Leveraging Synthetic Data to Advance Organizational Science

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Author Note

We have no known conflicts of interest to disclose.

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Abstract

The importance of data sharing in organizational science is well-acknowledged, yet the field faces hurdles that prevent this, including concerns around privacy, proprietary information, and data integrity. We propose that synthetic data generated using machine learning (ML) could offer one promising solution to surmount at least some of these hurdles. Although this technology has been widely researched in the field of computer science, most organizational scientists are not familiar with it. To address the lack of available information for organizational scientists, we propose a systematic framework for the generation and evaluation of synthetic data. This framework is designed to guide researchers and practitioners through the intricacies of applying ML technologies to create robust, privacy-preserving synthetic data. Additionally, we present two empirical demonstrations using the ML method of Generative Adversarial Networks (GANs) to illustrate the practical application and potential of synthetic data in organizational science. Through this exploration, we aim to furnish the community with a foundational understanding of synthetic data generation and encourage further investigation and adoption of these methodologies. By doing so, we hope to foster scientific advancement by enhancing datasharing initiatives within the field.

Keywords: synthetic data, machine learning, open science, data sharing

Leveraging Synthetic Data to Advance Organizational Science

Today's era of open science critically involves the sharing of data to strengthen scientific understanding, evidence-based practice, and policy making (Banks et al., 2019; Nosek et al., 2015). Yet, organizational researchers and other social scientists are often hesitant to share their data (e.g., Hardwicke et al., 2021; Towse et al., 2020; Vanpaemel et al., 2015; Wicherts et al., 2006). Vanpaemel et al. (2015) offered a telling example, by reporting that out of 394 data requests made across four American Psychological Association (APA) journals, a mere 150 researchers (38%) ultimately shared their data. The open science movement hopes to reverse this trend, where journals and the federal government are beginning to encourage, strongly recommend, or even require the sharing of data and materials, as found in the Transparency and Openness Promotion (TOP) guidelines of the Open Science Framework (Nosek et al., 2015). In the scholarly context, data-sharing activities seek to boost transparency, by allowing for analytic reanalysis and reproducibility, bolstering the credibility of scientific research (Pew Research Center, 2019; Towse et al., 2020). Moreover, the availability of open data allows for additional extended analyses, in addition to much greater flexibility and power when conducting metaanalyses across studies that provide the raw data.

Compounding this problem are many challenges to sharing data in organizations. Ensuring anonymity is one of them, given that organizations entrusted with employee and job applicant data seek to keep the identity of individuals not only anonymous but completely private. Other reasons are that organizations stand to gain a competitive advantage from the data they glean insights from and do not share; additionally, they avoid the risk of reputational damage by not sharing data that might reveal unfavorable information about the organization. Keeping these types of ethical, privacy, and proprietary issues well in mind, we believe that

synthetic data could offer one promising solution to surmounting at least some of these hurdles, for those organizations seeking to be thought leaders by participating in scientific activities in the aforementioned spirit of data sharing and open science.

Jordon et al. (2022) defined *synthetic data* as 'data that have been generated using a purpose-built mathematical model or algorithm, with the aim of solving a (set of) data science task(s).' If one were to rely on this definition, Monte Carlo simulation data could also be considered synthetic data. For example, researchers can simulate data for subsequent *t*-tests, ANOVAs, regression, SEM, and other forms of modeling and hypothesis testing (e.g., generating simulation data using the mvnorm function within the MASS package in R; Venables & Ripley, 2002). But simulations are based on specifying underlying parameters and distributions beforehand (e.g., a multivariate normal variance-covariance matrix and its associated mean structure). Thus, simulations generate data based on known parameters and attendant distributional assumptions; these data are then analyzed to see whether those parameters and assumptions can be well approximated by sample-based estimates.

In this paper, our definition of synthetic data slightly differs from that of Jordon et al. (2022). We emphasize the distinction between synthetic data and simulation data: while simulation data is generated based on multivariate distributional assumptions, synthetic data are generated by learning from the multivariate distribution of the original dataset itself. The goal is for analyses performed on synthetic data to closely mirror those performed on the original data. A synthetic dataset therefore serves as an alternative to the original dataset, allowing one to mirror the original data in its realism and complexity while still ensuring data privacy and protection for the original data owners (Raghunathan, 2021). With these advantages, synthetic data can promote open data sharing in organizational research, encouraging academic-

practitioner research partnerships that align with the recent and strengthening development of open science initiatives in the field (Castille et al., 2022).

At the same time, despite the strengths of synthetic data, it is essential to highlight that their security and substitutability are critically influenced by many important design factors. For example, for synthetic data to serve as a reasonable substitute for the original data, researchers need to determine their intended use, evaluate the efficacy and effectiveness of synthetic data generation techniques closely, and ensure stringent data anonymity and otherwise uphold ethical, privacy, and proprietary standards.

The primary goal of our paper is to develop a systematic framework that guides organizational researchers through the synthetic generation and evaluation processes, as we are unaware of any such resources available to organizational scientists. This framework helps readers consider, generate, interpret, and use synthetic data from a broad perspective. Through two specific examples, we will demonstrate how to apply machine learning (ML) generative models to learn from a given dataset. Although the machine learning method we explain and use is called generative adversarial networks (GANs), readers should know there are many other ML options for generating synthetic data; however, covering those here would detract from the central goal of our paper. Based on this framework, we also provide two empirical demonstrations. Ultimately, our goal is not to serve as a definitive resource, but rather to provide organizational scientists and practitioners with a general understanding and rationale behind generating synthetic data, hoping they will be motivated to pursue synthetic data methodologies further and expand upon our efforts.

We also discuss ideas for navigating potential ethical dilemmas and risks associated with developing and applying synthetic data (Porter, 2008; United Kingdom Statistics Authority,

2022). Taken as a whole, our research invites the broader integration of synthetic data within the organizational sciences, helping to unlock organizational data that has remained restricted, inaccessible, and thus ultimately lost over time. Ultimately, as more high-quality synthetic data are shared that strikes an appropriate balance between accessibility and privacy, we envision both organizational science and evidence-based practice to benefit greatly.

Synthetic Data: Answering Key Questions

The term 'synthetic data' is a relatively unfamiliar concept for most organizational scientists. When encountering a new research method, four main questions usually need answers: *What is this method? Why should we use this method? How does this method differ from previous methods? How should we implement this method?* Below, we will address these four questions in turn as they pertain to synthetic data.

What Are Synthetic Data?

In this paper, we define *synthetic data* as artificially generated data designed to emulate the original data as closely as possible without revealing actual observations in that data. The purpose is to provide an alternative to original data in situations where using original data is impractical, poses privacy concerns, is disallowed (e.g., organizationally, legally, ethically), or is otherwise restricted (Fonseca & Bacao, 2023; Jordon et al., 2022).

Consider an original dataset containing 1,000 data points. The corresponding synthetic dataset will also consist of 1,000 data points, but it will include carefully constructed noise to ensure that the two datasets do not exactly overlap, thus protecting the privacy of the data. At the same time, both datasets will have similar multivariate distributional properties, ensuring that the synthetic dataset can substitute for the original dataset with very similar analytic results, no matter what analysis is used.

Why Would One Synthesize Data?

Privacy issues have always been an obstacle to data sharing with researchers (Gabriel & Wessel, 2013; Leavitt, 2013). Rubin (1993) highlighted the privacy risks of sharing microdata (i.e., information about individual transactions) and the complex legal issues it presents. He suggested using imputed synthetic data as a solution, where confidential information in a dataset is replaced with estimates generated from an imputation model, using the same background variables without disclosing the original sensitive data. Whereas imputations require assuming and estimating a model that underlies the data, ML-based methods can learn the model from the data themselves, thus improving upon Rubin's ideas. We will illustrate the use of one type of ML generative model, Generative Adversarial Networks, or GANs (Goodfellow et al., 2014; Goodfellow et al., 2020). The GAN procedure begins as noisy data but then shapes itself into a synthetic dataset as it learns its distributional form from an actual dataset. Therefore, a synthetic dataset based on a GAN does not contain any actual individual data.

Note that although here we only introduce synthetic data as a potential approach to address the fundamental concern of data sharing—privacy issues, we also believe that the use of synthetic data is a promising solution to other obstacles preventing organizations from sharing their data. These obstacles are more nuanced, such as proprietary concerns (e.g., why should companies give up their competitive advantage?), legal issues (e.g., why should I share if it exposes an organization to legal liability?), and ethical considerations (e.g., do synthetic data break the contract made with employees about the use of their data?). These issues are important for organizational research but are often not considered in other disciplines (e.g., computer science) that study synthetic data extensively. We hope this paper can serve as a starting point for the use of synthetic data in organizational research, provide a general understanding and

rationale behind generating synthetic data, and call for more thought and research on synthetic data within the field.

How Do Synthetic Data Compare to Data Generated by Existing Methods?

In order to highlight the features of synthetic data, we compare it with similar but distinct data from two existing methods: anonymizing data and simulating data.

Anonymizing or De-identifying Data

Anonymization is the process of removing or altering personal identifiers from original data so that the individuals described by the original data become anonymous. Often, it involves changing or removing those variables that could directly or indirectly lead to identifying individuals in the dataset. Anonymized data have some use, but their value can be compromised due to having to remove, combine, or alter key features of the original dataset. For example, removing demographic information directly results in the inability to study these variables; yet data binning the data as a solution to keeping individual demographics anonymous would limit the variability of the data (Cohen, 1983) and limit the appropriate analyses and inferences that can be made as well. By contrast, synthetic data offer several advantages over simply anonymizing the original data. When produced well, synthetic data do not contain the original data of any individuals, thus offering a higher level of privacy than simply removing personal information from the original dataset. Likewise, synthetic data do not require removing or combining variables, thus retaining the essential qualities of the original data. In contrast with the previous example, demographic information can often still be retained as part of a synthetic dataset.

Simulating Data

Often researchers are unsure of the distinction between synthetic data and simulated data. Monte Carlo simulations, for example, are generated based on parameter estimates (e.g., a range of correlations or specific values, say estimates from a meta-analysis). These estimates are then incorporated into prespecified models (e.g., regression, ANOVA) to generate data with modeled distributional assumptions (e.g., multivariate normality with prespecified variances and covariances, specific proportions in each group, psychometric reliability and validity estimates, subgroup mean differences). Although this simulation-based approach affords the user tremendous flexibility and control over the data-generating mechanism, the simulated data (and its underlying model and parameters) may or may not be generalizable to the real world. By contrast, synthetic data are generated using an actual dataset to develop the best approximation of that dataset using ML models (in our case, GANs). Because synthetic data are derived from the original data, there are no distributional assumptions, and results are intended to reflect and thus generalize to the original dataset.

To further this comparison, let us use hamburgers as an accessible (and tasty) example. When using the synthetic data method, imagine we have a meat patty hamburger (representing the original data), which vegetarians cannot enjoy (analogous to data that cannot be shared due to privacy concerns). To address this, we use a plant-based hamburger (representing synthetic data) in place of the traditional meat-based one. Plant-based hamburgers these days can closely mimic the texture and taste of meat-based hamburgers, thus allowing everyone to enjoy them (paralleling the use of synthetic data to solve data-sharing issues).

Simulation-based methods, however, are more akin to creating a hamburger from a recipe. Thus, if we want to exactly reproduce an existing burger (perhaps so as to share it with

others), we need to know our diners' flavor preferences (sweet, salty, sour, spicy), the burger's texture (soft, hard), the types of ingredients used, the temperature at which the meat was cooked, all while considering existing market research data (known parameter distributions). Or if this were a Monte Carlo simulation, we might randomly select combinations of flavors, textures, and ingredients. For instance, we might randomly generate 10,000 "virtual" burgers, each with a randomly chosen set of characteristics (generating random samples). For each virtually generated burger, we calculate its popularity based on the assumed preference distribution. For example, if a virtual burger has tastes and textures that a high proportion of the population prefers, it is considered more popular. Conversely, with the synthetic burger (data), one might aim to reproduce the original, albeit imperfect, original burger.

How Can a Researcher Synthesize Data?

To facilitate the generation, use, and adoption of synthetic datasets within organizational research, we outline a general process to guide organizational researchers (see Figure 1). In general, this process consists of two major steps, data generation and evaluation, which we have color-coded accordingly. Next, we review each of these steps along with the specific considerations within each.

Figure 1

Flow Chart Summarizing the General Process Steps for Synthesizing Data

Note. GANs = generative adversarial networks; VAEs = variational autoencoders.

Examine Original Data and Determine Intended Use of Synthetic Data

The first step of data generation is to examine the original data and determine its intended use for synthesis. The features of the original data, and the intended use of the synthetic data, are both key factors in understanding and guiding the subsequent steps of the process.

As previously mentioned, synthetic data are generated by learning from the multivariate distribution of the original dataset itself. However, different ML models have their own strengths and adaptability in learning and capturing various features. For example, the Gaussian Copula models work particularly well for data that are approximately normal or can be made approximately normal through transformations. On the other hand, GANs work better for capturing complex, high-dimensional distributions, making them suitable for more complex data.

For different types of original data, the characteristics of different models determine how well they perform in learning them and generating corresponding synthetic data. Likewise, the complexity of relationships may limit the effectiveness of synthetic data methods. Greater complexity in the relationships between variables makes generating accurate synthetic data more challenging, leading to increased computational complexity and a higher risk of overfitting. Besides that, the intended use of the synthetic data also influences our choice of generative model selection and evaluation. Different intended uses mean that the synthetic data need to focus on learning different attributes of the original data, and different generation methods may be better suited for producing specific attributes.

We foresee at least three possible uses of synthetic data. First, researchers who cannot share their original data may generate and share synthetic data so that others can approximate and perhaps extend their original analyses (e.g., hypothesis tests, factor analyses, structural equation models). Note that the original data may not have satisfied the assumptions of the

statistical models used (e.g., homoscedasticity for regression analysis), and results may not have been statistically significant. Nonetheless, the goal for synthetic data is to be as close to the original data as possible, so that the properties of synthetic data and any analytic results conducted on them are as close to those from the original data as possible.

Second, researchers may generate synthetic data to help build, test, and train ML models. Synthetic data present an opportunity to access a version of the original data that previously could not be used for training, due to privacy concerns. Thus, many existing applications generate synthetic data as input into ML models whose primary goal is often similar levels of prediction or classification as with the original data, versus obtaining similar parameter estimates of a statistical model. It should be noted that researchers have generated artificial data to supplement an original dataset, increase its diversity, and train fairer ML models as a result (e.g., Feldman et al., 2014; Zhang et al., 2016). To be clear, this type of 'de-biased synthetic data' is different from the synthetic data discussed in this paper, which are designed to emulate the original dataset as closely as possible without any extensions of this nature.

Third, synthetic data may be generated to inform meta-analyses or integrative data analyses that summarize relationships or effect sizes within the existing literature (Curran & Hussong, 2009). In this application, synthetic data would allow researchers to more readily share their original data, which may help inform more nuanced summaries of a given field (e.g., just as item-level meta-analyses have, such as Carpenter et al., 2016).

For example, if the intended use of synthetic data is to help build, test, and train ML models, we will be more concerned with how closely the distribution of the synthetic data matches the original data. This includes the marginal and joint distributions of features, the correlation structure among features in the original data, and the proportions of various sample types in the original data. Given that GANs perform well in capturing complex distributions and correlations in data, using GANs might be a good choice.

Select Synthetic Data Generation Method

Once the researcher has a sufficient level of familiarity with the original data and has a clear goal for the use of synthetic data, they can select a generation method to use. We will mainly introduce methods based on generative adversarial networks (GANs) (Goodfellow et al., 2014; Goodfellow et al., 2020). GANs consist of two neural networks— the generator and the discriminator—that work together to produce high-quality synthetic data (see Figure 2). The generator creates data that is rewarded for generating and mimicking an original dataset, while the discriminator is rewarded whenever the data is correctly judged to be inauthentic. Through this adversarial process, the generator iteratively improves until it can produce data that serve as a substitute for the original data.

GANs can be combined with various statistical principles and other models to form more complex and powerful methods, such as Conditional Tabular GAN (CTGAN; Xu and Veeramachaneni, 2018; Xu et al., 2019) and Copula GAN (Kamthe et al., 2021). Readers should keep in mind that each method has its strengths and limitations, and what works well for one dataset or application might not be suitable for another. The right tool for the right job, understand and select the appropriate synthetic data generation method to ensure the preservation of original data characteristics and meet the intended use.

Figure 2

GANs Workflow

Note. All GAN-based models share a typical workflow consisting of two main components: the Generator and the Discriminator (or Critic). The Generator's primary role is to produce authentic data so the Discriminator cannot differentiate it from the original data. Conversely, the Discriminator's job is to identify whether the input data are actual or fabricated by the Generator. Both components enhance their capabilities through their competition, ultimately leading to data that more closely resemble the original dataset.

Identify Relevant Hyperparameters and Optimize Hyperparameters

Most ML-based synthetic data generative models, including GAN-based models, allow researchers to fine-tune various hyperparameters to help ensure that the synthesized data exhibits preferred qualities. For example, there are several options available, ranging from epoch (i.e., how many times the training data are used to train the model), batch size (i.e., the amount of data fed into the model during each training iteration), and learning rates (i.e., the speed at which

network parameters are updated during training). Appendix A provides more details on the differences between parameters and hyperparameters, as well as several hyperparameters and common methods for optimizing hyperparameters.

Interestingly, the tuning or adjusting of these hyperparameters is highly related to computational resources and time, which is also a consideration for generating synthetic data. Generally speaking, allowing the model to learn from and emulate the original data, spending more training rounds, and using more complex models results in better outcomes (see Appendix A). However, this also means investing more time and money; therefore, setting a minimum target performance standard is particularly important. The minimum target performance standard refers to the lowest acceptable threshold during evaluation, which means it essentially meets or nearly meets the intention of generating synthetic data.

Evaluate the Quality of Synthetic Data

An important question about synthetic data is how to evaluate its quality relative to the original data. Two important evaluation criteria are *security* and *substitutability*. We categorized the evaluation tests into 'basic tests' and 'use-specific tests.' Basic tests provide the fundamental checks for synthetic data, including descriptive statistics such as means and correlations, which are important for any synthetic data. Use-specific tests, on the other hand, focus on the performance of synthetic data in target applications. For instance, if the synthetic data are intended for training machine learning models, the results should be comparable to those obtained with the original data.

Synthetic Data Quality: Basic Tests. Four basic tests provide a general assessment of the security and substitutability of synthetic data.

Overlapped Sample Test. This test checks the uniqueness of the synthetic dataset, an important step to prevent data replication and overfitting while maintaining data security. Specifically, it assesses the proportion of cases in the original and synthetic datasets that share the same value. Lower values indicate less overlap, thereby reducing the risk of security concerns.

$$
Percentage = \frac{Number of same values}{Total number of values} \times 100
$$

Constrained Reflection Test. This test checks how well each generated value conforms to the range of the original variables. By calculating the minimum, maximum, mean, and standard deviation in both the original and synthetic datasets, as well as effect sizes capturing the differences in these measures, one can demonstrate whether there is sufficient alignment and consistency.

Distribution Kurtosis and Skewness Test. This test checks the distribution characteristics of the datasets, allowing one to understand the asymmetry and the 'tailedness' of the data distribution, which can be important in assessing the quality of the synthetic data. By analyzing the kurtosis and skewness, one can determine how closely the synthetic data mimic the original dataset in terms of distribution shape.

Variable Correlation Test. This test checks the correlation between datasets' variables, important for gauging the substitutability of the synthetic data. The datasets reveal interrelationships among the variables. We scrutinized how these correlations were shown in each generated dataset and computed the mean of these values.

Synthetic Data Quality: Use-Specific Tests. Along with the basic tests of synthetic data quality, researchers must also provide evidence that synthetic data provide reasonable

approximations of the parameters that will be of most interest or relevance to the eventual enduser. Some examples for each of the potential uses include:

Hypothesis Testing. Researchers intending to generate and share synthetic data as a means of allowing others to approximate and extend their work may be particularly concerned with whether the synthetic data reproduce the important parameters within their models. Within organizational research, these parameters often include factor loadings, regression coefficients, and covariances. Thus, demonstrating that these parameter estimates fail to exhibit bias (i.e., minimal differences between the values obtained in the original data and the synthetic data), have adequate coverage (i.e., overlapping confidence intervals for the synthetic and original data), and yield similar conclusions for significance testing across the synthetic and original data can help assure future users of the synthetic data of the reproducibility of the results.

Machine Learning. When using synthetic data to build, train, and test machine learning models, the most important criterion may be the model fit. With machine learning models, researchers are often less concerned with the value of specific parameter estimates and are seeking to identify efficient and accurate means by which they can classify cases or predict future values. Examples of model fit estimates, then, that a researcher could use to show that the original and synthetic data are returning comparable results include R^2 , mean square error (MSE), and mean absolute error (MAE).

Meta-Analyses. If using synthetic data to inform meta-analyses or integrative reviews, what likely becomes paramount is whether the effect size(s) obtained from synthetic data are similar to those from the original data, for all practical purposes, contributing to a meta-analysis in the same way as the original study would. Moreover, synthetic data provided across studies

might be combined to allow for more refined analyses of moderator effects through multilevel modeling, going beyond a moderator analysis of effect sizes in a traditional meta-analysis.

These examples above—hypothesis testing, machine learning, and meta-analysis illustrate that evaluating the quality of synthetic data involves reasoned demonstrations that their synthesized data are well-suited for their intended purpose(s). One can therefore never "collect stamps" (Landy, 1986) and say categorically that synthetic data are always as good as the original dataset.

Feedback Loop from Data Evaluation Back to Data Generation

It is likely that during this process researchers will obtain poor results with one, or perhaps several, of the basic or use-specific criteria. As such, researchers may adopt a paretooptimization approach when evaluating their synthetic data where they seek to reach defensible thresholds across multiple criteria and prioritize those that are most important given the intended use of the data. As depicted in Figure 1, to achieve such optimization, we anticipate that researchers will have to cycle back to some of the initial data generation steps after evaluating the synthetic data that are initially obtained.

This represents a broader process beyond just tuning hyperparameters. The iterative loop for hyperparameter optimization produces good results for a model within a specific range, guided by a statistical loss function (see Appendix A). The loss function is a fundamental measure for assessing synthetic data. It indicates the degree of inconsistency between the modelgenerated values with the original values (e.g., MSE, MAE). The loop from data evaluation back to data generation is an overall cycle of generating synthetic data. Through a more detailed evaluation, we may decide to adopt different models to improve the quality of the generated synthetic data.

Additional Considerations

Before proceeding, there are a few aspects of this workflow that are worth noting. First, we acknowledge that the techniques available for synthesizing data are developing rapidly (e.g., data generation models, and hyperparameter optimization). Thus, the specific approaches used within some of these steps will likely need to evolve as improved techniques emerge. Second, we do not presume that this process is solely the responsibility of the researchers (i.e., individual synthesizing the data), but should also be something that end-users consider before incorporating synthesized data into their own work. That is, the end-user of the synthesized data should use the proposed workflow to consider whether there is sufficient information available to determine the rigor and quality of the synthetic data given its stated purpose. Third, consistent with broader recommendations regarding transparency and open science, this workflow will be most effective if researchers disclose the steps used in the synthetic data generation process and provide a comprehensive summary of the results of the tests of the evaluation criteria.

Empirical Demonstration of Synthetic Data and Two Research Questions

As mentioned before, a primary benefit of a synthetic dataset is that it contains analytically interpretable raw data for conducting a wide range of analyses, without sacrificing the privacy of the individuals contributing to the dataset. Thus, an important question is assessing the extent to which a given synthetic dataset can sufficiently substitute for the original dataset that generated it. Addressing this question is important to support the broader use of synthetic datasets in organizational research. With the goal of trying to increase the synthetic data's similarity to the original dataset, this must be accomplished in a manner that safeguards the sensitive and personal information of respondents. Optimal synthetic data should precisely retain the statistical attributes of the original data while minimizing any resemblance, patterns, or

details that could inadvertently jeopardize the anonymity and security of participants and their data, as found in the original dataset.

Motivated by these goals, we present two empirical demonstrations of synthetic data that address the following research questions:

Research Question 1 (RQ1): To what extent do synthetic data possess sufficient substitutability, as captured original data patterns, to serve as a viable alternative to raw datasets?

Research Question 2 (RQ2): To what extent do synthetic data possess sufficient security and limit the percentage of duplicated cases with the original dataset?

The analytic codes for both studies are available on GitHub: https://github.com/wpengda/SyntheticData_OrganizationalScience. We used the Python SDV package (Patki et al., 2016) to generate synthetic data. Data were analyzed using R, version 4.4.0 (R Core Team, 2024) as well as the psych package version 2.4.6.26 (Revelle, 2024).

Study 1: Synthetic Data in the Context of Assessment

Our first study used the General Aptitude Test Battery (GATB) dataset (U.S. Department of Labor, 1970). The GATB is an expansive assessment tool that provides nine cognitive aptitude scale scores on the basis of 12 tests thought relevant to the prediction of job performance. These aptitudes are General Learning Ability (G), Verbal Aptitude (V), Numerical Aptitude (N), Spatial Aptitude (S), Form Perceptual (P), Clerical Perception (Q), Motor Coordination (K), Finger Dexterity (F), and Manual Dexterity (M) (see Table 2). In addition to GATB scores, the dataset contains job performance criterion scores and detailed job descriptions. Thus, the GATB dataset is akin to others commonly employed in the context of assessment, hiring, and selection (Bemis, 1968; Vevea et al., 1993).

Table 1

General Aptitude Test Battery (GATB): Aptitudes and Corresponding Subtests

Note. Adapted from U.S. Department of Labor (1970). as cited in Kato & Scherbaum (2023).

Participants and Procedure

The entire GATB dataset consists of 40,489 employees in various occupations who took the GATB. For the current study, just for the purpose of an example, we focus on a specific occupation: Gambling Dealers (O*NET SOC Code 39-3011.00), which comprises 1,056 employees. The sex distribution was 57.1% male and 42.9% female. In terms of ethnicity, it is predominantly White (85.8%), followed by Black (11.8%), with the remaining 2.4% representing other ethnic groups. The measures of the aforementioned nine aptitudes identified in the GATB data can also be seen in Table 1.

Analyses

To generate the synthetic data for the GATB dataset, we followed the process described earlier and depicted in Figure 1. First, we examined the original data and found that some variables were skewed and leptokurtic (i.e., non-normal). Subsequently, we hypothesized that the synthetic data's intended use was to assist in building, testing, and training machine learning models. We focused on the standardized scores for each of the nine aptitudes identified in the GATB data and also included the standard supervisory rating scale as the performance criterion (CRFIN) in the analysis. Essentially, the final performance criterion was predicted by these nine ability indices. Additionally, the GATB dataset includes demographic variables such as sex and race. Therefore, we also wanted to explore whether the original data and synthetic data produced similar results under the same demographic variables.

Based on these purposes, we selected the generative model CTGAN as the method for generating synthetic data and adjusting multiple hyperparameters, such as the number of epochs. As shown in Figure 1, optimizing hyperparameters is an interactive process, for the sake of parsimony, we only present the final results here (i.e., batch size $= 128$; epoch $= 5,000$).

Study 1 Results

Basic Test

Overlapped Sample Test. We began by conducting an overlapped sample test to ensure that the synthetic data did not inadvertently create potential security or privacy risks. This test indicated that there was no overlap in data cases between the synthetic and original data. This suggests a certain level of security in the synthetic data.

Constrained Reflection Test. Next, constrained reflection test findings are presented in Table 2. This table encompasses each variable's minimum and maximum values, median, mean, standard deviation, and Cohen's *d*. Cohen's *d*, which quantifies the effect size difference between original and synthetic data, was less than the small effect threshold of 0.20 in all cases. Some people may argue that even a tiny Cohen's *d*, like 0.10, reflects meaningful differences. However, we believe that if the goal is to detect any difference, regardless of size, then a small effect size like 0.10 may warrant attention. On the other hand, if the goal is to identify changes of a certain magnitude or greater—such as when we want to create synthetic data that is not the same as the original—then such a small effect size might be considered negligible.

Table 2

GATB Subtests and Performance Criterion Descriptive Statistics: Comparing Original Data and

Synthetic Data

Note. $n = 1,056$ for both the original dataset and the synthetic dataset. GATB = General Aptitude Test Battery. CRFIN = standard supervisory rating scale. $Ku =$ Kurtosis, $Sk =$ Skewness. Cohen's *d* represents the mean difference between the original data and synthetic data.

Distribution Kurtosis and Skewness Test. Table 2 also reports the skewness and kurtosis values. The kurtosis for both the original and synthetic data sets showed a high degree of similarity across variables, all close to three (Mesokurtic), indicating a nearly normal distribution. Although the skewness was also closely matched for most variables, exceptions such as V and P exhibited opposite signs, suggesting a divergence in their asymmetry. However, given that the skewness values were within the ± 0.5 range, we could infer that the distribution of these variables was approximately symmetric. This near-symmetry, coupled with the absence of pronounced features, might explain why the synthetic data failed to capture the more nuanced trends present in the original data.

Variable Correlation Test. We present the findings of the variable correlation test in Table 3. Most of the correlations between the original and synthetic data aligned closely, with only a few exhibiting minor differences. The mean absolute difference in the magnitude of correlation coefficients across the two datasets was .06, indicating a strong resemblance in relational dynamics. Significantly correlated variables in the original dataset generally retained their significance in the synthetic dataset. Instances of non-significant correlations or those that diverged in direction compared to the original data maintained absolute values below .30. These showed weak correlation, meaning that the linear relationship between the two variables was not very strong, implying that changes in one variable did not predictably lead to linear changes in the other. This also offered a plausible explanation for certain discrepancies observed in the synthetic data, where weak correlations were infrequent features.

Table 3

GATB Correlation Matrices: Comparing Original and Synthetic Data

Note. $n = 1,056$ for both original data and synthetic data. GATB = General Aptitude Test Battery. CRFIN = standard supervisory

rating scale. A correlation magnitude less than .05 is not statistically significant.

Use-Specific Tests

Because our purpose was to assist in building, testing, and training ML models, we wanted to explore whether the original data and synthetic data produced similar results under the same demographic variables. We have conducted several tests as described below:

Machine Learning Analyses. The ML findings are presented in Table 4, where we evaluated the efficacy of four different ML models by comparing their performance on both synthetic and original data. We used 80% of the original data to train the model and tested it on 20% of the original data and 100% synthetic data. The outcomes of the four ML models were very similar on both the original test data and the synthetic data, as reflected through metrics such as *R²*, MSE, and MAE. These findings suggest that the performance of machine learning models on original data closely mirrors that on synthetic data, indicating the interchangeability of synthetic data.

Table 4

Machine Learning Analyses: Comparing Original Data and Synthetic Data for CRFIN predicted

by GATB subtests

Note. $n = 1,056$ for both the original dataset and the synthetic dataset. GATB = General Aptitude

Test Battery. CRFIN = standard supervisory rating scale. We use five-fold cross-validation and

get an average for R^2 , MSE, and MAE. R^2 = coefficient of determination; MSE = mean squared error; MAE = mean absolute error.

Gender and Race Differences in Descriptive Statistics. Gender difference findings are summarized in Table 5. For both males and females, the mean and standard deviation of the synthetic dataset aligned closely with those of the original dataset. Additionally, the Cohen's *d* values were relatively consistent across both datasets. On average, the absolute difference in Cohen's *d* between the synthetic and original datasets for gender was 0.09.

Race difference findings are also presented in Table 5. As with gender, the differences between the White and Black groups in the synthetic data were close to those in the original data. The mean and standard deviation showed similar patterns, and Cohen's *d* maintained directional consistency and largely similar magnitudes. On average, the absolute difference in Cohen's *d* between the synthetic and original datasets for gender was 0.14.

Table 5

GATB Subtests and Performance Criterion Standardized Mean Differences: Comparing Original

and Synthetic Data by Gender and Race

Note. $n = 1,056$ for both the original dataset and the synthetic dataset. GATB = General Aptitude

Test Battery. Standard deviations are in parentheses. Cohen's *d* represents the difference between

male and female effect sizes and the difference between the white and black effect sizes.

Study 1 Discussion

This first empirical demonstration showed the application of synthetic data to GATB data. We conducted basic tests and use-specific tests to determine whether synthetic data based on an ML generative model possessed sufficient substitutability and security. It can be seen that the model estimates were generally quite close. Although we did not show the feedback loop from data evaluation back to data generation in this demonstration, it is important to note that whenever a creator of synthetic data is not satisfied with the evaluation results, they can choose to use different synthetic data generation methods or adjust hyperparameters (see Appendix A). This iterative process is important for improving the quality and accuracy of synthetic data. Furthermore, even when the same model and the same hyperparameters are employed, the resulting synthetic data can differ due to the random sampling of data. Differences might be reflected in the value of single data points rather than the overall structure and pattern of the dataset.

We now transition to demonstrate the iterative process with a very different dataset to illustrate the different analytic choices one must consider, depending on the dataset.

Study 2: Synthetic Data with Multi-source Ratings

For Study 2, we applied our synthetic data approach to a multi-source assessment of leadership. Such assessments, also referred to as *360-degree feedback assessments*, are commonly applied in leadership development programs and can help leaders understand how they perceive themselves and how they are perceived by others (Fleenor et al., 2010; Lee & Carpenter, 2018). Areas of consensus, as well as those where disagreements emerge (i.e., "blind spots"), can help inform subsequent leadership development (Atwater et al., 1998).

Because these assessments typically feature multiple rating sources as well as multiple dimensions of leadership, they represent a distinct data structure than what was synthesized in Study 1, with a structure that is similar to those found across several areas of the organizational sciences (e.g., assessment centers, performance appraisals; Meriac et al., 2014).

Participants and Procedure

Study 2 data consist of multi-source ratings of 16,752 leaders. Leaders and their colleagues completed a multi-source leadership assessment that measures dimensions relevant to entry-level leaders. Prior research has found that this assessment exhibits evidence of adequate internal consistency, interrater reliability, content validity, construct validity (e.g., patterns of correlations among dimensions), and criterion-related validity (e.g., correlations with measures of leader effectiveness; Leslie & Braddy, 2015).

The assessment includes two broad categories that organize the lower-order dimensions: Leading the Organization and Leading Others. These broad categories largely and respectively correspond to the prevailing theoretical models of task- vs. relationship-focused perceptions of leadership behaviors (Gerpott et al., 2019; Meriac et al., 2014; Shaffer et al., 2016). Within the Leading the Organization category, there are four dimensions (with corresponding sample items):

(1) strategic perspective – "Links their responsibilities with the mission of the whole organization";

(2) being a quick study – "Learns a new skill quickly;"

(3) decisiveness – "Is action-oriented;"

(4) change management – "Adapts plans as necessary."

The Leading Others category consists of seven dimensions:

(5) leading employees – "Is willing to delegate important tasks, not just things they don't want to do;"

(6) confronting problem employees – "Can deal effectively with resistant employees;"

(7) participative management – "Is open to the input of others;"

(8) building collaborative relationships - "Tries to understand what other people think before making judgments about them;"

(9) compassion and sensitivity – "Is sensitive to signs of overwork in others;"

(10) putting people at ease – "Has personal warmth."; and

([1](#page-32-0)1) respect for differences – "Treats people of all backgrounds fairly.".¹

The 11 scales were measured using three to thirteen items rated on a 5-point scale ranging from 1 ("To a very little extent") to 5 ("To a very great extent").

Raters also provide ratings of a leader's likelihood to derail, which reflects challenges or

issues that if, unaddressed, likely limit one's effectiveness in a leadership position (Atwater et

al., 1998). These include

(1) problems with interpersonal relationships – "Is dictatorial in their approach;"

(2) difficulty building and leading a team – "Does not resolve conflict among direct

reports.";

(3) difficulty changing or adapting – "Has not adapted to the culture of the organization;"

(4) failure to meet business objectives – "Is overwhelmed by complex tasks;"

(5) too narrow a functional orientation – "Could not handle management outside of current function."

Aside from the leader's self-ratings, an average of 9.95 raters (*SD* = 3.65) rated each leader. A total of 150,062 raters are reflected in the data, including 65,635 direct reports, 67,507

¹ The assessment also contained dimensions categorized as "Leading Yourself." However, for the sake of parsimony, and because these pertain to constructs beyond typical areas of emphasis within leadership literature (e.g., career management, work-life balance), we have excluded these from our analyses.

peers, and 16,920 superiors. For each source, we created aggregate scores for each type of rater and each dimension by averaging across all items within a given type of rater for each dimension. These aggregate scores served as input for our analyses.

Analyses

To generate synthetic multi-source leadership assessment data, we followed the process described earlier and depicted in Figure 1. First, we examined the original data and found that, much like other rating-based evaluations in the organizational sciences, most variables were significantly skewed and leptokurtic (i.e., non-normal). Thus, most leaders were rated above the midpoint along each competency and below the midpoint for the derailment ratings. Second, we also determined that our intended use of these synthetic data would be to allow others to examine and replicate prior hypothesis testing (Braddy et al., 2014). Specifically, our goal was to synthesize data that reproduced earlier findings, which could then be shared with other researchers interested in self-other agreement leadership research (Fleenor et al., 2010). These steps helped inform our decision to select a CTGAN synthetic data model and to tune several hyperparameters (i.e., epoch and batch size). Although this reflects an iterative process, for the sake of parsimony, we only share the results of the best-performing model (i.e., batch size $= 128$; $epoch = 3000$).

Study 2 Results

Basic Tests

Overlapped Sample Test. As with Study 1, we began by conducting an overlapped sample test to ensure that the synthetic data did not inadvertently create potential security or privacy risks. This test indicated that there was no overlap in data cases across the synthetic and original data. This provides more assurance of the security of the synthetic data.

Constrained Reflection Test. Next, we conducted a constrained reflection test, where we compared the mean and standard deviations for the original and synthetic data. Across the different competencies and measures of derailment, and rating sources, the average absolute Cohen's *d* value was 0.06 (*SD* = 0.04, min. = 0.00, max. = 0.19) (see Table 6). This suggests that, on average, the distributions of the variables in the synthetic data exhibited comparable measures of central tendency (i.e., mean) and variability (i.e., standard deviation) when compared to the original data.

Distribution Kurtosis and Skewness Test. Table 6 also reports the skewness and kurtosis values for each variable in the original and synthetic data. On average, the absolute difference in the skewness and kurtosis values were 0.22 and 0.92. Further inspection revealed that the items pertaining to derailment tended to exhibit the largest differences across the synthetic and original data.

Variable Correlation Test. We then considered the variable correlation test and examined the differences in the correlations obtained using the synthetic and original data. Across all items and rating sources, we compared 2,016 correlations (i.e., each cell in the complete matrix). On average, the absolute difference in the correlation estimates was .07 (*SD* $= .00$, min $= .00$, max $= .30$). Figure 3 provides a histogram summarizing these differences, which shows that 80% of the correlation estimates exhibited differences less than or equal to .10.

Taken as a whole, we found that, when compared to the original data, the synthetic data exhibited minimal differences in the means and standard deviations (i.e., Cohen's *d*), that for many variables there were comparable levels of skewness and kurtosis, and that the majority of correlations were reproduced with relatively small differences. Thus, we proceeded to our usespecific tests.

Table 6

360 Assessment Original Data and Synthetic Data Descriptive Statistics

Note. $n = 16,752$ for the original dataset and 15,000 for the synthetic dataset. Cohen's *d* represents the difference between the original

data and synthetic data's effect size.

Figure 3

Histogram of Absolute Differences in Correlation Estimates Between the Original and Synthetic

Data

Note. The complete correlation difference matrix, featuring differences across 2,080 cells, is provided in Appendix A.

Use-Specific Tests

As noted previously, our intended purpose of these synthetic data was to generate data that would reproduce findings previously reported pertaining to the relationship between selfother agreement for task and relationship leadership and derailment (Braddy et al., 2014). Specifically, this model regressed peers' ratings of derailment onto a leader's self-ratings and their superiors' ratings of task and relationship leadership.

To begin, we sought to reduce the number of competencies in the assessment to the twodimensional space reported in the earlier study (i.e., task and relationship leadership). Thus, we fit an exploratory factor analysis (EFA) that forced a two-factor solution onto the 11 leadership competencies for both self-ratings and superior's ratings.^{[2](#page-42-0)} Across the 22 factor loadings, we found that the average absolute difference between the original and synthetic data was $.03$ ($SD = .02$, min. $= .00$, max. $= .07$). This suggests that factor analyses returned comparable solutions across the original and synthetic data.

Next, we proceeded to identify more defensible measures of task and relationship leadership by identifying items that contributed to a clear factor structure and were not redundant. Thus, we selected items whose relative loadings (i.e., item loading for a factor/sum of all loadings) were greater than .70 for a given. This resulted in two competencies for the task leadership dimension (i.e., decisiveness and confronting problem employees) and two on the relationship leadership dimension (i.e., compassion and putting people at ease). We also

² The EFA was estimated using minimum residuals and varimax rotations (Revelle, 2024). We also inspected a scree plot for the EFA, which indicated that the elbow exhibited a marked flattening for two dimensions. Because each leader was evaluated by multiple raters (e.g., several peers), and we chose to average across multiple raters within a given category, systematic variance in ratings that can be attributable to types of raters are omitted from these models. Thus, these EFA results largely ignore this source of variability in the 360 evaluations.

calculated a mean derailment score by averaging across peers' ratings on the five derailment items.

Using these measures, we estimated polynomial regression models in both the original and synthetic data, which are direct replications of Braddy et al.'s (2014) models. Table 7 reports the model results for both data sets. In general, the two datasets produced models that largely yielded similar results. Specifically, both models indicated that the more a leader and their supervisor rated their task or relationship leadership higher, the less likely the leader's peers were to believe that the leader would derail. Ultimately, this yielded consistent estimates of the two primary response surface tests: the linear effects of the line of congruence (a1) and the linear effects of the line of incongruence (a3). Specifically, for both datasets, the more leaders and their superiors (dis)agreed about their level of task and relationship leadership, the (more) less likely their peers were to indicate that the leader was likely to derail. These findings are largely similar to those reported by Braddy et al. (2014) and, more importantly to our current work, are consistent across both datasets. To allow for further comparisons of the polynomial regression results, we generated response surfaces for each model using the original and synthetic data (see Figure 4). The surfaces generated when predicting leader derailment using task and relationship ratings are consistent when based on the original and synthetic data.

Table 7

Self-Other Agreement Polynomial Regression Models for Original and Synthetic Data

Note. $n = 16,752$ for the original dataset and 15,000 for the synthetic dataset. R^2 for ratings of

derailment based on the polynomial regression models was .12 when using the original data

and .10 for the synthetic data.

Figure 4

Response Surfaces for Polynomial Regression Models Based on Original and Synthetic Data

Note. Responses surfaces are based on the results of the polynomial regression models reported in Table 7. Surfaces on the left-hand side correspond to those based on models using the original data, while the surfaces on the right-hand side are based on models using the synthetic data. $n =$ 16,752 for the original dataset and 15,000 for the synthetic data.

Study 2 Discussion

Our second application of synthetic data to an organizational context drew on multisource leadership ratings. We believe this is a useful addition to Study 1 because these data are largely non-normally distributed (i.e., skewed and leptokurtic), reflect a higher dimensional space (i.e., several variables being synthesized at once), and exhibit fairly strong correlations among the measures. Thus, in many ways, we see these data as a relatively stringent test of the capabilities of synthetic data models and suspect that in many other situations (e.g., more normality, less measures, greater discrimination), state-of-the-art synthetic data models would perform even better.

Overall, the synthetic data were able to reproduce previously estimated models using 360 data (Braddy et al., 2014) and produce results that were quite similar to the original data. That said, there were some areas of imprecision. For example, the predictive relationship between self-ratings of task leadership are somewhat larger with the synthetic data than the original data (-0.20 vs. -0.04) and the non-linear effect of the line of incongruence (i.e., a⁴ response surface parameters) are non-significant only in the synthetic data for both task and relationship leadership. We suspect that further training of a synthetic data model with additional hyperparameter tuning may reduce these differences. Here, though, it is important to highlight that these comparisons are not based on simulated data. That is, we generated the data synthetically and then began conducting analyses and fitting potential models. Thus, the data are not geared towards a single analysis (e.g., exploratory factor analysis, polynomial regression model), but instead are intended to preserve many of the features of the original data.

Lastly, it is important to reemphasize that developing a suitable synthetic data generation model is usually an iterative process. Specifically, as indicated in Figure 1, we examined several

alternative synthetic data generation models (e.g., Copula GAN) and employed a range of hyperparameters (e.g., batch sizes that included 128, 256, and 500 and epochs including 500, 1,000, 2,000, and 3,000).[3](#page-47-0) For the sake of parsimony, though, we only share the results of the best-performing model (i.e., batch size $= 128$; epoch $= 3,000$). However, it is critical to highlight that researchers who generate synthetic data will likely need to consider several data generation models and employ a range of hyperparameters until they are satisfied with the results of the various quality tests.

General Discussion

In this research, we develop a system framework to guide the synthetic data generation and evaluation processes, facilitating the application of synthetic data in organizational research. Using this framework, we present two empirical demonstrations in Studies 1 and 2 to illustrate how synthetic data can serve as a potential alternative when the use of original data is impractical, restricted, or poses privacy concerns. Our goal is to provide organizational researchers and practitioners with a general understanding of the principles behind generating synthetic data, inspiring them to further explore synthetic data methodologies and their use in organizational research.

Potential Limitations and Ethical Considerations

The use of synthetic data offers a realm of fresh prospects for exploration and advancement. However, like every technological stride, it comes with its set of challenges. What we want to emphasize the most is that synthetic data offer an alternative when sharing original data is impractical, restricted, or poses privacy concerns, but it cannot completely replace original data. Synthetic data are inevitably a variation of the original data. Therefore, although

³ Complete results of the quality tests for these alternative synthetic data models are available on GitHub: https://github.com/wpengda/SyntheticData_OrganizationalScience.

modeling or analysis performed on synthetic data may approach the effectiveness of using original data, there will still be additional risks. We believe that synthetic data can be used as a tool to promote information sharing and research, but more regulations are needed as well as transparent reporting of the assumptions discussed in this work. For example, when presenting findings derived from synthetic data, researchers should very clearly state the source of the data to avoid it being misunderstood as the original data and explain the models and hyperparameters used to generate the synthetic data (see Appendix A for more information about hyperparameters).

In addition, the quality of synthetic data is highly dependent on the quality of the original data used to generate it; if the original data contains any errors in the quantitative information or in understanding the nature of the variables, the synthetic counterpart will also reflect those flaws. And generating high-quality synthetic data requires a high degree of technical and algorithmic knowledge. The quality of the synthesized data depends on the quality of the generative model used. If the model does not properly capture the key characteristics of the original data, the generated data may not provide accurate insights. For some specific applications or complex data structures, further research and development may be required to generate synthetic data effectively. Apart from that, even though synthetic data are not directly sourced from real-world individuals, the potential for disclosure exists (Abowd $&$ Vilhuber, 2008). Synthetic data are not automatically private and also require careful use and regulation. Nevertheless, we believe that through further research, organizational study can better understand and benefit from synthetic data.

Finally, we encourage researchers to ensure that they abide by rules and regulations regarding data sharing. When in doubt regarding data sharing, authors should contact their

oversight departments for clarification. For instance, institutional review boards may still require a statement such as this on consent forms for human subjects even if synthetic data are to be shared in place of original data: "For future research studies, we might use the survey data you provide to generate de-identified synthetic data. We might also share this non-identifiable synthetic data with other researchers for future research studies without requiring additional consent from you." Other entities, such as firms or database owners may have additional rules that may still need to be followed even with synthetic data.

Future Directions and Research Implications

We believe that synthetic data offer organizational researchers an opportunity to use previously inaccessible data. However, as emphasized in this paper, a myriad of factors including varied methodologies for generating synthetic data and the fine-tuning of hyperparameters - substantially influence both the substitutability and the security of the synthetic data produced. These elements significantly dictate the overall quality of the resultant datasets. This paper thus provides an overview of the nature of synthetic data and, via two empirical examples, how they are generated and tested for their quality. Also provided in Appendix A is a general overview of parameters, hyperparameters, and optimization when generating synthetic data. In future organizational research addressing synthetic data, these aspects also require further exploration and research.

Another idea in future research is to consider generating multiple synthetic datasets from an original dataset, and not just one. . Due to the inherent randomness of machine learning methods, each synthetic dataset generated from an original dataset is bound to be different. One could then conduct a comprehensive analysis of the set of synthetic datasets to shed further light on the nature of the original dataset and the robustness of the synthetic dataset generation.

Moreover, we think encouraging cross-disciplinary collaborations—such as facilitating exchanges between computer scientists, statisticians, and organizational scientists—can introduce unprecedented methods and ideas. Only through close cooperation among all parties can we fully explore and utilize the vast potential of synthetic data, driving the field of organizational research to new heights. As a final future direction, we suggest that there is a need and potential benefit to explore the use of synthetic data on unstructured, qualitative data (e.g., interview or focus group transcripts).

Conclusion

The open science movement has sought to promote the sharing of data as such a practice can serve to accelerate the advancement of theory, practice, and policy making. However, concerns remain about the need to protect human subjects and proprietary information. The creation of synthetic data is one means to promote open data while still honoring ethical and legal concerns. In the current paper, we reviewed the key steps in an iterative process needed to generate synthetic data. These include the consideration of a number of assumptions as well as basic and specific-use tests in order to evaluate the quality of synthetic data. We then demonstrated the use of these steps on two unique example datasets. We hope that this work serves to promote greater sharing of data in the organizational sciences.

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Appendix A

Parameters & Hyperparameters

Before we begin, it is important to define some terms commonly used in the field of ML, similar to how various terms are defined in psychology. We will introduce the concepts of parameters and hyperparameters in the sections below.

Parameters are elements that can be initialized and updated through the learning process, such as the weights of neurons in a neural network. In contrast, *hyperparameters*, which cannot be directly estimated from data, must be set before training a machine learning model. They also define the model's architecture (Kuhn & Johnson, 2013). The process of designing an ideal model architecture with the best configuration of hyperparameters is known as hyperparameter optimization/tuning. This tuning is considered an important component in building effective ML models (Hutter et al., 2019).

Common Hyperparameters

Common hyperparameters include (Hutter et al., 2019; Yang & Shami, 2020):

1. Learning rates: These rates determine the speed at which network parameters are updated during training, directly impacting learning efficiency.

2. Number of epochs: This defines how many times the complete dataset is used to train the model, which can affect both training duration and model accuracy.

3. Batch size: This hyperparameter sets the amount of data fed into the model during each training iteration, affecting both the speed and stability of the training process.

4. Optimization algorithms: Optimization algorithm refers to a method employed in ML to adjust the parameters of a model. The goal is to either minimize or maximize a specific function, often the loss function. Options such as Adam or SGD can significantly influence the effectiveness and speed of training.

5. Network architecture: Elements like the number of hidden layers and neurons per layer play important roles in determining the model's learning capability and complexity.

6. Noise dimension: The dimension of the input noise vector for the generator influences the diversity of the data generated.

Loss Function & Optimize Hyperparameters

In addition, we would like to briefly introduce how to optimize hyperparameters. Optimizing hyperparameters is usually aimed at minimizing the loss function. The loss function is a measure of the difference between the model's output and the true labels; for synthetic data, it measures how close the output is to the original data. By minimizing this function, the synthetic data generated by the model can be improved. Generally speaking, different goals and models will choose different loss functions. Common loss functions include the MSE and the MAE. GANs-based models have a generator and a discriminator, each with its own loss function. And following are common methods for optimizing hyperparameters (Yang & Shami, 2020).

1. Model-free algorithms optimization: These refer to optimization methods that do not rely on a clear mathematical description of the underlying model. For example, Manual Search is a very basic method where hyperparameters are manually adjusted by individuals based on their experience and intuition, also known as 'trial and error' or babysitting (Abreu, 2019). Another example is Grid Search, which is essentially a method of exhaustive search. For each hyperparameter, users select a small finite set to explore (Goodfellow et al., 2016). The Cartesian product of these hyperparameters results in several combinations, and Grid Search trains models

using each combination to select the one with the smallest loss function value as the best hyperparameters (Hutter et al., 2019).

2. Gradient-based optimization: This is a traditional optimization technique, which computes the gradient of variables to identify promising directions and move towards the optimal direction (Bengio, 2000). By randomly selecting a data point or a small subset of data, this technique updates the model parameters by moving in the opposite direction of the gradient computed for that sample or subset, thus taking a step towards minimizing the loss function. Therefore, after convergence, it can achieve a local optimum. For certain machine learning algorithms, the gradient of some hyperparameters can be computed, and then gradient descent is used to optimize these hyperparameters. However, it can only be used to optimize continuous hyperparameters, as other types of hyperparameters (e.g., the depth of the decision tree; the number of layers in the network structure; the choice of activation function) do not have a gradient direction. Moreover, this is only effective for convex functions, as non-convex functions might only reach a local rather than a global optimum.

3. Bayesian optimization: This method uses a probabilistic approach to predict the performance of various hyperparameters and updates the model as more results are observed (Snoek et al., 2012). The key idea is to balance exploration—testing hyperparameters where the model's predictions are uncertain—and exploitation—focusing on hyperparameters that are predicted to yield the best performance. In Bayesian optimization, a surrogate model, often a Gaussian process, is used to model the unknown function linking hyperparameters to an objective function, such as model accuracy. Gaussian processes are favored for their ability to provide a smooth estimate and naturally incorporate prediction uncertainty. An acquisition function, such as expected improvement, probability of improvement, or upper confidence bound, is then used

to select the next set of hyperparameters to be evaluated, optimizing the use of the surrogate model (Frazier, 2018). Compared to methods like grid search, Bayesian optimization can identify more effective hyperparameters with significantly fewer evaluations (Injadat et al., 2018).

Should We Worry About Overfitting for Synthetic Data?

Beyond that, overfitting is a common issue in ML, characterized by a model performing exceptionally well on training data but poorly on new, unseen data. This typically occurs because the model has learned the noise and specific details in the training data instead of the underlying true patterns of the data. But given our objective—to learn and mimic the training data as precisely as possible but not as same as the training data—generating synthetic data may mean that 'overfitting' is not necessarily a problem to be avoided. Common signs of overfitting, such as the model perfectly learning the training data, might actually be desirable. By this, here are several strategies that can help ensure the model learns from and emulates the training data.

1. Increase model complexity: Use more complex network architectures to ensure the network has sufficient capacity to capture and learn the complex patterns and details in the data.

2. Extend training duration: Increase the number of training iterations (number of epochs) until the model performs exceptionally well on the training set. This helps ensure the model learns as much information as possible from the training data.

We would like to emphasize again that the purpose here is to generate synthetic data as close to the original data as possible to protect privacy—not to predict the overall trend of a data. Therefore, the potential 'overfitting' associated with these methods should not be a concern in this context.