ON LEARNING REPRESENTATIONS FOR TABULAR DATA DISTILLATION

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ABSTRACT

Dataset distillation generates a small set of information-rich instances from a large dataset, resulting in reduced storage requirements, privacy or copyright risks, and computational costs for downstream modeling, though much of the research has focused on the image data modality. We study tabular data distillation, which brings in novel challenges such as the inherent feature heterogeneity and the common use of non-differentiable learning models (such as decision tree ensembles and nearest-neighbor predictors). To mitigate these challenges, we present **TDColER**, a tabular data distillation framework via column embeddings-based representation learning. To evaluate this framework, we also present a tabular data distillation benchmark, **TDBench**. Based on an elaborate evaluation on TDBench, resulting in 226,200 distilled datasets and 541,980 models trained on them, we demonstrate that **TDColER** is able to boost the distilled data quality of off-the-shelf distillation schemes by 0.5-143% across 7 different tabular learning models.

1 INTRODUCTION

Dataset distillation or dataset condensation is the process of creating a small set of extremely infor-027 mative samples (usually synthetic) from a large dataset such that a model trained on this set will have predictive performance comparable to that of a model trained on the original large dataset (Wang et al., 029 2020; Yu et al., 2023). First, data distillation reduces data storage costs and can mitigate the privacy and copyright concerns involved in keeping around (and continuously utilizing) large amounts of raw 031 data. Furthermore, the reduction in the data size implies a lower computational cost of model training, especially when multiple models need to be trained on any given dataset. The above advantages of 033 dataset distillation also facilitate various applications. Continual learning, where we need to learn 034 new tasks while avoiding forgetting older tasks sequentially, often makes use of a "replay buffer" of old task data to be used while learning new tasks to mitigate forgetting of the older tasks (Rolnick et al., 2019). Dataset distillation reduces the memory overhead of this replay buffer, allowing learning of a larger number of tasks without forgetting (Tiwari et al., 2022; Rosasco et al., 2022). 037

In federated learning, we need to train a model using data spread across multiple clients without ever moving the data 040 between clients and reducing the com-041 munication overhead. Dataset distilla-042 tion generates compact yet private syn-043 thetic data from the client data that can 044 be safely exchanged for communicationefficient model training (Song et al., 2023; Goetz & Tewari, 2020; Zhou et al., 2020). 046





Figure 1: **Overview of** TDBench. The benchmarking suite allows for flexible choice of datasets, distillation schemes, and downstream models that enables for modular evaluation of any new distillation method.

plication to other data modalities is limited. The problem of tabular data distillation has received very
little attention, though many real-world learning problems and applications involve tabular data (Guo
et al., 2017; Clements et al.; Borisov et al., 2024). Various image data distillation schemes have been
proposed in the literature, but their application to tabular data is not straightforward. First, all image
data distillation schemes rely on the choice of a *differentiable* "backbone model." While differentiable



(a) **Overview of TDColER.** The top describes a *vanilla* distil- (b) Snapshot of downstream classifiers' lation scheme that only uses standard preprocessing techniques before distillation. The highlighted box describes the proposed **TDColER**, which uses column embeddings after such preprocessing and encoder-decoder architectures to generate rich compact we observe a performance increase from representations.

performance increase when trained on data distilled k-means with and without TDColER. Throughout our experiments, 0.5% to as large as 143%.

Figure 2: Proposed approach – TDColER: Tabular Distillation Via Column Embeddings based 071 **R**epresentation Learning 072

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neural network-based schemes are standard for images, a wide variety of non-differentiable models 074 are used with tabular data, such as decision tree ensembles, nearest-neighbor models, and kernel 075 machines. Second, almost all data distillation methods for images generate distilled data in the 076 original pixel space. While pixels are homogeneous raw features of an image, the features in tabular 077 data can be extremely heterogeneous, creating a mismatch between what the image data distillation methods are designed for and what we have as an inherent property of tabular data. Finally, it is 079 standard to use vision-specific data augmentation schemes (such as rotation, reflection, cropping, and translation) to train the model on the distilled image data. Such standard augmentations are 081 not available for tabular data, thus creating another discrepancy in the expected conditions for the 082 problem.

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084 **Our contribution.** In this paper, we study tabular dataset distillation and present a novel scheme to enhance the distilled data quality of multiple off-the-shelf data distillation schemes across various 085 datasets, models, and distillation sizes. Specifically, we make the following contributions:

- We propose Tabular Distillation via Column Embeddings based Representation Learning or **TDColER** that can utilize modern neural-network architectures such as Transformers and graph neural networks to generate rich compact representations. **TDColER** improves the quality of 090 distilled data compared to existing distillation schemes. Figure 2a provides an overview of our proposed TDColER. 091
- We present TDBench, a Tabular Distillation Benchmark with 23 tabular datasets, 7 model classes, 092 and 4 distillation schemes. We present an overview of TDBench, an extensible and modular framework for measuring various aspects of data distillation on tabular data, in fig. 1. 094
- With the elaborate evaluation of our proposed TDColER on TDBench, resulting in over 226,200 095 distilled datasets and 541,980 model trainings, we show that, on aggregate across all datasets, 096 **TDColER** improves upon direct application of off-the-shelf distillation method on tabular data by 0.5-143% in terms of the distilled data quality across all models at the smallest distillation of 10 098 instances-per-class. Figure 2b presents a snapshot of our results.
- 099 Based on our thorough evaluation, we present various insights regarding tabular dataset distillation, 100 such as (i) k-means clustering in the learned representations make for an extremely favorable 101 distillation scheme, (ii) transformer-based tabular data representations obtain the highest distilled data quality on aggregate, while (iii) graph neural network based tabular data representations 102 perform slightly worse than transformers but are significantly more parameter efficient. 103
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- 105 1.1 RELATED WORK
- Dataset distillation was introduced by Wang et al. (2020) as a bilevel optimization problem (Feng 107 et al., 2024) and has been widely studied in the context of image data distillation. Most methods can

108 be categorized into approaches that match the original data by (i) backbone model performance, (ii) 109 backbone model parameters, or (iii) backbone representation distributions (Yu et al., 2023). Wang 110 et al. (2020) minimized performance differences between the original and distilled data, while Nguyen 111 et al. (2021) introduced kernel-induced points (KIP) using kernel ridge regression with a neural tangent kernel (Jacot et al., 2018). Alternatively, methods have focused on parameter or gradient 112 matching (Zhao et al., 2021; Lee et al., 2022; Jiang et al., 2023; Cazenavette et al., 2022). Gradient 113 matching (Zhao et al., 2021) aligns model gradients between original and synthetic data, while trajec-114 tory matching (Cazenavette et al., 2022) minimizes discrepancies between entire training trajectories. 115 Other approaches include distribution matching (Zhao & Bilen, 2023), which aligns per-class means, 116 and cross-layer feature embedding matching (Wang et al., 2022). However, the abovementioned 117 methods rely on differentiable backbones, limiting cross-architecture generalization (Cui et al., 2022; 118 Nguyen et al., 2021). As a result, research has focused primarily on images, leaving tabular data 119 distillation largely unexplored (Medvedev & Dyakonov, 2021). We address this gap by proposing a 120 more general distillation framework. 121

Dataset distillation aligns with coreset selection (Feldman, 2020), which aims to reduce data size, 122 typically selecting real data instances (potentially risking privacy). In contrast, distillation generates 123 synthetic data beyond the real data manifold. Notably, coreset selection is a subset of dataset 124 distillation, where the synthetic data lies on the real data manifold. Generative modeling (Goodfellow 125 et al., 2020; Kingma & Welling, 2013) is another related area, usually focused on generating realistic 126 data. In dataset distillation, the goal is to generate informative rather than realistic samples. Recently, 127 Cazenavette et al. (2023) demonstrated how generative modeling can be used to seed the dataset 128 distillation process, arguing that distillation methods should be applied to a latent representation 129 instead of the pixel space. This is aligned with our proposal, in which we demonstrate that distillation in the latent space is critical to obtaining meaningful distilled data quality with tabular datasets. 130 However, the proposed Generative Latent Distillation(GLaD) scheme is very focused on generative 131 vision models, requiring a careful choice of the latent representation from within the model for 132 trade-off in *realistic* distilled data or *expressivity*, thus limiting cross-architecture generalization. 133

Cui et al. (2022) benchmarked several distillation methods and found trajectory matching (Cazenavette et al., 2022) to be most effective, followed by KIP (Nguyen et al., 2021). Coreset methods, like *k*-means clustering, also outperformed many model-based distillation techniques, which we corroborate.
We focus on GM and KIP due to the high computational overhead of trajectory matching and omit data augmentation due to its limited applicability to tabular data. As noted before, data augmentation is not standard with tabular data, and we do not consider it in our evaluation with TDBench.

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2 TABLE DISTILLATION

143 Data distillation has been primarily studied in the context of images where each data point is 144 composed of a homogeneous set of features - pixels - and the downstream models are neu-145 ral networks. The two main distinctions with tabular data distillation are: (i) Feature Het-146 erogeneity: Features in tabular data are usually heterogeneous and can have vastly different 147 meanings, making it challenging to generate appropriate feature aggregations as usually done with neural networks. This is further exacerbated by the common presence of missing val-148 ues. (ii) Model Agnosticity: For tabular data, the downstream model that will use the distilled 149 data can be quite varied, with decision-tree-based models often being quite successful (Grin-150 sztajn et al., 2022), while linear and nearest-neighbor models are used for interpretability.

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Algorithm 1: Distill original data S with N sam-
ples given a preprocessor $P : \mathbb{R}^r \times \mathbb{C}^c \to \mathbb{R}^D$ and
a distiller $F : \mathbb{R}^{N \times D} \times Y^N \to \mathbb{R}^{n \times D} \times Y^n$.
1 $\overline{\tilde{S}} \leftarrow \{(P(x), y) \forall (x, y) \in S\}$ // Preprocess
2 $R \leftarrow F(\tilde{S})$ // Distill
3 return R

Various increasing competitive neuralnetwork-based models have also been developed for tabular data (Borisov et al., 2024; Gorishniy et al., 2021; McElfresh et al., 2023; Grinsztajn et al., 2022). However, in the most common cases, we cannot assume that the downstream model is differentiable and thus will be unable to perform a downstream model-specific dis-



162 We will consider a classification dataset $S = \{(x_1, y_1), \dots, (x_N, y_N)\}$ with N samples, r numerical 163 features and c categorical features, and L labels, where each $x_i \in \mathbb{R}^r \times \mathbb{C}^c$ and $y_i \in Y = \{1, \dots, L\}$. 164 Following Cui et al. (2022), we only consider classification tasks in this work, but it should be noted 165 that regression can be easily added into our framework. Note that features may contain missing 166 values. After appropriate preprocessing steps to convert the categorical variables to numerical ones and imputing the missing values, ¹ we can directly apply some existing distillation schemes such as 167 KIP (Nguyen et al., 2021) or GM (Zhao et al., 2021). This procedure is sketched in Algorithm 1. 168

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2.1 REPRESENTATION LEARNING VIA COLUMN EMBEDDING

171 A key ingredient in the development of neural networks for tabular data is the use of column 172 embeddings. First developed for categorical features, the idea is to learn an embedding for each 173 of the categories in a categorical feature (Guo & Berkhahn, 2016). This embedding would replace 174 the one-hot encoded numerical representation of the categories and be used in conjunction with the 175 (appropriately scaled and imputed) numerical features in standard and custom feed-forward networks 176 (FFNs) (Borisov et al., 2024). Column embeddings for numerical data were developed to use more 177 standard modern architectures such as graph neural networks (GNNs) and Transformers. As with 178 categorical data, each numerical value in a numerical feature of the table would be converted into a 179 learnable embedding. Thus, more precisely, a sample (row) in a table with r numerical features and ccategorical features is now represented as a set of (r+c) embeddings in \mathbb{R}^m each of size m (where 180 m is a user-specified hyperparameter), thus effectively as the $(m \times (r+c))$ matrix.² 181

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Encoder Architectures. Given the $\mathbb{R}^{m \times (r+c)}$ representation of a row (sample) using column 183 embeddings, our goal is to learn a more compact yet faithful representation of a row. One simple 184 strategy is to concatenate all the (r + c) column embeddings into a single vector in $\mathbb{R}^{m(r+c)}$ of 185 size m(r+c) and input it into an FFN which projects it down to a lower dimensionality (fig. 8). However, one of our main motivations for using column embeddings is to leverage the capabilities 187 of more modern architectures. For a given row, the (r + c) column embeddings can be treated as 188 initial token embeddings that are progressively updated through multiple Transformer blocks as 189 described by Gorishniy et al. (2021). Using a dummy [CLS] token, the above process can create a 190 m-dimensional representation of the row (fig. 11). An alternate procedure is to represent a table as 191 a bipartite graph between columns and rows (with column values and rows as vertices) and utilize 192 the column embeddings as representations for the column vertices (Wu et al., 2021). Then, the row 193 embeddings are obtained by filling in representations for the row vertices via multiple rounds of message passing in a multi-layered GNN (fig. 9). For our purposes, we consider all three architectures 194 – FFN, Transformer and GNN – as encoders that project the $\mathbb{R}^{m \times (r+c)}$ representation of row into an 195 196 embedding in \mathbb{R}^m . While categorical column embeddings are standard, there are multiple techniques for numerical column embeddings (Gorishniy et al., 2021; 2022). We discuss and ablate the effect 197 these different schemes have in appendix B.2. 198

Learning Objective. Our goal is to retain as much information regarding the original data in the 200 learned representation as possible. The need for high-fidelity learned representations is critical because we do not assume anything regarding the downstream model, which will be trained with 202 the distilled data. Thus, we try to reconstruct the original data from the learned representation as 203 well as possible. Formally, given column embeddings $C : \mathbb{R}^r \times \mathbb{C}^c \to \mathbb{R}^{m \times (r+c)}$, and an encoder 204 $\phi: \mathbb{R}^{m \times (r+c)} \to \mathbb{R}^m$, we utilize a decoder $\psi: \mathbb{R}^m \to \mathbb{R}^r \times \mathbb{C}^c$ to reconstruct the original data, and 205 solve the following optimization problem: 206

$$\min_{C,\phi,\psi} \sum_{(x,y)\in S} \ell\left(x,\psi(\phi(C(x)))\right),\tag{1}$$

where $\ell(\cdot, \cdot)$ is a reconstruction error (RE). Note that the above representation learning does not 210 use the label information in the data S. This representation learning framework allows us to infuse 211 class information in the representations while ensuring no loss of original information. Thus, after 212

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²¹³ ¹For example, using data science tools such as preprocessing.OneHotEncoder and 214 impute.SimpleImputer from the scikit-learn machine learning toolkit.

²While each feature can have column embeddings of different sizes, many neural network architectures require the column embedding size to match across all features.

obtaining the column embeddings C, encoder ϕ and decoder ψ by solving eq. (1), we fine-tune the encoder by learning a classifier $f : \mathbb{R}^m \to Y$ on top of the learned representations while keeping the reconstruction loss low:

$$\min_{C,\phi,\psi,f} \sum_{(x,y)\in S} \ell(x,\psi(\phi(C(x))) + \alpha \mathcal{L}(y,f(\phi(C(x))))),$$
(2)

where $\mathcal{L}(\cdot, \cdot)$ is the downstream learning loss function, and $\alpha > 0$ is a hyperparameter balancing the classification and reconstruction quality. Appendix A.4.2 discusses this procedure in more detail.

Algorithm 2: TDColER: Distill dataset S with N
samples given distiller $F : \mathbb{R}^{N \times m} \times Y^N \to \mathbb{R}^{n \times m} \times Y^N$, and learnable column embeddings $C : \mathbb{R}^r \times \mathbb{C}^c \to \mathbb{R}^{m \times (r+c)}$, encoder $\phi : \mathbb{R}^{m(r+c)} \to \mathbb{R}^m$,
decoder $\psi : \mathbb{R}^m \to \mathbb{R}^r \times \mathbb{C}^c$, classifier $f : \mathbb{R}^m \to Y$.1 $C, \phi, \psi \leftarrow$ solve eq. (1) // minimize RE
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 $C, \phi, \psi, f \leftarrow$ solve eq. (2) // fine-tune
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 $\tilde{S} \leftarrow \{(\phi(C(x)), y), (x, y) \in S\}$ // Encode
4
 $\tilde{R} \leftarrow F(\tilde{S})$ // Distill in latent space
5
 $R \leftarrow \{(\psi(x), y), (x, y) \in \tilde{R}\}$ // Decode
6
return $R, \tilde{R}, C, \phi, \psi$

Complete Distillation Pipeline. After the column embeddings C, encoder ϕ and decoder ψ are learned (with eq. (1)) and fine-tuned (with eq. (2)), we convert the input features of the whole original dataset (with N samples) into the learned representations in \mathbb{R}^m using C and ϕ and apply the aforementioned distillation schemes to this dataset (N samples in \mathbb{R}^m) to get n distilled samples in \mathbb{R}^m . At this point, we decode the distilled samples into the original representation using ψ . This whole pipeline is summarized in

Algorithm 2. Note that the distillation with the learned representation in \mathbb{R}^m , and the availability of 237 the decoder ψ , allows us to have two versions of the distilled data – one in the learned representation 238 $(\tilde{R} \text{ in Algorithm 2, Line 4})$, and one in the original representation (R in Algorithm 2, Line 5). We can 239 choose the appropriate distilled set based on the downstream application: If we require the distilled 240 data to be obfuscated with no explicit correspondence to the original features, we can use R. In this 241 setting, we are required to have the column embeddings C and the encoder ϕ during inference with 242 the downstream trained model to map the test points into the appropriate representation. If we require 243 the distilled data and the model trained on it to be interpretable in terms of the original features, we 244 should use the distilled set R in the original representation. In this case, we do not need the column 245 embeddings or the encoder during inference. 246

 Remark 1. Our contribution is a novel representation learning and distillation pipeline for modelagnostic tabular data distillation utilizing existing distillation schemes, column embeddings, and network architectures such as transformers and GNNs. In our thorough empirical evaluations, we will demonstrate the distilled data quality boost from this pipeline across multiple datasets and downstream models.

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3 EVALUATION BENCHMARK

To thoroughly evaluate the various configurations of the proposed distillation pipeline, we establish a comprehensive benchmark suite with a varied set of datasets and downstream models, evaluating the pipeline at various levels of distillation sizes. With 3 encoder architectures, 6 distillation schemes (including variants), 20+ datasets, 7 downstream models, 10 distillation sizes, 5 repetitions per distillation pipeline, and model training, we have generated over 226,200 distilled datasets and trained over 541,980 individual downstream models³

261 Datasets. We consider 23 datasets from OpenML (Vanschoren et al., 2013) with the number of 262 samples varying from 10,000 to over 110,000, and number of features varying from 7 to 54. Instead 263 of investigating a few *large* datasets, we choose to incorporate more datasets to generalize the findings 264 across a wider range of datasets. The datasets are chosen to be diverse in terms of the number of 265 samples, features, and the type of features (numerical, categorical, or mixed). There are 14/23 datasets

 ³The TDBench benchmarking suite (code provided in the supplement) can be extended to evaluate any new distillation method, tabular representation, and downstream model and compared against our current database of results (also provided in the supplement). The API requirements for each of these components in the distillation pipeline are described in appendix C, and the procedure to execute the benchmark suite can be found in appendix C.2, and the comparison using the current database of results can be found in appendix C.1.

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with only numerical features, 2/23 with only categorical features, and 7/23 with both numerical and categorical features. All these datasets correspond to binary classification problems. Class imbalance is a common feature of tabular datasets (Johnson & Khoshgoftaar, 2019; Thabtah et al., 2020), and we focus on binary classification to carefully study the effect of class imbalance on the distilled data quality. There are 9/23 almost perfectly balanced datasets and 10/23 datasets with a ratio of close to 1:2 between the smaller and larger classes, with the worst imbalance ratio smaller than 1:15. Note that while we only consider binary classification datasets, the distillation pipelines are natively applicable to multi-class classification problems.

Distillation Methods. Given our aforementioned desiderata for model-agnosticity, we have the following existing distillation schemes available, which take as input the set S of N samples and output a set R of $n \ll N$ distilled samples (further details regarding implementation of each distillation method is provided in appendix A.5.2):

- *k*-means Clustering (KM) finds n/L clusters for each of the L classes to produce a total of n distilled samples using Lloyd's k-means algorithm (Lloyd, 1982). We consider two variations here by (i) using the Euclidean center of each cluster to generate a synthetic sample or (ii) choosing the closest *real* point to the Euclidean center of each cluster. That is, R comprises n/L cluster centers (or closest real points) for each of the L classes.
- Agglomerative Clustering (AG) (Müllner, 2011) again generates n/L clusters for each of the L classes is similar to k-means. We use the Ward linkage scheme with the Euclidean distance metric. Similar to k-means, we generate (i) synthetic samples by using the Euclidean center of a cluster or (ii) real samples that are closest to the cluster centers.
- Kernel Induced Points (KIP) (Nguyen et al., 2021) uses the neural tangent kernel (NTK) (Jacot et al., 2018) of a wide neural network and kernel ridge regression to produce a distilled set of samples. Given the feature matrix $X \in \mathbb{R}^{N \times D}$ and the label vector $\mathbf{y} \in Y^N$, KIP learns the distilled feature matrix $\bar{X} \in \mathbb{R}^{n \times D}$ and label vector $\bar{\mathbf{y}} \in Y^n$ by solving the following problem:

$$\min_{\bar{X},\bar{\mathbf{y}}} \mathcal{L}\left(\mathbf{y}, K_{X\bar{X}}(K_{\bar{X}\bar{X}} + \lambda I)^{-1}\bar{\mathbf{y}}\right),\tag{3}$$

where \mathcal{L} is the downstream learning loss function, $K_{X\bar{X}} \in \mathbb{R}^{N \times n}$ is the NTK matrix between X and \bar{X} , $K_{\bar{X}\bar{X}} \in \mathbb{R}^{n \times n}$ is the NTK matrix of \bar{X} with itself, and $\lambda > 0$ is a regularization hyperparameter for the kernel ridge regression. Essentially, we are learning a set of synthetic samples such that the predictions made on the original dataset features using the distilled dataset via kernel ridge regression match the original labels.

Gradient Matching (GM) (Zhao et al., 2021) produces the distilled set R for a given "backbone model" M_θ (parameterized by θ) by directly optimizing for R to induce model parameter gradients that are similar to the gradients obtained while training M_θ on the full dataset S. Given a distance metric D(·, ·), and a distribution P_{θ0} over the random model parameter initializations θ₀, the distillation problem tries to minimize the distance between the model gradients computed on the full and distilled datasets over the T steps of model learning as follows:

$$\min_{R} \mathbb{E}_{\theta_0 \sim P_{\theta_0}} \left[\sum_{t=0}^{T-1} D\left(\nabla_{\theta} \mathcal{L}(\theta_t; S), \nabla_{\theta} \mathcal{L}(\theta_t; R) \right) \right], \tag{4}$$

where $\mathcal{L}(\theta; S)$ is the loss of the model M_{θ} on the original full dataset S, $\mathcal{L}(\theta; R)$ is the loss of M_{θ} evaluated on R, and the model parameters θ_t are updated at $\theta_{t+1} \leftarrow \theta_t - \eta_{\theta} \nabla_{\theta} \mathcal{L}(\theta_t; S)$ via gradient descent with a learning rate η_{θ} using the full original dataset.

We consider KIP and GM as representatives from previous data distillation literature that are *model-agnostic* and *model-centric*, respectively. Appendix A.5.1 further discusses our choice of distillation methods considered in this work. All the above distillation schemes require the data to be preprocessed into a numerical form, and can be used in Algorithm 1 to distill tables. But, as we will see, this is not a very useful scheme. Our evaluation of **TDColER** on TDBench will demonstrate how the performance of these distillation schemes are boosted via representation learning.

To study the ability of the distillation pipeline to generate really small but useful distilled datasets, we consider extremely small distilled datasets with 10-100 instances per class (IPC), corresponding to a distillation fraction of the order of 0.1-1.0% on the smallest datasets, and 0.01-0.1% for the largest datasets. This is comparable to the compression ratio of 0.02-1% used in Cui et al. (2022) and Cazenavette et al. (2023).



Figure 3: Change in relative regret of downstream classifiers when trained on distilled data over IPC \in [10, 100], aggregated over datasets and encoder architectures. Lower is better. Each column corresponds to a downstream classifier, and each row represents a representation scheme – original, encoded (Enc.), and reconstructed (Rec.). Data distilled by clustering methods (AG, KM) in the encoded space show the best performance for all classifiers. In many cases, using the encoded representation as the final output yields a performance comparable to using the original representation. Figure 12 shows a more detailed version of this plot that includes FTTransformer and ResNet.

347 **Downstream models.** We consider 7 downstream models to evaluate the distilled data quality. We 348 consider the Nearest-Neighbor Classifier (KNeighbors), Logistic Regression (LR), Gaussian Naive 349 Bayes (GNB), and the Multi-Layered Perceptron (MLP) from the scikit-learn library (Pe-350 dregosa et al., 2011). We also consider the popular XGBoost ensemble of gradient-boosted decision 351 trees (XGB) (Chen & Guestrin, 2016). We include two recent neural network models for tabular 352 data, the ResNet and the FTTransformer models (Gorishniy et al., 2021). Since our distillation 353 pipeline is deliberately model-agnostic, we train these models on the distilled data using the default 354 hyperparameters of the corresponding libraries. We also consider a hyperparameter optimization 355 (HPO) use case using the distilled datasets in our evaluations, which can be found in section 4.

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357 **Evaluation metric.** To have a standardized way to quantify the quality of the distilled data across 358 different models and datasets, we use the notion of *relative regret* which compares the model's balanced accuracy score when trained on the full, distilled and randomly sampled data points. 359 Precisely, the *relative regret* is defined as $(A_F - A)/(A_F - A_{R_{10}})$, where A_F is the balanced accuracy of 360 the model trained on the full training set, $A_{R_{10}}$ is the balanced accuracy on the same test set when 361 trained on 10 random samples per class averaged over 5 random repetitions, and A is the balanced 362 accuracy of the model when trained on the distilled dataset over random 5 repetitions. A relative regret of 1 matches the performance of random sampling at IPC=10, and a relative regret of 0 matches 364 the performance of the model trained on the full dataset (which is usually the gold standard) - lower 365 relative regret implies higher distilled data quality ⁴.

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4 RESULTS ANALYSIS

In this section, we present the analysis of the results obtained from our benchmarking experiments. For the sake of brevity, we will use the following acronyms – Instances Per Class: IPC, *k*-means: KM, agglomerative: AG, gradient matching: GM, kernel inducing points: KIP, feed-forward neural network: FFN, graph neural network: GNN, transformer: TF. Additionally, the supervised-fine-tuned variant of the autoencoder will be marked with a *. For example, the results of Algorithm 2 with a

 ⁴For all the downstream models, the aggregate (median across all datasets) relative regret of random samples at IPC=10 (smallest distillation size) is 1.0 by definition, while the aggregate relative regret of random samples at IPC=100 (largest distillation size) is around 0.5, indicating that the benchmark is challenging enough with significant room for improvement.

transformer architecture for ϕ as TF^* , whereas TF denotes the version that skips line 2 of Algorithm 2 to highlight the importance of the supervised fine-tuning.

382 How beneficial are the learned representations for distillation? As the first step of our analysis, we examine 383 the performance difference between pipelines that use 384 encoder's latent space and those that do not. To fully un-385 derstand the effect of our latent space projection step, we 386 analyze our results from two angles: 1) Is it better to distill 387 in the latent or original space? 2) If latent space is better, 388 is it better to decode the data back to the original space or 389 stay in the latent space? 390

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Figure 3 shows the relative regret score of distillation methods under different data representation schemes. We start by examining the downstream performance difference between pipelines that use the latent space to dis-

Table 1: Average rank and median relative regret of distillation pipelines that use the latent space of different encoder architectures evaluated at IPC=10, grouped over all datasets and classifiers.

Encoder	Mean Rank	Median R.R.
TF	4.1176	0.9439
FFN	4.3407	0.9746
GNN	4.2243	0.9695
TF*	2.3591	0.6149
FFN*	3.3652	0.8082
GNN*	2.5931	0.7135

394 till in vs. ones that do not (Algorithm 2 vs. Algorithm 1). The results show that using the latent space is highly beneficial in most cases with lower IPC values. This trend is most 396 apparent in classifiers such as KNN (44.96-108.79% improvement at IPC=10), Logistic Re-397 gression (22.14-62.64% improvement) or MLP (32.73-68.72% improvement), while XGBoost 398 shows the least improvement from any of the distillation methods (15.82-36.00% improvement). 399 k-means and agglomerative clustering also show a more apparent decrease in regret, while KIP and GM show noticeable improvements only when both the distillation and the final dataset are in 400 the latent space. With this in mind, we examine the performance difference when training on the 401 distilled data in the latent space or decoding to the original space before training the downstream 402 classifier (using \hat{R} or R from Algorithm 2). Figure 3 shows that training on the dataset in the 403 latent space improves the downstream performance for all distillation pipelines – in fact, it is the 404 best performer for almost every instance over classifiers and distillation methods. The change in 405 performance is more apparent in KNN (40.92-65.40%), Logistic Regression (33.75-67.29%) and 406 MLP (33.93-96.38%), while XGBoost shows a more subtle change (7.28-19.20%). This leads us to 407 conclude that distillation methods benefit the most when both distilling and downstream training 408 in on the latent representations. It is also worth noting that decoding the distilled data from the 409 latent space (Rec.) is also beneficial compared to random sampling in many cases. 410



Figure 4: Scatterplot of encoder parame-421 ter size and downstream classifier regret at 422 IPC=10 aggregated over datasets and classi-423 fiers. The dots represent the median values, 424 and the error bars span the 25% and 75% per-425 centile, respectively. Note that the encoder 426 sizes for both SFT and base versions are the 427 same for each dataset. 428

How do different encoders compare? Having observed that using the latent space is beneficial, we now seek to identify which encoder architecture leads to the best performance. Table 1 shows the average rank of distillation pipelines that use the latent space of different encoder architectures. Among the tested architectures and training objectives, the transformer architecture with supervised fine-tuning leads to the best downstream performance. We find that adding supervised fine-tuning improves the downstream performance of all encoders in general.

Another important aspect of data distillation is to improve downstream classifier efficiency providing a lightweight proxy. Thus, it is important to examine the resources required in the distillation pipeline. Specifically, one aspect of our distillation pipelines that can add an additional cost is the encoder. In

settings that require the data to be projected into latent space at inference time, the encoder can
be considered part of the distilled data. Figure 4 shows the parameter size of the different encoder
architectures vs. the downstream classifier regret scores. As noted before, the transformer architecture
leads to the best downstream performance. However, it is worth noting that *GNN architecture has the*

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Figure 5: Critical difference plot comparing ranks of distillation methods across datasets, encoders, and classifiers per IPC value. The x-axis denotes the average rank, and a black horizontal line connects groups of methods that are *not significantly different* in the rank distribution. k-means and agglomerative are indistinguishable from each other in IPC $\in \{10, 50\}$, but k-means gains an edge in IPC=100.

Table 3: Relative regret of pipelines that use different combinations of distill methods and encoders at IPC=10, aggregated over classifiers. The best value for each column is marked with **bold**, and the second best is marked with <u>underline</u>. The best in each distillation method group is marked with *italics*. On average, *k*-means with SFT transformer shows the best performance, but agglomerative clustering also shows comparable performance.

Distill Method	Encoder	Regret					
		Min	Q1	Mean	Median	Q3	Max
KM	TF* FFN* GNN*	<u>-14.4491</u> -11.9912 -12.1045	0.0733 0.2039 0.0973	-0.0464 0.1382 0.1054	0.4056 0.6035 0.5047	$\frac{0.7379}{0.8389}\\0.7887$	<u>1.1773</u> 1.5368 1.0494
AG	TF*	-15.3965	<u>0.0810</u>	<u>0.0187</u>	<u>0.4135</u>	0.6507	<i>1.4982</i>
	FFN*	-10.1288	0.2483	0.3695	0.6230	0.8823	4.1191
	GNN*	-13.1881	0.1397	0.2245	0.4793	0.7595	4.4801
KIP	TF*	-4.1619	0.5226	<i>1.1124</i>	0.9415	1.2966	11.1034
	FFN*	<i>-5.3973</i>	0.8053	1.6363	1.2502	1.6434	16.4137
	GNN*	-1.4649	0.7403	1.1957	1.0136	1.3329	<i>10.5175</i>
GM	TF*	-3.8002	0.4105	0.7273	0.7952	1.0564	<i>4.9450</i>
	FFN*	<i>-4.3269</i>	0.5975	1.2660	0.9938	1.3827	16.5044
	GNN*	-1.4776	0.4626	0.8073	0.8457	<i>0.9779</i>	8.4566

smallest overall parameter size while providing the second-best performance. Further discussion on the parameter size analysis of each encoder architecture can be found in appendix A.3.

Which distillation method leads to the best downstream 467 **performance?** We now compare the most critical piece 468 of the distillation pipeline – the distillation method.We 469 wish to understand which method leads to the best down-470 stream performance across datasets, encoders, and classi-471 fier configurations. To evaluate, we perform a Wilcoxon 472 signed-rank test to identify groups that stand out from the 473 rest, as shown in fig. 5. The results show that clustering-474 based methods (k-means, agglomerative) show the 475 strongest performance across datasets and encoder 476 configurations, consistently placing in the top two ranks. 477 While both methods show similar performance, we find 478 that k-means starts to outperform agglomerative as the 479 IPC increases. 480

Table 2: The best performers of each dataset are classifiers ranked by their appearance count at the top 3 of each comparison at IPC=10. *k*-means stands out as the strongest performer in combination with a supervised-fine-tuned transformer encoder.

Count	Encoder	D.M.	Output
67	TF*	KM	Enc.
63	GNN*	KM	Enc.
61	GNN*	AG	Enc.
61	TF*	AG	Enc.
42	FFN*	KM	Enc.

Which combination leads to best performance? Our previous analysis has revealed that transformer encoders with SFT and clustering-based distillation methods perform best in their respective
comparisons. Now, we aim to identify which combination of encoder and distillation method leads to
the best downstream performance. We approach this question by examining the detailed statistics
behind the combinations' performance and the top performers of each dataset, classifier, and n combinations. Table 3 shows detailed statistics about each distill method and encoder combination, while



Figure 6: Comparison of HPO validation performance vs. runtime when using full and distilled data. To better visualize the performance difference, we truncate the plot for the full data run at twice the runtime of the entire distilled run.

table 2 shows the count of the top 5 distillation pipelines that placed in the top 10 by performance in each comparison group. In line with our previous findings, the results show that *k*-means clustering with supervised-fine-tuned transformer encoder leads to the best overall performance. All of the top performers are clustering-based methods, and all of them use the latent space, again confirming that using the latent representation from the encoder greatly benefits distillation methods. In addition, the GNN encoder shows a comparative performance to that of the transformer encoder. This is especially noteworthy, considering that GNN has the smallest parameter size among the encoder architectures.



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Figure 7: Average median relative re-517 gret of distillation methods aggregated 518 over downstream classifiers and en-519 coders at IPC=10 with a least-squares 520 linear regression. Compared to KIP and 521 GM, k-means and agglomerative show 522 much stronger performance in imbal-523 anced data. 524

As mentioned in section 3, we additionally run a smallerscale HPO experiment to consider a use case for distilled data, as seen in fig. 6. Specifically, we consider a case where the validation and testing data is sampled from the original data, and the classifier is trained on the full or distilled data. In general, we note that training on the distilled data gives comparable performance to training on the full data in a fraction of the time, consuming on average 21.84% of the runtime and reaching 98.37% of the performance.

How does class imbalance affect performance? Finally, we examine the downstream performance of classifiers with respect to the label balance, or the imbalance, of the original dataset, shown fig. 7. Compared to other methods, including random sampling, clustering-based methods show impressive strength when distilling datasets with high label imbalance, highlighting their robustness under challenging data distributions. One possible explanation behind this phenomenon is that while NN-based

distillation methods may prioritize the majority class due to the imbalance, the clustering methods are forced to place equal emphasis on all classes, preventing an overfitting on the majority class.

5 DISCUSSION

530 This work introduced a tabular data distillation pipeline and evaluated it extensively leveraging various 531 distillation methods, with a focus on supporting both non-NN and NN ML classifiers. We introduce 532 a novel framework, **TDColER**, that leverages latent representation of tabular data in distillation, 533 and evaluate it thoroughly in our benchmark, TDBench, which included 23 datasets, 4 distillation 534 algorithms, 3 autoencoder architectures, and 7 downstream classifiers, resulting in over 226,200 distilled datasets and 541,980 downstream classifier instances. Our results show that TDColER 536 can induce superior performance in distillation methods on tabular data, improving the quality by 537 0.5-143%. We also show that k-means clustering and transformer autoencoder are a particularly strong combination for tabular data distillation. We hope that this work will serve as a starting point 538 for future research in tabular data distillation and plan to extend this benchmark further to incorporate new distillation pipelines.

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758	Dataset Name	Dataset URL
759	adult	https://api_oponml_org/d/1590
760	Amazon employee access	https://api.openml.org/d/1135
761	Bank marketing data set UCI	https://api.openml.org/d/44234
762	credit	https://api.openml.org/d/45027
762	default-of-credit-card-clients	https://api.openml.org/d/45020
703	Diabetes130US	https://api.openml.org/d/45022
764	electrcity	https://api.openml.org/d/151
765	elevators	https://api.openml.org/d/846
766	higgs	https://api.openml.org/d/23512
767	hcdr	https://api.openml.org/d/45071
768	house_16H	https://api.openml.org/d/821
769	jannis	https://api.openml.org/d/45021
770	law-school-admission-bianry	https://api.openml.org/d/43890
770	MagicTelescope	https://api.openml.org/d/1120
771	Medical-Appointment-No-Shows	https://api.openml.org/d/43439
772	MiniBooNE	https://api.openml.org/d/44088
773	numerai28.6	https://api.openml.org/d/23517
774	nursery	https://api.openml.org/d/959
775	PhishingWebsites	https://api.openml.org/d/4534
776	pol	https://api.openml.org/d/722
011	road-safety	https://api.openml.org/d/44161
777	Click_prediction_small	https://api.openml.org/d/1220
778	2dplanes	https://api.openml.org/d/727

Table 4: Dataset name and OpenML Vanschoren et al. (2013) url

Table 5: Metadata of each dataset seen in table 4

781							
782	Dataset	# Instances	# Features	# Cont.	# Cat.	# Class 0	# Class 1
783	2dplanes	40,768	10	10	0	20,420	20,348
784	Amazon_employee_access	32,769	9	8	1	1,897	30,872
785	Bank_marketing_data_set_UCI	45,211	16	7	9	39,922	5,289
786	Click_prediction_small	39,948	11	11	0	33,220	6,728
787	Diabetes130US	71,090	7	7	0	35,545	35,545
700	MagicTelescope	19,020	11	11	0	12,332	6,688
788	Medical-Appointment-No-Shows	110,527	13	10	3	88,208	22,319
789	MiniBooNE	72,998	50	50	0	36,499	36,499
790	PhishingWebsites	11,055	30	0	30	4,898	6,157
791	adult	48,842	14	6	8	37,155	11,687
792	credit	16,714	10	10	0	8,357	8,357
702	default-of-credit-card-clients	13,272	20	20	0	6,636	6,636
793	electrcity	45,312	8	7	1	26,075	19,237
794	elevators	16,599	18	18	0	5,130	11,469
795	hcdr	10,000	22	22	0	5,000	5,000
796	higgs	98,050	28	28	0	46,223	51,827
797	house_16H	22,784	16	16	0	6,744	16,040
700	jannis	57,580	54	54	0	28,790	28,790
790	law-school-admission-bianry	20,800	11	6	5	6,694	14,106
799	numerai28.6	96,320	21	21	0	47,662	48,658
800	nursery	12,960	8	0	8	8,640	4,320
801	pol	15,000	48	48	0	5,041	9,959
802	road-safety	111,762	32	29	3	55,881	55,881

A.1 DATASETS

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APPENDIX

Tables 4 and 5 show the information about datasets used in our experiments along with their OpenML Vanschoren et al. (2013) URLs.

Hyperparameter	Values
d_hidden	(100, 200)
n_hidden	[1, 4]
dropout	(0, 0.2, 0.4)
d_embedding	(10, 20, 50, 100, 200)
use_embedding	(True,False)
learning_rate	$10^{[-3,-1]}$
weight decay	$10^{[-4,-1]}$
lr_scheduler	(None, Plateau, Cosine)

Table 6: Hyperparameters tested for FFN encoder.

Table 7: Hyperparameters tested for GNN encoder.

Hyperparameter	Values
<pre>graph_layer graph_aggr n_graph edge_direction edge_dropout learning_rate weight_decay lr_scheduler</pre>	(graphsage, gcn, gat) (mean, softmax) [1, 15] (bidirectional, multipass) (0, 0.2, 0.4) $10^{[-3, -1]}$ $10^{[-4, -1]}$ (None, Plateau, Cosine)

A.2 HYPERPARAMETER OPTIMIZATION FOR ENCODERS

Tables 6 to 10 show the hyperparameters considered for different modules of the autoencoders. We use $\{x, y, z\}$ to denote a set of variables and [a, b] to denote an inclusive range of values. We conduct HPO for each autoencoder + dataset pair using an implementation of hyperopt Bergstra et al. (2015) from Ray Tune Liaw et al. (2018) with a maximum of 500 samples for each HPO run. As noted in section 2.1, we first train the vanilla autoencoders for each dataset using the encoder hyperparameters seen in tables 6 to 8 and decoder parameters seen in table 9. Once the vanilla autoencoders are trained, we then conduct an additional fine-tuning with a classifier head with hyperparameters seen in table 10 where α is used to balance the objective functions of the decoder and classifier heads.

Table 8: Hyperparameters tested for TF autoencoder.

Hyperparameter	Values
n_blocks	[1, 10]
n_attention_heads	$2^{[1,4]}$
d_qkv	$2^{[0,7]}$
layer_norm_eps	$10^{[-5,-1]}$
d_mlp	$2^{[7,11]}$
d_mlp_hidden	(100, 200)
n_mlp_hidden	[1, 4]
dropout	[0, 0.4]
learning_rate	$10^{[-3,-1]}$
weight_decay	$10^{[-4,-1]}$
lr_scheduler	(None, Plateau, Cosine)

Table 9: Hyperparameters tested for decoders. The decoder architecture is kept the same for all encoders and optimized individually.

Hyperparameter	Values
d_hidden	(100, 200)
n_hidden	[1,4]
learning_rate	$10^{[-3,-1]}$
eight_decay	$10^{[-4,-1]}$
r_scheduler	(None, Plateau, Cosine)

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A.3 DISCUSSION ON PARAMETER SIZE OF AUTOENCODERS

Here we expand on our parameter size of the encoder architectures of the autoencoders. This is worth noting because if the distilled data is in the latent space, the encoder module is required to project any new data to the same space. Thus, the encoder is considered to be a part of the distilled output.

We can characterize the parameter size of each encoder architecture given a D-dimensional binarized dataset with c categorical features and r continuous features that is projected to a d-dimensional latent space.

FFN. We used an FFN architecture with an M-dimensional embedding layer followed by H hidden layers that receive and output W-dimensional vectors. The parameter size of such an FFN is as follows:

$$O(DM + (c+r)MW + HW^2 + Wd)$$
⁽⁵⁾

The column embeddings are of size O(DM), the input layer maps the concatenated (c + r)Mdimensional vector to hidden layer dimension W with (c + r)MW size. The hidden layers are of sizes $O(W^2)$ each for H hidden layers. The output layer maps the W-dimensional hidden layer output to the desired d-dimensions.

GNN. We use a GNN encoder with H consecutive layers. The dimension of the vectors passed between the graph layers are fixed to d, meaning that M = d. Thus, each graph layer maintains a dby d matrix to handle a d-dimensional input vector and output a d-dimensional vector.

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$$O(Dd + Hd^2) \tag{6}$$

The column embeddings are of size O(Dd) since M = d. Each of the H GNN layers is of size $O(d^2)$.

Transformer. We consider an implementation of a transformer autoencoder inspired by the architecture of FT-Transformer Gorishniy et al. (2021). The encoder has an *M*-dimensional embedding 899 layer followed H transformer blocks. Each transformer block takes in a sequence of M-dimensional 900 embeddings and oututs a single d-dimensional vector. The block is composed of a multihead-attention 901 module with m heads and a FFN module to project the attention scores back to the input space. We 902 modify the architecture seen in (Gorishniy et al., 2021) by allowing the dimension of the attention 903 head to be configurable – i.e. instead of using M/m as the dimension of a single attention head, 904 we allow the module to compute the attention in d_{akv} . This choice is motivated by the fact that our 905 encoders were trained with a latent size of 16, which may not be wide enough for the TF encoder. 906 We then project the resulting embedding in $d_{qkv}m$ -dimension back to M-dimensionals with W_o . 907

Table 10: Hyperparameters tested for classifier head in SFT.

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911	Hyperparameter	Values
912	d_hidden	$\{100, 200\}$
913	n_hidden	[1, 3]
914	dropout	$\{0, 0.2, 0.4\}$
915	alpha	$\{0.3, 0.5, 0.7\}$
010	learning_rate	$10^{[-3,-1]}$
916	weight decay	$10^{[-4,-1]}$
917	lr_scheduler	(None, Plateau, Cosine)



Thus, each of W_q , W_k , W_v and W_o has $d_{qkv}mM$ parameters. The MHA module is then followed by an FFN module which takes a M-dimensional vector and projects it back to M-dimensions with a W-dimensional hidden layer.

$$O(H(4d_{qkv}Mm + 2MW)) \tag{7}$$

A.4 AUTOENCODER IMPLEMENTATION DETAILS

OPTIMIZATION FUNCTION A.4.1

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956 For the decoder $\psi : \mathbb{R}^d \to \mathbb{R}^D$, we consider a multi-layered fully-connected feed-forward network. Given the encoder ϕ and the decoder ψ , we use a group-wise softmax operator σ to map the output 958 of the decoder to a per-input-feature probability simplex: given an initial binary vector $b \in \{0,1\}^D$ constituting per-input-feature one-hot encodings b^i (that is $b = [b^1 \oplus \ldots \oplus b^{c+r}]$), and a decoder output $B \in \mathbb{R}^D$ with per-input-feature constituents B^i (that is $B = [B^1 \oplus \ldots \oplus B^{c+r}]$, we apply the 960 softmax operation to each per-input-feature constituent to get $\hat{b} = [\hat{b}^1 \oplus \ldots \oplus \hat{b}^{c+r}] \in [0, 1]^D$, where 962 $\hat{b}^i = \text{softmax}(B^i)$. We utilize the following per-sample reconstruction loss: 963

$$\ell(b,\hat{b}) = \frac{1}{c+r} \sum_{i=1}^{c+r} \frac{1}{\log_2 |b^i|} \mathsf{CE}(b^i,\hat{b}^i),\tag{8}$$

965 where CE is the standard cross-entropy loss between a one-hot vector and a softmax output, and 966 $|b^i|$ is the length of the *i*-th constituent one-hot encoding in b, corresponding to the number of 967 categories (or bins) in the *i*-th categorical (or numerical) feature. This loss is a weighted average 968 of the per-input-feature cross-entropy loss, with weights $(1/\log_2 |b^i|)$ to normalize the loss across all 969 features with varying number of categories or bins.

970 The encoder and decoder are then learned by optimizing the following unsupervised loss: 971

$$\mathcal{L}_R(\phi,\psi) = \frac{1}{N} \sum_{(x,y)\in S} \ell\left(P(x), \sigma(\psi(\phi(P(x))))\right), \tag{9}$$

972 where *P* is the data homogenizer, and σ is the aforementioned group-wise softmax operator. Learning 973 the latent representation in such an unsupervised manner makes this distillation pipeline agnostic 974 to the choice of downstream model. Another advantage of this choice is that the decoder allows 975 us to map the distilled artificial samples in the latent space to the original features, which might be 976 necessary in some applications (for interpretability reasons).

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A.4.2 SUPERVISED LATENT SPACE FINE-TUNING

Given the already learned encoder and decoder, we consider a supervised fine-tuning (FT) step where we utilize a classifier $f : \mathbb{R}^d \to Y$ that utilizes the latent representation. The classifier is learned, and the encoder and decoder are fine-tuned by minimizing the following loss to ensure that the latent space is quite predictive while the reconstruction loss stays low:

$$\mathcal{L}_{R}(\phi,\psi) + \frac{\alpha}{N} \sum_{(x,y)\in S} \mathsf{CE}(y, f(\phi(P(x)))),$$
(10)

where $\alpha > 0$ is penalty parameter to balance the two losses, and CE is the cross-entropy loss. We consider multi-layer FFN architecture as the classifier f.

988 A.4.3 ENCODER ARCHITECTURES

Fully-connected feed-forward network (FFN). This encoder first selects the column embeddings corresponding to nonzero entries in the binary representation *b*, concatenates them to get a (c+r)Mdimensional dense vectors (recall that *b* will only have c + r nonzeros out of the *D* dimensions), and inputs them to a fully-connected feed-forward network $\mu : \mathbb{R}^{(c+r)M} \to \mathbb{R}^d$. The encoder $\phi : \{0,1\}^D \to \mathbb{R}^d$ can be written as:

$$z = \phi(b) = \mu(\oplus([w_i, i \in \{1, \dots, D\} : b[i] = 1])), \tag{11}$$

where b[i] is the *i*-th entry of the *D*-dimensional vector, and \oplus is the concatenation operator. The FFN μ and the column embeddings $\{w_i, i \in \{1, ..., D\}\}$ constitute the parameters of the encoder ϕ . For a FFN with *H* hidden layers, each of width *W*, the total number of parameters in this encoder is $O(DM + (c+r)MW + HW^2 + Wd)$. Figure 8 shows a simplified architecture of the FFN encoder.

Graph neural network (GNN) encoder. We also consider a more recent encoder for tabular data proposed in Wu et al. (2021). A bipartite graph is constructed between the column embeddings $\{w_i, i \in \{1, ..., D\}\}$ and the (zero-initialized) row (sample) embeddings $\{z_j \in \mathbb{R}^d, j \in \{1, ..., N\}\}$, with a bidirectional edge between w_i and z_j if the $b_j[i] = 1$, where $b_j \in \{0, 1\}^D$ is the binary representation of the *j*-th sample. Given the (learned) column embeddings, the row embeddings are obtained via multiple rounds of message passing through multiple GNN layers. This can be written as:

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$$z_j^h = \mu_h(z_j^{h-1}, \mathsf{Agg}(w_i^{h-1}, i \in \mathcal{N}_j)),$$

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 $w_i^h = \mu_h(w_i^{h-1}, \mathsf{Agg}(z_j^h, j \in \mathcal{N}_i)),$
(12)

where μ_h is the *h*-th GNN layer, Agg is an aggregation, \mathcal{N}_i (or \mathcal{N}_j) is the neighbor set of the *i*-th column embedding (or *j*-th row embedding). We set the initial $z_j^0 = 0$ (zero-initialized row 1010 embeddings), $w_i^0 = w_i$, and utilize z_i^H as the latent representation for distillation after H GNN 1011 layers. While Wu et al. (2021) only considered Graph Convolutional Networks Kipf & Welling 1012 (2016) as GNN modules, we extend it to GraphSage Hamilton et al. (2017) and Graph Attention 1013 Networks Veličković et al. (2018). An important aspect of the GNN encoder is that the desired row 1014 embedding size d must match the column embedding size M, thus d = M. With H GNN layers, 1015 the total number of parameters in this encoder is usually $O(Dd + Hd^2)$, which can be significantly 1016 smaller than the FFN encoder with moderately sized FFN (large enough M, W). Figure 9 shows the 1017 graph formulation (left) and the GNN encoder architeture (right). 1018

Transformer encoder. Finally, we consider a transformer-based autoencoder inspired by the architecture of FT-Transformer Gorishniy et al. (2021). This encoder uses the same embedding layer as the FFN encoder, which is then followed by transformer blocks. We learn an additional *cls* embedding, which is placed before all other tokens in every sequence. Each block takes in a sequence (one row) of *d* embeddings, and is composed of a multihead-attention (MHA) module and a feed-forward network (FFN) module.

For a MHA module with m attention heads, we modify the architecture seen in (Gorishniy et al., 2021) by allowing the dimension of the attention head to be separately configurable – i.e. instead of

Method	Hyperparameter	Value	Description
0	distill space	-	Whether to use the encoder latent space or the raw binary representation.
Common	use_closest*	-	Whether to use <i>median</i> points instead of the euclidean center. Only applicable to clustering methods.
	output_space [†]	-	Whether to keep the encoder latent/ decode or use the raw binary space. The binary space is only applicable to clustering methods when use closest is set to True.
	$random_seed^{\ddagger}$	-	Random seed for distillation algorithm. Not applicable to agglomerative.
KIP	n_epochs mlp_dim	$\begin{array}{c} 1000 \\ 1024 \end{array}$	Number of epochs to train the <i>distilled data</i> . Width of the neural network to compute the NTK of.
	n_epochs	500	Number of epochs to train the distilled data.
C 14	mlp_dim	1024	Size of the hidden layer of the target model.
GM	n_layers	2	Number of hidden layers in the target model.
	lr_mlp	0.01	Learning rate for the target model.
	ir_uala	0.1	Learning rate for the <i>distilled data</i> .

Table 11: Parameters of distillation methods.

using d/m as the dimension of a single attention head, we allow the module to compute the attention 1047 in d_{akv} . This choice is motivated by the fact that our encoders were trained with a latent size of 1048 16, which may not be wide enough for the TF encoder. We then project the resulting embedding in 1049 $d_{qkv}m$ -dimension back to d-dimension with W_o . For an input w_i at the *i*th transformer block, the 1050 computation for the MHA module is as follows: 1051

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$$a_i = W_o^i(\operatorname{softmax}(\frac{W_q^i(w_i)W_k^i(w_i)}{\sqrt{d_{qkv}}})W_v^i(w_i))$$
(13)

1055 The resulting attention score a_i is then added with the original embedding and passed through an 1056 FFN module. Similarly to Gorishniy et al. (2021), the [cls] embedding is used as the final output 1057 of the encoder. Figure 10 shows our modified MHA component, and fig. 11 shows the TF encoder block. 1058

A.5 DISTILL METHODS 1061

1062 A.5.1 CHOICE OF DISTILL METHODS (KIP, GM)

The clustering-based distillation schemes and KIP are not explicitly tied to a specific model and thus 1064 satisfy our desiderata of model-agnosticity. In contrast, the Gradient Matching or GM distillation scheme heavily relies on the choice of the backbone model M_{θ} (as well as the learning algorithm 1066 parameters such as the learning rate), and there is no guarantee that the distilled samples R would 1067 be useful for any other model. Thus, this scheme is not model-agnostic. However, we consider GM 1068 to be representative of the model-specific distillation schemes for the sake of completeness of our 1069 evaluations. For our table distillation, we choose M_{θ} to be a multi-layered perceptron with a single 1070 hidden layer. This will pose a mismatch when we evaluate the quality of the distilled data R on standard tabular models such as decision tree ensembles and nearest-neighbor models, highlighting 1071 the need for model-agnosticity in tabular data distillation. 1072

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A.5.2 DISTILL METHOD IMPLEMENTAION

k-means We use the sklearn.cluster.KMeans from Pedregosa et al. (2011) with the 1076

- n_init set to "auto". 1077
- 1078
- Agglomerative We use sklearn.cluster.AgglomerativeClustering from Pe-1079 dregosa et al. (2011) with the linkage set to "ward". Because agglomerative clustering

1081			1		
1082		Classifier	Hyperparameter	Value	
1083			d token	128	
1084			n_blocks	2	
1085			attention_n_heads	8	
1086			attention_dropout	0.15	
1087		FT-Transformer	fin_d_nidden_multipiler	1.20	
1088			residual_dropout	0.05	
1089			learning_rate	10^{-4}	
1090			weight_decay	10^{-5}	
1091			early_stopping	True	
1092		Naive Bayes	var_smoothing	10^{-9}	
1093			n_neighbors	5	
1094		K-Nearest-Neighbors	leaf_size	30	
1095			р	2	
1090			penalty	12	
1007		Logistic Regression	tol	10^{-4}	
1090		Logistic Regression	С	1	
1100			solver	lbigs	
1101			d_hidden	100	
1102		MLP	n_hidden	$\frac{1}{10^{-4}}$	
1103			early stopping	IU True	
1104					
1105			n_plocks d block	4 128	
1106			d_hidden_multiplier	1.25	
1107		ResNet	dropout	0.2	
1108			learning_rate	0.0001	
1109			weight_decay	0.00001	
1110			patience	16	
1111			<u>Fact and c</u>		
1112 1113		"· · · · · · · · · · · · · · · · · · ·			
1114	does not have	a "centroid", we man	ually calculate a euclidean centre	old for each clu	ster by us-
1115	noint	.nergibors.neare			iosest real
1116	point.				
1117					
1118	KIP We use t	he implementation prov	ided by Nguyen et al. (2021) availa	ble at https:/	/github.
1119	com/google	-research/google	e-research/tree/master/	kip.	
1120					
1121	CM W	4		L1	/ / /]]
1122	GM we use	Ine implementation prov	vided by Znao et al. (2021) availat	ble at https://	/github.
1123		OE/DataSetConder	ISacion.		
1124	Table 11 shows	the parameters availab	le for each distillation methods. T	'he common para	imeters are
1120	used for every a	algorithm, with the exce	ptions marked on the right-most co	olumn. The meth	od-specific
1120	parameters for	KIP and GM are for the	original algorithms as proposed in	Nguyen et al. (2)	021); Znao
1128	et al. (2021).				
1120					
1130	A.6 DOWNS	TREAM CLASSIFIER H	YPERPARAMETERS		
1131	2.12 2.0.110				
1.1.1.1	T 1 1 1 0 1				

Table 12: Hyperparameters of downstream classifiers.

Table 12 shows the hyperparameters used for each downstream classifier. We use scikit-learn Pedregosa et al. (2011)'s implementation of Naive Bayes, *K*-Nearest-Neighbors, Logistic Regression, and MLP, and Gorishniy et al. (2021)'s implementation of FT-Transformer and ResNet.

Classifier	Train Time	Test Time	Test Perf.
FTTransformer	281.3431	0.17934	0.7879
NB	0.0030	0.00232	0.6624
KNN	0.0007	0.54309	0.7474
LR	0.4901	0.00646	0.7709
MLP	2.4444	0.00554	0.7826
ResNet	154.9824	0.08508	0.7833
XGB	11.4055	0.01439	0.8180

1134 Table 13: Average train/test times and test performance comparison for all downstream classifiers.

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1145 A.7 RESNET AND FT-TRANSFORMER PERFORMANCE

We test ResNet and FT-Transformer for 5 datasets. We found that even with early stopping, the two classifiers take significantly longer to train given the same computing resources. On average, we find that ResNet takes around 10 times longer to finish training, while FT-Transformer takes around 28 times when compared to XGBoost. We also find that the performance of resnet and FT-Transformer does not stand out – in fact, the average test performance when trained on the full dataset shows that both ResNet and FTTransformer show a similar performance to MLP, and are outperformed by XGBoost.

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1155 A.8 DETERMINING THE BEST OVERALL PERFORMANCE

1156 We describe the best overall pipeline in section 4 and table 2. Here, we provide a more detailed 1157 explanation of how we determined the best overall pipeline. The runs are grouped by their classifier, 1158 dataset and distill size n. Similar to other parts of analysis, the grouping is done in order to ensure 1159 that the comparisons are *fair*. In this instance, we are interested in only the pipeline components that 1160 lead to the best classifier performance, regardless of the exact classifier kind. Thus, we group every 1161 run by their non-pipeline-specific parameters, which are the classifier, dataset and distill size n. In 1162 each group, we then count the instances the pipeline places on the top 3 in terms of the regret score 1163 and sum up the counts for each pipeline.

Following the previous findings, table 2 shows that *k*-means based methods have the best performance, placing in the top 3 with all SFT encoder variants. Surprisingly, we also find pipelines that use KIP and GM as the 4th and 5th best performers. While we were not able to determine any specific conditions that cause KIP and GM to place on top, this result shows that there are exist some conditions which leads the pipelines using gradient-based methods (KIP, GM) to be the top performer. On the other hand, the consistent rank placement of pipelines that use the autoencoder latent space shows that fine-tuned autoencoders can indeed boost the performance of distillation methods significantly.

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¹¹⁷² B ADDITIONAL ANALYSIS

1174 B.1 FULL RESULTS OF DISTILLATION METHODS BY DOWNSTREAM CLASSIFIERS

1176 B.2 EFFECT OF COLUMN EMBEDDING SCHEME ON DOWNSTREAM PERFORMANCE

1177 While column embeddings are standard for categorical columns – each category is represented with 1178 a vector, there are various ways of embedding numerical columns: (i) A numerical feature can be 1179 binned, and each bin treated as a category with an embedding $\mathbf{w} \in \mathbb{R}^m$ corresponding to each bin. 1180 (ii) With linearly scaled column embeddings, a single column embedding $\mathbf{w} \in \mathbb{R}^m$ is used for each 1181 numerical column, and the column embedding for a particular numerical value $v \in \mathbb{R}$ is obtained 1182 by scaling w to $v \cdot w$. (iii) Piecewise linear encoding or PLE (Gorishniy et al., 2022) also bin the 1183 numerical feature but use a more sophisticated way of generating the column embeddings for a given numerical value. We considered binned numerical features in the main paper for a couple of 1184 1185 reasons: (a) Binned numerical features naturally handle missing values (quite prevalent in tabular data) by maintaining a "missing" bin instead of relying on a heuristic intermediate imputation step; 1186 sometimes, the fact that a value is missing is in itself a signal, and heuristic imputation schemes often 1187 lose this information. (b) The binned features can be used for all architectures we consider here –



Figure 12: Full results of distillation methods by downstream classifiers.

1215 Table 14: A comparison of relative regret scores of distillation pipelines that use the encoded space 1216 of autoencoders trained with different column embeddings, tested on 5 datasets (Adult, Amazon 1217 Employee Access, Credit, House, Phishing Websites). The center value shows the median relative 1218 regret, and smaller values on each side refers to the first and third quantile, respectively. In general, 1219 PLE embeddings show the strongest performance. However, it is worth noting that PLE embeddings are not applicable to GNN encoders, and that binary embeddings also show superior performance to 1220 scaled embeddings. 1221

2 3	Col. Emb.	KM	AG	GM	KIP
	Binary	$_{0.1082} 0.5645 \ _{0.7886}$	$_{0.0976}$ 0.4633 $_{0.7181}$	$_{0.5504}$ 0.9038 $_{1.0063}$	$_{0.6551}$ 0.9254 $_{1.1918}$
	Scaled	$_{0.7214}\ 0.8613\ _{1.0671}$	$_{0.4908} 0.6939 \ _{1.0249}$	$_{1.0092} 1.4412 \ _{1.8658}$	$_{1.3304} 1.6137 \ _{2.2985}$
	PLE	$_{-0.2428} 0.1976 \ _{0.9305}$	$_{-0.2698}\ 0.2173\ _{0.6752}$	$_{-0.0865}\ 0.2747\ _{1.0524}$	$_{-0.0263}\ 0.7398\ _{1.3923}$

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FFN, Transformer, and GNN – and using a common embedding scheme allows us to ablate the effect 1232 of the different architectures. The other numerical embedding schemes do not apply to GNNs.

To understand the effect of different kinds of column embeddings schemes, we conduct a smaller 1234 scale experiment on 5 datasets. Specifically, we compare scaled embeddings as seen in Gorishniy 1235 et al. (2021), piecewise linear encoding (PLE) as seen in Gorishniy et al. (2022), against using binary 1236 column embeddings where continuous features are binarized by binning, and examine the downstream 1237 performance of distillation pipelines that use the latent space of the autoencoders trained with the corresponding column embedding scheme. Table 14 shows that using the **both binary column** embeddings and PLE consistently leads to lower regret scores compared to scaled column 1239 **embeddings**. While PLE embeddings show the strongest performance, they are not applicable to 1240 the GNN autoencoder architecture. Thus, we conduct most of our experiments using binary column 1241 embeddings for a fair comparison across different autoencoder architectures for a fair comparison.





1296 B.4 PAIRWISE COMPARISION OF DISTILLATION METHODS.

1298 In addition, we compare the downstream classifier performance with every pair of pipelines that use different distillation methods under otherwise equal settings. The left table of fig. 15 reveals that KIP 1299 had the highest tendency to underperform other distillation methods, while k-means had the highest 1300 tendency to outperform other distillation methods. This is consistent with our previous findings, 1301 where k-means outranked other distillation methods most frequently. In order to gain further insights 1302 behind the performance lag of graident-based distillation methods, we conduct a pairwise comparison 1303 of the distillation methods for different classifiers as well. The center and right tables of fig. 15 1304 shows the pairwise comparison of distillation methods for XGBoost and MLP as downstream models. 1305 This suggests that gradient-based methods' underperformance is not solely due to its kernel, but that 1306 tabular data itself may pose a unique challenge in distillation that is not seen in image data. It is also 1307 worth noting that while the clustering-based approaches had the best overall rank, random sampling 1308 proved to be a strong baseline with a near 50% win ratio against them.

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C DOCUMENTATION OF TDBENCH

The information in this section is also available in a markdown format in the README.md file of the supplementary material.

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1316 C.1 REPRODUCING RESULTS

Every plot and table in the main paper can be reconstructed using the following scripts:

- 1319 Q0_experiment_scale.py
- Q1_1_col_embeds.py
- Q1_encoding.py
- Q2_distill_methods.py
- Q3_autoencoders.py
- Q4_1_runtime.py
- Q4_2_get_hpo_dirs.py
 - Q4_2_hpo.py
- Q4_combinations.py
- 1327 Q5_class_imbal.py

The scripts are organized in order of the question addressed in section 4 and will be populated in iclr-figures directory. These can be simply ran by calling python SCRIPT_NAME.

The following files are included in the supplementary material and contain all the necessary information for the scripts:

- 1333 dataset_stats.csv
- 1334 enc_stats.csv
- 1335 *data_mode_switch_results.csv
- 1336 hpo-measure/
- 1337 *mixed_tf_results.csv
- 1338 *ple_tf_results.csv

The files marked with an asterisk (*) are not included in the repository, but can be downloaded from this url: https://drive.google.com/drive/folders/ 1tJ5eliCvaz-UbxEgpmuCPj-58crgYRJW?usp=share_link

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C.2 DESCRIPTION OF THE WORKFLOW

1345The ## Running the Code section of README.md file discusses the actual commands and1346available options for running each stage in detail.

- The procedure is as follows:
- Train the autoencoder with the desired configuration.
 - (Optional) Fine-tune the autoencoder with a classifier head.

Run distillation methods against specified downstream classifiers.

1352 C.3 CONSTRUCTING A NEW PIPELINE

1354 Changing default parameters The configurations for this project are managed by hydra and can
 1355 be modified by adding new files/directories under the 'config' directory.
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Adding new datasets Adding new datasets is as simple as adding a new config/data/datasets/DATASET_NAME.yaml file. Currently, only openml datasets are supported.

	Field	Туре	
	dataget name	string	
	download url	string	
	label	string	
	n_classes	int	
	source_type	string	
	Table 15: Configuration d	etails for da	atasets
FT1 0.11 1 0			
The following flags must	be specified for the dataset t	o be correct	tly loaded as seen in table 15
	Field	Type	
		<u></u>	
	parse_mode	string	
	bin strat	string	
	n_bins	int	
Ta	ble 16: Configuration details	for data pr	reprocessing
	-	_	
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to work correctly. One ca	an additionally define any ty	pe of scal	e_mode or bin_strat,
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• is_random: Whether there is randomness in the method. If true, the pipeline will be ran multiple times. • is_cluster: Whether the method is a clustering method. If true, an option that uses the nearest-to-center method will be included. • can_use_encoder: Whether the method can be applied in the latent space. • args: any additional arguments to the actual function. Once the configuration is created, it will be consumed by load_distilled_data method of tabdd/distill/load_distilled_data.py. This method can then be modified to include the new distillation method. Adding new encoders All encoders used in the benchmark are subclasses BaseEncoder from tabdd/models/encoder/base_encoder.py. A simple example of how to implement can be seen in tabdd/models/encoder/mlp_autoencoder.py. The module needs to encoder the following methods: __init__(), encode, decode and forward. The autoencoders are specified by the configuration files in config/encoder/models/. The class of the encoder is specified by cls, and the hyperparameters are specified by tune_params.



Figure 16: Critical difference plot comparing ranks of distillation methods across datasets per IPC value when applied with TF-SFT encoder for XGBoost classifier with additional baselines The x-axis denotes the average rank, and a black horizontal line connects groups of methods that are *not significantly different* in the rank distribution. *k*-means and agglomerative are indistinguishable from each other in IPC $\in \{10, 50\}$, but *k*-means gains an edge in IPC=100. (FG: Forgetting, GN: GraNd, GL: Glister, GC: Graph Cut)

Table 18: Relative regret of pipelines that use different combinations of distill methods and encoders at IPC=10, aggregated over classifiers. The best value for each column is marked with **bold**, and the second best is marked with <u>underline</u>. (FG: Forgetting, GN: GraNd, GL: Glister, GC: Graph Cut)

Distill Method			Re	egret		
	Min	Q1	Mean	Median	Q3	Max
Random Sample	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
KM	0.0597	0.5256	0.6682	0.6654	0.8186	1.1094
AG	0.0000	0.5177	0.6301	0.6036	0.8914	0.9965
KIP	0.6728	0.8483	1.1109	1.0544	1.2523	2.2713
GM	0.4175	0.7707	0.9858	0.9377	1.1461	1.7292
FG	0.8705	1.1400	2.3837	1.4465	1.8731	16.0146
GN	0.7748	1.1498	2.0530	1.3704	2.2624	10.6670
GL	0.8376	1.1000	2.0907	1.3146	1.6823	14.1625
GC	0.6361	0.9077	1.5084	1.1031	1.5998	6.8392
MTT	0.4175	0.7707	1.0340	0.9699	1.2176	2.3026
DATM	0.4175	0.7707	1.0340	0.9699	1.2176	2.3026

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D ADDITIONAL ANALYSIS

1491 D.1 ADDITIONAL DISTILLATION METHODS

1493 We conduct a further comparison of more recent distillation methods against the methods compared 1494 in section 4 to verify whether these methods will show superior performance. Specifically, we incorporate four representative NN-based coreset selection methods examined in Deepcore (Guo 1495 et al., 2022) - Forgetting (Toneva et al., 2018), GraNd (Paul et al., 2021), Glister (Killamsetty et al., 1496 2021), Graph Cut (Iyer & Bilmes, 2013)) and MTT (Cazenavette et al., 2022) and DATM (Guo et al., 1497 2023). The results are presented in Table 18 and Figure 16. Consistent to our findings in section 4, 1498 we find that more recent distillation methods that rely on NNs do not fair well on non-differentiable 1499 downstream classifier (XGBoost), and that clustering methods still show dominance. It is also 1500 interesting to note that GM shows superior performance to MTT and DATM, suggesting that the 1501 latter two methods may actually be overfitting to the teacher network's architecture.

D.2 DATASET FEATURE CORRELATION

We further investigate the presevation of feature correlation in the distilled data. Figure 17 shows the change in feature correlation in the original, randomly sampled and distilled with k-means in the latent space of TF-SFT in 3 datasets – Credit, Magic Telescope and Tencent CTR.

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1509 D.3 RELATION TO PREVIOUS WORK

1511 Kang et al. (2024) presented a preliminary abstract on work that explores data distillation for tabular data. The authors utilize an MLP and GNN based autoencoder networks to transform the data

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Figure 17: A side-by-side comparison of correlation of numerical features in the training data before distillation, after random sampling@IPC=100, and after distillation@ICP=100. While some weaker correlations are not entirely accurately portrayed, the distilled data preserves the stronger correlations remarkably well.

to before distilling and show that simple clusetering-based methods can outperform competetive distillation algorithms proposed in computer vision (KIP (Nguyen et al., 2021))

Building upon this work, our work provides a comprehensive analysis of distillation methods on tabular data, and provides a detailed comparison of distillation methods across a wide range of datasets and classifiers. We also provide a detailed analysis of the effect of IPC on the performance of distillation methods, and provide insights into the effect of distillation on the feature correlation of the data.

- Below, we provide a detailed comparison of our work with the preliminary abstract presented by Kang et al. (2024):
- We conduct a comprehensive comparison of different binning methods and their effect on down stream performance.
- We test with a transformer-based autoencoder, and show that it outperforms MLP and GNN based autoencoders.
- We additionally consider gradient matching Zhao et al. (2021) as an additional baseline to represent the gradient-based family of distillation methods Cazenavette et al. (2022); Zhao & Bilen (2023); Guo et al. (2023)
- We provide a complete python package, TDBench, that can be used and extended by anyone in the community.
 - We explore a realistic use case for data distillation in the context of HPO and show the trade-offs in utility and cost saving.
- We introduce a relative regret metric to compare the performance of different distillation methods across datasets and classifiers.
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D.4 RAW BALANCED ACCURACY SCORE

Below is a comparison of the raw balanced accuracy of each distillation pipelines averaged over
random iterations. Table 19 shows a comparison of all 10 distillation methods that were ran with
TF-SFT encoder and tested on XGB downstream classifier, and table 20 shows the performance of the
baseline methods when applied without the encoders. Tables 21 and 22 show the same comparison
that with and without TF-SFT encoder for the 4 baselines methods (*k*-means, aggloermative, KIP,
GM) on KNN classifier, and tables 23 and 24 show the same for MLP classifier.

The last two rows of the tables each denote the number of instances that the pipeline ranked at the top, and the number of times it outperformed random sampling. The results show that random sampling is not a trivial baseline for many methods, and that both clustering methods, AG and KM, show the strongest performance. We also see that adding the encoder to the pipeline significantly increases the downstream performer of all 3 representative models.

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Table 19: Comparison of raw balanced accuracy scores of distillation methods applied with TF-SFT on XGB classifier. Last two rows of the tables each denote the number of instances that the pipeline ranked at the top, and the number of times it outperformed random sampling. Best performance at for each dataset is marked in bold, and second-best performance is marked with underline.

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Dataset	AG	GM	KIP	KM
AD	$0.6078 {\pm} 0.0354$	$0.7175 {\pm} 0.0423$	$0.5353 {\pm} 0.0562$	0.5949 ± 0.0644
AE	0.5252 ± 0.0195	$0.5304{\pm}0.0167$	0.5060 ± 0.0066	0.5007 ± 0.0126
BM	0.5599 ± 0.0525	0.5816 ± 0.0448	0.5114 ± 0.0179	$0.5842 {\pm} 0.0914$
CR	$0.5667 {\pm} 0.0491$	$\overline{0.5394 \pm 0.0334}$	$0.5106 {\pm} 0.0383$	0.5612 ± 0.0578
CD	$0.5887 {\pm} 0.0310$	0.5607 ± 0.0448	0.5309 ± 0.0466	0.5526 ± 0.0382
DB	$0.5133 {\pm} 0.0157$	$\overline{0.5053 \pm 0.0265}$	$0.5008 {\pm} 0.0140$	0.5146±0.0137
EL	$\overline{0.5929 \pm 0.0782}$	0.5617 ± 0.0545	0.5093 ± 0.0290	0.5866 ± 0.0741
EV	$0.6120 {\pm} 0.0658$	$0.5968 {\pm} 0.0567$	$0.5730 {\pm} 0.0590$	0.6009 ± 0.0754
HG	$0.5159 {\pm} 0.0107$	0.5130 ± 0.0143	$0.5028 {\pm} 0.0094$	0.5141 ± 0.0196
HE	0.5909 ± 0.0372	$0.5918 {\pm} 0.0378$	$0.5112 {\pm} 0.0396$	0.5790 ± 0.0608
HS	0.6770 ± 0.0526	0.6257 ± 0.0567	$0.5288 {\pm} 0.0671$	0.6484 ± 0.0956
JN	0.6076 ± 0.0176	$0.6111 {\pm} 0.0262$	0.5759 ± 0.0654	0.5755 ± 0.0511
LA	0.8079 ± 0.1752	0.8006 ± 0.1236	$0.7352 {\pm} 0.1598$	0.8101±0.1533
MT	$\overline{0.8217 \pm 0.1813}$	$0.9581 {\pm} 0.0285$	0.8029 ± 0.1473	0.8082 ± 0.1785
MA	0.5146 ± 0.0185	$0.5585 {\pm} 0.0324$	0.4991 ± 0.0108	0.5112 ± 0.0222
MB	0.6715 ± 0.0942	$0.6480 {\pm} 0.0710$	$0.5559 {\pm} 0.0732$	0.6476 ± 0.1124
NU	0.5047±0.0079	$\overline{0.5005 \pm 0.0060}$	0.5004 ± 0.0041	0.5022 ± 0.0050
NS	$1.0000 {\pm} 0.0000$	1.0000 ± 0.0000	$1.0000 {\pm} 0.0000$	1.0000 ± 0.0000
PW	0.7665 ± 0.1429	0.8466±0.0613	0.6758 ± 0.1216	0.7918 ± 0.1242
PL	0.5966 ± 0.0441	0.6813 ± 0.0515	0.6045 ± 0.1043	0.6834±0.0898
RS	$0.6469 {\pm} 0.0546$	$\overline{0.5810 \pm 0.0373}$	0.5200 ± 0.0350	0.6469 ± 0.0541
TC	$0.5343 {\pm} 0.0295$	$0.5118 {\pm} 0.0357$	$0.5031 {\pm} 0.0228$	0.5301 ± 0.0245
TD	$0.8162 {\pm} 0.0100$	0.7790 ± 0.0270	$0.6355 {\pm} 0.0884$	0.7736 ± 0.0584
# Best	12/23	8/23	1/23	5/23
vs RND	15/23	16/23	3/23	15/23

Table 20: Comparison of raw balanced accuracy scores of distillation methods applied in the original space (no encoder) on XGB classifier. Last two rows of the tables each denote the number of instances that the pipeline ranked at the top, and the number of times it outperformed random sampling. Best performance at for each dataset is marked in bold, and second-best performance is marked with underline.

1730 Dataset AG GM KIP KM 1731 AD $0.7904 {\pm} 0.0171$ 0.7609 ± 0.0170 $0.6645 {\pm} 0.0662$ $0.7940 {\pm} 0.0078$ 1732 0.5371±0.0022 0.5246 ± 0.0244 0.5129 ± 0.0130 0.5365 ± 0.0192 AE 0.6997 ± 0.0556 BM 0.7898±0.0052 0.7546 ± 0.0317 0.7897 ± 0.0083 1733 $0.5437 {\pm} 0.0127$ 0.5500±0.0170 0.5219 ± 0.0199 CR 0.5337 ± 0.0260 1734 CD 0.6490 ± 0.0302 0.6449 ± 0.0471 0.5819 ± 0.0483 0.6674 ± 0.0112 DB 1735 0.5607 ± 0.0019 0.5054 ± 0.0474 0.5408 ± 0.0335 0.5565 ± 0.0064 EL 0.6163 ± 0.0173 $0.5758 {\pm} 0.0423$ 0.5655 ± 0.0241 0.6276±0.0126 1736 $\overline{0.7152 \pm 0.0017}$ EV 0.6621 ± 0.0319 $0.6205 {\pm} 0.0448$ 0.7130 ± 0.0193 1737 HG $0.5796 {\pm} 0.0338$ $0.5239 {\pm} 0.0128$ $0.5205 \!\pm\! 0.0106$ $\overline{0.5792 \pm 0.0130}$ HE $0.6870 {\pm} 0.0061$ $0.6588 {\pm} 0.0174$ $0.6325 {\pm} 0.0600$ 0.6786 ± 0.0103 1738 HS $0.7759 {\pm} 0.0119$ 0.7211 ± 0.0279 $0.6575 {\pm} 0.0831$ $\overline{0.7721 \pm 0.0128}$ 1739 JN $0.7383 {\pm} 0.0050$ 0.6972 ± 0.0111 $0.6795 {\pm} 0.0142$ 0.7308±0.0035 LA $0.9979 {\pm} 0.0000$ $0.9654 {\pm} 0.0255$ $0.9395 {\pm} 0.0760$ $\overline{0.9935 \pm 0.0055}$ 1740 $0.9717 {\pm} 0.0002$ 0.9674 ± 0.0040 0.9715±0.0026 MT $0.9714 {\pm} 0.0065$ 1741 $0.5570 {\pm} 0.0096$ 0.5587 ± 0.0252 0.5063 ± 0.0160 $\overline{0.5683 \pm 0.0083}$ MA $0.6478 {\pm} 0.0156$ $\overline{0.6871 \pm 0.0152}$ 0.6307 ± 0.0494 $0.6939 {\pm} 0.0241$ MB 1742 NU 0.4971 ± 0.0083 0.4994 ± 0.0060 0.4967 ± 0.0058 0.5075±0.0020 1743 0.9573±0.0063 NS 0.9944±0.0063 0.9716 ± 0.0095 0.9941 ± 0.0056 PW $0.8964 {\pm} 0.0158$ 0.8620 ± 0.0170 0.6696 ± 0.0283 0.9016±0.0158 1744 PL. 0.8277±0.0313 $\underline{0.7829 {\pm} 0.0206}$ 0.7505 ± 0.0500 0.6717 ± 0.0584 1745 RS 0.7154 ± 0.0216 0.6357 ± 0.0386 0.6679 ± 0.0459 0.7208+0.0134 TC 0.5530 ± 0.0256 0.5261 ± 0.0222 $0.5173 {\pm} 0.0106$ $0.5609 {\pm} 0.0138$ 1746 TD 0.9230 ± 0.0012 0.9117 ± 0.0167 0.8204 ± 0.0502 0.9242 ± 0.0052 1747 # Best 11/23 0/231/23 11/23 1748 vs RND 22/23 21/23 15/23 22/23 1749

Table 21: Comparison of raw balanced accuracy scores of distillation methods with TF-SFT and
 KNN downstream classifier. Best performance at for each dataset is marked in bold, and second-best
 performance is marked with underline.

Dataset	AG	GM	KIP	KM
AD	$0.7352 {\pm} 0.0212$	$0.7292 {\pm} 0.0136$	$0.5600 {\pm} 0.0599$	$0.7246 {\pm} 0.0309$
AE	$0.5309 {\pm} 0.0252$	$\overline{0.5204 \pm 0.0109}$	0.5131 ± 0.0235	0.5143 ± 0.0162
BM	0.7111 ± 0.0136	$\overline{0.6352 \pm 0.0335}$	$0.5374 {\pm} 0.0504$	$0.7210 {\pm} 0.0277$
CR	$\overline{0.5364 \pm 0.0178}$	0.5393 ± 0.0256	0.5161 ± 0.0210	$0.5508 {\pm} 0.0180$
CD	$0.6082{\pm}0.0252$	$\overline{0.6005 \pm 0.0292}$	$0.5525 {\pm} 0.0275$	0.6005 ± 0.0312
DB	0.5154 ± 0.0162	0.5139 ± 0.0261	0.5049 ± 0.0213	$0.5288 {\pm} 0.0178$
EL	$\overline{0.6300 \pm 0.0314}$	$0.5630 {\pm} 0.0346$	$0.5273 {\pm} 0.0463$	0.6210 ± 0.0331
EV	0.6840 ± 0.0477	$0.6380 {\pm} 0.0361$	0.5907 ± 0.0423	0.6949±0.0317
HG	$\overline{0.5397 \pm 0.0181}$	0.5121 ± 0.0124	$0.5118 {\pm} 0.0064$	0.5281 ± 0.0128
HE	0.6442 ± 0.0253	$0.5837 {\pm} 0.0354$	0.5194 ± 0.0449	0.6546 ± 0.0183
HS	0.6954 ± 0.0497	0.6340 ± 0.0532	0.5274 ± 0.0498	0.7115±0.0275
JN	$\overline{0.6555 \pm 0.0197}$	$0.6320 {\pm} 0.0185$	$0.5891 {\pm} 0.0515$	0.6597±0.0211
LA	$\overline{0.8267 \pm 0.0424}$	$0.7451 {\pm} 0.0585$	$0.8233 {\pm} 0.0684$	0.8039 ± 0.0672
MT	0.8070 ± 0.0590	0.7332 ± 0.0815	0.7098 ± 0.0900	0.8236±0.0855
MA	0.5756 ± 0.0098	0.5632 ± 0.0237	0.5111 ± 0.0340	$0.5676 {\pm} 0.0186$
MB	0.6712 ± 0.0703	0.6122 ± 0.0577	0.5565 ± 0.0573	0.6731±0.0627
NU	$\overline{0.5065 \pm 0.0033}$	0.5019 ± 0.0050	0.5005 ± 0.0054	0.5035 ± 0.0049
NS	0.9278 ± 0.0753	0.8064 ± 0.0162	$0.9775 {\pm} 0.0140$	0.8876 ± 0.0842
PW	0.8700±0.0175	0.8128 ± 0.0311	0.6291 ± 0.0598	0.8678 ± 0.0240
PL	0.6327 ± 0.0557	0.5675 ± 0.0262	0.5634 ± 0.0362	0.6554 ± 0.0705
RS	0.6350 ± 0.0324	0.5440 ± 0.0214	0.5213 ± 0.0200	0.6261 ± 0.0304
TC	0.5129 ± 0.0285	0.5152 ± 0.0240	0.4953 ± 0.0155	0.5205+0.0195
TD	0.7632 ± 0.0386	0.7125 ± 0.0293	0.6139 ± 0.0481	0.7814 ± 0.0377
# Best	10/23	0/23	1/23	12/23
vs RND	22/23	18/23	3/23	22/23

1775 1776 1777

1728 1729

Table 22: Comparison of raw balanced accuracy scores of distillation methods in the original space
(no encoder) KNN downstream classifier. Best performance at for each dataset is marked in bold, and
second-best performance is marked with underline.

1783					
1784	Dataset	AG	GM	KIP	KM
1785	Dataset	710	OM	KII	
1706	AD	0.7627 ± 0.0039	$0.7406 {\pm} 0.0168$	$0.7318 {\pm} 0.0212$	$0.7628 {\pm} 0.0210$
1700	AE	0.5467 ± 0.0250	0.5324 ± 0.0090	$0.5189 {\pm} 0.0063$	$0.5630 {\pm} 0.0212$
1787	BM	0.7894±0.0319	0.7685 ± 0.0210	0.7632 ± 0.0312	0.7887 ± 0.0142
1788	CR	0.5299 ± 0.0242	0.5443 ± 0.0228	$0.5525 {\pm} 0.0185$	0.5349 ± 0.0134
1700	CD	0.6323 ± 0.0845	0.6358 ± 0.0411	0.6138 ± 0.0261	$0.6542 {\pm} 0.0414$
1789	DB	0.5364 ± 0.0051	0.5211 ± 0.0278	0.5348 ± 0.0349	0.5405±0.0139
1790	EL	0.6432 ± 0.0317	0.5690 ± 0.0326	0.6131 ± 0.0309	0.6543±0.0187
1150	EV	0.7310±0.0019	0.6792 ± 0.0421	0.6742 ± 0.0347	0.7202 ± 0.0350
1791	HG	$0.6058 {\pm} 0.0126$	0.5302 ± 0.0068	0.5477 ± 0.0254	0.5997 ± 0.0152
1792	HE	0.6540 ± 0.0057	0.6364 ± 0.0225	0.6256 ± 0.0370	$0.6580 {\pm} 0.0157$
	HS	$0.7801 {\pm} 0.0029$	0.7257 ± 0.0336	0.7478 ± 0.0149	0.7768 ± 0.0141
1793	JN	$0.7192{\pm}0.0036$	0.6911 ± 0.0130	0.6952 ± 0.0315	0.7153 ± 0.0102
1794	LA	0.9983±0.0010	0.9893 ± 0.0192	0.9883 ± 0.0238	0.9980 ± 0.0017
	MT	0.9698 ± 0.0055	0.9627 ± 0.0056	0.9697 ± 0.0050	0.9733±0.0032
1795	MA	0.5694 ± 0.0127	0.5571 ± 0.0283	0.5160 ± 0.0107	0.5878±0.0149
1796	MB	$0.6818 {\pm} 0.0092$	0.6555 ± 0.0568	0.6697 ± 0.0217	0.6707 ± 0.0169
1202	NU	0.4958 ± 0.0047	0.5012 ± 0.0057	0.4987 ± 0.0060	0.5071 ± 0.0045
1/9/	NS	0.9749 ± 0.0153	0.9731 ± 0.0179	0.9838 ± 0.0139	$0.9842 {\pm} 0.0129$
1798	PW	0.8804 ± 0.0107	0.8466 ± 0.0383	0.7921 ± 0.0523	0.9046±0.0108
1700	PL	0.9010 ± 0.0198	0.8502 ± 0.0175	0.8198 ± 0.0426	0.9000 ± 0.0059
1799	RS	0.6842 ± 0.0019	0.6210 ± 0.0500	0.6627 ± 0.0714	0.6877 ± 0.0205
1800	TC	$0.5785 {\pm} 0.0231$	0.5150 ± 0.0307	0.5366 ± 0.0251	0.5734 ± 0.0197
1901	TD	0.9191 ± 0.0104	0.9010 ± 0.0260	0.8999 ± 0.0213	0.9200±0.0037
1001	# Best	9/23	0/23	1/23	13/23
1802	vs RND	21/23	19/23	18/23	23/23
1803					

Table 23: Comparison of raw balanced accuracy scores of distillation methods with TF-SFT and MLP downstream classifier. Best performance at for each dataset is marked in bold, and second-best performance is marked with underline.

Dataset	AG	GM	KIP	KM
AD	$0.7183 {\pm} 0.0392$	0.7576±0.0148	$0.6756 {\pm} 0.0604$	0.7385±0.0276
AE	$0.5743 {\pm} 0.0265$	0.5444 ± 0.0153	0.5267 ± 0.0241	0.5618 ± 0.0410
BM	$0.7406 {\pm} 0.0224$	$0.6573 {\pm} 0.0312$	0.5776 ± 0.0569	0.7351 ± 0.0311
CR	0.5607 ± 0.0216	$0.5388 {\pm} 0.0272$	$0.5037 {\pm} 0.0440$	0.5618 ± 0.0277
CD	$\overline{0.6146 \pm 0.0276}$	$0.5920 {\pm} 0.0524$	$0.5706 {\pm} 0.0564$	0.6040 ± 0.0332
DB	$0.5168 {\pm} 0.0171$	0.5203 ± 0.0207	$0.5052 {\pm} 0.0281$	0.5329±0.0203
EL	$0.6713 {\pm} 0.0315$	$\overline{0.5904 \pm 0.0363}$	$0.5568 {\pm} 0.0787$	0.6573 ± 0.0347
EV	$0.6828 {\pm} 0.0270$	$0.6570 {\pm} 0.0289$	$0.6380 {\pm} 0.0651$	0.6900±0.0255
HG	$\overline{0.5463 \pm 0.0218}$	$0.5184 {\pm} 0.0120$	0.5190 ± 0.0163	0.5423 ± 0.0221
HE	0.6221 ± 0.0210	0.6213 ± 0.0397	$0.5369 {\pm} 0.0574$	0.6309±0.022
HS	0.7514±0.0159	0.6746 ± 0.0321	$0.5970 {\pm} 0.0850$	0.7397 ± 0.0390
JN	$0.6352{\pm}0.0188$	$0.6328 {\pm} 0.0214$	0.6209 ± 0.0370	0.6339 ± 0.013
LA	$0.8530 {\pm} 0.0389$	0.7621 ± 0.0419	$0.8924{\pm}0.1000$	0.7970 ± 0.044
MT	0.9008 ± 0.0332	0.8068 ± 0.0741	0.8904 ± 0.0269	0.8839 ± 0.0584
MA	$0.5710 {\pm} 0.0124$	$0.5591 {\pm} 0.0198$	$\overline{0.5294 \pm 0.0387}$	0.5640 ± 0.015
MB	0.7411±0.0577	$0.6768 {\pm} 0.0636$	0.5995 ± 0.0945	0.7248 ± 0.065
NU	$0.5076 {\pm} 0.0025$	0.5009 ± 0.0057	0.5004 ± 0.0028	0.5063 ± 0.005
NS	$0.9799 {\pm} 0.0208$	$0.8159 {\pm} 0.0102$	0.9967±0.0038	0.9006 ± 0.074
PW	0.9018 ± 0.0178	$0.8248 {\pm} 0.0253$	$0.8084 {\pm} 0.0546$	0.8775 ± 0.032
PL	0.7934 ± 0.0946	0.6883 ± 0.0491	0.7319 ± 0.0239	0.7961±0.071
RS	$\overline{0.6304 \pm 0.0134}$	0.5567 ± 0.0191	$0.5386 {\pm} 0.0350$	0.6305±0.022
TC	$\overline{0.5404 \pm 0.0253}$	0.5177 ± 0.0141	$0.5016 {\pm} 0.0358$	0.5154 ± 0.032
TD	$0.7924{\pm}0.0154$	$\overline{0.7164 \pm 0.0507}$	$0.6930 {\pm} 0.0413$	0.7751 ± 0.026
# Best	14/23	1/23	2/23	6/23
vs RND	22/23	19/23	6/23	21/23

Table 24: Comparison of raw balanced accuracy scores of distillation methods with in the original space (no encoder) MLP downstream classifier. Best performance at for each dataset is marked in bold, and second-best performance is marked with underline.