Bayesian Non-parametric Generation of Fully Synthetic Multivariate Categorical Data in the Presence of Structural Zeros

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Summary. Statistical agencies are increasingly adopting synthetic data methods for disseminating microdata without compromising the privacy of respondents. Crucial to the implementation of these approaches are flexible models, able of capturing the nuances of the multivariate structure present in the original data. In the case of multivariate categorical data, preserving this multivariate structure also often involves satisfying constrains in the form of combinations of responses that cannot logically be present in any dataset—like married toddlers or pregnant men—also known as structural zeros. Ignoring structural zeros can result in both logically inconsistent synthetic data and biased estimates. Here we propose the use of a Bayesian non-parametric method for generating discrete multivariate synthetic data subject to structural zeros. This method can preserve complex multivariate relationships between variables; can be applied to high dimensional datasets with massive collections of structural zeros; requires minimal tuning from the user; and is computationally efficient. We demonstrate our approach by synthesizing an extract of 17 variables from the 2000 U.S. Census. Our method produces synthetic samples with high analytic utility and low disclosure risk.

Keywords: Bayesian Nonparametric, Dirichlet Process, Contingency Tables, Multiple Imputation, MCMC, Disclosure Risk

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1. Introduction

The use of synthetic data (Rubin, 1993) is an attractive option for statistical agencies and other organizations that wish to share individual-level data with third parties, but at the same wish to protect the identities and sensitive attributes of respondents. The idea is simple. The data custodian (henceforth "the agency") uses the sensitive data to fit a statistical model, and releases samples from its predictive distribution instead of the original data. Secondary analysts can then perform analyses on the synthetic data without having access to the original data. In order to account for the uncertainty associated with the sampling and estimation procedures, the agency can release a set of M approximately independent samples from the predictive distribution, which then analysts can combine using the rules developed specifically for synthetic data by Raghunathan et al. (2003).

The utility of synthetic data schemes depends heavily on the quality of the models used to generate the data: analysts will be unable to detect features that the synthesis model did not adequately capture in the first place. In the case of multivariate data, synthesis models have to be prepared to preserve complex—and often unexplored—relationships between variables. A popular synthesis technique is the sequential modeling or full conditional specification (FCS) approach (Van Buuren and Oudshoorn, 1999; Van Buuren et al., 2006). Here the agency fits regression models to each of the variables conditional on the rest, and then use them for sampling each variable, one at a time. Greater flexibility can be achieved by using non-parametric regression models such as CART and random forests (Reiter, 2005; Caiola and Reiter, 2010). This approach has the advantage of simplicity, replacing the problem of specifying a complex multivariate distribution with the simpler problem of specifying several univariate conditional models. However, as has been noted (e.g. Raghunathan et al., 2001; Vermunt et al., 2008; White et al., 2011), this procedure lacks guarantees that the resulting set of regression models will correspond to any well-defined joint distribution. Moreover, when dealing with certain configurations of categorical data, it lacks the ability of sampling from the whole support of the distribution. We comment on this specific problem in the discussion.

A second approach to synthetic data generation is the use of joint probability models. This approach avoids most of the pitfalls of sequential conditional modeling, but has the drawbacks of estimation complexity, and the need of finding and selecting models with good predictive performance. In the case of discrete data, most early proposals using joint modeling have focused on simple models, like the

discretized multivariate normal (Matthews et al., 2010). More recently, Hu et al. (2014) proposed the use of a Bayesian non-parametric version of the Latent Class (NPLCM) model proposed by Dunson and Xing (2009) to synthesize multivariate categorical data. They showed that this model enjoys a good predictive performance, scalability, and low disclosure risk.

An important issue that Hu et al. (2014) did not address was the case of structural restrictions in the form of responses that are known to be impossible *a priori*, known as structural zeros (Bishop et al., 1975)—for example, it is impossible for a toddler to be a widower. An obvious problem with not explicitly accounting for structural zeros is the risk of assigning positive probability to impossible combinations, and thus of generating and disseminating synthetic data with inconsistent responses (like widower toddlers). Such synthetic data could cause confusion in analysts, and ultimately lead to the public's losing of confidence in the agency's work. Additionally, as Manrique-Vallier and Reiter (2014) noted, failing to account for structural zeros can lead to biased estimates.

In this article we propose and evaluate the use of an extension of the NPLCM, originally introduced by Manrique-Vallier and Reiter (2014), for the task of synthesizing discrete multivariate data subject to structural zeros. This extension, called the Truncated NPLCM (TNPLCM), retains most of the advantages described by Hu et al. (2014) while adding the ability of handling complex patterns of structural zeros. We present a considerably improved computational method to fit the TNPLCM (Sections 2.2 and 2.3), and extend it to the task of generating fully synthetic data (Section 2.4). We illustrate the use of our approach by synthesizing an extract of 17 categorical variables from the U.S. 2000 census, which results in a contingency table of about 55×10^9 cells from which about 52×10^9 correspond to structural zeros. Through a demanding battery of tests we show that the TNPLCM generates high-utility synthetic data (Section 3.1) with low-disclosure risk (Section 3.2).

2. Nonparametric Latent Class Models for Categorical Data Synthesis

Suppose that the agency has collected a sample of n individual confidential records, each detailing J attributes with finitely many possible values. Let $\mathcal{X} = (\mathbf{x}_1, ..., \mathbf{x}_n)$ be the original sample, $\mathbf{x}_i = (x_{i1,}, ..., x_{iJ})$ each record, and $\mathcal{C}_j = \{1, ..., L_j\}$ the set of possible values of x_{ij}. Thus for any individual $i \in \{1, ..., n\}$ we have that in principle $\mathbf{x}_i \in \mathcal{C} = \prod_{j=1}^{J} \mathcal{C}_j$. Following standard terminology we call each of the elements of $\mathcal{C}$ a *cell*. Let $S \subset \mathcal{C}$ be a set for which it is known *a priori* that $\Pr(\mathbf{x} \in S) = 0$. We

call the cells in S *structural zeros* (Bishop et al., 1975). Our objective is to use $\mathcal{X}$ to generate M fully synthetic datasets $\boldsymbol{\mathcal{Y}} = (\mathcal{Y}_1, .., \mathcal{Y}_M)$, with support in $\mathcal{C} \setminus S$, which can be safely disseminated, and that lead to inferences close to those which would be obtained from $\mathcal{X}$ itself.

2.1. Nonparametric Latent class models

Hu et al. (2014) proposed the use of the nonparametric latent class model (NPLCM) as a data-synthesizer for high-dimensional discrete categorical data without structural zeros. Here we describe it in preparation for discussing the issues involved in considering the structural zeros. The NPLCM is a Dirichlet process mixture of product-multinomial distributions, originally proposed by Dunson and Xing (2009) as a general-purpose tool for modeling complex contingency tables. As Dunson and Xing (2009) show, the NPLCM has full support in $\mathcal{C}$. Thus it is consistent for estimating cell probabilities in any contingency table. Additional practical advantages include its computational tractability and scalability, its tolerance to severely sparse contingency tables, and its minimal need for tuning by the user (see e.g. Si and Reiter, 2013; Manrique-Vallier and Reiter, 2014; Manrique-Vallier, 2016, for example applications in different domains).

The construction of the NPLCM model in Dunson and Xing (2009) is similar to the classic Latent Class model (Goodman, 1974). We assume that the population can be partitioned into a finite number of homogeneous classes, and that within each of these classes item responses can be considered independent—conditional independence given class membership. This can be expressed as the following generative model

$$x_{ij} \overset{ind}{\sim} \text{Discrete}(\{1, ..., L_j\}, (\lambda_{jz_i}[1], ..., \lambda_{jz_i}[L_j])), \text{ for } i = 1, .., n,\ j = 1, ..., J \tag{1}$$

$$z_i \sim \text{Discrete}(\{1, ..., K\}, (\pi_1, ..., \pi_K)),\ \text{for } i = 1, ..., n\ , \tag{2}$$

where the class assignment labels, z_i, and their probabilities, π_i are unknown. Dunson and Xing (2009) construct the NPLCM by considering an infinite number of classes, and assigning a stick-breaking prior (Sethuraman, 1994) for their (infinite dimensional) probability vector. The version of the NPLCM proposed by Hu et al. (2014) for data synthesis is a computationally convenient finite-dimensional

approximation to this model. We describe it by completing the LCM model in (1)-(2) with

$$\boldsymbol{\pi} = (\pi_1, ..., \pi_K) \sim SB_K(\alpha) \tag{3}$$

$$\lambda_{jk}[\cdot] \overset{iid}{\sim} \text{Dirichlet}(\mathbf{1}_{L_j}), \text{for } j = 1, ..., J \text{ and } k = 1, ..., K \tag{4}$$

$$\alpha \sim \text{Gamma}(a, b) \tag{5}$$

where $SB_K(\alpha)$ is the finite dimensional stick-breaking process (Ishwaran and James, 2001): for $k = 1, ..., K$ make $\pi_k = V_k \prod_{h<K}(1 - V_h)$, where $V_K = 1$ and $V_k \sim \text{Beta}(1, \alpha)$ for $k < K$. Here $SB_K(\alpha)$ replaces the infinite-dimensional stick breaking process from Dunson and Xing (2009); see Si and Reiter (2013) and Manrique-Vallier and Reiter (2014) for guidance about choosing K. We also follow Dunson and Xing (2009) in setting $a = b = 0.25$ as a weak prior that favors a data-dominated inference.

2.2. NPLCM with Structural Zeros

Manrique-Vallier and Reiter (2014) developed an extension to the NPLCM, henceforth denoted TNPLCM (Truncated NPLCM), which allows to enforce the restriction $\Pr(\mathbf{x} \in S) = 0$ for some known set of structural zeros $S \subset \mathcal{C}$. Their computational method relies on a sample augmentation technique whereby we assume the existence of an unobserved sample $\mathcal{X}^0 = (\mathbf{x}_1, ..., \mathbf{x}_{n_0})$ of unknown size $n_0 = N - n$, generated from the unrestricted NPLCM, but which contains only records whose values fall into S. Manrique-Vallier and Reiter (2014) showed that setting the improper prior distribution $P(N) \propto 1/N$ and estimating $\mathcal{X}^0$ and their corresponding latent variables $\mathcal{Z}^0 = (z_1, ..., z_{n_0})$ simultaneously with the rest of the parameters involved in the model in (1)-(2), results in the same marginal posterior distribution of $(\boldsymbol{\lambda}, \boldsymbol{\pi})$ corresponding to the TNPLCM. We note that under this scheme, computing the predictive distribution of the TNPLCM for a given set of parameters $(\boldsymbol{\lambda}, \boldsymbol{\pi})$ requires truncating and re-normalizing the pmf so that $f^{TNPLCM}(\mathbf{x}|\pi, \boldsymbol{\lambda}, S) \propto I(\mathbf{x} \notin S) \sum_{k=1}^{K} \pi_k \prod_{j=1}^{J} \lambda_{jk}[x_j]$.

Manrique-Vallier and Reiter (2014) also noted that significant computational gains can be realized whenever s can be expressed as the union of a relatively small (with respect to the size of s) collection of disjoint *table slices*. A table slice is the collection of cells that result from fixing some of the j response components, while letting the rest take any possible value—for example the set $\{\mathbf{x} = (x_1, ..., x_6) \in \mathcal{C} : x_1 = 1, x_3 = 4\}$. Real situations in which this is possible are frequent; it is common that structural

zeros arise from specific combinations of levels of a few (often just two) variables at a time. When the resulting collection of slices is not disjoint, we need to transform them into a disjoint collection using the specialized algorithm developed for this task by Manrique-Vallier and Reiter (2014), and improved in Manrique-Vallier and Reiter (to appear). We detail this algorithm in Section 3 of the supplemental materials. Manrique-Vallier and Reiter (2014) developed a specialized notation for operating with table slices that we now describe, as we will need it to develop our estimation algorithms. Consider the set $\mathcal{C}^* = \prod_{j=1}^{j} \mathcal{C}_j^*$ for $\mathcal{C}_j^* = \mathcal{C}_j \cup \{*\}$. We call the elements of $\mathcal{C}^*$ *slice definitions*—or "margin conditions" in Manrique-Vallier and Reiter (2014) terminology. We use slice definitions to represent and operate with table slices. For example, we use the slice definition $(1, *, 4, *, *, *)$ to represent the table slice that results from fixing $x_1 = 1$ and $x_3 = 4$. We use the symbol '*' in the j-th place of a vector $\boldsymbol{\mu} \in \mathcal{C}^*$ as a placeholder to indicate that that coordinate is free to vary in the range $1...l_j$. More formally, we define the mapping that takes slice definition $\boldsymbol{\mu} = (\mu_1, ..., \mu_j)$ to its corresponding table slice as $\bar{\boldsymbol{\mu}} = \{\mathbf{x} \in \mathcal{C} : x_j = \mu_j \text{ for } \mu_j \neq *\}$. We call $\bar{\boldsymbol{\mu}}$ the *slice defined by* $\boldsymbol{\mu}$.

2.3. Estimation using MCMC

Here we present an improved version of the algorithm from Manrique-Vallier and Reiter (2014) for obtaining samples from the posterior distribution of the TNPLCM. Assume that the set of structural zeros can be represented as $S = \cup_{c=1}^{C^0} \bar{\boldsymbol{\mu}}_c$, where $\{\overline{\boldsymbol{\mu}_c}\}$ is a collection of disjoint table slices. Let $\delta_c \in \mathcal{C}$ $(c = 1, ..., C^1)$ be the non-empty cells in the contingency table generated by $\mathcal{X}$, and $n_c^1 = \sum_{i=1}^{n} I(\mathbf{x}_i = \delta_c)$ be the corresponding cell counts. Let $m_{ck}^1 = \sum_{i=1}^{J} I(\mathbf{x}_i = \delta_c, z_i = k)$ be the number of individuals in cell δ_c that belong to latent class k, and $\Omega_{jkl}^1 = \sum_{j=1}^{J} I(x_{ij} = l, z_i = k)$ the number responses to item j at level l for observed individuals in class k. We define analogous quantities $n_c^0 = \sum_{i=1}^{n_0} I(\mathbf{x}_i^0 \in \bar{\boldsymbol{\mu}}_c)$, $m_{ck}^0 = \sum_{i=1}^{J} I(\mathbf{x}_i^0 \in \bar{\boldsymbol{\mu}}_c, z_i^0 = k)$ and $\Omega_{jkl}^0 = \sum_{j=1}^{J} I(x_{ij}^0 = l, z_i^0 = k)$ for the n_0 individuals in the augmented sample.

Our MCMC algorithm is as follows:

(a) For $c = 1, ..., C^1$, sample $(m_{c1}^1, ..., m_{cK}^1) \sim \text{Multinomial}(n_c^1, (p_1, ..., p_K))$, with $p_k \propto \pi_k \prod_{j=1}^{J} \lambda_{jk}[\delta_{cj}]$. Make $\Omega_{jkl}^1 = \sum_{c=1}^{C^1} m_{ck}^1 I(\delta_{cj} = l)$.

(b) For $j = 1, ..., J$ and $k = 1, ..., K$, sample $\lambda_{jk}[\cdot] \sim \text{Dirichlet}(\xi_{jk1}, ..., \xi_{jkL_j})$, with $\xi_{jkl} = 1 + \Omega_{jkl}^0 + \Omega_{jkl}^1$.

(c) For $k = 1, ..., K-1$, sample $V_k \sim \text{Beta}(1 + \nu_k, a + \sum_{h=k+1}^{K} \nu_k)$ where $\nu_k = \sum_{c=1}^{C^1} m_{ck}^1 + \sum_{c=1}^{C^0} m_{ck}^0$. Let $V_K = 1$ and make $\pi_k = V_k \prod_{h<k}(1 - V_h)$ for all $k = 1, ..., K$.

(d) Sample $(n_1^0, ..., n_{C^0}^0) \sim NM(n, (\omega_1, ..., \omega_c))$, where $\omega_c = \Pr(\mathbf{x} \in \boldsymbol{\mu}_c | \boldsymbol{\lambda}, \boldsymbol{\pi}) = \sum_{k=1}^{K} \pi_k \prod_{\mu_{cj} \neq *} \lambda_{jk}[\mu_{cj}]$, and $NM(n, \cdot)$ is the negative multinomial distribution.

(e) For each $c = 1, ..., C^0$, sample $(m_{c1}^0, ..., m_{cK}^0) \sim \text{Multinomial}(n_c^0, (p_1, ..., p_k))$, where $p_k \propto \pi_k \prod_{j:\mu_{cj} \neq *} \lambda_{jk}[\mu_{cj}]$.

(f) For $c = 1, ..., C^0$, $k = 1, ..., K$ and $j = 1, ..., J$:
if $\mu_{cj} = *$, sample $(\gamma_{cjk}[1], ..., \gamma_{cjk}[L_j]) \sim \text{Multinomial}(m_{ck}^0, (\lambda_{jk}[1], ..., \lambda_{jk}[L_j]))$;
otherwise make $\gamma_{cjk}[l] = m_{ck}^0 I(\mu_{cj} = l)$ for $l = 1, ..., L_j$. Make $\Omega_{jkl}^0 = \sum_{c=1}^{C^0} \gamma_{cjk}[l]$.

Different from Manrique-Vallier and Reiter (2014), this algorithm works by directly sampling total counts within C^0 table slices, instead of imputing the responses and class assignments of n_0 augmented data points in the region S. This change of strategy has important consequences. In practice n_0 can sometimes be very large—in our example (see next section) a dataset of $n = 10,000$ and $C^0 = 3803$ results in a n_0 in the order of $\approx 700,000$, with some samples as large as $880,000$. Thus the proposed strategy change can drastically reduce both the number of operations and the storage needs. In our example in Section 3, these effects resulted in a speedup of approximately 300% and a reduction of 97% in RAM allocation. Furthermore, since n_0 is not known in advance but estimated simultaneously with the rest of the parameters, our modifications result in an algorithm with predictable speed and allocation needs. Similarly, we have also modified the algorithm to sample total counts within the contingency table cells with observed counts, instead of imputing n latent class labels z_i for each observed record. This modification brings some computational savings, although more modest.

2.4. Synthetic Data Generation

To obtain M synthetic datasets, $\boldsymbol{\mathcal{Y}} = (\mathcal{Y}_1, ..., \mathcal{Y}_M)$, the agency can run steps (a)-(f) until convergence, and pick M samples $\theta^{(m)} = (\boldsymbol{\lambda}^{(m)}, \boldsymbol{\pi}^{(m)})$, sufficiently spaced to minimize correlation effects. Then, for each $\theta^{(m)}$, the agency can generate its corresponding synthetic dataset, $\mathcal{Y}_m$, by generating N_{synth} samples from the predictive distribution, $p(\mathbf{x}^* | \boldsymbol{\lambda}^{(m)}, \boldsymbol{\pi}^{(m)}, S) \propto I(\mathbf{x}^* \notin S) \sum_{k=1}^{K} \pi_k^{(m)} \prod_{j=1}^{J} \lambda_{jk}^{(m)}[x_{ij}^*]$. This can be done using a simple rejection sampling scheme: for $i = 1, ..., N_{synth}$ we obtain each $\mathbf{y}_i$ by

(a) Sample $z \sim \text{Discrete}(\{1, ..., K\}, (\pi_1, ..., \pi_K))$

(b) For $j = 1, ..., J$ sample $y_j^* \overset{ind}{\sim} \text{Discrete}(\{1, ..., L_j\}, (\lambda_{jz}[1], ..., \lambda_{jz}[L_j]))$

(c) If $\mathbf{y}^* = (y_1^*, ..., y_J^*) \in S$, discard it and go back to step 1. Otherwise make $\mathbf{y}_i = \mathbf{y}^*$.

3. Empirical Study: Synthesizing U.S. Census Data

Here we empirically illustrate the performance of our TNPLCM synthesizer under repeated sampling. For this we use an extract from the 5% public use microdata from the 2000 United States census for the state of California (Ruggles et al., 2010) which comprises $H = 1,690,642$ records measured in $J = 17$ categorical variables with between 2 and 11 levels each. We detail the variables and the number of levels for each variable in the Supplemental Materials. This results in a massive contingency table of approximately 5.52×10^{10} cells. Analysis of impossible combinations of variables reveals 73 overlapping sets of slices defined by the levels of two variables at a time; e.g. the slice that results from fixing the levels of mortgage status (MORTGAGE) and ownership of dwelling (OWNERSHP) at the combination 'No, owned free and clear' and 'renting', respectively, maps to approximately 4.6 billion cells. We transform this collection of 73 overlapping slices into an equivalent collection of 3803 disjoint ones using a variant of the algorithm from Manrique-Vallier and Reiter (2014). This analysis finally reveals that approximately 5.38×10^{10} of the table's cells correspond to structural zeros.

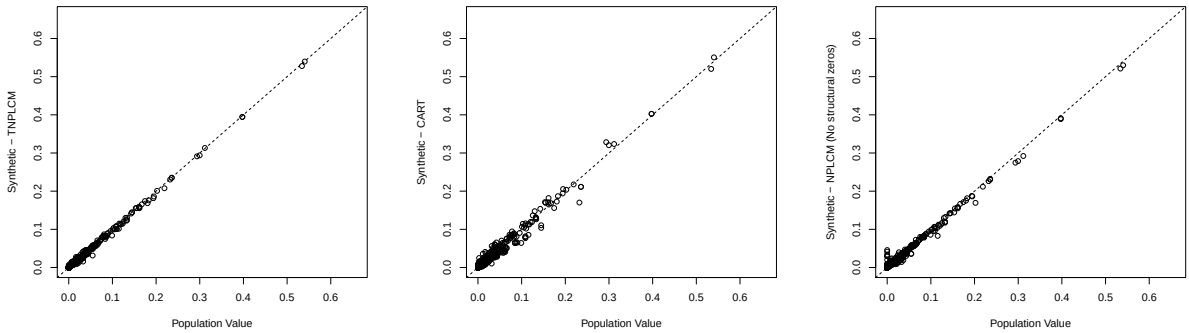
3.1. Utility of the synthetic data

We conduct a repeated sampling experiment considering the H original records as a population, and randomly obtaining 200 datasets of size $n = 10,000$. We use our TNPLCM synthesizer on each subsample to generate 200 groups of $M = 5$ synthetic datasets of size $N_{synth} = 10,000$. For this we have run chains with 15,000 iterations burn-in periods, after which we generated one synthetic dataset every 2000 iterations, due to the high autocorrelation of parameters. We noted, however, that we obtain essentially the same results by generating one synthetic dataset every 200 samples; meaning that we actually may have used shorter runs. We evaluate the utility of our synthetic data by using the synthetic datasets to estimate a large group of population quantities, and comparing them to their actual values computed from the complete $H = 1,690,642$ records. Our target quantities are all the 12,780 3-way marginal proportions that involve cells with structural zeros—corresponding to the cells

of the 119 3-way marginal tables with structural zeros. From these individual proportions, 5617 have population value of exactly zero—because of the presence of either random or structural zeros. For comparison, we also have generated synthetic data using an FCS approach using classification and regression trees (CARTs), similar to the scheme proposed by Reiter (2005) and evaluated by Drechsler and Reiter (2011) for partially synthetic data generation, and using random forests (Caiola and Reiter, 2010). Results using the latter FCS method are presented in the Online Supplement. In order to better understand the effect of the structural zeros, we have also fitted the NPLCM directly as proposed by Hu et al. (2014), without accounting for impossible combinations. For each trial, we have obtained all the estimates from the $M = 5$ synthetic datasets using the combination rules from Reiter and Raghunathan (2007).

For the CART synthesizer we have used a minimum terminal node size of 5 and an impurity parameter (specified as a fraction of the root node) of 0.01. As noted by the the Associate Editor, Drechsler and Reiter (2011) have empirically shown that smaller impurity parameters can lead to substantially better utility results. However, we have found that using our data such synthesizers can lead to synthetic data that in large part reproduces the original sample—thus leading to potential disclosures. We have conducted an empirical investigation onto this issue which we present in the Supplemental Materials #2. We believe that this phenomenon is related to the large size of the structural zeros region in our example data, and a structural phenomenon with FCS synthesizers in the presence of structural zeros that we discuss in Section 4. However, more research is needed to fully understand this issue.

Figure 1 shows the resulting estimates using synthetic data from our TNPLCM and the comparison approaches versus the true population values. We see that results from the TNPLCM line almost perfectly within the main diagonal, indicating that these estimates are very close to their population values (Figure 1a). In contrast, our comparison approach using sequential regression synthesis with CART tuned with default parameters (Figure 1b) produces biased estimates, both overestimating and underestimating. Our last comparison, fitting the NPLCM without truncating the support of the distribution (Figure 1c) illustrates the effect of the structural zeros. NPLCM estimates are relatively good, although they exhibit a small but noticeable bias. However, the main difference with the TNPLCM are a set of several estimates of population quantities (near the origin of Figure 1c) which should be exactly zero, but are estimated with positive probability. These mostly result from structural zeros

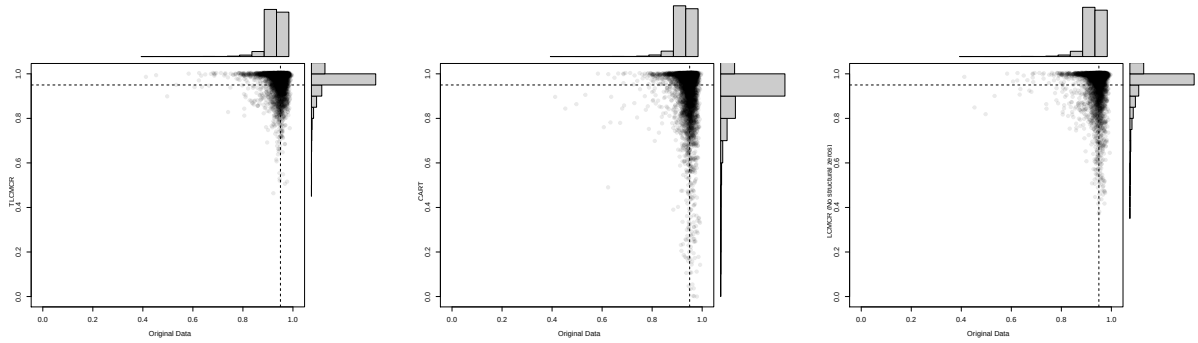


(a) TNPLCM (b) CART (c) NPLCM (no structural zeros)

Fig. 1: Mean estimates (over 200 experimental trials) of the test 3-way margin proportions estimated from synthetic data vs. their actual population values (plots show a random sample of 2000 estimands for clarity).

being estimated with positive probability due to the lack of truncation of the support.

We have also computed the empirical coverage (over the 200 replications of the experiment) of 95% intervals computed from the synthetic data, as well as from the original data for calibration. In this comparison we have omitted the structural zeros, which in the case of the TNPLCM are not being estimated—and are trivially set at their correct value of 0. Figure 2 shows these results. The coverage obtained with the TNPLCM (Figure 2a) is comparable to that obtained using the original data, and in general well within Monte Carlo error of their nominal value of 95%. In fact, 98.6% of the intervals obtained from the TNPLCM have coverage above 80% (which is an even larger proportion than the 98.4% using the original data); moreover, 91% of the TNPLCM intervals have coverage above 90% (c.f. 91.8% using original data). The coverage obtained using the comparison FCS synthesizers, using CART and random forests is notably inferior (see online supplement for plots for the latter). In the case of CART, 89.3% of intervals have coverage greater than 80%, and only 74.5% greater than 90%. We note that in the case of CART it is possible to get much better utility by using a smaller contamination parameter, although the disclosure risk properties of such procedure are somewhat dubious (see Supplemental materials #2 for more information). Random forests fared much worse, with 64.3% of intervals having coverage greater than 80% and 49.3% of them with coverage larger than 90%. In



(a) TNPLCM (b) CART (c) NPLCM (no structural zeros)

Fig. 2: Empirical coverage (over 200 experimental trials) of 95% intervals for the test quantities (not including structural zeros) estimated from the synthetic data vs. estimated from the original dataset. Discontinuous lines mark the nominal 95% coverage levels. Random Uniform[-0.005, 0.005] noise added for clarity.

the case of the NPLCM without structural zeros the situation is better than with CART and random forests, but still noticeably inferior to the TNPLCM. In this case, only 85.0% of intervals have coverage greater than 90%. We note that these numbers do not include all the wrongly estimated structural zeros. Their inclusion would make the comparison even more favorable to the TNPLCM.

3.2. Evaluation of Disclosure Risk

Having shown the utility of our TNPLCM synthesizer we now evaluate the disclosure risk posed by the release of a single set of $M = 5$ synthetic datasets generated from it. Here we follow a variant of the strategy developed by Reiter et al. (2014) and implemented by Hu et al. (2014) for the NPLCM without structural zeros, which we now briefly describe.

Different from partially synthetic datatsets, for which the original confidential records are preserved in a modified form, fully synthetic datasets are composed exclusively by simulated records. Therefore disclosure risk for fully synthetic data cannot be assessed in terms of the risk of correctly matching released and external records. Instead, Reiter et al. (2014) considered measuring the risk of intruders correctly guessing that a particular record is in the original data, based on the synthetic data and

additional information. More specifically, they proposed to evaluate and compare probabilities of the form $\rho_i(\mathbf{x}) = p(\mathbf{x}|\boldsymbol{\mathcal{Y}}, \mathcal{X}_{-i}, \mathcal{K}) \propto p(\boldsymbol{\mathcal{Y}}|\mathbf{x}, \mathcal{X}_{-i}, \mathcal{K})p(\mathbf{x}|\mathcal{X}_{-i}, \mathcal{K})$, where $\boldsymbol{\mathcal{Y}} = (\mathcal{Y}_1, \ldots, \mathcal{Y}_M)$ is the set of all released synthetic datasets, $\mathcal{X}_{-i}$ is the original data except for the i-th record, and $\mathcal{K}$ is the knowledge of the intruder about the process that generated $\boldsymbol{\mathcal{Y}}$. Given an original record $\mathbf{x}_i$, $\rho_i(\mathbf{x})$ is the probability that an intruder who possesses the entire original dataset except for the i-th record, guesses that the missing value is $\mathbf{x}$. Therefore, whenever $\rho_i(\mathbf{x}_i)$ ranks at the top (or among the top) of the set $\{\rho_i(\mathbf{x})\}_{\mathbf{x}\in\mathcal{U}(\mathbf{x}_i)}$ where $\mathcal{U}(\mathbf{x}_i)$ is a set of suitable alternative candidates, we can consider the record at risk. We repeat this procedure for all unique responses in the original sample; non unique responses are already known to the intruder. We note that this is an extremely conservative approach, as it is unlikely that actual intruders will ever have such detailed knowledge of the original sample. The purpose of such evaluation is to obtain a sort of upper bound for the risks.

As Reiter et al. (2014) recommends, for each $\mathbf{x}_i$ we take $\mathcal{U}(\mathbf{x}_i)$ to be the set of all responses that result from varying one single value from $\mathbf{x}_i$ at a time. This results in sets of $\sum_j L_j$ potential guesses, from which we remove the structural zeros. We assume that the intruders know the set of structural zeros, S, and the fact that $\boldsymbol{\mathcal{Y}}$ was generated from the TNPLCM. Additionally we assume that intruders do not have any *a priori* preference for particular guesses as long as they correspond to valid answers. Thus we take $p(\mathbf{x}|\mathcal{X}_{-i}, \mathcal{K}) \propto 1\{\mathbf{x} \notin S\}$. As the Associate Editor pointed out, other sensible prior specifications could be employed here. In particular, intruders could base their prior distribution on the observed frequencies in $\mathcal{X}_{-i}$. Such prior, however, would underweight sample uniques (which cannot be present in $\mathcal{X}_{-i}$) resulting in less conservative disclosure risk measures. We direct readers to Reiter et al. (2014) for further discussion about prior specifications and their effect.

We follow Hu et al. (2014) in computing the disclosure risks using an importance sampling approach, recycling posterior samples from the TNPLCM's parameters obtained from the MCMC algorithm. We note, however, that these computations entail considerable difficulties. In our implementation we have been unable to compute the actual guessing probabilities; we resorted instead to an indirect bootstrap hypothesis testing framework aimed at approximating the ranking of each $\rho_i(\mathbf{x}_i)$ among its comparison class, $\mathcal{U}(\mathbf{x}_i)$. We detail our full procedure in Appendix 1.

Table 3 shows the 21 records that we have evaluated to be at risk, based on their ranking at the top of their corresponding comparison class. All these records are sample uniques by design. However it is

Fig. 3: List of records from the original sample that are considered at risk, based on their probabilities $\rho_i(\mathbf{x}_i)$ being ranked at the top of their comparison class $\mathcal{U}(\mathbf{x}_i)$.

Response vector	Population Frequency
(2,2,1,5,1,1,3,1,2,8,1,2,2,2,1,2,3)	124
(2,2,1,5,1,1,3,1,2,11,1,2,2,3,1,2,3)	277
(2,2,1,7,5,1,3,1,2,8,1,2,4,1,2,2,3)	196
(2,2,1,7,5,3,2,1,2,1,1,2,4,1,2,2,2)	3
(2,2,2,6,6,1,1,1,2,1,1,2,1,1,1,1,1)	442
(2,2,2,7,5,1,3,1,2,10,1,2,4,1,2,2,3)	34
(2,3,1,2,6,1,4,1,3,6,6,3,2,3,1,2,2)	88
(2,3,1,5,1,1,3,1,2,9,1,2,2,2,1,2,3)	222
(2,3,1,5,4,1,3,1,2,10,1,2,2,2,1,2,3)	94
(2,3,1,5,4,1,3,1,2,11,1,2,2,3,1,2,3)	189
(2,3,1,5,5,1,3,1,2,9,1,2,2,3,1,2,2)	11
(2,3,1,5,5,1,3,1,2,9,1,2,2,3,1,2,3)	20
(2,3,1,6,6,1,3,4,3,2,4,4,1,1,1,1,1)	238
(2,3,2,6,6,1,3,4,3,2,4,4,1,1,1,1,1)	226
(2,3,2,6,6,3,1,1,3,1,2,3,1,1,1,1,1)	6
(2,3,2,6,6,4,1,1,2,1,1,2,1,1,1,1,1)	73
(2,4,1,5,1,1,3,1,2,9,1,2,2,3,1,2,3)	6
(3,1,1,1,6,1,3,2,3,5,6,3,1,1,1,1,1)	79
(3,1,1,5,1,3,6,4,2,10,1,2,2,3,1,2,2)	18
(3,1,2,6,6,1,1,3,1,1,1,1,1,1,1,1,1)	304
(3,1,2,6,6,3,1,1,1,1,1,1,1,1,1,1,1)	45

interesting to note that their population frequencies are modestly large, ranging from 3 to 442. This means that even though theoretical intruders could correctly guess the presence of these responses in the original data, they will be unable to link these responses to uniquely identified individuals in the population. Following the suggestion from Reiter et al. (2014) we use the proportion of unique records that rank first in their identification probabilities as a file-level disclosure measure. This results in $\tau_1 = n^{-1} \sum_{i:n(\mathbf{x}_i)=1} I(\underset{\mathbf{x}\in\mathcal{U}(\mathbf{x}_i)}{argmax}\, \rho_i(\mathbf{x}) = \mathbf{x}_i) = 0.0021$, which means that around 0.21% of unique records in $\mathbf{x}$ are at risk, according to our criterion. We can obtain more conservative file-level assessments by considering τ_k, the proportion of unique records whose identification probabilities rank among the k highest in their comparison class. For example, considering the two highest probabilities results in $\tau_2 = 0.0104$. Based on these evaluations we conclude that our TNPLCM synthesizer provides a reasonably high level of protection against accidental disclosure.

4. Discussion

The TNPLCM is a promising tool for agencies seeking to generate high-utility multivariate categorical synthetic data that can be shared with the public at a low disclosure risk. In our tests, using real data from a 17-variable extract of the 2000 U.S. Census involving contingency tables with more than 5.5×10^{10} cells and more than 5.2×10^{10} structural zeros, the TNPLCM synthesizer did an excellent job at preserving inferences for a battery of more than 12,000 population quantities, while simultaneously enforcing the structural zero restrictions. The TNPLCM clearly outperformed the comparison methods based on FCS using CART, random forests and plain NPLCM in terms of utility. Furthermore, our evaluation of the disclosure risk indicates that in our example synthetic samples generated from the TNPLCM posed a low disclosure risk.

We believe that the TNPCLM's ability of seamlessly handling complex and extremely large sets structural zeros in both model fitting and synthetic data generation is currently unmatched by other synthetic data generation proposals. In particular, being a joint probability modeling method, it is immune to several limitations of FCS-based methods. One of such limitations, which has not received much attention in the literature, is the fact that some patterns of structural zeros can cause FCS synthesizers to fail producing samples from certain regions of the support of the distribution. Specifically, since FCS approaches work by updating one variable at a time while keeping the rest fixed, reaching any point that differs by more than one coordinate from the current position requires passing through intermediate points in the support. However, if those intermediate points are all structural zeros, reaching that destination from the current position would be impossible, effectively leading to a reducible Markov Chain. As a simple but non-trivial example consider a survey with binary variables so that $\mathcal{C} = \{1, 2\}^J$, where structural restrictions state that x_1 cannot be equal to x_2. Under such configuration, a FCS synthesizer that starts on any value where $(x_1, x_2) = (1, 2)$ cannot sample values where $(x_1, x_2) = (2, 1)$, since doing so would require passing through either $(1, 1)$ or $(2, 2)$, which are structural zeros. The same considerations apply if the starting point were such that $(x_1, x_2) = (2, 1)$. We can construct more complex examples if we consider variables with more than two levels. We note that this behavior is restricted to strict FCS approaches (e.g Reiter, 2005; Matthews et al., 2010), and is a direct consequence of the particular way in which strict FCS approaches work: by sequentially regressing one variable at a time conditional on the current value of the rest of the multivariate vector.

The TNPLCM, in contrast, does not suffer such limitation as it can just sample all the coordinates at a time.

Our MCMC sampler for the TNPLCM is computationally efficient and requires small to no tuning from the users. In our examples, our algorithm took approximately 375 seconds to generate a set of $M = 5$ synthetic datasets of size $n = 10,000$ using a standard desktop computer. Moreover, our improvements over Manrique-Vallier and Reiter (2014) result in a drastic reduction, on the order of 97%, of memory allocation needs. Such level of computational efficiency is crucial in synthetic data generation applications. Real-life datasets of the type agencies are interested in synthesizing are usually generally large and highly multivariate. Synthesis methods should be able to scale appropriately. Therefore we believe that our proposal should be an attractive candidate for routine real-life applications by statistical agencies and other organizations that wish to disseminate sensitive data. We further note that future implementations of our algorithm can achieve even greater speeds by exploiting parallelism. In particular, steps 1, 5 and 6 in the algorithm described in Section 2.3 involve the sampling of large numbers of (conditionally) independent multinomial variates, all of which can be done in parallel.

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Appendix: Computation of disclosure risk

Following Hu et al. (2014) we note that evaluating the disclosure risk of a single unique combination $\mathbf{x}_i$ from the original sample involves obtaining the probabilities

$$p(\mathbf{x}|\boldsymbol{\mathcal{Y}}, \mathcal{X}_{-i}, \mathcal{K}) \propto \prod_{m=1}^{M} \int p(\mathcal{Y}_m|\mathcal{X}_{-i}^{\mathbf{x}}, \mathcal{K}, \theta) p(\theta|\mathcal{X}_{-i}^{\mathbf{x}}, \mathcal{K}) d\theta \times p(\mathbf{x}|\mathcal{X}_{-i}, \mathcal{K}) \tag{6}$$

for all potential guesses $\mathbf{x}$ (including $\mathbf{x}_i$) in a comparison class $\mathcal{U}(\mathbf{x}_i) \subset \mathcal{C} \setminus S$. Here $\mathcal{Y}_m$ is the m-th synthetic dataset, $\mathcal{X}_{-i}$ is the original data without its i-th element, $\mathcal{X}_{-i}^{\mathbf{x}}$ is the dataset that results from replacing the i-th element of $\mathcal{X}$ with $\mathbf{x}$, and θ is the vector of parameters from the TNPLCM. As noted in Section 3.2 we assume that intruders do not have any preference *a priori* about records from $\mathcal{U}(\mathbf{x}_i)$ so $p(\mathbf{x}|\mathcal{X}_{-i}, \mathcal{K}) \propto 1\{\mathbf{x} \notin S\}$.

Hu et al. (2014) proposed approximating the M integrals in (6) through importance sampling, using T samples obtained from the NPLCM posterior distribution conditional on the original data, $p(\theta|\mathcal{X})$. The resulting Monte Carlo approximation for the TNPLCM is:

$$\int p(\mathcal{Y}_m|\mathcal{X}_{-i}^{\mathbf{x}}, \mathcal{K}, \theta) p(\theta|\mathcal{X}_{-i}^{\mathbf{x}}, \mathcal{K}) d\theta = E_\theta[\mathcal{L}(\theta; \mathcal{Y}_m)|\mathcal{X}_{-i}^{\mathbf{x}}] \approx \sum_{t=1}^{T} w(t; \mathbf{x}_i, \mathbf{x}) \mathcal{L}(\theta^{(t)}; \mathcal{Y}_m) \tag{7}$$

where $\mathcal{L}(\theta; \mathcal{Y}_m) = \prod_{\mathbf{x} \in \mathcal{Y}_m} f^{TNPLCM}(\mathbf{x}|\theta)$, and $w(t; \mathbf{x}_i, \mathbf{x})$ are self-normalized importance weights $w(t; \mathbf{x}_i, \mathbf{x}) \propto f^{TNPCLM}(\mathbf{x}|\theta^{(t)}) / f^{TNPCLM}(\mathbf{x}_i|\theta^{(t)})$ such that $\sum_t w(t; \mathbf{x}_i, \mathbf{x}) = 1$ (see Robert and Casella, 2004, p.95).

Unfortunately, the resulting estimator in (7) has serious stability issues which makes it unsuitable for risk calculations. In particular, values of $\mathcal{L}(\theta^{(t)}; \mathcal{Y}_m)$ vary by several thousands in the log scale from one sample $\theta^{(t)}$ to another, resulting in an estimator with an enormous mean squared error. As an alternative we propose to estimate the distribution of $g(\theta) = \log \mathcal{L}(\theta; \mathcal{Y}_m)$, for $\theta \sim p(\theta|\mathcal{X}_{-i}^{\mathbf{x}}, \mathcal{K})$, by assuming that it belongs to a simple parametric family with density $h(\cdot|\phi)$, so that we can compute the expectation $E[\exp g(\theta)|\hat{\phi}]$ analytically. Inspection of the samples from $g(\theta)$, using importance re-sampling, suggest

that a normal approximation might be adequate. However, since the behavior of $\exp g(\theta)$ is heavily influenced by the assumptions about the right tail of the distribution, and the log-likelihood must be upper-bounded by zero, we instead opted for assuming that $-g(\theta) \sim \text{Gamma}(\cdot|a, b)$, where $E[-g(\theta)] = a/b$, so that $\log E[\exp g(\theta)|a, b] = -a \log(1 + 1/b)$. We note that assuming that $g(\theta)$ follows a normal distribution results in the same conclusions about the ranking of probabilities. We obtain a method of moments estimator for a and b, by approximating the first and second moments of $g(\theta)$ using the importance sampling estimators $\hat{\mu}_1 = \sum_t w(t; \mathbf{x}_i, \mathbf{x}) g(\theta^{(t)})$ and $\hat{\mu}_2 = \sum_t w(t; \mathbf{x}_i, \mathbf{x}) g(\theta^{(t)})^2$.

An additional problem presents when we try to rank the resulting probabilities. Experiments suggest that the variances of the resulting estimators, while much smaller than those obtained from the naive approach from (7), are still considerable. Furthermore, since we compute all the probabilities from the same posterior sample of θ, these estimates are correlated. For these reasons, instead of simply considering a ranking of point estimators, we resort to a bootstrap approach whereby we consider the joint sampling distribution of all the probabilities in the comparison set $\mathcal{U}(\mathbf{x}_i)$. We then compute p-values for hypotheses $H_0(i, k)$ stating that the probability of guessing the true missing value, $\mathbf{x}_i$, is among the largest k probabilities in $\mathcal{U}(\mathbf{x}_i)$. For example $H_0(i, 1)$ states that the probability associated with $\mathbf{x}_i$ is the largest in $\mathcal{U}(\mathbf{x}_i)$ or, equivalently, that the record is ranked first. Larger values of k result in more conservative statements about the disclosure risk. Finally, when considering several $\mathbf{x}_i$s simultaneously (for example, when evaluating all the records in the original dataset) we need to account for the possibility of false positives resulting from multiple comparisons. We account for this problem by using the Benjamini and Hochberg (1995) procedure with a false discovery rate of 0.005, meaning that we accept the risk that about 0.5% of the records deemed safe could actually be at risk.