# DIFFUSION-NESTED AUTO-REGRESSIVE SYNTHESIS OF HETEROGENEOUS TABULAR DATA

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# Abstract

Autoregressive models are predominant in natural language generation, while their application in tabular data remains underexplored. We posit that this can be attributed to two factors: 1) tabular data contains heterogeneous data type, while the autoregressive model is primarily designed to model discrete-valued data; 2) tabular data is column permutation-invariant, requiring a generation model to generate columns in arbitrary order. This paper proposes a Diffusion-nested Autoregressive model (TABDAR) to address these issues. To enable autoregressive methods for continuous columns, TABDAR employs a diffusion model to parameterize the conditional distribution of continuous features. To ensure arbitrary generation order, TABDAR resorts to masked transformers with bi-directional attention, which simulate various permutations of column order, hence enabling it to learn the conditional distribution of a target column given an arbitrary combination of other columns. These designs enable TABDAR to not only freely handle heterogeneous tabular data but also support convenient and flexible unconditional/conditional sampling. We conduct extensive experiments on ten datasets with distinct properties, and the proposed TABDAR outperforms previous state-of-the-art methods by 18% to 45% on eight metrics across three distinct aspects.

#### 1 INTRODUCTION



Figure 1: Challenges in Auto-Regressive tabular data generation. (a) The conditional distribution of continuous columns is hard to express. (b) Tabular data is column-permutation-invariant.

Due to the widespread application of synthetic tabular data in real-world scenarios, such as data 042 augmentation, privacy protection, and missing value prediction (Fonseca & Bacao, 2023; Assefa 043 et al., 2021; Hernandez et al., 2022), an increasing number of studies have begun to focus on 044 deep generative models for synthetic tabular data generation. In this domain, various approaches, 045 including Variational Autoencoders (VAEs)(Liu et al., 2023), Generative Adversarial Networks 046 (GANs)(Xu et al., 2019), Diffusion Models (Zhang et al., 2024b), and even Large Language Models 047 (LLMs)(Borisov et al., 2023), have demonstrated significant progress. However, Auto-Regressive 048 models, a crucial category of generative models, have been largely overlooked in this process. In language modeling, autoregressive models have become the *de facto* solution (e.g., GPTs (Mann et al., 2020; Achiam et al., 2023)). Tabular data shares similarities with natural language in its discrete 051 structure, making an autoregressive decomposition of its distribution a natural approach, i.e.,

$$p(\mathbf{x}) = p(x^1) \prod_{i=2}^{D} p(x^i | x^1, x^2, \cdots, x^{i-1}) = p(x^1) \prod_{i=2}^{D} p(x^i | \mathbf{x}^{< i})$$
(1)

where each  $x^i$  represents the value at the *i*-th column,  $\mathbf{x}^{\leq i} = \{x^1, x^2, \dots, x^{i-1}\}$ . However, research on autoregressive models for tabular data generation has not received adequate attention.

We posit that this is primarily due to two key challenges (see Fig. 1): 1) Modeling continuous 057 distribution: Autoregressive models aim to learn the per-token (conditional) probability distribution, which is convenient for discrete tokens (such as words in Natural Languages) because their probability can be represented as a categorical distribution. However, the same approach is challenging to apply to 060 continuous tokens unless there are strong prior assumptions about their distribution, such as assuming 061 they follow Gaussian distributions. 2) No fixed order: Unlike natural language, which possesses 062 an inherent causal order from left to right, tabular data exhibits column permutation invariance . 063 To reflect this property in the autoregressive model, we need to ensure a sequence of tokens can 064 be generated in arbitrary order. Existing autoregressive models for tabular data generation adopt simplistic approaches to address these challenges. For instance, they discretize continuous columns, 065 allowing them to learn corresponding categorical distributions (Castellon et al., 2023; Gulati & 066 Roysdon, 2023). However, this method inevitably leads to information loss. Regarding the generation 067 order, these models typically default to a left-to-right column sequence (Castellon et al., 2023), failing 068 to reflect the column permutation invariant property. 069

To address these challenges, this paper proposes  $\underline{D}$  iffusion-nested AutoRegressive Tabular Data Generation (TABDAR in short). TABDAR addresses the aforementioned issues through two design 071 features: 1) Nested diffusion models for modeling the conditional probability distributions of 072 the next continuous-valued tokens. TABDAR nests a small diffusion model (Ho et al., 2020; 073 Karras et al., 2022) into the autoregressive framework for learning the conditional distribution of 074 a continuous-valued column. Specifically, we employ two distinct loss functions for learning the 075 distribution of the next continuous/discrete-valued tokens, respectively. For discrete columns, their 076 conditional distribution is learned by directly minimizing the KL divergence between the prediction 077 vector and the ground-truth one-hot category embedding. For continuous columns, we learn their 078 distribution through a diffusion model conditioned on the output of the current location. In this 079 way, TABDAR can flexibly learn the distribution of tabular data containing arbitrary data types. 2) Masked Transformers with bi-directional attention. TABDAR simulates arbitrary sequence orders 081 via a transformer-architectured model with bi-directional attention mechanisms and masked inputs. The masked/unmasked locations indicate the columns that are missing/observed, ensuring that when predicting a new token, the model has only access to the known tokens. During training, TABDAR 083 follows the form of masked language modeling, predicting the distribution of masked tokens based 084 on unmasked tokens. During testing, TABDAR generates entire rows of data in an autoregressive 085 manner according to a given order. 086

087 TABDAR offers several advantages. 1) TABDAR employs the most appropriate generative models 880 for different data types, i.e., diffusion models for continuous columns and categorical prediction for discrete columns, seamlessly integrating them into a unified framework. This avoids contrived 089 processing methods such as discrete diffusion models (Lee et al., 2023; Kotelnikov et al., 2023), 090 continuous tokenization of categorical columns (Zhang et al., 2024b), and ineffective discretiza-091 tion (Castellon et al., 2023). 2) Through an autoregressive approach, TABDAR models the conditional 092 distribution between different columns, thereby better capturing the dependency relationships among 093 various columns and achieving superior density estimation. 3) Combining autoregression and masked 094 Transformers enables a trained TABDAR to compute and sample from the conditional distribution of target columns given an arbitrary set of observable columns, enabling generation in arbitrary order. 096 This capability facilitates precise and convenient posterior inference (e.g., conditional sampling and missing data imputation).

098 We conduct comprehensive experiments on ten tabular datasets of various data types and scales to 099 verify the efficacy of the proposed TABDAR. Experimental results comprehensively demonstrate 100 TABDAR's superior performance in: 1) Statistical Fidelity: The ability of synthetic data to faithfully 101 recover the ground-truth data distribution; 2) Data Utility: The performance of synthetic data 102 in downstream Machine Learning tasks, such as Machine Learning Efficiency; and 3) Privacy 103 Protection: Whether the synthetic data is sampled from the underlying distribution of the training data rather than being a simple copy. In missing value imputation tasks, TABDAR exhibits remarkable 104 performance, even surpassing state-of-the-art methods that are specially designed for missing data 105 imputation tasks. For a genuine and fair comparison, we have released the code to reproduce 106 our method and all baseline results. The code is available at https://anonymous.4open. 107 science/r/ICLR-TabDAR.

#### 108 **RELATED WORKS** 2

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110 **Synthetic Tabular Data Generation** Generative models for tabular data have become increasingly 111 important and have widespread applications Assefa et al. (2021); Zheng & Charoenphakdee (2022); 112 Hernandez et al. (2022). For example, CTGAN and TAVE (Xu et al., 2019) deal with mixed-type 113 tabular data generation using the basic GAN (Goodfellow et al., 2014) and VAE (Kingma & Welling, 114 2013) framework. GOGGLE (Liu et al., 2023) incorporates Graph Attention Networks in a VAE framework such that the correlation between different data columns can be explicitly learned. DP-115 116 TBART (Castellon et al., 2023) and TabMT (Gulati & Roysdon, 2023) use discretization techniques to numerical columns and then apply autoregressive transformers for a generation. Recently, inspired 117 by the success of Diffusion models in image generation, a lot of diffusion-based methods have been 118 proposed, such as TabDDPM (Kotelnikov et al., 2023), STaSy (Kim et al., 2023), CoDi (Lee et al., 119 2023), and TabSyn (Zhang et al., 2024b), which have achieved SOTA synthesis quality. 120

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Autoregressive Models for Continuous Space Data In text generation, autoregressive next-token 122 generation is undoubtedly the dominant approach (Mann et al., 2020; Achiam et al., 2023). However, 123 in image generation, although autoregressive models (Van den Oord et al., 2016; Salimans et al., 124 2017) were proposed early on, their pixel-level characteristics limited their further development. 125 Subsequently, diffusion models, which are naturally suited to modeling continuous distributions, have 126 become the most popular method in the field of image generation. In recent years, some studies have 127 attempted to use discrete-value image tokens (van den Oord et al., 2017; Razavi et al., 2019) and 128 employ autoregressive transformers for image-generation tasks (Kolesnikov et al., 2022). However, 129 discrete tokenizers are both difficult to train and inevitably cause information loss. To this end, recent work has attempted to combine continuous space diffusion models with autoregressive methods. 130 For example, Li et al. (2024b) employs an autoregressive diffusion loss in a causal Transformer 131 for learning image representations; Li et al. (2024a) proposes using a diffusion model to model the 132 conditional distribution of the next continuous image and employs a masked bidirectional attention 133 mechanism to enable the generation of any number of tokens in arbitrary order. 134

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#### **PRELIMINARIES** 3

#### 3.1 DEFINITIONS AND NOTATIONS

In this paper, we always use uppercase boldface (e.g.,  $\mathbf{X}$ ) letters to represent matrices, lowercase 140 boldface letters (e.g.,  $\mathbf{x}$ ) to represent vectors, and regular italics (e.g., x) to denote scalar entries 141 in matrices or vectors. Tabular data refers to data organized in a tabular format consisting of rows 142 and columns. Each row represents an instance or observation, while each column represents a 143 feature or variable. In this work, we consider heterogeneous tabular data that may contain both 144 numerical and categorical columns or only one of these types. Let  $\mathcal{D} = \{\mathbf{x}_i\}_{i=1}^N$  denote a tabular 145 dataset comprising N instances, where each instance  $\mathbf{x} = (x^1, x^2, \dots, x^D)$  is a D-dimensional 146 vector representing the values of D features or variables. We further categorize the features into 147 two types: 1) Numerical/continuous features:  $\mathcal{N} = \{i \mid x^i \in \mathbb{R}\}$  is the set of indices corresponding 148 to numerical features. 2) Categorical/discrete features:  $C = \{i \mid x^i \in C_i\}$  is the set of indices 149 corresponding to categorical features, where  $C_i$  is the set of possible categories for the *i*-th feature. 150 Note that  $\mathcal{N} \cup \mathcal{C} = 1, 2, \dots, D$  and  $\mathcal{N} \cap \mathcal{C} = \emptyset$ .

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## 3.2 DIFFUSION MODELS

154 Diffusion models (Ho et al., 2020; Song et al., 2021; Karras et al., 2022) learn the data distribution 155  $p(\mathbf{x})$  through a diffusion SDE, which consists of a forward process that gradually adds Gaussian noises of increasing scales to x (which are pre-normalized to have zero-mean and unit-variance), and 156 a reverse process that recovers the clean data from the noisy one<sup>1</sup>: 157

$\mathbf{x}_t = \mathbf{x}_0 + \sigma(t)\boldsymbol{\varepsilon}, \ \boldsymbol{\varepsilon} \sim \mathcal{N}(0, \mathbf{I}),$	(Forward Process)	(2)
$\mathrm{d}\mathbf{x}_t = -2\dot{\sigma}(t)\sigma(t)\nabla_{\mathbf{x}_t}\log p(\mathbf{x}_t)\mathrm{d}t + \sqrt{2\dot{\sigma}(t)\sigma(t)}\mathrm{d}\boldsymbol{\omega}_t,$	(Reverse Process)	(3)

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<sup>1</sup>This formulation is a simplified version of VE-SDE (Song et al., 2021). See Appendix B for details.

162 where  $\omega_t$  is the standard Wiener process.  $\sigma(t)$  is the noise schedule, and  $\dot{\sigma}(t)$  is the derivative of  $\sigma(t)$ 163 w.r.t. t A diffusion model is learned by using a denoising/score network  $\epsilon_{\theta}(\mathbf{x}_t, t)$  to approximate the 164 conditional score function  $\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t | \mathbf{x}_0)$  (named score-matching). The final loss function could 165 be reduced to a simple formulation where the denoising network is optimized to approximate the 166 added noise  $\varepsilon$ , i.e.,

$$\mathcal{L}(\mathbf{x}) = \mathbb{E}_{t \sim p(t)} \mathbb{E}_{\boldsymbol{\varepsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \| \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t, t) - \boldsymbol{\varepsilon} \|^2.$$
(4)

The sampling process starts from a large timestep T such that  $\mathbf{x}_T \approx \mathcal{N}(\mathbf{0}, \sigma^2(T)\mathbf{I})$  recovers  $\mathbf{x}_0$  via solving the reverse SDE in Eq. 3, using mature numerical solution tools.

**METHODS** 4

#### 4.1 KEY INGREDIENTS OF TABDAR

Modeling tabular data using autoregression. TABDAR follows the autoregressive criteria for 176 modeling the distribution of tabular data. Autoregressive modeling decomposes the joint data distribution into the product of a series of conditional distributions in raster order, and the optimization 178 is achieved by minimizing the standard negative log-likelihood: 179

$$p(\mathbf{x}) = \prod_{i=1}^{D} p(x^{i} | \mathbf{x}^{< i}), \ \mathcal{L} = -\log p(\mathbf{x}) = -\sum_{i=1}^{D} \log p(x^{i} | \mathbf{x}^{< i})$$
(5)

183 Therefore, instead of directly modeling the complicated joint distribution, one can seek to model each conditional distribution, i.e.,  $p(x^i|\mathbf{x}^{< i})$ , separately, which is intuitively much simpler. 185

Autoregression is natural for language modeling, as language inherently possesses a left-to-right 186 (L2R in short) order, and we can expect that the generation of a new word depends entirely on the 187 observed words preceding it. Therefore, Transformers (Vaswani et al., 2017) with causal attention 188 (where only the previous tokens are observable to predict the following tokens) are widely used for 189 text generation. Unlike text data, tabular data has long been considered column permutation invariant. 190 In this case, one has to randomly shuffle the columns many times and then apply causal attention to 191 each generated order, which is conceptually complicated.

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Simulate arbitrary order using masked Bi-194 directional Attention. To deal with this, an inter-195 esting observation is that even if given the default 196 order of data, we can simulate arbitrary-order causal 197 attention using masked bi-directional attention. As illustrated in Fig. 2, giving the tabular data arranged in the default order ['age', 'capital gain', 'work', 'ed-199 ucation', 'income'] and a shuffled generation order 200 ['education'  $\rightarrow$  'income'  $\rightarrow$  'capital gain',  $\rightarrow$  'age', 201  $\rightarrow$  'work'], the prediction of 'capital gain' can be 202 equivalently achieved by 1) causal attention based on 203 the previous columns 'education' and 'income'; 2) 204 bidirectional attention where all other columns ('age, 205 'capital gain', and 'work') are masked. 206



Figure 2: With appropriate masking, bidirectional attention is equivalent to causal attention in arbitrary order.

207 Column-specific losses for discrete/continuous columns Autoregressive models aim at learning 208 the conditional distribution of the target column given the observations of previous columns, i.e., 209  $p(x^i|\mathbf{x}^{< i})$ . Take  $\mathbf{x}^{< i}$  as input, Transformers are able to generate column-specific output vectors, i.e., 210  $\mathbf{z}^i$  for column *i*. Then we only need to model the conditional distribution  $p(x^i | \mathbf{z}^i)$ .

211 Discrete Columns. For a discrete column  $x^i$ , the target distribution is a categorical distribution, 212 which could be represented by a  $|C_i|$ -dimensional vector. Consequently, we can directly project  $z^i$ 213 to a  $|C_i|$ -way classifier using a prediction head  $f_i(\cdot)$  (e.g., a shallow MLP:  $\mathbb{R}^d \to \mathbb{R}^{|C_i|}$ ), and then 214 minimize the KL-divergence between the predicted distribution and the one-hot encoding of a sample: 215

$$\mathcal{L}(x^{i}, \mathbf{z}^{i}) = -\log p(x^{i} | \mathbf{z}^{i}) = \text{Cross-Entropy}(x^{i}, \text{softmax}(f_{i}(\mathbf{z}^{i})), i \in \mathcal{C}$$
(6)





227 Figure 3: Framework of TABDAR. An embedding laver first encodes each column into a vector. The masks are 228 then added to the target columns ('age' and 'education'). 229 With Bi-direction Transformers' decoding, the output 230 vectors z are used as conditions for predicting the distri-231 bution of current columns. TABDAR nests a diffusion 232 model in the autoregressive framework to learn the con-233 ditional distribution of a continuous column. 234

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Figure 4: An illustration of TABDAR's generation process. Given a random generation order, e.g., 'capital gain'  $\rightarrow$  'education'  $\rightarrow \cdots$  'income', TABDAR generates the value for each column in a row according to the conditional distribution learned by the masked Transformers.

*Continuous Columns.* Unlike discrete columns, a continuous column might have infinite value states and, therefore, cannot be modeled by a categorical distribution<sup>2</sup>. Inspired by the prominent capacity of Diffusion models in modeling arbitrary continuous distributions, we hereby adopt a conditional diffusion model to learn the conditional continuous distribution (Li et al., 2024a)  $p(x^i | z^i)$ . Compared with the unconditional diffusion loss in Eq. 4, the denoising function  $\epsilon_{\theta}$  takes the condition vector  $z^i$  as an additional input. The final loss function is expressed as follows:

$$\mathcal{L}(x^{i}, \mathbf{z}^{i}) = -\log p(x^{i} | \mathbf{z}^{i}) = -\log \mathbb{E}_{t \sim p(t)} \mathbb{E}_{\boldsymbol{\varepsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \| \boldsymbol{\epsilon}_{\theta}(x_{t}^{i}, t, \mathbf{z}^{i}) - \boldsymbol{\varepsilon} \|^{2}, \quad i \in \mathcal{N}$$
(7)

#### 4.2 DETAILED ARCHITECTURE OF TABDAR

In this section, we introduce the detailed architecture and implementations of TABDAR. The overall
 framework of TABDAR is presented in Fig. 3.

**Tokenization layer.** Given a row of tabular data  $\mathbf{x} = (x^1, x^2, \dots, x^D)$ , the tokenization layer embeds each feature to a *d*-dimensional vector using column-specific learnable linear transformation. For a continuous column, the linear transformation is  $\mathbf{W}^i \in \mathbb{R}^{1 \times d}$ , while for a discrete column, the transformation matrix is  $\mathbf{W}^i \in \mathbb{R}^{|\mathcal{C}_i| \times d}$ . The output token of column *i* is denoted by  $\mathbf{h}^i$ , and we obtain an embedding matrix of *D* tokens  $\mathbf{H} \in \mathbb{R}^{D \times d}$ . We also add column-specific learnable positional encoding so that the token embeddings at different locations can be discriminated.

**Input masking.** As illustrated in Section 4.1, we can use masked bidirectional attention to simulate arbitrary causal attention. Therefore, we first uniformly sample the number of tokens to mask/predict  $M \sim \mathcal{U}(1, D)$ . Given M, we randomly sample a masking vector  $\mathbf{m} \in \{0, 1\}^D$ , s.t.,  $\sum_i m^i = M$ .  $m^i = 1$  indicates that column i is masked and vice versa. Then, the input embeddings of masked columns are set as zero, making them unobservable when predicting the target columns.

 $\mathbf{H}' = (1 - \mathbf{m}) \odot \mathbf{H}.$ 

(8)

**Bi-directional Transformers.** Given the masked token sequence, we then follow the standard pipeline of Transformer implementations. We first pad the embedding of the class token [pad] at the beginning of the sequence. The [pad] tokens not only enable class-conditional generation but also help stabilize the training process (Li et al., 2024a). By default, we use one unique [pad] token, equivalent to unconditional generation (we may use class-specific [pad] tokens for class-conditional distribution). Afterward, these tokens are processed by a series of standard Transformer blocks and will finally output column-wise latent vectors  $\{z^i\}_{i=1}^{D}$ .

<sup>&</sup>lt;sup>2</sup>MSE loss is also not acceptable since it is a deterministic mapping rather than a conditional distribution

Loss function and model training. After obtaining the latent vector  $\mathbf{z}^i$  for a target/masked column *i*, we use it as the condition for predicting the distribution of  $\mathbf{x}^i$ , i.e.,  $p(x^i | \mathbf{z}^i)$ .

Discrete columns. As presented in Eq. 6, we use a column-specific prediction head  $f_i(\cdot)$  to obtain the  $|C_i|$ -dimensional prediction then compute the cross-entropy loss.

275 *Continuous columns.* For predicting the distribution of the continuous column  $x^i$ , we use the 276 conditional diffusion loss described in Eq. 7. The training of the conditional diffusion model follows 277 the standard process of diffusion models (Karras et al., 2022). To be specific, we first randomly 278 sample a timestep  $t \sim p(t)$ , and standard Gaussian noise  $\varepsilon \sim \mathcal{N}(0, 1)$ , obtaining  $x_t^i = x^i + \sigma(t) \cdot \varepsilon$ . 279 Then, a denoising neural network  $\epsilon_{\theta}(x_t^i, t, \mathbf{z}^i)$  takes  $x_t^i, t$ , and  $\mathbf{z}^i$  as input to predict the added noise  $\varepsilon$ 280 (via the MSE loss in Eq. 7). The denoising neural network is implemented as a shallow MLP, and its 281 detailed architecture is presented in Appendix C.

Model Training. The training of TABDAR is end-to-end: all the model parameters, including the
 Embedding layer, transformers, prediction heads for discrete columns, and diffusion models for the
 continuous columns, are jointly trained via gradient descent on the summation of the losses of the
 target/masked columns in the current batch.

Model inference. After TABDAR is trained, we can easily perform a variety of inference tasks, e.g.,
 unconditional and conditional generation. An illustration of TABDAR's auto-regressive sampling
 process is presented in Fig. 4.

289 Unconditional Sampling. To generate unconditional data examples  $\mathbf{x} \sim p(\mathbf{x})$ , we can first randomly 290 sample a generation order. Then, starting with all columns masked (except the [pad] token), we can 291 generate the value of each column one by one according to the sampled order.

Conditional Sampling. One important advantage of TABDAR's autoregressive generation manner is that one can perform flexible conditional sampling, such as simple class-conditional generation. This can be achieved by directly setting the corresponding column values to the desired ones and then randomly sampling the generation order of other columns. Missing value imputation can be regarded as a special case of conditional sampling by resorting to the conditional distribution of missing columns given observed values. More implementation details can be found in Appendix D.4.

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## 5 EXPERIMENTS

- **302** 5.1 EXPERIMENTAL SETUPS
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Datasets. We select ten real-world tabular datasets of varying data types and sizes: 1) two contain
 only continuous features - California and Letter; 2) two contain only categorical features - Car
 and Nursery; 3) six datasets of mixed continuous and discrete features - Adult, Default, Shoppers,
 Magic, News, and Beijing. The detailed introduction of these datasets can be found Appendix D.2.

308 Baselines. We compare the proposed TABDAR with ten powerful synthetic tabular data generation 309 methods belonging to six categories. 1) The non-parametric interpolation method SMOTE (Chawla et al., 2002). 2) VAE-based methods TVAE (Xu et al., 2019) and GOGGLE (Liu et al., 2023). 3) GAN-310 based method CTGAN (Xu et al., 2019). 4) LLM-based method GReaT (Borisov et al., 2023). 5) 311 Diffusion-based methods: STaSy (Kim et al., 2023), CoDi (Lee et al., 2023), TabDDPM (Kotelnikov 312 et al., 2023), and TabSyn (Zhang et al., 2024b). 6) Autoregressive methods DP-TBART (Castellon 313 et al., 2023) and Tab-MT (Gulati & Roysdon, 2023). The proposed TABDAR belongs to the 314 autoregressive family, yet it utilizes a diffusion model for modeling continuous columns. 315

Evaluation Methods. We evaluate the quality of synthetic tabular data from three distinct dimensions:
1) *Fidelity* - if the synthetic data faithfully recovers the ground-truth data distribution. 2) *Utility* - the performance when applied to downstream tasks, and we focus on Machine Learning Efficiency (MLE). 3) *Privacy* - if the synthetic data is not copied from the real records. More introduction of these metrics is in Appendix D.6.

**Implementations.** Since TABDAR's diffusion loss is applied to each single column, the denoising network  $\varepsilon_{\theta}$  can be light-weighted, and we implement it as a three-layer MLP with 256 hidden dimension. For the diffusion model, we follow Zhang et al. (2024b) and set  $\sigma(t) = t$ , which enables a small number of diffusion step, i.e., NFE = 50.

Method	Marginal $\downarrow\%$	Joint↓ %	$\alpha\text{-}\mathbf{Precision}{\downarrow}~\%$	$\beta\text{-}\mathbf{Recall}{\downarrow}~\%$	$\textbf{C2ST}{\downarrow}~\%$	$JSD\downarrow 10^{-2}$
Interpolation SMOTE (Chawla et al., 2002)	$1.72 \pm 1.36$	$2.95 \pm 1.66$	$3.78 \pm 3.94$	16.7±9.16	3.00±3.66	0.11±0.10
VAE-based						
TVAE (Xu et al., 2019)	$15.8 \pm 17.1$	$17.4 \pm 18.3$	$18.2 \pm 20.1$	$70.9 \pm 26.3$	$43.9 \pm 22.7$	$1.01 \pm 0.70$
GOGGLE (Liu et al., 2023)	$17.2 \pm 6.28$	$29.1{\scriptstyle \pm 11.8}$	$21.8 \pm 17.3$	$90.8 {\pm} 5.64$	-	-
GAN-based						
CTGAN (Xu et al., 2019)	$17.9{\pm}6.99$	$18.4 {\pm} 9.11$	$17.7 \pm 15.1$	$69.1 \pm 33.8$	$53.0{\pm}_{22.5}$	$1.18 \pm 0.6$
LLM-based						
GReaT (Borisov et al., 2023)	$12.9 {\pm} 6.05$	$44.3 \pm 27.3$	$17.2 \pm 12.8$	$53.2 \pm 26.0$	$42.4{\scriptstyle \pm 19.2}$	$1.43 \pm 1.1$
Diffusion-based						
STaSy (Kim et al., 2023)	$14.3 \pm 7.40$	$13.5 \pm 9.76$	$21.8 \pm 24.7$	$55.6 \pm 29.6$	$53.9 \pm 16.6$	$1.25 \pm 1.1$
CoDi (Lee et al., 2023)	$17.4 \pm 11.3$	$15.2 \pm 19.8$	$10.0 \pm 5.93$	$51.7 \pm 31.1$	$44.0 \pm 33.3$	$0.76 \pm 0.5$
TabDDPM (Kotelnikov et al., 2023)	$15.0 \pm 25.3$	$7.92 \pm 8.16$	$23.6 \pm 2.93$	$49.6 \pm 34.5$	$24.6 \pm 38.9$	$1.03 \pm 1.6$
TabSyn (Zhang et al., 2024b)	$1.73 \pm 0.76$	$2.53 \pm 1.45$	$2.52 \pm 2.93$	$44.1 \pm 24.5$	$2.76 \pm 2.19$	$.12 \pm 0.09$
Autoregressive-based						
DP-TBART (Castellon et al., 2023)	$3.24 \pm 1.76$	$2.71 \pm 1.56$	$2.11 \pm 2.15$	$48.0 \pm 27.8$	$5.36 {\pm} 4.58$	$0.16 \pm 0.1$
Tab-MT (Gulati & Roysdon, 2023)	$14.9 {\pm} {}_{15.1}$	$8.11 \pm 10.8$	$23.2 \pm 31.9$	$63.5{\pm}_{38.3}$	$48.6{\scriptstyle \pm 47.7}$	$0.60 \pm 0.8$
TABDAR (ours)	$1.21_{\pm 0.51}$	$1.80{\scriptstyle \pm 0.72}$	$1.33_{\pm 1.10}$	$37.2_{\pm 20.1}$	$1.50_{\pm 1.42}$	$0.09_{\pm 0.0}$
Improvement	29.65%	28.85%	36.97%	-	45.65%	18.18%

Table 1: Comparison of different methods regarding the statistical fidelity of the synthetic data.
 All metrics have been scaled so that lower numbers indicate better performance, to facilitate better numerical comparison.

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#### 5.2 MAIN RESULTS

346 Statistical Fidelity We first investigate whether synthetic data can faithfully reproduce the distribu-347 tion of the original data. We use various statistical metrics to reflect the degree to which synthetic 348 data estimates the distribution density of the original data. These metrics include univariate density 349 estimation (i.e., the marginal distribution of a single column), the correlation between any two vari-350 ables (which reflects the **joint** probability distribution),  $\alpha$ -Precision (reflecting whether a synthetic 351 data example is close to the true distribution),  $\beta$ -Recall (reflecting the coverage of synthetic data 352 over the original data), Classifier Two Sample Test (C2ST, reflecting the difficulty in distinguishing 353 between synthetic data and real data), and Jensen-Shannon divergence (JSD, estimating the distance 354 between the distributions of real data and synthetic data). Due to space limitations, in this section, we 355 only present the average performance with standard deviation on each metric across all ten datasets. The detailed performance on each individual dataset is in Appendix E. 356

357 In Table 1, we present the performance comparison on these fidelity metrics. As demonstrated, our 358 model achieved performance far surpassing the second-best method in five out of six fidelity metrics, 359 with advantages ranging from 18.18% to 45.65%. Considering that these metrics have already been 360 elevated to a considerably high level due to the explosive development of recent deep generative 361 models for tabular data, our improvement is very significant. The only exception is  $\beta$ -Recall, which measures the degree of coverage of the synthetic data over the entire data distribution. On this metric, 362 the simple classical interpolation method SMOTE achieved the best performance, far surpassing 363 other generative models. On the other hand, SMOTE also achieves very good performance on other 364 metrics, surpassing many generative methods. These phenomena indicate that simple interpolation methods can indeed obtain synthetic data with a distribution close to that of real data. However, the 366 limitation of interpolation methods lies in the fact that the synthetic data is too close to the real data, 367 making it resemble a copy from the training set rather than a sample from the underlying distribution, 368 which may cause privacy issues. Detailed experiments are in the Privacy Protection section. 369

370 **Utility on Downstream Tasks** We then evaluate the quality of synthetic data by assessing their 371 performance in Machine Learning Efficiency (MLE) tasks. Following previous settings (Zhang 372 et al., 2024b), we first split a real table into a real training and a real testing set. The generative 373 models are trained on the real training set, from which a synthetic set of equivalent size is sampled. 374 This synthetic data is then used to train a classification/regression model (XGBoost Classifier and 375 XGBoost Regressor (Chen & Guestrin, 2016)), which will be evaluated using the real testing set. The performance of MLE is measured by the AUC score for classification tasks and RMSE for regression 376 tasks. As demonstrated in Table 2, the proposed TABDAR gives a fairly satisfying performance on 377 the MLE tasks, and the classification/regression performance obtained via training on the synthetic

Method	Continuo	us only	Discre	ete only	Heterogeous					
	California AUC↑	Letter AUC↑	Car AUC↑	Nursery AUC↑	Adult AUC↑	<b>Default</b> AUC↑	Shoppers AUC↑	<b>Magic</b> AUC↑	<b>News</b> RMSE↓	Beijing RMSE
Real data	0.999	0.989	0.999	1.000	0.927	0.770	0.926	0.946	0.842	0.423
<i>VAE-based</i> TVAE GOGGLE	0.986	0.989	0.746	0.939	$0.846 \\ 0.778$	$0.744 \\ 0.584$	$0.898 \\ 0.658$	$0.912 \\ 0.654$	$0.979 \\ 1.09$	$1.010 \\ 0.877$
<i>GAN-based</i> CTGAN	0.925	0.729	0.899	1.000	0.874	0.736	0.868	0.874	0.845	1.065
<i>LLM-based</i> GReaT	0.996	0.983	0.979	0.999	0.913	0.755	0.902	0.888	-	0.653
Diffusion-based STaSy CoDi TabDDPM TabSyn	<b>0.997</b> 0.981 0.992 0.993	$\begin{array}{c} 0.990 \\ 0.998 \\ 0.513 \\ 0.990 \end{array}$	$\begin{array}{c} 0.927 \\ 0.995 \\ 0.995 \\ 0.971 \end{array}$	$\begin{array}{c} 0.982 \\ 1.000 \\ 1.000 \\ 0.997 \end{array}$	$\begin{array}{c} 0.903 \\ 0.829 \\ 0.911 \\ 0.904 \end{array}$	$\begin{array}{c} 0.749 \\ 0.497 \\ 0.763 \\ 0.764 \end{array}$	$\begin{array}{c} 0.909 \\ 0.855 \\ 0.915 \\ 0.913 \end{array}$	$\begin{array}{c} 0.923 \\ 0.930 \\ 0.933 \\ 0.934 \end{array}$	$0.933 \\ 0.999 \\ - 0.862$	$0.672 \\ 0.750 \\ 2.665 \\ 0.669$
Autoregressive DP-TBART Tab-MT	$0.993 \\ 0.988$	$\begin{array}{c} 0.985 \\ 0.985 \end{array}$	$\begin{array}{c} 0.990 \\ 0.981 \end{array}$	$0.917 \\ 1.000$	<mark>0.918</mark> 0.873	$\begin{array}{c} 0.717 \\ 0.714 \end{array}$	$0.896 \\ 0.912$	$0.924 \\ 0.822$	$0.896 \\ 1.002$	$0.676 \\ 2.098$
TABDAR	0.994	0.994	0.996	1.000	0.904	0.764	0.916	0.935	0.856	0.579

Table 2: AUC (classification task) and RMSE (regression task) scores of Machine Learning Efficiency.  $\uparrow$  ( $\downarrow$ ) indicates that the higher (lower) the score, the better the performance.

Table 3: Probability that a synthetic example's DCR to the training set rather than that of the holdout set), a score closer to 50% is better.

Method	Default	Shoppers
SMOTE	91.41%	96.40%
TabDDPM	51.30%	51.74%
TabSyn	50.88%	51.50%
TABDAR	51.13%	50.97%



Figure 5: Distributions of the DCR scores between the synthetic dataset and the training/holdout datasets.

set is rather close to that on the original training set. Also, similar to the observations in (Zhang et al., 2024b), the differences between various methods on MLE tasks are very small, even though some methods may not correctly learn the distribution of the original data. Therefore, it is important to combine this with the fidelity metrics in Table 1 to obtain a more comprehensive evaluation of synthetic data. 

**Privacy Protection** Finally, a good synthetic dataset should not only faithfully reproduce the original data distribution but also ensure that it is sampled from the underlying distribution of the real data rather than being a copy. To this end, we use the Distance to Closest Record (DCR) score for measurement. Specifically, we divide the real data equally into two parts of the same size, namely the training set and the holdout set. We train the model based on the training set and obtain the sampled synthetic dataset. Afterward, we calculate the distribution of distances between each synthetic data example and its closest sample in both the training set and the holdout set. Intuitively, if the training set and holdout set are both drawn uniformly from the same distribution and if the synthetic data has learned the true distribution, then on average, the proportion of synthetic data samples that are closer to the training set should be the same as those closer to the holdout set (both 50%). Conversely, if the synthetic data is copied from the training set, the probability of it being closer to samples in the training set would far exceed 50%. 

In Table 3 and Figure 5, we present the probability comparison and the distributions of the DCR scores of SMOTE, TabDDPM, TabSyn, and the proposed TABDAR. As demonstrated, SMOTE is poor at privacy protection, as its synthetic sample tends to be closer to the training set rather than the holdout set, as its synthetic examples are obtained via interpolation between training examples. By contrast, the remaining deep generative methods are all good at preserving the privacy of training data, leading to almost completely overlapped DCR distributions.

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Figure 6: (30% MCAR) Comparison of missing value imputation performance with 4 competitive baselines.

Table 4: Ablation Studies: Effects of the Diffusion loss and random order sampling.

Variants	Margin	Joint
w/o. both w/o. Diff. loss w/o. rand. order	$\begin{array}{c c} 14.82\% \\ 12.35\% \\ 1.83\% \end{array}$	$\begin{array}{c} 8.94\% \\ 6.11\% \\ 2.05\% \end{array}$
TABDAR	1.21%	1.80%

Table 5: Impacts of the model depth (number of Transformer layers) on Adult and Beijing.

Table 6: Impacts of the embedding dimension don Adult and Beijing.

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8         0.96%         2.09%         1.02%         46.84%         64         1.05%         2.24%         1.62%         42.2	۱%

#### 5.3 MISSING DATA IMPUTATION

Since TABDAR directly models the factorized conditional probability of the target column(s) given the observation of other columns, it has a strong potential for missing data imputation. In this section, 455 we compare the proposed TABDAR with the current state-of-the-art (SOTA) methods for missing 456 data imputation, including KNN (Pujianto et al., 2019), GRAPE (You et al., 2020), MOT (Muzellec et al., 2020), and Remakser (Du et al., 2024). We consider the task of training the model on the complete training data and then imputing the missing values of testing data. The missing mechanism 459 is Missing Completely at Random (MCAR), and the missing ratio of testing data is set at 30%. In Figure 6, we present the performance comparison on four datasets: Letter, Adult, Default, and Shoppers (as well as the average imputation performance). The proposed TABDAR demonstrates superior performance on these four datasets, significantly outperforming the current best methods on three out of four datasets. On the Adult dataset, it was slightly inferior. These results confirm that TABDAR is not only suitable for unconditional generation but also applicable to other conditional generation tasks, demonstrating a wide range of application values.

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#### 5.4 ABLATION STUDIES

Effects of diffusion loss and random ordering. We first study if the two key ingredients of 469 TABDAR-1) the diffusion loss and 2) random ordering – are indeed beneficial. We consider three 470 variants of TABDAR: 'w/o. Diff. Loss', which indicates that we discretize the continuous columns 471 into 100 uniform bins, treating them as discrete ones, such that we can apply the cross-entropy loss; 472 'w/o rand. order,' which indicates that we follow the default left-to-right order in both the training 473 and generation phases using a causal attention Transformer model; 'w/o. both', which indicates the 474 version that combines the two variants. In Table 4, we compare TABDAR with the three variants on 475 the average synthetic data's fidelity across all the datasets. We can observe that both the diffusion loss 476 and random training/generation order are important to TABDAR's success. Specifically, the diffusion loss targeting the modeling of the conditional distribution of the continuous columns contributes the 477 most, and the random ordering further improves TABDAR's performance. Furthermore, random 478 ordering enables TABDAR to perform flexible conditional inference tasks like imputation. 479

480 Sensitivity to hyperparameters. We then study TABDAR's sensitivity to its hyperparameters 481 that specify its transformer architecture: the model depth (number of Transformer layers) and the 482 embedding dimension d. From Table 5 and Table 6 (grey cells indicate the default setting), we can observe that although there exists an optimal hyperparameter setting (i.e., depth = 6, d = 32), 483 the change of the two hyperparameters has little impact on the model performance. These results 484 demonstrate that our model is relatively robust to these hyperparameters. Therefore, good results can 485 be obtained for different datasets without the need for specific hyperparameter tuning.

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Figure 8: 2D joint distribution density of 'Longitude' and 'Latitude' of California dataset.

#### 6 VISUALIZATIONS

In this section, we visualize the synthetic data to demonstrate that the proposed TABDAR can generate synthetic data that closely resembles the ground-truth distribution. In Figure 7 and Figure 8, we plot the 2D joint distribution of two columns of the Adult and California datasets to investigate if the ground-truth joint distribution density can be learned by the synthetic data. In Figure 9, 519 we further plot the heatmaps of the 520 estimation error of column pair cor-521 relations. These results visually 522 demonstrate that TABDAR can gen-523 erate synthetic samples very close 524 to the distribution of real data and faithfully reflect the correlations be-526 tween different columns of the data.



Figure 9: Heatmaps of the joint column correlation estimation error. Lighter areas indicate a lower error in estimating the correlation between two columns.

#### 7 CONCLUSION

532 This paper has presented TABDAR, a generative model that embeds a diffusion model within an 533 autoregressive transformer framework used for multi-modal tabular data synthesis. TABDAR uses 534 a novel diffusion loss and traditional cross-entropy loss to learn the conditional distributions of 535 continuous columns and discrete columns, respectively, enabling a single autoregressive model to 536 generate both continuous and discrete features simultaneously. Furthermore, TABDAR employs 537 masked bidirectional attention to simulate arbitrary autoregressive orders, allowing the model to generate in any direction. This not only enhances the accuracy of joint probability modeling but 538 also enables more flexible conditional generation. Extensive experimental results demonstrate the effectiveness of the proposed method.

# 540 REPRODUCIBILITY STATEMENT

We describe the algorithm of TABDAR in Appendix A. The detailed implementations are provided in Appendix C and Appendix D. The codes for implementing baselines and the proposed TAB-DAR are provided in the anonymous github repo https://anonymous.4open.science/r/ ICLR-TabDAR. 

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# 756 A ALGORITHMS

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762 763 In this section, we provide detailed algorithms of TABDAR. Algorithm 3 provides the training algorithm of TABDAR. Algorithm 4 and 5 provide the unconditional and conditional generation algorithm of TABDAR, respectively. For simplicity, the algorithms are presented with a single data as input, it is straightforward to extend to batch setting.

Algorithm 1: Loss for continuous columns

764 1: Input: Condition vector  $\mathbf{z}^i$ , target continuous value  $x^i$ , denoising network  $\boldsymbol{\epsilon}_{\theta}$ 765 2: Output: Loss  $\mathcal{L}(p(x^i | \mathbf{z}^i))$ 766 3: Sample  $t \sim p(t)$ 767 4: Sample  $\varepsilon \sim \mathcal{N}(0, 1)$ 768 5: Get  $x_t^i = x^i + \sigma(t) \cdot \varepsilon$ 769 6: Compute loss:  $\mathcal{L}(p(x^i|\mathbf{z}^i)) = \|\boldsymbol{\epsilon}_{\theta}(x_t^i, t, \mathbf{z}^i) - \varepsilon\|_2^2$ 770 771 772 Algorithm 2: Loss for discrete columns 773 1: Input: Condition vector  $\mathbf{z}^i$ , target discrete value  $x^i$ , prediction head  $f_i(\theta)$ 774 2: Output: Loss  $\mathcal{L}(p(x^i|\mathbf{z}^i))$ 775 3: Get  $\hat{\mathbf{x}}^i = f_i(\mathbf{z}^i)$ 776 4: Compute loss:  $\mathcal{L}(p(x^i|\mathbf{z}^i)) = \text{CrossEntropy}(x^i, \text{Softmax}(\hat{\mathbf{x}}^i))$ 777 778 779 Algorithm 3: TABDAR: Training 780 1: Input: data  $\mathbf{x} = (x^1, x^2, \cdots x^D)$ 781 2: Output: Model parameters 782 3: 1. Tokenization 783 4: for  $i \in 1, 2, \dots, D$  do 784  $\mathbf{h}^i = \mathbf{W}^i x^i$ 5: 785 6: end for 786 7: Let  $\mathbf{H} = [\mathbf{h}^1, \mathbf{h}^2, \cdots, \mathbf{h}^D]$ 787 8: Add positional encoding 788 9: 789 10: 2. Adding mask 11: Sample the masking number  $M \sim \text{Uniform}(1, D)$ 790 12: Sample the masking vector  $\boldsymbol{m} \in \{0,1\}^D$ , s.t.,  $\sum_i m^i = M$ 791 13: Let  $\mathbf{H}' = (1 - \mathbf{m}) \odot \mathbf{H}$ 792 14: 793 15: 3. Transformer layers 794 16: Append padding token [pad] 17:  $\mathbf{Z} = \text{Transformers}(\mathbf{H}')$ 796 18: 797 19: 4. Compute Losses 798 20: for  $i \in 1, 2, \dots, D$  do 799 if  $m^i == 1$  then 21: 800 22: if  $i \in C$  then 801 Compute  $\mathcal{L}(p(x^i|\mathbf{z}^i))$  as discrete columns ; ▷ Algorithm 2 23: 24: 802 else 25: Compute  $\mathcal{L}(p(x^i|\mathbf{z}^i))$  as continuous columns ; ⊳ Algorithm 1 26: end if 804 end if 27: 805 28: end for 806 29: Compute  $\mathcal{L} = \sum_{i=1}^{D} \mathcal{L}(p(x^{i}|\mathbf{z}^{i})) \cdot m^{i};$ 807 ▷ Compute losses only for target/masked columns 30: Back-propagation to optimize model parameters 809

	<b>Input:</b> A generation order $\mathbf{o} = [o_1, o_2, \cdots, o_n]$	$[p_D] = $ Shuffle $([1, 2, 3, \cdots D])$
	<b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$	
	$\mathbf{m} \leftarrow 1 \in \mathbb{R}^{D}$ ;	All tokens are unknown initia
	$\mathrm{H}=0$	
5:	for $i \in 1, 2, \cdots, D$ do	
6:	Add positional encoding	
7:	$\mathbf{H}' = (1 - \mathbf{m}) \odot \mathbf{H} = 0 \in \mathbb{R}^{D \times d}$ ;	▷ All token embedding are set z
8:	$\mathbf{Z} = \text{Transformers}(\mathbf{H}')$	
9:	Sample $\tilde{x}^{o_i}$ from $p(x^{o_i} \mathbf{z}^{o_i})$ ;	▷ Sample for location
10:	if $i \in \mathcal{C}$ then	
11:	Compute $\hat{\mathbf{x}}^{o_i} = f_{o_i}(\mathbf{z}^{o_i}) \in \mathbb{R}^{\mathcal{C}_i}$	
12:	Sample $\tilde{x}^{o_i} \sim \text{Multi}(\tilde{\mathbf{x}}^{o_i})$ ;	Sample discrete comport
13:	else	
14:	Sample $\tilde{x}^{o_i}$ from the diffusion sampler :	Sample continuous componies
15:	end if	
16:	$ ilde{\mathbf{h}}^{o_i} = \mathbf{W}^{o_i}  ilde{x}^{o_i}  ext{ ; }  agence  extsf{k}$	Tokenization for the newly sampled column va
17:	$\mathbf{H}_{o_i}^\prime \gets  ilde{\mathbf{h}}^{o_i}$ ;	⊳ Update the in
18:	$m^{o_i} \leftarrow 1;$	▷ Update the m
	end for	v opute the in
	The finally sampled data is $\tilde{\mathbf{x}} = (\tilde{x}^1, \tilde{x}^2, \cdots, \tilde{x}^n)$	$(\tilde{x}^D)$
-0.		,~ )
2: 3:	$o_1, \dots, o_{D-M}$ are the indices of $D - M$ obsorbed of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$	served columns, $o_{D-M+1}, \cdots, o_D$ are the indition the $D-M$ observed values.
2: 3: 4:	$o_1, \dots, o_{D-M}$ are the indices of $D - M$ obsorbed of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ for $i \in 1, \dots, D$ do	served columns, $o_{D-M+1}, \dots, o_D$ are the indicate the $D-M$ observed values.
2: 3: 4: 5:	$o_1, \dots, o_{D-M}$ are the indices of $D - M$ obsorbed of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ for $i \in 1, \dots, D$ do if $i <= D - M$ then	served columns, $o_{D-M+1}, \dots, o_D$ are the indicate the $D-M$ observed values.
2: 3: 4: 5: 6:	$o_1, \dots, o_{D-M}$ are the indices of $D - M$ obsorbed of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ for $i \in 1, \dots, D$ do if $i <= D - M$ then $\tilde{x}^{o_i} = x^{o_i}$	served columns, $o_{D-M+1}, \dots, o_D$ are the indicate the $D-M$ observed values.
2: 3: 4: 5: 6: 7:	$o_1, \dots, o_{D-M}$ are the indices of $D - M$ obsolution of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ for $i \in 1, \dots, D$ do if $i \leq D - M$ then $\tilde{x}^{o_i} = x^{o_i}$ else	served columns, $o_{D-M+1}, \dots, o_D$ are the indicate the $D-M$ observed values.
2: 3: 4: 5: 6: 7: 8:	$o_1, \dots, o_{D-M}$ are the indices of $D - M$ obsolution of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ for $i \in 1, \dots, D$ do if $i <= D - M$ then $\tilde{x}^{o_i} = x^{o_i}$ else $\tilde{x}^{o_i} = 0$	served columns, $o_{D-M+1}, \dots, o_D$ are the indicate the $D-M$ observed values.
2: 3: 4: 5: 6: 7: 8: 9:	$o_1, \dots, o_{D-M}$ are the indices of $D - M$ obsolution of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ for $i \in 1, \dots, D$ do if $i <= D - M$ then $\tilde{x}^{o_i} = x^{o_i}$ else $\tilde{x}^{o_i} = 0$ end if	served columns, $o_{D-M+1}, \dots, o_D$ are the indicate the $D-M$ observed values.
2: 3: 4: 5: 6: 7: 8: 9: 10:	$o_1, \dots, o_{D-M}$ are the indices of $D - M$ obsolution of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ <b>for</b> $i \in 1, \dots, D$ <b>do</b> <b>if</b> $i \leq D - M$ <b>then</b> $\tilde{x}^{o_i} = x^{o_i}$ <b>else</b> $\tilde{x}^{o_i} = 0$ <b>end if</b> $\mathbf{h}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$	served columns, $o_{D-M+1}, \dots, o_D$ are the indicate the $D-M$ observed values.
2: 3: 4: 5: 6: 7: 8: 9: 10: 11:	$o_1, \dots, o_{D-M}$ are the indices of $D - M$ obsolution of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ for $i \in 1, \dots, D$ do if $i <= D - M$ then $\tilde{x}^{o_i} = x^{o_i}$ else $\tilde{x}^{o_i} = 0$ end if $\mathbf{h}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ end for	served columns, $o_{D-M+1}, \cdots, o_D$ are the indic the $D-M$ observed values. $x^{o_1}, \cdots, \tilde{x}^{o_{D-M}} = x^{o_{D-M}}$
2: 3: 4: 5: 6: 7: 8: 9: 10: 11: 12:	$o_1, \dots, o_{D-M}$ are the indices of $D - M$ obsolution of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ <b>for</b> $i \in 1, \dots, D$ <b>do</b> <b>if</b> $i <= D - M$ <b>then</b> $\tilde{x}^{o_i} = x^{o_i}$ <b>else</b> $\tilde{x}^{o_i} = 0$ <b>end if</b> $\mathbf{h}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ <b>end for</b> Initialize the mask vector $\mathbf{m} = [0^{D-M}, 1^M]$	$x^{o_1}, \cdots, \tilde{x}^{o_{D-M}} = x^{o_{D-M}}$
2: 3: 4: 5: 6: 7: 8: 9: 10: 11: 12: 13:	$o_1, \dots, o_{D-M}$ are the indices of $D - M$ obsolution of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ <b>for</b> $i \in 1, \dots, D$ <b>do</b> <b>if</b> $i <= D - M$ <b>then</b> $\tilde{x}^{o_i} = x^{o_i}$ <b>else</b> $\tilde{x}^{o_i} = 0$ <b>end if</b> $\mathbf{h}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ <b>end for</b> Initialize the mask vector $\mathbf{m} = [0^{D-M}, 1^M]$	served columns, $o_{D-M+1}, \cdots, o_D$ are the indic the $D-M$ observed values. $x^{o_1}, \cdots, \tilde{x}^{o_{D-M}} = x^{o_{D-M}}$
2: 3: 4: 5: 6: 7: 8: 9: 10: 11: 12: 13:	$o_1, \dots, o_{D-M}$ are the indices of $D - M$ obsolution of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ <b>for</b> $i \in 1, \dots, D$ <b>do</b> <b>if</b> $i <= D - M$ <b>then</b> $\tilde{x}^{o_i} = x^{o_i}$ <b>else</b> $\tilde{x}^{o_i} = 0$ <b>end if</b> $\mathbf{h}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ <b>end for</b> Initialize the mask vector $\mathbf{m} = [0^{D-M}, 1^M]$ <b>for</b> $i \in D - M + 1, \dots, D$ <b>do</b>	served columns, $o_{D-M+1}, \cdots, o_D$ are the indic the $D-M$ observed values. $x^{o_1}, \cdots, \tilde{x}^{o_{D-M}} = x^{o_{D-M}}$
2: 3: 4: 5: 6: 7: 8: 9: 10: 11: 12: 13: 14: 15:	$o_1, \dots, o_{D-M}$ are the indices of $D - M$ obsolution of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ <b>for</b> $i \in 1, \dots, D$ <b>do</b> <b>if</b> $i <= D - M$ <b>then</b> $\tilde{x}^{o_i} = x^{o_i}$ <b>else</b> $\tilde{x}^{o_i} = 0$ <b>end if</b> $\mathbf{h}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ <b>end for</b> Initialize the mask vector $\mathbf{m} = [0^{D-M}, 1^M]$ <b>for</b> $i \in D - M + 1, \dots, D$ <b>do</b> $\mathbf{H}' = (1 - \mathbf{m}) \odot \mathbf{H}$	served columns, $o_{D-M+1}, \cdots, o_D$ are the indic the $D-M$ observed values. $x^{o_1}, \cdots, \tilde{x}^{o_{D-M}} = x^{o_{D-M}}$
2: 3: 4: 5: 6: 7: 8: 9: 10: 11: 12: 13: 14: 15: 16:	$o_1, \dots, o_{D-M}$ are the indices of $D - M$ obsolution of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ <b>for</b> $i \in 1, \dots, D$ <b>do</b> <b>if</b> $i <= D - M$ <b>then</b> $\tilde{x}^{o_i} = x^{o_i}$ <b>else</b> $\tilde{x}^{o_i} = 0$ <b>end if</b> $\mathbf{h}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ <b>end for</b> Initialize the mask vector $\mathbf{m} = [0^{D-M}, 1^M]$ <b>for</b> $i \in D - M + 1, \dots, D$ <b>do</b> $\mathbf{H}' = (1 - \mathbf{m}) \odot \mathbf{H}$ $\mathbf{Z} = \text{Transformers}(\mathbf{H}')$	served columns, $o_{D-M+1}, \dots, o_D$ are the indic the $D - M$ observed values. $x^{o_1}, \dots, \tilde{x}^{o_{D-M}} = x^{o_{D-M}}$ ; $\triangleright$ Tokens at missing positions are mast
2: 3: 4: 5: 6: 7: 8: 9: 10: 11: 12: 13: 14: 15: 16: 17:	$o_1, \dots, o_{D-M}$ are the indices of $D - M$ obsolution of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ <b>for</b> $i \in 1, \dots, D$ <b>do</b> <b>if</b> $i \leq D - M$ <b>then</b> $\tilde{x}^{o_i} = x^{o_i}$ <b>else</b> $\tilde{x}^{o_i} = 0$ <b>end if</b> $\mathbf{h}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ <b>end for</b> Initialize the mask vector $\mathbf{m} = [0^{D-M}, 1^M]$ <b>for</b> $i \in D - M + 1, \dots, D$ <b>do</b> $\mathbf{H}' = (1 - \mathbf{m}) \odot \mathbf{H}$ $\mathbf{Z} = \text{Transformers}(\mathbf{H}')$ Sample $\tilde{x}^{o_i}$ from $p(x^{o_i}   \mathbf{z}^{o_i})$ ;	served columns, $o_{D-M+1}, \dots, o_D$ are the indic the $D - M$ observed values. $x^{o_1}, \dots, \tilde{x}^{o_{D-M}} = x^{o_{D-M}}$ ; $\triangleright$ Tokens at missing positions are mas
2: 3: 4: 5: 6: 7: 8: 9: 10: 11: 12: 13: 14: 15: 16: 17: 18: 18: 19: 11: 13: 14: 15: 11: 13: 11: 13: 14: 15: 15: 10: 11: 13: 14: 15: 15: 15: 15: 15: 15: 15: 15	$o_1, \dots, o_{D-M}$ are the indices of $D - M$ obsolution of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ <b>for</b> $i \in 1, \dots, D$ <b>do</b> <b>if</b> $i \leq D - M$ <b>then</b> $\tilde{x}^{o_i} = x^{o_i}$ <b>else</b> $\tilde{x}^{o_i} = 0$ <b>end if</b> $\mathbf{h}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ <b>end for</b> Initialize the mask vector $\mathbf{m} = [0^{D-M}, 1^M]$ <b>for</b> $i \in D - M + 1, \dots, D$ <b>do</b> $\mathbf{H}' = (1 - \mathbf{m}) \odot \mathbf{H}$ $\mathbf{Z} = \text{Transformers}(\mathbf{H}')$ Sample $\tilde{x}^{o_i}$ from $p(x^{o_i}   \mathbf{z}^{o_i})$ ; <b>if</b> $i \in C$ <b>then</b>	served columns, $o_{D-M+1}, \dots, o_D$ are the indic the $D - M$ observed values. $x^{o_1}, \dots, \tilde{x}^{o_{D-M}} = x^{o_{D-M}}$ ; $\triangleright$ Tokens at missing positions are mas
2: 3: 4: 5: 6: 7: 8: 9: 10: 11: 12: 13: 14: 15: 16: 17: 18: 19: 19: 11: 11: 12: 13: 14: 11: 11: 11: 12: 13: 14: 15: 11: 11: 12: 13: 14: 15: 15: 15: 15: 15: 15: 15: 15	$o_1, \dots, o_{D-M}$ are the indices of $D - M$ obsolution of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ <b>for</b> $i \in 1, \dots, D$ <b>do</b> <b>if</b> $i \leq D - M$ <b>then</b> $\tilde{x}^{o_i} = x^{o_i}$ <b>else</b> $\tilde{x}^{o_i} = 0$ <b>end if</b> $\mathbf{h}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ <b>end for</b> Initialize the mask vector $\mathbf{m} = [0^{D-M}, 1^M]$ <b>for</b> $i \in D - M + 1, \dots, D$ <b>do</b> $\mathbf{H}' = (1 - \mathbf{m}) \odot \mathbf{H}$ $\mathbf{Z} = \text{Transformers}(\mathbf{H}')$ Sample $\tilde{x}^{o_i}$ from $p(x^{o_i}   \mathbf{z}^{o_i})$ ; <b>if</b> $i \in C$ <b>then</b> Compute $\hat{\mathbf{x}}^{o_i} = f_{o_i}(\mathbf{z}^{o_i}) \in \mathbb{R}^{C_i}$	served columns, $o_{D-M+1}, \dots, o_D$ are the indic the $D - M$ observed values. $x^{o_1}, \dots, \tilde{x}^{o_{D-M}} = x^{o_{D-M}}$ ; $\triangleright$ Tokens at missing positions are mask $\triangleright$ Sample for location
2: 3: 4: 5: 6: 7: 8: 9: 10: 11: 12: 13: 14: 15: 16: 17: 18: 19: 20:	$o_1, \dots, o_{D-M} \text{ are the indices of } D - M \text{ obs}$ of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ <b>for</b> $i \in 1, \dots, D$ <b>do</b> <b>if</b> $i <= D - M$ <b>then</b> $\tilde{x}^{o_i} = x^{o_i}$ <b>else</b> $\tilde{x}^{o_i} = 0$ <b>end if</b> $\mathbf{h}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ <b>end for</b> Initialize the mask vector $\mathbf{m} = [0^{D-M}, 1^M]$ <b>for</b> $i \in D - M + 1, \dots, D$ <b>do</b> $\mathbf{H}' = (1 - \mathbf{m}) \odot \mathbf{H}$ $\mathbf{Z} = \text{Transformers}(\mathbf{H}')$ Sample $\tilde{x}^{o_i}$ from $p(x^{o_i}   \mathbf{z}^{o_i})$ ; <b>if</b> $i \in C$ <b>then</b> Compute $\hat{\mathbf{x}}^{o_i} = f_{o_i}(\mathbf{z}^{o_i}) \in \mathbb{R}^{C_i}$ Sample $\tilde{x}^{o_i} \sim \text{Multi}(\tilde{\mathbf{x}}^{o_i})$ ;	served columns, $o_{D-M+1}, \dots, o_D$ are the indic the $D - M$ observed values. $x^{o_1}, \dots, \tilde{x}^{o_{D-M}} = x^{o_{D-M}}$ ; $\triangleright$ Tokens at missing positions are mask $\triangleright$ Sample for location
2: 3: 4: 5: 6: 7: 8: 9: 10: 11: 12: 13: 14: 15: 16: 17: 18: 19: 20: 21:	$o_1, \dots, o_{D-M} \text{ are the indices of } D - M \text{ obs}$ of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ <b>for</b> $i \in 1, \dots, D$ <b>do</b> <b>if</b> $i <= D - M$ <b>then</b> $\tilde{x}^{o_i} = x^{o_i}$ <b>else</b> $\tilde{x}^{o_i} = 0$ <b>end if</b> $\mathbf{h}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ <b>end for</b> Initialize the mask vector $\mathbf{m} = [0^{D-M}, 1^M]$ <b>for</b> $i \in D - M + 1, \dots, D$ <b>do</b> $\mathbf{H}' = (1 - \mathbf{m}) \odot \mathbf{H}$ $\mathbf{Z} = \text{Transformers}(\mathbf{H}')$ Sample $\tilde{x}^{o_i}$ from $p(x^{o_i}   \mathbf{z}^{o_i})$ ; <b>if</b> $i \in C$ <b>then</b> Compute $\hat{\mathbf{x}}^{o_i} = f_{o_i}(\mathbf{z}^{o_i}) \in \mathbb{R}^{C_i}$ Sample $\tilde{x}^{o_i} \sim \text{Multi}(\tilde{\mathbf{x}}^{o_i})$ ; <b>else</b>	served columns, $o_{D-M+1}, \dots, o_D$ are the indic the $D - M$ observed values. $x^{o_1}, \dots, \tilde{x}^{o_{D-M}} = x^{o_{D-M}}$ ; > Tokens at missing positions are mask $\triangleright$ Sample for location $\triangleright$ Sample discrete component
2: 3: 4: 5: 6: 7: 8: 9: 10: 11: 12: 13: 14: 15: 16: 17: 18: 19: 20: 21: 22:	$o_1, \dots, o_{D-M} \text{ are the indices of } D - M \text{ obs}$ of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ <b>for</b> $i \in 1, \dots, D$ <b>do</b> <b>if</b> $i <= D - M$ <b>then</b> $\tilde{x}^{o_i} = x^{o_i}$ <b>else</b> $\tilde{x}^{o_i} = 0$ <b>end if</b> $\mathbf{h}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ <b>end for</b> Initialize the mask vector $\mathbf{m} = [0^{D-M}, 1^M]$ <b>for</b> $i \in D - M + 1, \dots, D$ <b>do</b> $\mathbf{H}' = (1 - \mathbf{m}) \odot \mathbf{H}$ $\mathbf{Z} = \text{Transformers}(\mathbf{H}')$ Sample $\tilde{x}^{o_i}$ from $p(x^{o_i}   \mathbf{z}^{o_i})$ ; <b>if</b> $i \in C$ <b>then</b> Compute $\hat{\mathbf{x}}^{o_i} = f_{o_i}(\mathbf{z}^{o_i}) \in \mathbb{R}^{C_i}$ Sample $\tilde{x}^{o_i} \sim \text{Multi}(\tilde{\mathbf{x}}^{o_i})$ ;	served columns, $o_{D-M+1}, \dots, o_D$ are the indic the $D - M$ observed values. $x^{o_1}, \dots, \tilde{x}^{o_{D-M}} = x^{o_{D-M}}$ ; > Tokens at missing positions are mask $\triangleright$ Sample for location $\triangleright$ Sample discrete compon
2: 3: 4: 5: 6: 7: 8: 9: 10: 11: 12: 13: 14: 15: 16: 17: 18: 19: 20: 21: 22: 23:	$o_1, \dots, o_{D-M} \text{ are the indices of } D - M \text{ obs}$ of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ <b>for</b> $i \in 1, \dots, D$ <b>do</b> <b>if</b> $i <= D - M$ <b>then</b> $\tilde{x}^{o_i} = x^{o_i}$ <b>else</b> $\tilde{x}^{o_i} = 0$ <b>end if</b> $\mathbf{h}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ <b>end for</b> Initialize the mask vector $\mathbf{m} = [0^{D-M}, 1^M]$ <b>for</b> $i \in D - M + 1, \dots, D$ <b>do</b> $\mathbf{H}' = (1 - \mathbf{m}) \odot \mathbf{H}$ $\mathbf{Z} = \text{Transformers}(\mathbf{H}')$ Sample $\tilde{x}^{o_i}$ from $p(x^{o_i}   \mathbf{z}^{o_i})$ ; <b>if</b> $i \in C$ <b>then</b> Compute $\hat{\mathbf{x}}^{o_i} = f_{o_i}(\mathbf{z}^{o_i}) \in \mathbb{R}^{C_i}$ Sample $\tilde{x}^{o_i} \sim \text{Multi}(\tilde{\mathbf{x}}^{o_i})$ ; <b>else</b> Sample $\tilde{x}^{o_i}$ from the diffusion sampler ; <b>end if</b>	served columns, $o_{D-M+1}, \dots, o_D$ are the indic the $D - M$ observed values. $x^{o_1}, \dots, \tilde{x}^{o_{D-M}} = x^{o_{D-M}}$ ; > Tokens at missing positions are mask $\triangleright$ Sample for location $\triangleright$ Sample discrete components $\triangleright$ Sample continuous components
2: 3: 4: 5: 6: 7: 8: 9: 10: 11: 12: 13: 14: 15: 16: 17: 18: 19: 20: 21: 22: 23: 24:	$o_1, \dots, o_{D-M} \text{ are the indices of } D - M \text{ obs}$ of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ <b>for</b> $i \in 1, \dots, D$ <b>do</b> <b>if</b> $i <= D - M$ <b>then</b> $\tilde{x}^{o_i} = x^{o_i}$ <b>else</b> $\tilde{x}^{o_i} = 0$ <b>end if</b> $\mathbf{h}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ <b>end for</b> Initialize the mask vector $\mathbf{m} = [0^{D-M}, 1^M]$ <b>for</b> $i \in D - M + 1, \dots, D$ <b>do</b> $\mathbf{H}' = (1 - \mathbf{m}) \odot \mathbf{H}$ $\mathbf{Z} = \text{Transformers}(\mathbf{H}')$ Sample $\tilde{x}^{o_i}$ from $p(x^{o_i}   \mathbf{z}^{o_i})$ ; <b>if</b> $i \in C$ <b>then</b> Compute $\hat{\mathbf{x}}^{o_i} = f_{o_i}(\mathbf{z}^{o_i}) \in \mathbb{R}^{C_i}$ Sample $\tilde{x}^{o_i}$ from the diffusion sampler ; <b>end if</b> $\tilde{\mathbf{h}}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ ;	served columns, $o_{D-M+1}, \dots, o_D$ are the indic the $D - M$ observed values. $x^{o_1}, \dots, \tilde{x}^{o_{D-M}} = x^{o_{D-M}}$ ; > Tokens at missing positions are mast $\triangleright$ Sample for location $\triangleright$ Sample discrete component Sample continuous component Tokenization for the newly sampled column variables.
2: 3: 4: 5: 6: 7: 8: 9: 10: 11: 12: 13: 14: 15: 16: 17: 18: 19: 20: 21: 22: 22: 22: 25:	$o_1, \dots, o_{D-M} \text{ are the indices of } D - M \text{ obs}$ of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ <b>for</b> $i \in 1, \dots, D$ <b>do</b> <b>if</b> $i <= D - M$ <b>then</b> $\tilde{x}^{o_i} = x^{o_i}$ <b>else</b> $\tilde{x}^{o_i} = 0$ <b>end if</b> $\mathbf{h}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ <b>end for</b> Initialize the mask vector $\mathbf{m} = [0^{D-M}, 1^M]$ <b>for</b> $i \in D - M + 1, \dots, D$ <b>do</b> $\mathbf{H}' = (1 - \mathbf{m}) \odot \mathbf{H}$ $\mathbf{Z} = \text{Transformers}(\mathbf{H}')$ Sample $\tilde{x}^{o_i}$ from $p(x^{o_i}   \mathbf{z}^{o_i})$ ; <b>if</b> $i \in C$ <b>then</b> Compute $\hat{\mathbf{x}}^{o_i} = f_{o_i}(\mathbf{z}^{o_i}) \in \mathbb{R}^{C_i}$ Sample $\tilde{x}^{o_i}$ from the diffusion sampler ; <b>end if</b> $\tilde{\mathbf{h}}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ ; $\triangleright$	served columns, $o_{D-M+1}, \dots, o_D$ are the indic the $D - M$ observed values. $x^{o_1}, \dots, \tilde{x}^{o_{D-M}} = x^{o_{D-M}}$ ; > Tokens at missing positions are mast $\triangleright$ Sample for location $\triangleright$ Sample discrete component $\triangleright$ Sample continuous component Tokenization for the newly sampled column va $\triangleright$ Update the in
2: 3: 4: 5: 6: 7: 8: 9: 10: 11: 12: 13: 14: 15: 16: 17: 18: 19: 20: 21: 22: 22: 22: 22: 22: 22: 22: 22: 22	$o_1, \dots, o_{D-M} \text{ are the indices of } D - M \text{ obs}$ of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ <b>for</b> $i \in 1, \dots, D$ <b>do</b> <b>if</b> $i <= D - M$ <b>then</b> $\tilde{x}^{o_i} = x^{o_i}$ <b>else</b> $\tilde{x}^{o_i} = 0$ <b>end if</b> $\mathbf{h}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ <b>end for</b> Initialize the mask vector $\mathbf{m} = [0^{D-M}, 1^M]$ <b>for</b> $i \in D - M + 1, \dots, D$ <b>do</b> $\mathbf{H}' = (1 - \mathbf{m}) \odot \mathbf{H}$ $\mathbf{Z} = \text{Transformers}(\mathbf{H}')$ Sample $\tilde{x}^{o_i}$ from $p(x^{o_i}   \mathbf{z}^{o_i})$ ; <b>if</b> $i \in C$ <b>then</b> Compute $\hat{\mathbf{x}}^{o_i} = f_{o_i}(\mathbf{z}^{o_i}) \in \mathbb{R}^{C_i}$ Sample $\tilde{x}^{o_i}$ from the diffusion sampler ; <b>end if</b> $\tilde{\mathbf{h}}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ ; $\bowtie$ $\mathbf{H}'_{o_i} \leftarrow \tilde{\mathbf{h}}^{o_i}$ ; $m^{o_i} \leftarrow 1$ ;	served columns, $o_{D-M+1}, \dots, o_D$ are the indic the $D - M$ observed values. $x^{o_1}, \dots, \tilde{x}^{o_{D-M}} = x^{o_{D-M}}$ ; > Tokens at missing positions are mast $\triangleright$ Sample for location $\triangleright$ Sample discrete component $\triangleright$ Sample continuous component Tokenization for the newly sampled column va $\triangleright$ Update the in
2: 3: 4: 5: 6: 7: 8: 9: 10: 11: 12: 13: 14: 15: 16: 17: 18: 19: 20: 21: 22: 22: 22: 22: 22: 22: 22: 22: 22	$o_1, \dots, o_{D-M} \text{ are the indices of } D - M \text{ obs}$ of $M$ columns to impute. $x^{o_1}, \dots x^{o_{D-M}}$ are <b>Output:</b> A sample $\tilde{\mathbf{x}} \in \mathbb{R}^D$ , such that $\tilde{x}^{o_1} =$ <b>for</b> $i \in 1, \dots, D$ <b>do</b> <b>if</b> $i <= D - M$ <b>then</b> $\tilde{x}^{o_i} = x^{o_i}$ <b>else</b> $\tilde{x}^{o_i} = 0$ <b>end if</b> $\mathbf{h}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ <b>end for</b> Initialize the mask vector $\mathbf{m} = [0^{D-M}, 1^M]$ <b>for</b> $i \in D - M + 1, \dots, D$ <b>do</b> $\mathbf{H}' = (1 - \mathbf{m}) \odot \mathbf{H}$ $\mathbf{Z} = \text{Transformers}(\mathbf{H}')$ Sample $\tilde{x}^{o_i}$ from $p(x^{o_i}   \mathbf{z}^{o_i})$ ; <b>if</b> $i \in C$ <b>then</b> Compute $\hat{\mathbf{x}}^{o_i} = f_{o_i}(\mathbf{z}^{o_i}) \in \mathbb{R}^{C_i}$ Sample $\tilde{x}^{o_i}$ from the diffusion sampler ; <b>end if</b> $\tilde{\mathbf{h}}^{o_i} = \mathbf{W}^{o_i} \tilde{x}^{o_i}$ ; $\triangleright$	served columns, $o_{D-M+1}, \dots, o_D$ are the indic the $D - M$ observed values. $x^{o_1}, \dots, \tilde{x}^{o_{D-M}} = x^{o_{D-M}}$ ; > Tokens at missing positions are mask $\triangleright$ Sample for location $\triangleright$ Sample discrete component $\triangleright$ Sample continuous component Tokenization for the newly sampled column va $\triangleright$ Update the in $\triangleright$ Update the m

## B DIFFUSION SDES

This paper adopts the simplified version of the Variance-Exploding SDE in (Song et al., 2021). Song et al. (2021) has proposed the following general-form forward SDE:

$$d\mathbf{x} = \boldsymbol{f}(\mathbf{x}, t)dt + g(t) d\boldsymbol{w}_t = d\mathbf{x} = f(t) \mathbf{x} dt + g(t) d\boldsymbol{w}_t.$$
(9)

Then the conditional distribution of  $\mathbf{x}_t$  given  $\mathbf{x}_0$  (named as the perturbation kernel of the SDE) could be formulated as:

$$p(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; s(t)\mathbf{x}_0, s^2(t)\sigma^2(t)\mathbf{I}),$$
(10)

where

$$s(t) = \exp\left(\int_0^t f(\xi) \mathrm{d}\xi\right), \text{ and } \sigma(t) = \sqrt{\int_0^t \frac{g^2(\xi)}{s^2(\xi)} \mathrm{d}\xi}.$$
 (11)

Therefore, the forward diffusion process could be equivalently formulated by defining the perturbation kernels (via defining appropriate s(t) and  $\sigma(t)$ ).

Variance Exploding (VE) implements the perturbation kernel Eq. 10 by setting s(t) = 1, indicating that the noise is directly added to the data rather than weighted mixing. Therefore, The noise variance (the noise level) is totally decided by  $\sigma(t)$ . When s(t) = 1, the perturbation kernels become:

$$p(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \mathbf{0}, \sigma^2(t)\mathbf{I}) \implies \mathbf{x}_t = \mathbf{x}_0 + \sigma(t)\boldsymbol{\varepsilon},$$
(12)

which aligns with the forward diffusion process in Eq. 2.

The sampling process of diffusion SDE is given by:

$$d\mathbf{x} = [\boldsymbol{f}(\mathbf{x},t) - g^2(t)\nabla_{\mathbf{x}}\log p_t(\mathbf{x})]dt + g(t)d\boldsymbol{w}_t.$$
(13)

For VE-SDE,  $s(t) = 1 \Leftrightarrow f(\mathbf{x}, t) = f(t) \cdot \mathbf{x} = \mathbf{0}$ , and

$$\sigma(t) = \sqrt{\int_0^t g^2(\xi) d\xi} \Rightarrow \int_0^t g^2(\xi) d\xi = \sigma^2(t),$$

$$g^2(t) = \frac{d\sigma^2(t)}{dt} = 2\sigma(t)\dot{\sigma}(t),$$
(14)

 $g(t) = \sqrt{2\sigma(t)\dot{\sigma}(t)}.$ 

Plugging g(t) into Eq. 13, the reverse process in Eq. 3 is recovered:

$$d\mathbf{x}_t = -2\sigma(t)\dot{\sigma}(t)\nabla_{\mathbf{x}_t}\log p(\mathbf{x}_t)dt + \sqrt{2\sigma(t)\dot{\sigma}(t)}d\boldsymbol{\omega}_t.$$
(15)

### C DETAILED MODEL ARCHITECTURES

In this section, we introduce the detailed architecture of TABDAR, which consists of a tokenization layer, several transformer blocks, and two (group of) predictors for numerical and categorical features, respectively.

#### C.1 TOKENIZERS AND TRANSFORMERS

**Tokenization.** We first apply one-hot encoding to the categorical features and then project both numerical and categorical features into the embedding space. We employ column-wise tokenizers for the feature of every single column, respectively, following the setup in Zhang et al. (2024b).

912	• For a numerical column, we use a simple linear projection to map the sc	alar into a d-
913	dimensional vector.	
914	$\mathbf{h}^i = \mathbf{W}^i x^i,  ext{ where } \mathbf{W}^i \in \mathbb{R}^{1  imes d}$	(16)
915	• For a categorical column, we use a simple linear projection to map the one-ho	t encoding of
916	$x^i$ into a d-dimensional vector.	t cheoding of
917		

$$\mathbf{h}^{i} = \mathbf{W}^{i} x^{i}, \text{ where } \mathbf{W}^{i} \in \mathbb{R}^{\mathcal{C}_{i} \times d}$$
 (17)

918 **Transformer layers** After tokenization, we add column-wise positional encoding to each token 919 embedding, and then we apply a]the zero mask to the predefined masked/target tokens. Furthermore, 920 we append the [pad] token embedding at the beginning of the obtained data sequence. The proposed 921 data will be further processed by a series of Transformer blocks.

922 We use ViT (Dosovitskiy, 2021) as the backbone of the Transformer layers, which consists of 923 multiple Transformer blocks (Vaswani et al., 2017). Each Transformer block contains a multi-head 924 self-attention mechanism and a feed-forward network. Specifically, we use a stack of six Transformer 925 blocks with four attention heads. 926

927 **Predictors.** Given the output token embeddings from the Transformer layers, i.e.,  $z^i$ , we further 928 use additional predictors such that it is tailored for learning the conditional distribution  $p(x^i|\mathbf{z}^i)$ 

929 We apply a simple MLP predictor  $f_i(\cdot)$  for each token. For each discrete column,  $f_i(\cdot)$  is a 4-layer 930 MLP with ReLU activation. 931

932 For each continuous column, the output token embedding  $z^i$  be further fed into the denoising neural 933 network to predict the noise. We defer this part to Appendix C.2.

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C.2 DIFFUSION MODEL

In this section, we introduce the architecture of the diffusion model. In a nutshell, we use simple 937 MLPs as our denoising neural network, which is similar to the design in Zhang et al. (2024b) and 938 (Kotelnikov et al., 2023), the only difference is our denoising network takes an additional input  $z^i$  as the conditional information. 940

Denoising neural network. The denoising neural network takes three inputs: the noisy data  $x_t^i = x^i + \sigma(t) \cdot \varepsilon$  (note that we let  $\sigma(t) = t$ ), the current timestep t, and the conditional information  $z^i$ . Following the practice in (Kotelnikov et al., 2023), the current timestep t is first embedded with sinusoidal positional embedding, then further embedded with a 2-layer fully connected MLP with SiLU activation;

$$e_{pe} = PE(t), e_t = MLP_t(e_{pe})$$

where PE denotes the sinusoidal positional embedding (Vaswani et al., 2017). 948

949 Similarly, the conditional information  $z^i$  is embedded with a similar 2-layer MLP with SiLU activa-950 tion.

$$e_z = \mathrm{MLP}_z(\mathbf{z}^i)$$

952 Now we have the embeddings of current timestep and conditional information, we add them together as the final condition embedding  $e^*$ . 954

$$e^* = e_t + e_a$$

For the noisy data  $x_t^i$ , we first project it with a single linear layer to align the dimension with the conditional embedding, then add it with  $e^*$  and feed into a 4-layer MLP with SiLU activation for the final prediction of the denoised data.

$$\boldsymbol{\epsilon}_{\theta}(x_t^i, t, \mathbf{z}^i) = \text{MLP}(\text{Linear}(x_t^i) + e^*)$$

Finally, we minimize the MSE loss between the output of the denoising neural network and the added noise:

$$\min \|\boldsymbol{\epsilon}_{\theta}(x_t^i, t, \mathbf{z}^i) - \boldsymbol{\varepsilon}\|_2^2$$

D DETAILED EXPERIMENTAL SETUPS

D.1 HARDWARE SPECIFICATION AND ENVIRONMENT

We run our experiments on a single machine with Intel i9-14900K, Nvidia RTX 4090 GPU with 24 970 GB memory. The code is written in Python 3.10.14 and we use PyTorch 2.2.2 on CUDA 12.2 to train 971 the model on the GPU.

#### 972 D.2 DATASETS

The dataset used in this paper could be automatically downloaded using the script in the provided code. We use 10 tabular datasets from Kaggle<sup>3</sup> or UCI Machine Learning Repository<sup>4</sup>: Adult<sup>5</sup>, Default<sup>6</sup>, Shoppers<sup>7</sup>, Magic<sup>8</sup>, Beijing<sup>9</sup>, and News<sup>10</sup>, California<sup>11</sup>, Letter<sup>12</sup>, Car<sup>13</sup>, and Nursery<sup>14</sup>, which contains varies number of numerical and categorical features. The statistics of the datasets are presented in Table 7.

Table 7: Dataset statistics.

Dataset	# Rows	# Continuous	# Discrete	# Target	# Train	# Test	Task
California	20,640	9	-	1	18,390	2,520	Classification
Letter	20,000	16	-	1	18,000	2,000	Classification
Car	1,728	-	7	1	1,555	173	Classification
Nursery	12,960	-	9	1	11,664	1,296	Classification
Adult	32,561	6	8	1	22,792	16,281	Classification
Default	30,000	14	10	1	27,000	3,000	Classification
Shoppers	12,330	10	7	1	11,098	1,232	Classification
Magic	19,021	10	1	1	17,118	1,903	Classification
Beijing	43,824	7	5	1	39,441	4,383	Regression
News	39,644	46	2	1	35,679	3,965	Regression

In Table 7, # Rows denote the number of rows (records) in the table. # Continuous and # Discrete denote the number of continuous features and discrete features, respectively. Note that there is an additional # Target column. The target columns are either continuous or discrete, depending on the task type. All datasets (except Adult) are split into training and testing sets with the ratio 9 : 1 with a fixed random seed. As Adult has its official testing set, we directly use it as the testing set. For Machine Learning Efficiency (MLE) evaluation, the training set will be further split into training and validation split with the ratio 8 : 1.

# 

# 1003 D.3 TABDAR IMPLEMENTATION DETAILS

Data Preprocessing. We first fill the missing values with the columns's average for numerical columns. For categorical columns, missing cells are treated as an additional category. Then numerical columns are transformed to follow a normal distribution by QuantileTransformer<sup>15</sup> and categorical columns are encoded as integers by OrdinalEncoder<sup>16</sup>. Finally, we normalize the numerical features to have 0 mean and 0.5 variance, following (Karras et al., 2022).

1011	
1011	<sup>3</sup> https://www.kaggle.com
1012	<sup>4</sup> https://archive.ics.uci.edu/datasets
1013	<sup>5</sup> https://archive.ics.uci.edu/dataset/2/adult
1014	<sup>6</sup> https://archive.ics.uci.edu/dataset/350/default+of+credit+card+clients
1015	<sup>7</sup> https://archive.ics.uci.edu/dataset/468/online+shoppers+purchasing+
1016	intention+dataset
1017	<sup>8</sup> https://archive.ics.uci.edu/dataset/159/magic+gamma+telescope
1018	<pre>https://archive.ics.uci.edu/dataset/381/beijing+pm2+5+data</pre>
1019	<sup>10</sup> https://archive.ics.uci.edu/dataset/332/online+news+popularity
1020	<sup>11</sup> https://www.kaggle.com/datasets/camnugent/california-housing-prices
	<sup>12</sup> https://archive.ics.uci.edu/dataset/59/letter+recognition
1021	<sup>13</sup> https://archive.ics.uci.edu/dataset/19/car+evaluation
1022	<sup>14</sup> https://archive.ics.uci.edu/dataset/76/nursery
1023	<sup>15</sup> https://scikit-learn.org/stable/modules/generated/sklearn.
1024	preprocessing.QuantileTransformer.html
1025	<sup>16</sup> https://scikit-learn.org/stable/modules/generated/sklearn.
	preprocessing.OrdinalEncoder.html

Hyperparameters. TABDAR uses a fixed set of hyperparameters for all datasets. Table 8 shows the hyperparameters. Our experiments show that TABDAR is robust to the choice of hyperparameters, saving the time of meticulous hyperparameter tuning for each dataset. 

Туре	Parameter	Value
	optimizer	Adam
	initial learning rate	1e-3
Training	weight decay	1e-6
Training	LR scheduler	ReduceLROnPlateau
	training epochs	5000
	batch size	4096
	#Transformer blocks	6
Transformers	embedding dim	32
	#heads	4

Table 8: Default hyperparameter setting of TABDAR.

#### D.4 MISSING VALUE IMPUTATION

Following (Zhang et al., 2024a), we use the *Expected A Posteriori* (EAP) estimator to impute the missing values. Specifically, denote a sample x with missing values as  $\mathbf{x} = (\mathbf{x}_{obs}, \mathbf{x}_{mis})$  where  $\mathbf{x}_{obs}$ and  $\mathbf{x}_{mis}$  are the observed and missing values, respectively. Our goal is to compute the expectation of the missing values conditioned on the observed values: 

$$\mathbb{E}_{\mathbf{x}_{\min} \sim p(\mathbf{x}_{\min} | \mathbf{x}_{obs})}[\mathbf{x}_{\min}]$$

To estimate the expectation, we sample k times from the posterior distribution  $p(\mathbf{x}_{\text{mis}}|\mathbf{x}_{\text{obs}})$  (with Algorithm 5) and obtain a set of samples  $\{\hat{\mathbf{x}}_{mis}^i\}_{i=1}^k$ 

For numerical features, the imputation  $\hat{\mathbf{x}}_{mis}$  is set to the mean of the samples:

 $\hat{\mathbf{x}}_{\text{mis}} = \frac{1}{k} \sum_{i=1}^{k} \hat{\mathbf{x}}_{\text{mis}}^{i}$ 

For categorical features, we apply a majority vote on every column to approximate the expectation. Suppose the column has categories  $\mathcal{C} = \{c_1, c_2, \cdots, c_m\}$ , the imputation  $\hat{\mathbf{x}}_{mis}$  is set to the most frequent category:

$$\hat{\mathbf{x}}_{\text{mis}} = \arg \max_{c_j \in \mathcal{C}} \frac{1}{k} \sum_{i=1}^k \delta(\hat{\mathbf{x}}_{\text{mis}}^i = c_j)$$

where  $\delta(\cdot)$  is an indicator function that equals to 1 if the input is true and 0 otherwise. The majority vote can be understood as a mean estimator that is more robust to outliers.

Finally, we concatenate the observed values with the imputed missing values to obtain the final imputed sample: 

$$\mathbf{x}_{\text{imputed}} = (\mathbf{x}_{\text{obs}}, \hat{\mathbf{x}}_{\text{mis}})$$

In our experiments, we find that k = 10 is a good trade-off between performance and efficiency. 

**D.5 BASELINE IMPLEMENTATIONS** 

Tab-MT and DP-TBART. Tab-MT (Gulati & Roysdon, 2023) and DP-TBART (Castellon et al., 2023) are two recently proposed tabular data generation models based on MAE. To handle numerical features (with continuous distribution), Tab-MT quantizes the numerical features into 100 uniform bins, and DP-TBART quantizes the numerical features into 100 bins where each bin has the same nearest center determined by K-means. Additionally, DP-TBART employs DP-SGD (Abadi et al., 2016) to enhance the differential privacy performance. Since the focus of this paper is not on differential privacy, in our implementation, we use Adam (Kingma & Ba, 2015) optimizer.

1080 1081 1082	<b>Other Baselines.</b> The implementations of SMOTE (Chawla et al., 2002), CTGAN (Xu et al., 2019), TVAE (Xu et al., 2019), GOOGLE <sup>17</sup> (Liu et al., 2023), GReaT (Borisov et al., 2023), CoDi (Lee et al., 2023), STaSy (Kim et al., 2023), TabDDPM (Kotelnikov et al., 2023), TabSyn (Zhang et al.,
1083 1084	2024b) follows the codebase of Zhang et al. $(2024b)^{18}$ .
1085 1086	D.6 METRICS
1087 1088 1089	Most of the metrics (including Marginal, Joint, $\alpha$ -Precision, $\beta$ -Recall, C2ST, MLE, and DCR) used in this paper directly follow the setups in Zhang et al. (2024b). Here is a reference:
1090	• Marginal: Appendix E.3.1 in Zhang et al. (2024b).
1091 1092	• Joint: Appendix E.3.2 in Zhang et al. (2024b).
1093	• $\alpha$ -Precision and $\beta$ -Recall: Appendix F.2 in Zhang et al. (2024b).
1094	• C2ST: Appendix F.3 in Zhang et al. (2024b).
1095 1096	• MLE: Appendix E.4 in Zhang et al. (2024b).
1097	• DCR: Appendix F.6 in Zhang et al. (2024b).
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1100	Below is a summary of how these metrics work.
1101	D.6.1 MARGINAL DISTRIBUTION
1102	
1103 1104	The <b>Marginal</b> metric evaluates if each column's marginal distribution is faithfully recovered by the synthetic data. We use Kolmogorov-Sirnov Test for continuous data and Total Variation Distance for
1105	discrete data.
1106	
1107 1108 1109	<b>Kolmogorov-Sirnov Test (KST)</b> Given two (continuous) distributions $p_r(x)$ and $p_s(x)$ (r denotes real and s denotes synthetic), KST quantifies the distance between the two distributions using the upper bound of the discrepancy between two corresponding Cumulative Distribution Functions
1110	(CDFs):
1111 1112	$KST = \sup_{x}  F_r(x) - F_s(x) , \tag{18}$
1113	where $F_r(x)$ and $F_s(x)$ are the CDFs of $p_r(x)$ and $p_s(x)$ , respectively:
1114	
1115 1116	$F(x) = \int_{-\infty}^{x} p(x) \mathrm{d}x.$ (19)
1117	$J_{-\infty}$
1118	Total Variation Distance (TVD) TVD computes the frequency of each category value and ex-
1119	presses it as a probability. Then, the TVD score is the average difference between the probabilities of
1120	the categories:
1121 1122	$TVD = \frac{1}{2} \sum_{\omega \in \Omega}  R(\omega) - S(\omega) , \qquad (20)$
1123	$2\sum_{\omega\in\Omega}$
1124	where $\omega$ describes all possible categories in a column $\Omega$ . $R(\cdot)$ and $S(\cdot)$ denotes the real and synthetic
1125	frequencies of these categories.
1126	
1127 1128	D.6.2 JOINT DISTRIBUTION
1129	The <b>Joint</b> metric evaluates if the correlation of every two columns in the real data is captured by the
1130	synthetic data.
1131	

<sup>&</sup>lt;sup>17</sup>We find the result of GOOGLE is hard to reproduce due to memory issues, so we directly use the results 1132 in Zhang et al. (2024b)
 <sup>18</sup>https://github.com/amazon-science/tabsyn/tree/main/baselines 1133

Pearson Correlation Coefficient The Pearson correlation coefficient measures whether two continuous distributions are linearly correlated and is computed as:

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- 1138 1139

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where x and y are two continuous columns. Cov is the covariance, and  $\sigma$  is the standard deviation.

 $\rho_{x,y} = \frac{\operatorname{Cov}(x,y)}{\sigma_x \sigma_y},$ 

1141 Then, the performance of correlation estimation is measured by the average differences between the 1142 real data's correlations and the synthetic data's corrections:

Pearson Score =  $\frac{1}{2}\mathbb{E}_{x,y}|\rho^R(x,y) - \rho^S(x,y)|,$  (22)

(21)

(23)

1146 where  $\rho^R(x, y)$  and  $\rho^S(x, y)$ ) denotes the Pearson correlation coefficient between column x and 1147 column y of the real data and synthetic data, respectively. As  $\rho \in [-1, 1]$ , the average score is divided 1148 by 2 to ensure that it falls in the range of [0, 1], then the smaller the score, the better the estimation.

Contingency similarity For a pair of categorical columns A and B, the contingency similarity score computes the difference between the contingency tables using the Total Variation Distance. The process is summarized by the formula below:

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where  $\alpha$  and  $\beta$  describe all the possible categories in column A and column B, respectively.  $R_{\alpha,\beta}$ and  $S_{\alpha,\beta}$  are the joint frequency of  $\alpha$  and  $\beta$  in the real data and synthetic data, respectively.

Contingency Score =  $\frac{1}{2} \sum_{\alpha \in A} \sum_{\beta \in B} |R_{\alpha,\beta} - S_{\alpha,\beta}|,$ 

1159 1160 D.6.3  $\alpha$ -Precision and  $\beta$ -Recall

1161  $\alpha$ -Precision and  $\beta$ -Recall are two sample-level metrics quantifying how faithful the synthetic data 1162 is proposed in Alaa et al. (2022). In general,  $\alpha$ -Precision evaluates the fidelity of synthetic data 1163 – whether each synthetic example comes from the real-data distribution,  $\beta$ -Recall evaluates the 1164 coverage of the synthetic data, e.g., whether the synthetic data can cover the entire distribution of the 1165 real data (In other words, whether a real data sample is close to the synthetic data).

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1167 D.6.4 CLASSIFIER-TWO-SAMPLE-TEST (C2ST)

C2ST studies how difficult it is to distinguish real data from synthetic data, therefore evaluating
 whether synthetic data can recover real data distribution. The C2ST metric used in this paper is
 implemented by the SDMetrics<sup>19</sup> package.

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1173 D.6.5 MACHINE LEARNING EFFICIENCY (MLE)

In MLE, each dataset is first split into the real training and testing set. The generative models are learned on the real training set. After the models are learned, a synthetic set of equivalent size is sampled.

The performance of synthetic data on MLE tasks is evaluated based on the divergence of test scores 1178 using the real and synthetic training data. Therefore, we first train the machine learning model on the 1179 real training set, split into training and validation sets with a 8 : 1 ratio. The classifier/regressor is 1180 trained on the training set, and the optimal hyperparameter setting is selected according to the perfor-1181 mance on the validation set. After the optimal hyperparameter setting is obtained, the corresponding 1182 classifier/regressor is retrained on the training set and evaluated on the real testing set. We create 1183 20 random splits for training and validation sets, and the performance reported is the mean of the 1184 AUC/RMSE score over the 20 random trails. The performance of synthetic data is obtained in the 1185 same way.

<sup>1187 &</sup>lt;sup>19</sup>https://docs.sdv.dev/sdmetrics/metrics/metrics-in-beta/ detection-single-table

#### D.6.6 DISTANCE TO CLOSEST RECORD

We follow the 'synthetic vs. holdout' setting  $^{20}$ . We initially divide the dataset into two equal parts: the first part served as the training set for training our generative model, while the second part was designated as the holdout set, which is not used for training. After completing model training, we sample a synthetic set of the same size as the training set (and the holdout set). 

We then calculate the DCR scores for each sample in the synthetic set concerning both the training set and the holdout set. We further calculate the probability that a synthetic sample is closer to the training set (rather than the holdout set). When this probability is close to 50% (i.e., 0.5), it indicates that the distribution of distances between synthetic and training instances is very similar (or at least not systematically smaller) than the distribution of distances between synthetic and holdout instances, which is a positive indicator in terms of privacy risk. 

#### Ε ADDITIONAL EXPERIMENTAL RESULTS

In this section, we provide a more detailed empirical comparison between the proposed TABDAR and other baseline methods. 

E.1 DETAILED RESULTS ON THE FIDELITY METRICS 

Note that in Table 1, we only present the average performance of each method on the six fidelity metrics across the ten datasets. In this section, we present a detailed performance comparison of each individual dataset: 

- Marginal Distribution: Table 9
- Joint Correlation: Table 10
  - $\alpha$ -Precision: Table 11
  - $\beta$ -Recall: Table 12
  - Classifier-Two-Sample-Test: Table 13
  - Jensen-Shannon Divergence: Table 14

Table 9: Performance comparison on the Marginal Distribution Density metric. Numbers represent the error rate in %, the lower the better. 

	Method	Continuou	is only	Discre	ete only			Heter	ogeous		
		California	Letter	Car	Nursery	Adult	Beijing	Default	Magic	News	Shoppers
	erpolation SMOTE	0.99	0.97	1.00	0.57	1.59	1.78	1.49	1.07	5.28	2.48
	<i>E-based</i> TVAE	5.37	16.70	24.12	9.81	24.32	25.13	9.94	4.39	18.48	23.93
	<i>N-based</i> CTGAN	12.84	18.79	16.46	12.33	19.32	21.98	18.25	5.69	13.90	25.71
	<i>M-based</i> GReaT	14.93	4.88	2.22	5.08	12.12	8.25	19.94	16.16	_	14.51
55	<i>fusion-based</i> STaSy CoDi TabDDPM TabSyn	$10.82 \\ 18.98 \\ 57.34 \\ 1.00$	$11.93 \\ 22.62 \\ 61.43 \\ 2.53$	$24.38 \\ 1.53 \\ 1.53 \\ 2.48$	$10.93 \\ 0.65 \\ 0.65 \\ 1.04$	$10.41 \\ 24.84 \\ 1.32 \\ 2.75$	$\begin{array}{c} 6.38 \\ 12.54 \\ 1.20 \\ 2.43 \end{array}$	$11.34 \\ 16.54 \\ 7.59 \\ 0.95$	$13.02 \\ 11.64 \\ 1.09 \\ 0.79$	8.54 28.13 - 1.77	$16.14 \\ 36.48 \\ 2.86 \\ 1.52$
	oregressive DP-TBART Tab-MT	$3.30 \\ 5.87$	$4.46 \\ 3.29$	$1.98 \\ 0.96$	$0.53 \\ 0.70$	$1.17 \\ 17.20$	$2.68 \\ 25.10$	$5.03 \\ 25.17$	$3.90 \\ 21.88$	$6.28 \\ 46.54$	$3.05 \\ 2.20$
_	TABDAR	0.99	1.79	1.31	0.73	0.59	0.80	1.74	0.80	2.03	1.32

> <sup>20</sup>https://www.clearbox.ai/blog/2022-06-07-synthetic-data-for-privacy-\ preservation-part-2

Method	Continuous only		Discr	ete only	Heterogeous					
	California	Letter	Car	Nursery	Adult	Beijing	Default	Magic	News	Shoppers
interpolation SMOTE	2.70	1.19	3.16	1.21	3.56	1.53	6.93	2.84	2.87	3.53
<i>VAE-based</i> TVAE	5.85	5.28	38.66	18.34	36.65	31.12	19.37	4.46	6.45	20.12
<i>GAN-based</i> CTGAN	14.49	11.40	25.63	18.14	27.35	27.08	30.52	5.04	5.22	24.24
<i>LLM-based</i> GReaT	9.66	3.46	4.72	8.38	17.59	59.60	70.02	59.96	_	45.16
Diffusion-based STaSy CoDi TabDDPM TabSyn	$3.59 \\ 6.89 \\ 19.83 \\ 0.78$	$5.34 \\ 5.25 \\ 22.35 \\ 1.78$	$36.40 \\ 3.52 \\ 3.52 \\ 4.28$	$15.02 \\ 1.31 \\ 1.31 \\ 1.85$	$13.50 \\ 22.72 \\ 2.50 \\ 4.64$	$8.71 \\ 6.42 \\ 3.31 \\ 4.16$	$\begin{array}{c} 10.65 \\ 67.88 \\ 11.55 \\ 3.30 \end{array}$	$5.58 \\ 6.93 \\ 0.67 \\ 0.91$	$3.06 \\ 10.81 \\ - \\ 1.43$	$15.29 \\ 20.18 \\ 6.23 \\ 2.18$
Autoregressive DP-TBART Tab-MT	$2.52 \\ 5.87$	$1.94 \\ 3.29$	$3.54 \\ 0.96$	$\begin{array}{c} 1.19 \\ 0.70 \end{array}$	$2.50 \\ 17.20$	$2.55 \\ 25.10$	$6.70 \\ 25.17$	$1.73 \\ 21.88$	$1.60 \\ 46.54$	$2.83 \\ 2.20$
TABDAR	0.61	1.45	2.99	1.36	1.36	2.27	2.83	1.86	1.50	1.89

Table 10: Performance comparison on the Joint Column Correlation metric. Numbers represent the error rate in %, the low the better.

1261Table 11: Performance comparison on the  $\alpha$ -**Precision** metric. Numbers represent  $1 - \alpha$ -**Precision**.1262The lower the better. Note that the numbers in Table 1 are in % while numbers in this table are in raw1263scale.

264	Method	Continuo	Continuous only Discrete only				Heterogeous						
265	Methou	California	Letter	Car	Nursery	Adult	Beijing	Default	Magic	News	Shoppers		
66 67	interpolation SMOTE	0.0173	0.0222	0.0103	0.0040	0.0729	0.0118	0.0228	0.0186	0.1256	0.0725		
68	VAE-based TVAE	0.0191	0.0937	0.2322	0.0972	0.4124	0.1100	0.1610	0.0338	0.1530	0.5655		
69 70	<i>GAN-based</i> CTGAN	0.2933	0.0522	0.1023	0.0677	0.2528	0.0723	0.3595	0.1106	0.0177	0.1292		
71 72	<i>LLM-based</i> GReaT	0.1665	0.0891	0.0262	0.0836	0.4421	0.0168	0.1410	0.1454	1.0000	0.2112		
2 3 4 5	Diffusion-based STaSy CoDi TabDDPM TabSyn	$\begin{array}{c} 0.8385 \\ 0.1333 \\ 0.8385 \\ 0.0062 \end{array}$	$\begin{array}{c} 0.0158 \\ 0.0963 \\ 1.0000 \\ 0.0998 \end{array}$	$\begin{array}{c} 0.3347 \\ 0.0323 \\ 0.0323 \\ 0.0206 \end{array}$	$\begin{array}{c} 0.1385 \\ 0.0037 \\ 0.0037 \\ 0.0056 \end{array}$	$\begin{array}{c} 0.2250 \\ 0.1805 \\ 0.0444 \\ 0.0239 \end{array}$	$\begin{array}{c} 0.0350 \\ 0.0471 \\ 0.0130 \\ 0.0049 \end{array}$	$\begin{array}{c} 0.1320 \\ 0.1722 \\ 0.0924 \\ 0.0123 \end{array}$	$\begin{array}{c} 0.1853 \\ 0.1434 \\ 0.0146 \\ 0.0053 \end{array}$	$\begin{array}{c} 0.0809 \\ 0.1041 \\ 1.0000 \\ 0.0457 \end{array}$	$\begin{array}{c} 0.1656 \\ 0.0825 \\ 0.0807 \\ 0.0279 \end{array}$		
'6 '7	Autoregressive DP-TBART Tab-MT	$\begin{array}{c} 0.0256 \\ 0.0239 \end{array}$	$\begin{array}{c} 0.0427 \\ 0.0415 \end{array}$	$\begin{array}{c} 0.0093 \\ 0.0140 \end{array}$	$\begin{array}{c} 0.0054 \\ 0.0146 \end{array}$	$\begin{array}{c} 0.0054 \\ 0.1776 \end{array}$	$\begin{array}{c} 0.0049 \\ 0.4839 \end{array}$	$\begin{array}{c} 0.0727 \\ 0.0581 \end{array}$	$\begin{array}{c} 0.0160 \\ 0.5507 \end{array}$	$\begin{array}{c} 0.0149 \\ 0.9369 \end{array}$	$\begin{array}{c} 0.0145 \\ 0.0158 \end{array}$		
8	TABDAR	0.0080	0.0383	0.0190	0.0052	0.0029	0.0070	0.0133	0.0147	0.0218	0.0025		

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#### E.2 TRAINING / SAMPLING TIME

In Table 15, we compare the training and sampling time of TABDAR with other methods on the
Adult dataset.

1285 E.3 ADDITIONAL VISUALIZATIONS

We present the 2D visualizations (Figure 7 and Figure 8) of the synthetic data generated by all baseline methods in Figure 10 and Figure 11, respectively. We also present the heat maps of all methods on the four datasets (Figure 9) in Figure 12, Figure 13, Figure 14, and Figure 15, respectively.

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Table 12: Performance comparison on the  $\beta$ -Recall metric. Numbers represent  $1 - \beta$ -Recall. The lower the better. Note that the numbers in Table 1 are in % while numbers in this table are in raw scale.

Method	Continuous only		Discrete only		Heterogeous					
inteniou	California	Letter	Car	Nursery	Adult	Beijing	Default	Magic	News	Shopper
Interpolation SMOTE	0.2157	0.1338	0.0045	0.0012	0.2325	0.2080	0.2390	0.1934	0.2011	0.2386
VAE-based TVAE	0.6512	0.8324	0.4369	0.2625	0.8969	0.9392	0.7078	0.6243	0.7413	0.7672
<i>GAN-based</i> CTGAN	0.8412	0.9903	0.9879	0.0530	0.8246	0.6230	0.8889	0.8472	0.7732	0.7441
<i>LLM-based</i> GReaT	0.5515	0.6643	0.0034	0.0024	0.5088	0.5666	0.5796	0.6509	1.0000	0.5510
Diffusion-based STaSy CoDi TabDDPM TabSyn	$\begin{array}{c} 0.9288 \\ 0.5998 \\ 0.9288 \\ 0.5706 \end{array}$	$\begin{array}{c} 0.7332 \\ 0.4551 \\ 1.0000 \\ 0.7486 \end{array}$	$\begin{array}{c} 0.1075 \\ 0.0040 \\ 0.0040 \\ 0.0031 \end{array}$	$\begin{array}{c} 0.0029 \\ 0.0009 \\ 0.0009 \\ 0.0007 \end{array}$	$\begin{array}{c} 0.6812 \\ 0.9032 \\ 0.5152 \\ 0.5484 \end{array}$	$\begin{array}{c} 0.5061 \\ 0.4472 \\ 0.4335 \\ 0.4847 \end{array}$	$\begin{array}{c} 0.6421 \\ 0.7811 \\ 0.6150 \\ 0.5365 \end{array}$	$\begin{array}{c} 0.5686 \\ 0.5139 \\ 0.5206 \\ 0.5146 \end{array}$	$\begin{array}{c} 0.6033 \\ 0.6505 \\ 1.0000 \\ 0.5602 \end{array}$	$\begin{array}{c} 0.7174 \\ 0.8187 \\ 0.4492 \\ 0.4399 \end{array}$
Autoregressive DP-TBART Tab-MT	$\begin{array}{c} 0.6138 \\ 0.6272 \end{array}$	$\begin{array}{c} 0.8859 \\ 0.8385 \end{array}$	$\begin{array}{c} 0.0038 \\ 0.0067 \end{array}$	$\begin{array}{c} 0.0010 \\ 0.0008 \end{array}$	$\begin{array}{c} 0.5033 \\ 0.9681 \end{array}$	$\begin{array}{c} 0.4536 \\ 0.4930 \end{array}$	$\begin{array}{c} 0.5562 \\ 0.9179 \end{array}$	$\begin{array}{c} 0.6044 \\ 0.9844 \end{array}$	$\begin{array}{c} 0.6532 \\ 1.0000 \end{array}$	$0.5285 \\ 0.5105$
	0.5038	0.4562	0.0040	0.0008	0.4928	0.4249	0.5162	0.3887	0.5277	0.4078

Table 13: Performance comparison on the C2ST metric. Numbers represent  $100 \times (1 - C2ST)$  (i.e. in base of  $10^{-2}$ ). The lower the better.

Method	Continuou	is only	Discr	ete only			Het	erogeous		
Wiethou	California	Letter	Car	Nursery	Adult	Beijing	Default	Magic	News	Shoppers
interpolation SMOTE	0.61	0.00	0.00	0.00	3.05	0.44	7.69	1.93	6.49	9.80
VAE-based TVAE	12.48	22.27	70.30	52.73	72.39	45.53	41.65	12.07	60.27	70.04
<i>GAN-based</i> CTGAN	50.11	82.40	59.59	48.63	36.79	56.82	64.60	14.15	27.64	48.86
<i>LLM-based</i> GReaT	28.38	16.14	6.05	18.41	46.24	31.07	52.90	56.74	_	57.15
Diffusion-based STaSy CoDi TabDDPM TabSyn	$54.61 \\ 47.48 \\ 88.01 \\ 0.71$	$47.75 \\ 42.85 \\ 96.86 \\ 3.18$	$78.52 \\ 0.00 \\ 0.00 \\ 2.90$	$\begin{array}{c} 40.43 \\ 0.22 \\ 0.22 \\ 2.88 \end{array}$	$54.02 \\ 80.02 \\ 3.95 \\ 8.05$	$23.48 \\ 15.70 \\ 3.29 \\ 3.60$	$\begin{array}{c} 49.29 \\ 52.37 \\ 11.75 \\ 1.33 \end{array}$	$53.97 \\ 27.70 \\ 0.95 \\ 0.08$	$50.21 \\ 91.62 \\ - \\ 1.77$	$62.20 \\ 81.84 \\ 16.37 \\ 3.05$
Autoregressive DP-TBART Tab-MT	$3.89 \\ 8.71$	$\begin{array}{c} 11.07\\ 9.34 \end{array}$	$\begin{array}{c} 0.07\\ 0.37\end{array}$	$\begin{array}{c} 0.00 \\ 0.00 \end{array}$	$0.81 \\ 99.86$	$3.63 \\ 99.97$	$7.41 \\ 91.62$	$5.01 \\ 74.47$	$12.96 \\ 100.00$	$8.73 \\ 1.47$
TABDAR	1.27	0.55	0.00	0.74	0.47	1.55	3.43	0.1100	3.12	3.74

Table 14: Performance comparison on the Jensen-Shannon Divergence (**JSD**) metric. The lower the better. Note that the numbers in Table 1 are in % while numbers in this table are in raw scale.

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Method	Continuo	us only	Discre	te only	Heterogeous					
	California	Letter	Car	Nursery	Adult	Beijing	Default	Magic	News	Shoppers
interpolation SMOTE	0.0006	0.0006	0.0013	0.0008	0.0008	0.0003	0.0006	0.0008	0.0040	0.0015
VAE-based TVAE	0.0041	0.0072	0.0323	0.0132	0.0078	0.0077	0.0052	0.0036	0.0109	0.0107
<i>GAN-based</i> CTGAN	0.0182	0.0135	0.0220	0.0165	0.0038	0.0033	0.0114	0.0056	0.0078	0.0066
<i>LLM-based</i> GReaT	0.0111	0.0022	0.0030	0.0068	0.0182	0.0023	0.0076	0.0107	_	0.0056
Diffusion-based STaSy CoDi TabDDPM TabSyn	$\begin{array}{c} 0.0380 \\ 0.0152 \\ 0.0380 \\ 0.0006 \end{array}$	$\begin{array}{c} 0.0057 \\ 0.0085 \\ 0.0382 \\ 0.0017 \end{array}$	$\begin{array}{c} 0.0326 \\ 0.0020 \\ 0.0020 \\ 0.0033 \end{array}$	$\begin{array}{c} 0.0146 \\ 0.0009 \\ 0.0009 \\ 0.0014 \end{array}$	$\begin{array}{c} 0.0041 \\ 0.0073 \\ 0.0004 \\ 0.0004 \end{array}$	$\begin{array}{c} 0.0030 \\ 0.0017 \\ 0.0092 \\ 0.0012 \end{array}$	$\begin{array}{c} 0.0055 \\ 0.0067 \\ 0.0008 \\ 0.0003 \end{array}$	$\begin{array}{c} 0.0107 \\ 0.0142 \\ 0.0013 \\ 0.0007 \end{array}$	$0.0070 \\ 0.0092 \\ - 0.0016$	$\begin{array}{c} 0.0086 \\ 0.0103 \\ 0.0019 \\ 0.0007 \end{array}$
Autoregressive DP-TBART Tab-MT	$\begin{array}{c} 0.0023 \\ 0.0038 \end{array}$	$\begin{array}{c} 0.0010 \\ 0.0019 \end{array}$	$\begin{array}{c} 0.0023 \\ 0.0013 \end{array}$	$\begin{array}{c} 0.0008 \\ 0.0009 \end{array}$	$0.0004 \\ 0.0026$	$\begin{array}{c} 0.0006 \\ 0.0024 \end{array}$	$\begin{array}{c} 0.0025 \\ 0.0034 \end{array}$	$\begin{array}{c} 0.0018 \\ 0.0211 \end{array}$	$\begin{array}{c} 0.0036 \\ 0.0221 \end{array}$	$\begin{array}{c} 0.0008 \\ 0.0007 \end{array}$
TABDAR	0.0004	0.0010	0.0018	0.0010	0.0003	0.0004	0.0007	0.0011	0.0015	0.0008

Table 15: Comparison of training and sampling time of different methods, on Adult dataset.

Method	Training	Sampling
CTGAN	1029.8s	0.8621s
TVAE	352.6s	0.5118s
GReaT	2h 27min	2min 19s
STaSy	2283s	8.941s
CoDi	2h 56min	4.616s
TabDDPM	1031s	28.92s
TabSyn	2422s	11.84s
DP-TBART	2355.8s	2.11s
Tab-MT	2352.23s	2.18s
TABDAR	2701.5s	21.66s



Figure 10: Kernel density estimation (KDE) plot of the 2D joint density of 'education.num' and 'age' features in the Adult dataset. The results from GOGGLE and Tab-MT are not plotted since they either fail to generate or generate singleton synthetic data on one feature (e.g. always generate 'education.num' equals one).



Figure 11: Scatter plots of the 2D joint density of the Longitude and Latitude features in the CaliforniaHousing dataset. Blue lines represent the geographical border of California.



Figure 12: Heat map of synthetic data of Letter dataset.



Figure 13: Heat map of synthetic data of Adult dataset.



Figure 14: Heat map of synthetic data of Default dataset.

