Generating Realistic Synthetic Relational Data through Graph Variational Autoencoders

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Abstract

Synthetic data generation has recently gained widespread attention as a more reliable alternative to traditional data anonymization. The involved methods are originally developed for image synthesis. Hence, their application to the typically tabular and relational datasets from healthcare, finance and other industries is non-trivial. While substantial research has been devoted to the generation of realistic tabular datasets, the study of synthetic relational databases is still in its infancy. In this paper, we combine the variational autoencoder framework with graph neural networks to generate realistic synthetic relational databases. We then apply the obtained method to two publicly available databases in computational experiments. The results indicate that real databases' structures are accurately preserved in the resulting synthetic datasets, even for large datasets with advanced data types.

1 Introduction

1.1 Motivation

Increases in computational power as well as general awareness have brought data sciences to the forefront of modern business management. However, with the upsurge in data usage came an upsurge in privacy concerns and protocols. Since the introduction of the General Data Protection Regulation (GDPR) in the European Union, over 1100 fines have been issued [1], a number that grows steadily.

Legal (see, e.g. [2, 3]), scientific (see, e.g., [4, 5]) and anecdotal evidence indicates that traditional anonymization techniques offer insufficient protection against data breaches. A famous example is the 2014 New York City Taxi and Limousine Commission data breach [6], in which hackers could infer drivers' addresses and incomes. Deep-learning generative models (DLGMs) have gained attention as a more reliable alternative to anonymization [7, 8, 9]. Rather than distorting existing datasets to mask its subjects, these methods create entirely synthetic new datasets. However, these synthetic datasets retain all the intricate patterns of the real datasets used in the DLGM's training.

DGLMs such as variational autoencoders (VAE) have been applied succesfully for realistic image generation [10, 11] and more recently for generating realistic tabular data with statistically independent rows [12, 13, 14, 15, 16]. However, the lack of methods for more advanced database structures such as relational databases limits the use cases to which DLGMs can be applied. In this paper, we introduce graph-VAE, a method based on graph neural networks and VAE to generate realistic synthetic tabular data. We also evaluate the effectiveness of the method using a publicly available dataset through model compatibility metrics. Results indicate that graph-VAE generates relational databases that accurately preserve real databases' structures, even for large datasets with advanced data types.

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2 Background

2.1 Variational autoencoders

Given a table of data T, the objective of a deep-learning generative model (DLGM) is to construct a new dataset T' such that T and T' have the same distribution. A variational autoencoder (VAE) does this by connecting *encoder* and *decoder* neural networks [12, 16]. Encoder $q_\phi(z|x)$, $x \in T$, parameterized by ϕ, maps T to a probability distribution ("code"). Decoder $p_\psi(x|z)$, parameterized by ψ, maps *latent variables* z to the data space. Training a VAE is maximizing the (log-)likelihood that code samples are taken from the original data's distribution. Structure is imposed on the encoder by minimizing its KL-divergence with a prior P (typically Gaussian). This gives the loss function in expression (1), for D_{KL} the KL-divergence and β a hyperparameter.

$$\mathcal{L}(\phi, \psi) = -\sum_{x \in T} \mathbb{E}_{z \sim q_\phi(z|x)} \log p_\psi(x|z) + \beta \cdot D_{KL}(q_\phi || P) \tag{1}$$

2.2 Graph neural networks

Graph neural networks (GNN) are structures designed to reconcile neural networks with advances data types modeled through graph theory. GNN models typically involve a *message passing* step [17, 18]. Such a step distributes information contained in feature values of a specific vertex to its neighborhood, allowing subsequent neural network layers to infer patterns on a larger structural level than that of mere individual node features. Several layers of message passing can be cascaded.

Let $G = (V, E)$ be a graph, in which each vertex $t \in V$ has a set of *vertex features* X_t and each edge $\{s, t\} \in E$ has a set of *edge features* $X_{\{s,t\}}$. Additionally, a collection H_s^l of hidden vertex variables is associated with each vertex $t \in V$. Let $N(t)$ denote the neighborhood of vertex $t \in V$, that is: $N(t) := \{s \in V : \{s, t\} \in E\}$. Suppose there are L message layers. In each layer l and for each vertex $s \in V$, vertex features $h_s^l \in H_s^l$ are updated through a differentiable *message function* M_l and a differentiable *update function* U_l according to equation (2).

$$\begin{aligned} h_t^{l+1} &= U_l(h_t^l, m_t^{l+1}) \\ m_t^{l+1} &= \textstyle\sum_{s \in N(t)} M_l(h_t^l, h_s^l, X_{\{s,t\}}) \end{aligned} \tag{2}$$

For a given vertex, the message function computes messages from adjacent vertices, which are then aggregated over the vertex' neighborhood. We aggregate through summation, though other aggregation operations may also be chosen. The update function uses the aggregated messages to update the vertex attributes.

3 Graph Variational Autoencoders for Realistic Synthetic Relational Data

3.1 Relational data

Our graph variational autoencoder (graphVAE) combines VAE with GNN to generate realistic tabular data. A *dataset* D is a collection of one or more tables $\{T_1, T_2, \ldots\}$. A *table* T is a collection of rows $\{t_1, \ldots, t_n\}$. A row t is a tuple defined over a sequence of attributes $A(T) = (a_1, \ldots, a_p)$ and represents an *entity* in the real world: we denote by $v(t, a) \in V(T, a) \cup \emptyset$ the value of the attribute a for the row t, with $V(T, a)$ being the *domain* of the attribute a and $\emptyset$ representing the undefined value (i.e., $v(t, a) = \emptyset$ means that a is not defined for t). We say that an attribute a is *unique* for a table T if and only if the mapping $t_i \mapsto v(t_i, a)$ is injective for all $t_i \in T$ and a is always defined in T.

We say that a dataset D is *relational* if the following conditions hold:

1. it contains at least two tables;
2. at least one *primary table* $T^\star$ has a unique attribute $a^\star$;
3. for each other *secondary* table T in the dataset, $A(T) \ni a^\star$ and $\forall t \in T, \exists t^\star \in T^\star : v(t, a^\star) = v(t^\star, a^\star)$.

Intuitively, a relational dataset is a dataset with a primary table $T^\star$ describing some entities, one row per entity, and other tables describing some other entities, each one linked to one specific entity of $T^\star$. For example, a primary table may contain information about customers, and a secondary table may contain data about specific purchases. We refer to the attribute a^* as the *identifier attribute*.

3.2 Graph theoretic representation of relational data

To model relational databases as graphs, we follow [19]. Consider a relational dataset D with a primary table T^* and special attribute a^*. Define the *relational graph* $G(D) = (V(D), E(D))$ according to equation (3).

$$\begin{aligned} V(D) &= \{t|\ \exists T \in D : t \in T\} \\ E(D) &= \{\{s,t\}\,|(s \in T^*) \wedge (\exists T \in D \setminus T^* : t \in T) \wedge (v(s,a^*) = v(t,a^*))\} \end{aligned} \tag{3}$$

So that the identifier attribute a^* (unique in T^*) links records in secondary tables back to the specific row in the primary table with the corresponding identifier value. We note that the definition of a relational graph also applies to relational databases with multiple primary tables and identifier attributes, by computing the edge set for all identifier attributes (including nested structures where a table T may serve as a primary table to a table T', but as a secondary table to a table T'').

For a relational graph $G(D)$ of a relational dataset D, we define the *edge list attribute*, denoted by $a^\dagger$ for all $T \in D$ according to equation (4)

$$v(t, a^\dagger) = \{s|\ \{s,t\} \in E(D)\} \tag{4}$$

3.3 GraphVAE architecture

Let D be a relational dataset with a primary table T^*, secondary tables $T^1, T^2, ...$ and relational graph $G(D) = (V(D), E(D))$. Let $\phi_\dagger$ be the mapping such that $\phi_\dagger(G(D)) = a^\dagger$, for $a^\dagger$ the edge list of $G(D)$. Use this mapping to obtain and store $a^\dagger$. Next, follow the preprocessing steps detailed in [20] for each table $T \in D$. Particularly, an invertible function ϕ_{type} maps tables containing numeric, categorical and date-time attributes to normalized tables of only numeric attributes. Subsequently, an invertible function ϕ_v maps all tables $T \in D$ to a single table as follows. First, add the edge list attribute $a^\dagger$ to all tables. Next, initialize a table X with attribute set $A(X) = \bigcup_{T \in D} A(T) \cup \{a^\dagger\}$. Note that, as each table contains the special attribute a^*, we have $|A(X)| = \sum_{T \in D} A(T) - |D| + 2$. Subsequently, all rows of all tables $T \in D$ are added to X through vertical concatenation, where

$$\forall a \in A(X): \quad v(x,a) = \begin{cases} v(t,a), & \text{if } a \in A(T) \cup \{a^\dagger\} \\ 0, & \text{otherwise} \end{cases} \tag{5}$$

And $v(t, a^\dagger)$ is the adjacency list of the vertex corresponding to vertex (row of some table) t. The table X is a representation of a graph with vertex features and adjacency lists.

Subsequently, k_1 message passing layers are applied to the graph represented by X. The number k_1 is a hyperparameter determined by the user. Larger values of k_1 result in information being more distributed throughout the graph. The message and update functions are provided in equation (6).

$$\begin{aligned} U_l(h_t^l, h_t^{l+1}) &= \text{GRU}(h_t^l, m_t^{l+1}) \\ M_l(h_s^l, h_t^l, x_{\{s,t\}}) &= A(X_{\{s,t\}})h_s^l \end{aligned} \tag{6}$$

Where GRU is a gated recurrent unit (cf. [19]); A is a a matrix of learned parameters that map edge features to the appropriate dimensions; and h_t^l is the value $v(t,a)$ for $t \in X$ in message passing layer l.

After the message passing phase, attribute $a^\dagger$ is discarded and the remaining table, say X', is entered into a variational autoencoder with a standard multivariate normal Gaussian prior, the dimension of which is a hyperparameter chosen by the user. Random samples $\hat{Y}'$ in the latent space are taken and transferred back to the data space by the decoder. Subsequently, a user-specified number k_2 of additional message passing layers are applied before the data is transferred to the original primary and secondary table structure through the inverse preprocessing functions. A standard VAE loss function is invoked during training (see equation (1)). This is illustrated in a computational diagram in Figure 1.

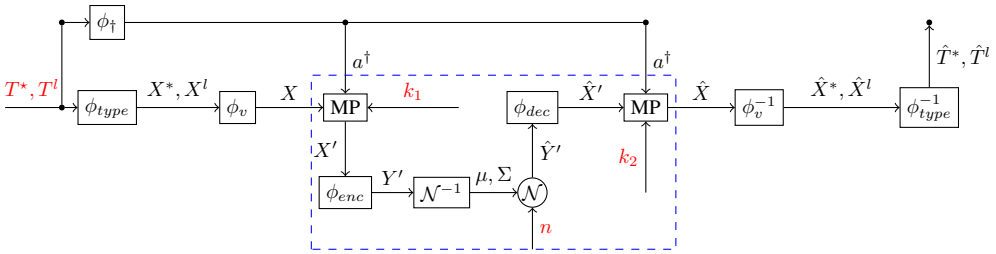

Figure 1: Schematic representation of the steps for going from a relational dataset $D = (T^\star, T^1, \ldots, T^h)$ to a compatible synthetic relational dataset $\hat{D} = (\hat{T}^\star, \hat{T}^1, \ldots, \hat{T}^h)$. In red, the parameter and inputs provided by the user; in blue dashed rectangles, the core steps of the graphVAE, other steps having to do with pre- and post-processing. Abbreviation "MP" indicates a cascade of four message passing layers.

4 Experimental Results

4.1 Datasets

We applied our method to two publicly available datasets: the BasketballMen dataset from the Relational Dataset Repository [21] and the Rossmann Store Sales dataset from Kaggle [22]. These sets have a single primary table and two and one secondary tables, respectively. All attribute types (numeric, categorical, date-time) are represented in these sets. Both secondary tables of the BasketballMen dataset are linked to the primary dataset through the same identifier attribute. While the Rossmann dataset has only one child table, it has a large data volume and a more complex mixture of datatypes. Table 1 summarizes the salient information of the datasets.

Dataset	$\lvert T \rvert$	$\lvert A(T) \rvert$	N	C	T
BasketballMen					
Primary	5 062	4	2	2	0
Secondary 1	1 608	7	7	0	0
Secondary 2	23 751	6	5	1	0
Rossmann Store					
Primary	1 004	9	5	4	0
Secondary	915 223	8	2	5	1

Table 1: Overview of the datasets used in the experiments, one row per table. Column $|T|$ indicates the number of rows in the table. Column $|A(T)|$ indicates the number of attributes. Columns N, C, and T indicate the number of numeric, categorical, and time attributes respectively.

4.2 Experimental set-up

We used the architecture from Figure 1 to generate synthetic data with each of the two datasets as input. Hyperparameters were tuned manually. The obtained hyperparameters are provided in Table 2.

To measure the degree to which generated synthetic data preserves the structure of the input data, we used model compatibility (MC). The procedure we used was the following: 1) we divided the input dataset into a training set (80%) and a test set (20%); 2) We trained the graphVAE using the training set; 3) We used the trained model to construct the synthetic dataset; 4) We train a classifier on the outer-join of the training set tables; 5) We train a gradient boosted trees (XGBoost) classifier on the outer-join of the synthetic primary and secondary tables with choice of target column based on domain knowledge; 6) We apply both models to the test set and evaluate standard machine learning metrics (ROC AUC and F1-score) of the trained models; 7) We compare the performance metrics of the model built on the training set to those built on the test set. If the synthetic data accurately mimics the properties of the input dataset, the performances of both models should be roughly equal.

Param	Description	Basketball	Rossmann
n	VAE latent space dimensionality	[8, 10, 10]	[8, 8]
k_1	# message passing layers	4	4
k_2	# message passing layers	4	4
β	VAE loss terms tradeoff	[1,1,1]	[5,5,5]

Table 2: Summary of hyperparameter values. Vectors provide separate parameter values for the primary table in the first entry, followed by those of the secondary table(s).

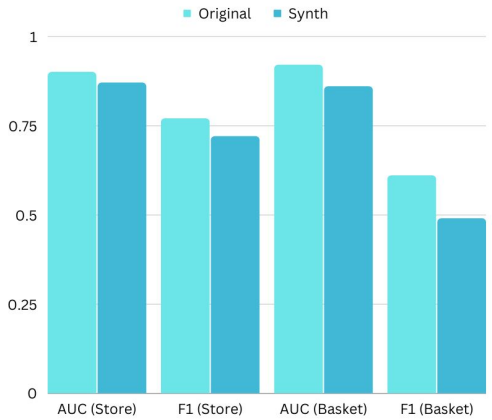

Figure 2: Effectiveness metrics evaluated on training (light blue) and synthetic data (dark blue)

As a quantitative indicator of model compatibility, we use the metric

$$MC(D, \hat{D}) = \left| 1 - \frac{e(m, D_{test})}{e(\hat{m}, D_{test}} \right|$$

Where D and $\hat{D}$ are the real and synthetic datasets, respectively; m and $\hat{m}$ are the model built on the training and synthetic datasets, respectively; and e is the effectiveness metric (ROC AUC or F1-score). The closer $MC(D, \hat{D})$ is to zero, the more similar the performance of the two models is on the test data.

4.3 Results and discussion

The model compatibilitiies for the BasketballMen dataset are 0.07 (ROC AUC) and 0.24 (F1-score). For the Rossmann Store Sales dataset, they are 0.03 (ROC AUC) and 0.07 (F1-score). Figure 2 shows the performance metrics of the models evaluated on the test dataset. Results indicate that the method can generate accurate synthetic relational data. The model compatability metric value is significantly smaller for the Rossman data (especially the F1-score). This indicates that the number of secondary tables has a bigger impact on the results than the volume of the data and the complexity of its datatypes. Nonetheless, the metric value is sufficiently small for the synthetic data to be of use in testing, analytic and machine learning contexts.

5 Conclusion

We propose a novel deep learning method for the generation of realistic synthetic relational data based on graph neural networks and variational autoencoders. By treating links between tables in a relational database as edges in a graph, message passing layers enable information to propagate through the database. Subsequently, the encoder can infer inter-table patterns, which are reproduced during synthesis. Computational experiments on publicly available datasets indicate that our method creates synthetic relational data with a high degree of similarity to the databases they were modeled after.

The proposed method works well, even for a database with a large data volume and complex data types. The quantity of tables in the relational database may render synthesis more problematic, though the results were promising also for a set with two secondary tables. Improved hyperparameter optimization may improve the results further. Future research should inspect whether there is a correlation between the number of tables in the database and the performance of graphVAE. Dedicated heuristics for hyperparameter optimization should also be explored.

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