data is very similar. This results were expected as the generative algorithm used non-conditional Wassertein-GAN) is trained to learn the probability distributions of original data. w-GAN training involve fitting a probability distribution over a vector of observations from the real data.

 In table 4 we can show the results of applying global metrics. Propensity score is very close to 0 (0.00356) but Maximum Mean Discrepancy has higher values than other datasets (SOFC and e-scotter). So using global metrics comparison does not reveal a clear conclusion to the assessment task. Results of applying our proposed method illustrates that both datasets are not similar. Bottleneck distance is very high in comparison with other dataset, and the results from the univariate tests reveals that synthetic datasets can't be considered as an real data substitute.

 A visual comparison of original and synthetic samples (Figure 1 – Appendix 2) reveals certain differences. Some features like Surface area and Radius shows important differences in its shape. Visual comparing variables is not an easy task as we have nine samples in the original data and ninety in synthetic data. This differences can be seen in Figure 4 – Appendix 2.
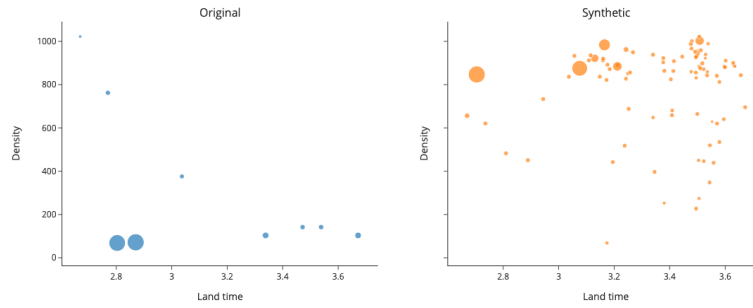

Figure 4 - **Appendix 2** : Representation of Density versus Land Time. The points size corresponds to balls radius.