

Deep Neural Networks and Tabular Data: A Survey

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ABSTRACT

Heterogeneous tabular data are the most commonly used form of data and are essential for numerous critical and computationally demanding applications. On homogeneous data sets, deep neural networks have repeatedly shown excellent performance and have therefore been widely adopted. However, their application to modeling tabular data (inference or generation) remains highly challenging. This work provides an overview of state-of-the-art deep learning methods for tabular data. We start by categorizing them into three groups: data transformations, specialized architectures, and regularization models. We then provide a comprehensive overview of the main approaches in each group. A discussion of deep learning approaches for generating tabular data is complemented by strategies for explaining deep models on tabular data. Our primary contribution is to address the main research streams and existing methodologies in this area, while highlighting relevant challenges and open research questions. To the best of our knowledge, this is the first in-depth look at deep learning approaches for tabular data. This work can serve as a valuable starting point and guide for researchers and practitioners interested in deep learning with tabular data.

1. Introduction

The success of deep neural networks — particularly those based on convolutions, recurrent deep learning mechanisms (Hochreiter and Schmidhuber, 1997), or transformer networks (Vaswani et al., 2017) - has been accelerated through affordable computational and storage resources and the availability of large, labeled data sets (Schmidhuber, 2015; Goodfellow et al., 2016). Although deep learning methods perform outstandingly well for classification or data generation tasks on homogeneous data (e.g., image, audio, and text data), tabular data still pose a challenge to these models (Arik and Pfister, 2019; Popov et al., 2019; Shwartz-Ziv and Armon, 2021). Kadra et al. (2021) named the tabular data sets the last “unconquered castle” for deep neural network models.

Tabular data – in contrast to image or language data – are heterogeneous, leading to dense numerical and sparse categorical features. Furthermore, the correlation among the features is weaker than the spatial or semantic relationship in images or speech data. Variables can be correlated or independent, and the features have no positional information. Hence, it is necessary to discover and exploit correlation without relying on spatial information (Somepalli et al., 2021).


Heterogeneous data are the most commonly used form of data (Shwartz-Ziv and Armon, 2021), and it is ubiquitous in many crucial applications, such as medical diagnosis based on patient history (Ulmer et al., 2020; Somani et al., 2021; Borisov et al., 2021), predictive analytics for financial applications (e.g., risk analysis, estimation of creditworthiness, the recommendation of investment strategies, and portfolio management) (Clements et al., 2020), click-through rate (CTR)

prediction (Guo et al., 2017), user recommendation systems (Zhang et al., 2019), customer churn prediction (Ahmed et al., 2017; Tang et al., 2020), cybersecurity (Buczak and Guven, 2015), fraud detection (Cartella et al., 2021), identity protection (Liu et al., 2021a), psychology (Urban and Gates, 2021), delay estimations (Shoman et al., 2020), anomaly detection (Pang et al., 2021), and so forth. In all these applications, a boost in predictive performance and robustness may have considerable benefits for both end users and companies that provide such solutions. Simultaneously, this requires handling many data-related pitfalls, such as noise, impreciseness, different attribute types and value ranges, or the non-availability of values.

Meanwhile, deep neural networks offer multiple advantages over traditional machine learning methods. They are highly flexible (Sahoo et al., 2017) and allow for efficient and iterative training. Deep neural networks are particularly valuable for AutoML (He et al., 2021; Artzi et al., 2021; Shi et al., 2021; Fakoor et al., 2020; Gijssbers et al., 2019; Yin et al., 2020). Tabular data generation is possible using deep neural networks and can, for instance, help mitigate class imbalance problems (Wang et al., 2019c). Finally, neural networks can be deployed for multimodal learning problems where tabular data can be one of many input modalities (Baltrušaitis et al., 2018; Lichtenwaller et al., 2021; Shi et al., 2021; Pölsterl et al., 2021; Soares et al., 2021), for tabular data distillation (Medvedev and D'yakonov, 2020; Li et al., 2020a), for federated learning (Roschewitz et al., 2021), and in many more scenarios.

As the data collection step, especially for heterogeneous data, is costly and time-consuming, there are many approaches for synthetic tabular data generation. However, modeling the probability distribution of rows in tabular data and generating realistic synthetic data are challenging since heterogeneous tabular data typically includes a mix of

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discrete and continuous variables. Continuous variables may have multiple modes, whereas discrete columns are often imbalanced. All these pitfalls in combination with missing, noisy, or unbounded values make the issue of tabular data generation quite complex, even for modern deep generative architectures. We discuss the state-of-the-art approaches for tabular data generation in Section 5.

Another important aspect is the interpretation of deep neural networks on tabular data (Grisci et al., 2021). Many popular approaches for the interpretation of deep neural networks stem from the computer vision domain, where a pixel group is highlighted, creating a so-called saliency map. Nevertheless, for tabular data sets, highlighting a variable relationship is also essential. Many existing methods – especially those based on attention mechanisms (Vaswani et al., 2017) – offer a highlighting of relationships by design and their attention maps can be easily visualized.

The aims of this survey are to provide

1. a thorough review of existing scientific literature on deep learning for tabular data
2. a taxonomic categorization of the available approaches for classification and regression tasks on heterogeneous tabular data
3. a presentation of the state-of-the-art as well as an outlook on promising paths towards tabular data generation
4. an overview of existing explanation approaches for deep models for tabular data
5. a discussion on the main reasons for the limited success of deep learning on tabular data.
6. a list of open challenges related to deep learning for tabular data.

Thus, data science practitioners and researchers will be able to quickly identify promising starting points and guidance for the use cases or research questions at hand.

The remainder of the survey is organized as follows: Section 2 discusses the related work. To introduce the Reader to the field, in Section 3 we provide the used formalism, a brief outline of the domain's history, list the main challenges that are typically encountered, and propose a unified taxonomy of possible approaches to deep learning with tabular data. Section 4 covers the main methods for modeling tabular data using the deep neural networks in detail. Section 5 presents an overview on tabular data generation using deep neural networks. An overview of explanation mechanisms for deep models for tabular data is presented in Section 6. In Section 7, we summarize the state of the field and give future perspectives. We list open research questions before concluding in Section 8.

To help improve the survey, please do not hesitate to send corrections and suggestions to corresponding authors.

2. Related Work

To the best of our knowledge, there is no study dedicated exclusively to the application of deep neural networks to tabular data, spanning the areas of supervised and unsupervised learning and data synthesis. Prior works cover some of these aspects, but none of them systematically discusses the existing approaches in the broadness of this survey. We also could not find any work that reviews state-of-the-art approaches for synthesizing tabular data using deep neural networks.

However, there are some works that cover parts of the domain. There is a comprehensive analysis of common approaches for categorical data encoding as a preprocessing step for deep neural networks by Hancock and Khoshgoftaar (2020). The survey's authors compared existing methods for categorical data encoding on various tabular data sets and different deep learning architectures. We also discuss the key categorical data encoding methods in Section 4.1.1.

Gorishniy et al. (2021) empirically evaluated a large number of state-of-the-art deep learning approaches for tabular data on a wide range of data sets. Interestingly, the authors demonstrated that a tuned deep neural network model with the ResNet-like architecture (He et al., 2016) shows comparable performance to some state-of-the-art deep learning approaches for tabular data.

Recently, Shwartz-Ziv and Armon (2021) published a study on several different deep models for tabular data including TabNet (Arik and Pfister, 2019), NODE (Popov et al., 2019), Net-DNF (Katzir et al., 2021). Additionally, they compared the deep learning approaches to the gradient boosting decision tree algorithm regarding the accuracy, training effort, inference efficiency, and also hyperparameter optimization time. They observed that the deep models had the best results on the data sets used in their original paper, however, no deep model could exceed the others in general. They were challenged by the gradient boosting decision trees, which was why the authors concluded that efficient tabular data modeling using deep neural networks is still an open question. With our survey, we aim to provide the background necessary for future work on this question.

A quantitative study by Gupta et al. (2021) analyzed the robustness of neural networks also considering different state-of-the-art regularization techniques. To fool a prediction model, tabular data can be corrupted, and adversarial examples can be produced. Using this data, it is possible to mislead fraud detection models as well as humans as shown by Cartella et al. (2021). Before using deep learning models for tabular data in a critical environment, one should be aware of the possible susceptibility to attacks.

Finally, a recent survey by Sahakyan et al. (2021) summarizes explanation techniques in the context of tabular data. Hence, we do not provide a detailed discussion of explainable machine learning for tabular data in this paper. However, for the sake of completeness, we highlight some of the most relevant works in Section 6.

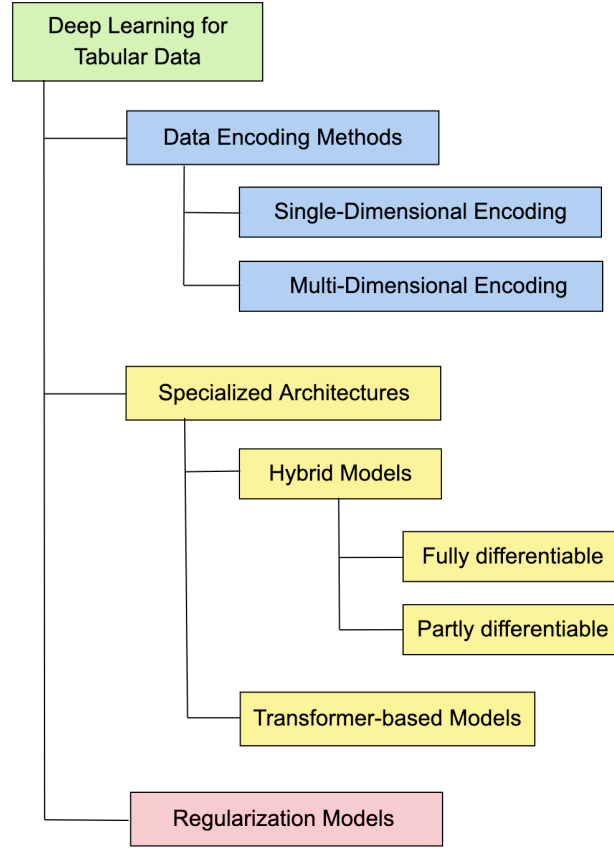


Figure 1: Unified taxonomy of deep neural network models for heterogeneous tabular data.

3. Tabular Data and Deep Neural Networks

3.1. Definitions

In this section, we give definitions for central terms used in this work. We also provide references for a more detailed explanation of the methods.

One important concept in this survey is the one of (*deep*) *neural networks*. In most passages of this work we use this concept as a synonym for feed-forward networks, as described by Goodfellow et al. (2016), and name the concrete model whenever we deviate from this concept.

A deep neural network defines a mapping \hat{f}

$$y = f(x) \approx \hat{f}(x; W), \quad (1)$$

that learns the value of the parameters W (the “weights” of a neural network) that results in the best approximation of f . The network is called feed-forward if the input information flows in one direction to the output without any feedback connections.

This survey has a focus on *heterogeneous data*, which distinguishes itself from *homogeneous* data modalities, such as images, audio, or text data, by containing a variety of attribute types, such as continuous or discrete numerical attributes from different distributions (e.g., binary values,

ordinal values, high-cardinality categorical values). According to Lane’s definition (David M. Lane, 2003), categorical variables are qualitative values. They “do not imply a numerical ordering”, unlike quantitative values, which are “measured in terms of numbers”. Also, there is a limited unique set of values a categorical variable can take. Examples of categorical variables in a tabular data set are *gender*, *user_id*, *product_type*, *topic*.

Tabular data (sometimes *structured data* in the literature) is a subcategory of the heterogeneous data format, that usually is presented in a table (Cvitkovic et al., 2020) with data points as rows and features as columns. Hence, for the scope of this work, we also define a tabular data set as a table which contains n numerical columns $\{N_1, \dots, N_n\}$ and c categorical columns $\{C_1, \dots, C_c\}$. All columns are random variables following a joint distribution $\mathbb{P}(N_{1:n}, C_{1:c})$. Each data point can be understood as a row in the table, or – taking a probabilistic view – as a sample from the unknown joint distribution. When working with tabular data we have limited prior knowledge regarding the structure and relationships between its features. Tabular data are widely used in practical machine learning and data science.

3.2. Brief History of Deep Learning on Tabular Data

Tabular data are the oldest form of data. Before digital collection of text, images, and sound was possible, almost all data were tabular. Therefore, it was the target of early machine learning research. However, deep neural networks became popular in the digital age and were further developed with a focus on homogeneous data. In recent years, various supervised, self-supervised, and semi-supervised deep learning approaches have been proposed that explicitly address the issue of tabular data modeling again. Early works mostly focused on data transformation techniques for preprocessing (Giles et al., 1992; Horne and Giles, 1995; Willenborg and De Waal, 1996), which are still important today (Hancock and Khoshgoftaar, 2020).

A huge stimulus was the rise of e-commerce, which demanded novel solutions, especially in advertising (Richardson et al., 2007; Guo et al., 2017). These tasks required fast and accurate estimation on heterogeneous data sets with many categorical variables, for which the traditional machine learning approaches are not well suited (e.g., categorical features that have high cardinality can lead to very sparse high-dimensional feature vectors and non-robust models). As a result, researchers and data scientists started looking for more flexible solutions, e.g., based on deep neural networks, that are able to capture complex non-linear dependencies in the data.

In particular, the click-through rate prediction problem has received a lot of attention (Guo et al., 2017; Ke et al., 2019; Wang et al., 2021). A large variety of approaches were proposed, most of them relying on specialized neural network architectures for heterogeneous tabular data. The most important methods for click-through rate estimation are included in our survey.

A newer line of research evolved based on idea that regularization may improve the performance of deep neural networks on tabular data (Kadra et al., 2021). The idea was sparked by Shavitt and Segal (2018), leading to an intensification of research on regularization approaches.

Due to the tremendous success of attention-based approaches such as transformers on textual (Brown et al., 2020) and visual data (Dosovitskiy et al., 2021; Khan et al., 2021), researchers have started applying attention-based methods and self-supervised learning techniques to tabular data recently. After the first and the most influential work by Arik and Pfister (2019) raised the reasearch interest, transformers are quickly gaining popularity, especially for large tabular data sets.

3.3. Challenges of Learning With Tabular Data

As mentioned above, deep neural networks are usually inferior to more traditional (e.g. linear or tree-based) machine learning methods when dealing with tabular data. However, it is often unclear why deep learning cannot achieve the same level of predictive quality as in other domains such as image classification and natural language processing. In the following, we identify and discuss four possible reasons:

1. **Inappropriate Training Data:** The data quality is a common issue for real-world tabular data sets. They often include missing values (Sánchez-Morales et al., 2020), extreme data (outliers) (Pang et al., 2021), erroneous or inconsistent data (Karr et al., 2006), and have small overall size relative to the high-dimensional feature vectors generated from the data (Xu and Veeramachaneni, 2018). Also, due to the expensive nature of data collection, tabular data are frequently class-imbalanced.
2. **Missing or Complex Irregular Spatial Dependencies:** There is often no spatial correlation between the variables in tabular data sets (Zhu et al., 2021), or the dependencies between features are rather complex and irregular. Thus, the *inductive biases* used in popular models for homogeneous data, such as convolutional neural networks, are unsuitable for modeling this data type (Katzir et al., 2021; Rahaman et al., 2019; Mitchell et al., 2017).
3. **Extensive Preprocessing:** One of the main challenges when working with tabular data is how to handle categorical features (Hancock and Khoshgoftaar, 2020). In most cases, the first step is to convert the categories into a numerical representation, for example, using a simple one-hot or ordinal encoding scheme. However, as categorical features may be very sparse (a problem known as *curse of dimensionality*), this can lead to a very sparse feature matrix (using the one-hot encoding scheme) or a synthetic alignment of unordered values (using the ordinal encoding scheme). Hancock and Khoshgoftaar (2020) have analyzed different embedding techniques for categorical variables. Dealing with categorical features is also one of the main aspects we discuss in Section 4. Applications that work with homogeneous data have effectively used data augmentation (Perez and Wang, 2017), transfer learning (Tan et al., 2018) and test-time augmentation (Shanmugam et al., 2020). For heterogeneous tabular data, these techniques are often difficult to apply. However, some frameworks for learning with tabular data, such as VIME (Yoon et al., 2020) and SAINT (Somepalli et al., 2021), use data augmentation strategies in the embedding space. Lastly, note that we often lose information with respect to the original data when applying preprocessing methods for deep neural networks, leading to a reduction in predictive performance (Fitkov-Norris et al., 2012).
4. **Model Sensitivity:** Deep neural networks can be extremely fragile to tiny perturbations of the input data (Szegedy et al., 2013; Levy et al., 2020). The smallest possible change of a categorical (or binary) feature might already have a large impact on the prediction. This is usually less problematic for homogeneous (continuous) data sets. In contrast to deep neural networks, decision-tree algorithms can handle perturbations exceptionally well by selecting a feature and threshold value and "ignoring"

the rest of the data sample. As a consequence of their extreme sensitivity, artificial neural network models have high curvature decision boundaries (Poole et al., 2016; Achille et al., 2019), whereas decision tree-based algorithms can learn hyperplane-like boundaries. In order to reduce the input-related sensitivity of deep neural networks, some approaches propose to apply strong regularization to learning parameters (Shavitt and Segal, 2018; Kadra et al., 2021). We discuss these methods in Section 4.3 in more detail.

Finally, deep neural networks usually have an excessive number of hyperparameters (Goodfellow et al., 2016), where traditional machine learning approaches on tabular data (e.g., decision-tree-based models, support-vector machines (Cortes and Vapnik, 1995)) typically have significantly fewer hyperparameters. As a consequence, the tuning time for deep learning models is vastly higher than that of decision tree-based approaches. In addition, neural networks tend to be sensitive to the choice of hyperparameters (e.g. learning rate, number of hidden layers or activation function). In general, fewer hyperparameters are preferable to reduce the risk of non-robust predictions.

3.4. Unified Taxonomy

In this section, we introduce a taxonomy of approaches, that allows for a unifying view of the field. We observed that the works we encountered while preparing this survey fall into three main categories: *data transformation methods*, *specialized architectures*, and *regularization models*. The unified taxonomy of deep learning for tabular data methods is shown in Fig. 1.

The methods in the first group transform categorical and numerical data, thus a deep neural network model is able to better extract the information signal. These methods do not require new architectures or adapting the existing data processing pipeline. Nevertheless, the transformation step comes at the cost of an increased preprocessing time. This might be an issue for high-load systems (Baylor et al., 2017), in the case of categorical variables with high cardinality and growing data set size. We can further subdivide this field into *Single-Dimensional Encodings*, which are employed to transform each feature independently or *Multi-Dimensional Encodings*, which are used to map an entire data record to another representation.

The biggest share of works investigates specialized architectures and suggests that a different deep neural network architecture is required for tabular data. Two types of architectures are of particular importance: *hybrid models* fuse classical machine learning approaches (e.g., decision trees) with neural networks, while *transformer-based models* rely on the attention mechanism.

Lastly, the group of regularization models claims that one of the main reasons for the moderate performance of deep learning models on tabular is their extreme non-linearity and model complexity. Therefore, strong regularization schemes

are proposed as a solution. They are mainly implemented in the form of special-purpose loss functions.

We believe our taxonomy may help practitioners find the methods of choice, that can be easily integrated into their existing tool chain. For instance, the data transformations can result in performance improvements while maintaining the current model architecture. With specialized architectures, the data preprocessing pipeline can be kept intact.

4. Deep Neural Networks for Tabular Data

In this section, we discuss the use of deep neural networks on tabular data for classification or regression tasks according to the taxonomy presented in the previous section.

We provide an overview of existing deep learning approaches in this area of research in Table 1 and discuss the three methodological categories in detail: data transformation methods (Subsection 4.1), architecture-based methods (Subsection 4.2.1), and regularization-based models (Subsection 4.3).

4.1. Data Transformation Methods

Most traditional approaches for deep neural networks on tabular data fall into this group. Interestingly, data preprocessing plays a relatively minor role in computer vision, even though the field is currently dominated by deep learning solutions. (Goodfellow et al., 2016). There are many different possibilities to transform tabular data, and each may have an impact on the learning results (Hancock and Khoshgoftaar, 2020).

4.1.1. Single-Dimensional Encoding

One of the critical obstacles for deep learning with tabular data are categorical variables. Since neural networks only accept real number vectors as input, these values must be transformed before a model can use them. Therefore, approaches from this group try to encode categorical variables in a way suitable for deep learning models.

As Hancock and Khoshgoftaar (2020) state in their survey, approaches in this group, are divided into *deterministic* techniques, which can be used before training the model, and more complicated *automatic* techniques that are part of the model architecture. There are many ways for deterministic data encoding, so we restrict ourselves to the most common ones without the claim of completeness.

The most simple data encoding technique might be ordinal or label encoding. Every category is just mapped to a discrete numeric value, e.g., {"Apple", "Banana"} are encoded as {0, 1}. Unfortunately, this method introduces an artificial order to previously unordered categories. Another straightforward method that does not include any order is the one-hot encoding. One column for each unique category is added to the data. Only the column corresponding to the observed category is assigned the value one, with the other values being zero. In our example, "Apple" could be encoded as (1, 0) and "Banana" as (0, 1). Having a diverse set of categories in the data, this method, of course, can lead to

high-dimensional sparse feature vectors (and the “curse of dimensionality” problem).

Binary encoding limits the number of new columns by transforming the qualitative data into a numerical representation (as the label encoding does) and using the binary format of the number. Again the digits are split into different columns, but there are only $\log(c)$ new columns if c is the number of unique categorical values. If we extend our example to three fruits, e.g., {“Apple”, “Banana”, “Pear”}, we only need two columns to represent them: (01), (10), (11).

One approach that needs no extra columns and does not include any artificial order is the so-called leave-one-out encoding. It is based on the target encoding technique proposed in the work by Micci-Barreca (2001), where every category is replaced with the mean of the target variable of that category. The leave-one-out encoding excludes the current row when computing the mean of the target variable to avoid overfitting. This approach is quite generic and is also used in the CatBoost framework (Prokhorenkova et al., 2018), a state-of-the-art machine learning library for heterogeneous tabular data based on the gradient boosting algorithm (Friedman, 2002).

A different strategy is hash-based encoding. Every category is transformed into a fixed-size value via a deterministic hash function. The output size is not directly dependent on the number of input categories but can be chosen manually.

4.1.2. Multi-Dimensional Encoding

One way of applying an automatic encoding is used by the VIME approach (Yoon et al., 2020). The authors propose a self- and semi-supervised deep learning framework for tabular data that trains an encoder in a self-supervised fashion by using two pretext tasks. Those tasks that are independent from the concrete downstream task which the predictor has to solve. The first task of VIME is called mask vector estimation; its goal is to determine which values in a sample are corrupted. The second task, i.e., feature vector estimation, is to recover the original values of the sample. The encoder itself is a simple multilayer perceptron. This automatic encoding makes use of the fact that there is often much more unlabeled than labeled data. The encoder learns how to construct an informative homogeneous representation of the raw input data. In the semi-supervised step, a predictive model (which is also a deep neural network model) is trained, using the labeled and unlabeled data transformed by the encoder. For the latter, a novel data augmentation method is used, corrupting one (unlabeled) data point multiple times with different masks. On the predictions from all augmented samples from one original data point, a consistency loss \mathcal{L}_u can be computed that rewards similar outputs. Combined with a supervised loss \mathcal{L}_s from the labeled data, the predictive model minimizes the final loss $\mathcal{L} = \mathcal{L}_s + \beta \cdot \mathcal{L}_u$. To summarize, the VIME network trains an encoder, which is responsible to transform the categorical (and also numerical) features into a new homogeneous and informative representation. This transformed feature vector is used as an input to the predictive model. For the encoder itself, the categorical data

can be transformed by a simple one-hot-encoding and binary encoding.

Another stream of research aims at transforming the tabular input into a more homogeneous format. Since the revival of deep learning, convolutional neural networks have shown tremendous success in computer vision tasks. Therefore, the work by (Sun et al., 2019) proposed the SuperTML method, which is a data conversion technique for tabular data into visual data format (2-d matrices), i.e., an equivalent to black-and-white images.

The image generator for tabular data (IGTD) by Zhu et al. (2021) follows an idea similar to SuperTML. The IGTD framework converts tabular data into images to make use of classical convolutional architectures. As convolutional neural networks rely on spatial dependencies, the transformation into images is optimized by minimizing the difference between the feature distance ranking of the tabular data and the pixel distance ranking of the generated image. Every feature corresponds to one pixel, which leads to compact images with similar features close at neighboring pixels. Thus, IGTDs can be used in the absence of domain knowledge. The authors show relatively solid results for data with strong feature relationships but the method may fail if the features are independent or feature similarities can not characterize the relationships. In their experiments, the authors used only gene expression profiles and molecular descriptors of drugs as data. This kind of data may lead to a favorable inductive bias, so the general viability of the approach remains unclear.

4.2. Specialized Architectures

Specialized architectures form the largest group of approaches for deep tabular data learning. Hence, in this group, the focus is on the development and investigation of novel deep neural network architectures designed specifically for heterogeneous tabular data. Guided by the types of available models, we divide this group into two sub-groups: Hybrid models (presented in 4.2.1) and transformer-based models (discussed in 4.2.2).

4.2.1. Hybrid Models

Most approaches for deep neural networks on tabular data are hybrid models. They transform the data and fuse successful classical machine learning approaches, often decision trees, with neural networks. We distinguish between fully differentiable models, that can be differentiated w.r.t. all their parameters and partly differentiable models.

Fully differentiable Models

The fully differentiable models in this category offer a valuable property: They permit end-to-end deep learning for training and inference by means of gradient descent optimizers. Thus, they allow for highly efficient implementations in modern deep learning frameworks that exploit GPU or TPU acceleration throughout the code.

Popov et al. (2019) propose an ensemble of differentiable oblivious decision trees (Langley and Sage, 1994) – the NODE framework for deep learning on tabular data. Oblivious decision trees use the same splitting function for all nodes on the same level and can therefore be easily

parallelized. NODE generalizes the successful CatBoost (Prokhorenkova et al., 2018) framework. To make the whole architecture fully differentiable and benefit from end-to-end optimization, NODE utilizes the entmax transformation (Peters et al., 2019) and soft splits. In their experiments, the NODE framework outperforms XGBoost and other GBDT models on many data sets. As NODE is based on decision tree ensembles, there is no preprocessing or transformation of the categorical data necessary. Decision trees are known to handle discrete features well. In the official implementation strings are converted to integers using the leave-one-out encoding scheme. The NODE framework is widely used and provides a sound implementation that can be readily deployed.

Frosst and Hinton (2017) contributed another model relying on soft decision trees (SDT) to make neural networks more interpretable. They investigated training a deep neural network first, before using a mixture of its outputs and the ground truth labels to train the SDT model in a second step. This also allows for semi-supervised learning with unlabeled samples that are labeled by the deep neural network and used to train a more robust decision tree along with the labeled data. The authors showed that training a neural model first increases accuracy over SDTs that are directly learned from the data. However, their distilled trees still exhibit a performance gap to the neural networks that were fitted in the initial step. Nevertheless, the model itself shows a clear relationship among different classes in a hierarchical fashion. It groups different categorical values based on the common patterns, e.g., the digits 8 and 9 from the MNIST data set (LeCun and Cortes, 2010). To summarize, the proposed method allows for high interpretability and efficient inference, at the cost of slightly reduced accuracy.

The follow-up work (Luo et al., 2021) extended this line of research to heterogeneous tabular data and regression tasks and presents the soft decision tree regressor (SDTR) framework. The SDTR is a neural network which tries to imitate a binary decision. Therefore all neurons, like all nodes in a tree, get the same input from the data instead of the output from previous layers. In the case of deep networks, the SDTR could not beat other state-of-the-art models, but it has shown good result in a low-memory setting, where single tree models and shallow architectures were compared.

An interesting idea was introduced by Katzir et al. (2021). Their Net-DNF takes into account that every decision tree is merely a form of a Boolean formula, more precisely a disjunctive normal form. They use this inductive bias to design the architecture of a neural network, which is able to imitate the characteristics of the gradient boosting decision trees algorithm. The resulting Net-DNF was tested for classification tasks on data sets with no missing values, where it showed results that are comparable to those of XGBoost (Chen and Guestrin, 2016). Not mentioned, however, is how to handle high-cardinality categorical data, as the used data sets contained mostly numerical and few binary features.

Linear models (e.g., linear and logistic regression) provide global interpretability but are inferior to complex deep

neural networks. Usually, handcrafted feature engineering is required to improve the accuracy of linear models. (Liu et al., 2020) use a deep neural network to combine the features in a possibly non-linear way; the resulting combination then serves as input to the linear model. This enhances the simple model while still providing interpretability.

The work by Cheng et al. (2016) proposes a hybrid architecture that consists of linear and deep neural network models - Wide&Deep. A linear model that takes single features and a wide selection of hand-crafted logical expressions on features as an input is enhanced by a deep neural network to improve the generalization capabilities. Additionally, Wide&Deep learns an n -dimensional embedding vector for each categorical feature. All embeddings are concatenated resulting in a dense vector used as input to the neural network. The final prediction can be understood as a sum of both models. A similar work from Guo and Berkahn (2016) proposes an embedding using deep neural networks for categorical variables.

Another contribution to the realm of Wide&Deep models is DeepFM Guo et al. (2017). The authors demonstrate that it is possible to replace the hand-crafted feature transformations with learned Factorization Machines (FMs) (Rendle, 2010), leading to an improvement of the overall performance. The FM is an extension of a linear model designed to capture interactions between features within high-dimensional and sparse data efficiently. Similar to the original Wide&Deep model, DeepFM also relies on the same embedding vectors for its “wide” and “deep” parts. In contrast to the original Wide&Deep model, however, DeepFM alleviates the need for manual feature engineering.

Lastly, Network-on-Network (NON) (Luo et al., 2020) is a classification model for tabular data, which focuses on capturing the intra-feature information efficiently. It consists of three components: a field-wise network consisting of one unique deep neural network for every column to capture the column-specific information, an across-field-network, which chooses the optimal operations based on the data set, and an operation fusion network, connecting the chosen operations allowing for non-linearities. As the optimal operations for the specific data are selected, the performance is considerably better than that of other deep learning models. However, the authors did not include decision trees in their baselines, the current state-of-the-art models on tabular data. Also, training as many neural networks as columns and selecting the operations on the fly may lead to a long computation time.

Partly differentiable Models

This subgroup of hybrid models aims at combining non-differentiable approaches with deep neural networks. Usually models from this group utilize decision trees for the non-differentiable part.

The DeepGBM model (Ke et al., 2019) combines the flexibility of deep neural networks with the preprocessing capabilities of gradient boosting decision trees. DeepGBM consists of two neural networks - CatNN and GBDT2NN.

While CatNN is specialized to handle sparse categorical features, GBDT2NN is specialized to deal with dense numerical features.

In the preprocessing step for the CatNN network, the categorical data are transformed via an ordinal encoding (to convert the potential strings into integers), and the numerical features are discretized, as this network is specialized for categorical data. The GBDT2NN network distills the knowledge about the underlying data set from a model based on gradient boosting decision trees by accessing the leaf indices of the decision trees. This embedding based on decision tree leaves was first proposed by Moosmann et al. (2006) for the random forest algorithm. Later, the same knowledge distillation strategy has been adopted for gradient boosting decision trees (He et al., 2014).

Using the proposed combination of two deep neural networks, DeepGBM has a strong learning capacity for both categorical and numerical features. Unique about the network is that the authors explicitly implemented and tested the online prediction performance, where DeepGBM significantly outperforms gradient boosting decision trees. On the downside, the leaf indices can be seen as meta categorical features since we cannot directly compare these numbers. Also, it is not clear how other data-related issues, such as missing values, different scaling of numeric features, and noise, influence the predictions produced by the models.

The TabNN architecture, introduced by Ke et al. (2018), is based on two principles: explicitly leveraging expressive feature combinations and reducing model complexity. It distills the knowledge from gradient boosting decision trees to retrieve feature groups, it clusters them and then constructs the neural network based on those feature combinations. Also structural knowledge from the trees is transferred to provide an effective initialization. However, the construction of the network already takes different extensive computation steps (where one is only a heuristic to avoid an NP-hard problem). Furthermore, in light of the construction challenges and since an implementation of TabNN was not provided, the practical use of the network seems limited.

In similar spirit to DeepGBM and TabNN, the work from Ivanov and Prokhorenkova (2021) proposes using gradient boosting decision trees for the data preprocessing step. The authors show that a decision tree structure has the form of a directed graph. Thus, the proposed framework exploits the topology information from the decision trees using graph neural networks (Scarselli et al., 2008). The resulting architecture is coined Boosted Graph Neural Network (BGNN). In multiple experiments, BGNN demonstrates that the proposed architecture is superior to existing solid competitors in terms of predictive performance and training time.

4.2.2. Transformer-based Models

Transformer-based approaches form another subgroup of model-based deep neural methods for tabular data. Inspired by the recent explosive interest in transformer-based methods and their successes on text and visual data (Wang et al.,

2019a; Khan et al., 2021), researchers and practitioners have proposed multiple approaches using deep attention mechanisms (Vaswani et al., 2017) for heterogeneous tabular data.

TabNet (Arik and Pfister, 2019) is one of the first transformer-based models for tabular data. Similar to a decision tree, the TabNet architecture comprises multiple subnetworks that are processed in a sequential hierarchical manner. According to Arik and Pfister (2019), each subnetwork corresponds to one particular *decision step*. To train TabNet, each decision step (subnetwork) receives the current data batch as input. TabNet aggregates the outputs of all decision steps to obtain the final prediction. At each decision step, TabNet first applies a sparse feature mask (Martins and Astudillo, 2016) to perform soft instance-wise feature selection. Arik and Pfister (2019) claim that the feature selection can save valuable resources, as the network may focus on the most important features. The feature mask of a decision step is trained using attentive information from the previous decision step. To this end, a *feature transformer* module decides which features should be passed to the next decision step and which features should be used to obtain the output at the current decision step. Some layers of the feature transformers are shared across all decision steps. The obtained feature masks correspond to local feature weights and can also be combined into a global importance score. Accordingly, TabNet is one of the few deep neural networks that offers different levels of interpretability by design. Indeed, experiments show that each decision step of TabNet tends to focus on a particular subdomain of the learning problem (i.e., one particular subset of features). This behaviour is similar to convolutional neural networks. TabNet also provides a decoder module that is able to preprocess input data (e.g., replace missing values) in an unsupervised way. Accordingly, TabNet can be used in a two-stage self-supervised learning procedure, which improves the overall predictive quality. Recently, TabNet has also been investigated in the context of fair machine learning (Boughorbel et al., 2021; Mehrabi et al., 2021).

One supervised and semi-supervised approach is introduced by Huang et al. (2020). Their TabTransformer architecture uses self-attention-based transformers to map the categorical features into a contextual embedding. This embedding is more robust to missing or noisy data and enables interpretability. The embedded categorical features are then together with the numerical ones fed into a simple multilayer perceptron. If, in addition, there is an extra amount of unlabeled data, unsupervised pre-training can improve the results, using masked language modeling or replace token detection. Extensive experiments show that TabTransformer matches the performance of tree-based ensemble techniques, showing success also when dealing with missing or noisy data. The TabTransformer network puts a significant focus on the categorical features. It transforms the embedding of those features into a contextual embedding which is then used as

input for the multilayer perceptron. This embedding is implemented by different multi-head attention-based transformers, which are optimized during training.

ARM-net, introduced by Cai et al. (2021), is an adaptive neural network for relation modeling tailored for tabular data. The key idea of the ARM-net framework is to model feature interactions with combined features (feature crosses) selectively and dynamically by first transforming the input features into exponential space and then determining the interaction order and interaction weights adaptively for each feature cross. Furthermore, the authors propose a novel sparse attention mechanism to generate the interaction weights given the input data dynamically. Thus, users can explicitly model feature crosses of arbitrary orders with noisy features filtered selectively.

SAINT (Self-Attention and Intersample Attention Transformer) (Somepalli et al., 2021) is a hybrid attention approach, combining self-attention (Vaswani et al., 2017) with inter-sample attention over multiple rows. When handling missing or noisy data, this mechanism allows the model to borrow the corresponding information from similar samples, which improves the model's robustness. The technique is reminiscent of nearest-neighbor classification. In addition, all features are embedded into a combined dense latent vector, enhancing existing correlations between values from one data point. To exploit the presence of unlabeled data, a self-supervised contrastive pre-training can further improve the result, minimizing the distance between two views of the same sample and maximizing the distance between different ones. Similar to the VIME framework (Section 4.1.1), SAINT uses CutMix (Yun et al., 2019) to augment samples in the input space and uses mixup (Zhang et al., 2017a) in the embedding space. Attention-based architectures offer mechanisms for interpretability, which is an essential advantage over many hybrid models. Figure 2 shows attention maps on the MNIST (LeCun and Cortes, 2010) and volkert (Gijssbers et al., 2019) data sets, which can be found using different attention mechanisms.

4.3. Regularization Models

The third group of approaches argues that extreme flexibility of deep learning models for tabular data is one of the main learning obstacles and strong regularization of learned parameters may improve the overall performance.

One of the first methods in this category was the Regularization Learning Network (RLN) proposed by Shavitt and Segal (2018), which uses a learned regularization scheme. The main idea is to apply trainable regularization coefficients λ_i to each single weight w_i in a neural network and, by this, lower the high sensitivity:

$$\mathcal{L}_C(Z, W, \lambda) = \mathcal{L}(Z, W) + \sum_{i=1}^n \exp(\lambda_i) \cdot \|w_i\|, \quad (2)$$

where $Z = \{(x_m, y_m)\}_{m=1}^M$ are the training samples, \mathcal{L} is the classification loss given the model with weights, $W = \{w_i\}_{i=1}^n$. The norm, $\|\cdot\|$, can be chosen according

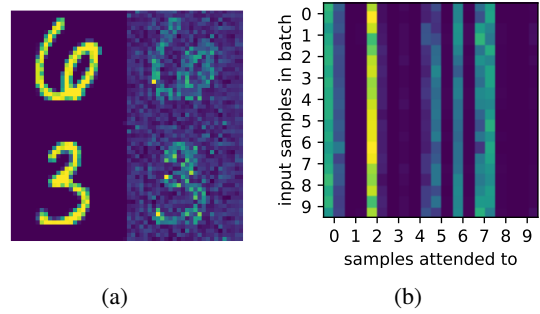


Figure 2: Interpretable learning with the SAINT architecture from Somepalli et al. (2021) by visual representations of various attention maps, (a) MNIST (LeCun and Cortes, 2010) and (b) a tabular data set (Somepalli et al., 2021).

to use-case-specific sparsity requirements, and the λ_i , i.e., the regularization coefficients, are learned for each weight w_i . To efficiently determine the corresponding coefficients, the authors propose a novel loss function termed ‘‘Counterfactual Loss’’, $\mathcal{L}_C(Z, W, \lambda)$. The regularization coefficients lead to a very sparse network, which also provides the importance of the remaining input features.

In their experiments, RLNs outperform deep neural networks and obtain results comparable to those of the gradient boosting decision trees algorithm, but they used only one data set with mainly numerical data to compare the models. The RLN paper does not address the issues of categorical data. For the experiments and the example implementation data sets with exclusively numerical data (except for gender attribute) were used. A similar idea is proposed in (Borisov et al., 2019), where regularization coefficients are learned only in the first layer with a goal to extract feature importance.

Kadra et al. (2021) state that simple multilayer perceptrons can outperform state-of-the-art algorithms on tabular data if deep learning networks are properly regularized. The authors of the work propose a ‘‘cocktail’’ of regularization with thirteen different techniques that are applied jointly. From those, the optimal subset and their subsidiary hyperparameters are selected. They demonstrate in extensive experiments that the ‘‘cocktails’’ regularization can not only improve the performance of multilayer perceptrons, but these simple models also outperform tree-based architectures. On the downside, the extensive per-data set regularization and hyperparameter optimization take much more computation time than the gradient boosting decision trees algorithm.

There are several other works (Valdes et al., 2021; Fiedler, 2021) showing that strong regularization of deep neural networks is beneficial for tabular data.

5. Tabular Data Generation

For many applications, the generation of realistic tabular data is fundamental. These include data augmentation (Chen et al., 2019) with data imputation (the filling of missing values values) (Gondara and Wang, 2018; Camino et al., 2020) and

	Method	Interpr.	Key Characteristics
Encoding	SuperTML Sun et al. (2019)		Transform tabular data into images for CNNs
	VIME Yoon et al. (2020)	✓	Self-supervised learning and contextual embedding
	IGTD Zhu et al. (2021)		Transform tabular data into images for CNNs
	SCARF Bahri et al. (2021)		Self-supervised contrastive learning
Architectures, Hybrid	Wide&Deep Cheng et al. (2016)		Embedding layer for categorical features
	DeepFM Guo et al. (2017)		Factorization machine for categorical data
	SDT Frosst and Hinton (2017)	✓	Distill neural network into interpretable decision tree
	xDeepFM Lian et al. (2018)		Compressed interaction network
	TabNN Ke et al. (2018)		DNNs based on feature groups distilled from GBDT
	DeepGBM Ke et al. (2019)		Two DNNs, distill knowledge from decision tree
	NODE Popov et al. (2019)		Differentiable oblivious decision trees ensemble
	NON Luo et al. (2020)		Network-on-network model
	DNN2LR Liu et al. (2020)		Calculate cross feature fields with DNNs for LR
	Net-DNF Katzir et al. (2021)		Structure based on disjunctive normal form
	Boost-GNN Ivanov and Prokhorenkova (2021)		GNN on top decision trees from the GBDT algorithm
	SDTR Luo et al. (2021)		Hierarchical differentiable neural regression model
Architectures, Transformer	TabNet Arik and Pfister (2019)	✓	Sequential attention structure
	TabTransformer Huang et al. (2020)	✓	Transformer network for categorical data
	SAINT Somepalli et al. (2021)	✓	Attention over both rows and columns
	ARM-Net Cai et al. (2021)		Adaptive relational modeling with multi-headgated attention network
Regular.	RLN Shavitt and Segal (2018)	✓	Hyperparameters regularization scheme
	Regularized DNNs Kadra et al. (2021)		A "cocktail" of regularization techniques

Table 1

Overview over deep learning approaches for tabular data. We organize them in categories ordered chronologically inside the groups. The interpretable column indicates whether the approach offers some form interpretability for the model's decisions. The key characteristics of every model are summarized.

rebalancing (Engelmann and Lessmann, 2021; Quintana and Miller, 2019; Koivu et al., 2020; Darabi and Elor, 2021) in particular. Another highly relevant topic is privacy-aware machine learning (Choi et al., 2017; Fan et al., 2020; Kamthe et al., 2021) where generated data can be used to overcome privacy concerns.

5.1. Methods

While the generation of images and text is highly explored (Karras et al., 2020; Lin et al., 2017; Subramanian et al., 2017), generating synthetic tabular data is still a challenge. The mixed structure of discrete and continuous features along with their different value distributions has to be managed.

Classical approaches for the data generation task include Copulas (Patki et al., 2016; Li et al., 2020b) and Bayesian Networks (Zhang et al., 2017b), where for the latter those based on the approximation proposed by Chow and Liu (1968) are especially popular. In the deep-learning era, Generative Adversarial Networks (GANs) (Goodfellow et al., 2014) have proven highly successful for the generation of images (Radford et al., 2016; Karras et al., 2020).

GANs were recently introduced as an original way to train a generative deep neural network model. They consist of two separate models: a generator G that generates samples from the data distribution, and a discriminator D that estimates the probability that a sample came from the ground truth distribution. Both G and D are usually chosen to be a non-linear mapping function, such as a multilayer perceptron. To learn a generator distribution p_g over data \mathbf{x} , the generator $G(\mathbf{z}; \theta_g)$ maps samples from a noise distribution $p_z(\mathbf{z})$ (usually the Gaussian distribution) to the input data space. The discriminator $D(\mathbf{x}; \theta_d)$, outputs the probability that a data point \mathbf{x} come from the training data's distribution p_{data} rather than from the generator's output distribution p_g . Both samples from the ground truth data and from the generator are fed to the discriminator.

G and D are both trained together: we adjust parameters for G to minimize $\log(1 - D(G(\mathbf{z})))$ and adjust parameters for D to minimize $\log D(\mathbf{x})$, as if they are following the two-player min-max game with value function $V(G, D)$:

$$\min_G \max_D V(G, D) = \min_G \max_D \mathbb{E}_{\mathbf{x} \sim p_{data}(\mathbf{x})} [\log D(\mathbf{x})] + \mathbb{E}_{\mathbf{z} \sim p_z(\mathbf{z})} [\log(1 - D(G(\mathbf{z})))]. \quad (3)$$

For more details on GANs, we refer the interested reader to the original paper (Goodfellow et al., 2014).

Although it is noted that GANs lag behind at the generation of discrete outputs such as natural language (Subramanian et al., 2017), they are frequently chosen for the tabular data generation task. Vanilla GANs or derivatives such as the Wasserstein GAN (WGAN) (Arjovsky et al., 2017), WGAN with gradient penalty (WGAN-GP) (Gulrajani et al., 2017), Cramér GAN (Bellemare et al., 2017) or the Boundary seeking GAN (Hjelm et al., 2018) which is specifically designed with discrete data in mind are common in the literature. Also, VeeGAN (Srivastava et al., 2017) is frequently used for

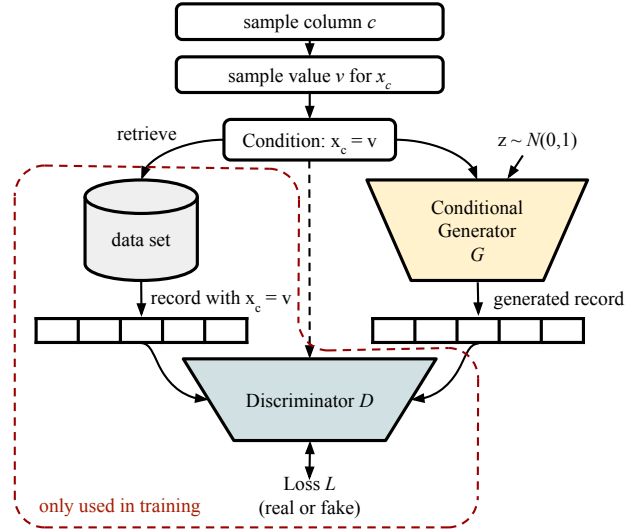


Figure 3: Overview of the CTGAN model. A condition is sampled first and passed to the conditional generator G along with a random input z . The generated sample is opposed to a randomly picked example from the data set that also fulfills the condition and assessed by the conditional discriminator D . This approach allows to preserve dependency relations. Adapted from (Xu et al., 2019).

tabular data. Apart from GANs, autoencoders – in particular Variational Autoencoders (VAEs) proposed by Kingma and Welling (2014) – are investigated (Ma et al., 2020; Xu et al., 2019).

We provide an overview of tabular generation approaches, that use deep learning techniques in Table 2. Note that due to the sheer number of approaches, we list only the most influential works that address the problem of data generation and focus on tabular data in particular. Also, we exclude works that are targeted towards highly domain-specific tasks. An extensive review of existing approaches can also be found in (Engelmann and Lessmann, 2021).

In the following section, we will briefly discuss the most relevant approaches, that helped shape the domain. MedGAN by Choi et al. (2017) was one of the first works and provides a deep learning model to generate patient records. As all the features there are discrete, this model can not be easily transferred to general tabular data. The table-GAN approach by (Park et al., 2018) adapts Deep Convolutional GAN for tabular data. Specifically, the features from one record are converted into a matrix, so that they can be processed by convolutional filters of a convolutional neural network. However, it remains unclear to which extent the inductive bias used for images is suitable for tabular data.

A holistic approach by Xu et al. (2019) focuses on the correlation between the features of one data point. The authors first propose the *mode-specific normalization* technique for data preprocessing, that allows to transform non-Gaussian distributions in the continuous columns. They express numeric values in terms of a mixture component number and the deviation from that component's center. This

allows to represent multi-modal skewed distributions. Their generative solution, coined CTGAN, uses the conditional GAN architecture depicted in Fig. 3 to enforce the learning of proper conditional distributions for each column. To obtain categorical values and to allow for backpropagation in the presence of categorical values, the so-called gumbel-softmax trick (Jang et al., 2017) is utilized. The authors also propose a model based on Variational Autoencoders, named TVAE (for Tabular Variational Autoencoder), that even outperforms the GAN approach. Both approaches can be considered state-of-the-art.

While GANs and VAEs are prevalent, other recently proposed architectures include machine-learned Causal Models (Wen et al., 2021) and Invertible Flows (Kamthe et al., 2021). When privacy is the main factor of concern, models such as PATE-GAN (Jordon et al., 2018) provide generative models with certain differential privacy guarantees. Although very interesting and relevant for practical applications, such privacy guarantees and related federated learning approaches with tabular data are outside the scope of this review.

Fan et al. (Fan et al., 2020) compare a variety of different GAN architectures for tabular data synthesis and recommend using a simple, fully-connected architecture with a vanilla GAN loss with minor changes to prevent mode-collapse. They also use the normalization proposed by (Xu et al., 2019). In their experiments, the Wasserstein GAN loss or the use of convolutional architectures on tabular data does boost the generative performance.

5.2. Assessing Generative Quality

To assess the quality of the generated data, several performance measures are used. The most common approach is to define a proxy classification task and train one model for it on the real training set and another on the artificially generated data set. With a highly capable generator, the predictive performance of the artificial-data model on the real-data test set should be almost on par with its real-data counterpart. This measure is often referred to as *machine learning efficacy* and used in (Choi et al., 2017; Mottini et al., 2018; Xu et al., 2019). In non-obvious classification tasks, an arbitrary feature can be used as a label and predicted (Choi et al., 2017; Camino et al., 2018; Baowaly et al., 2019). Another approach is to visually inspect the modeled distributions per-feature, e.g., the cumulative distribution functions (Chen et al., 2019) or compare the expected values in scatter plots (Choi et al., 2017; Camino et al., 2018). A more quantitative approach is the use of statistical tests, such as the Kolmogorov-Smirnov test (Massey Jr, 1951), to assess the distributional difference (Baowaly et al., 2019). On synthetic data sets, the output distribution can be compared to the ground truth, e.g. in terms of log-likelihood (Xu et al., 2019; Wen et al., 2021). Because overfitted models can also obtain good scores, (Xu et al., 2019) propose evaluating the likelihood of a test set under an estimate of the GAN's output distribution. Especially in a privacy-preserving context, the distribution of the *Distance to Closest Record* (DCR) can be

calculated and compared to the respective distances on the test set (Park et al., 2018).

6. Explanation Mechanisms for Deep Learning with Tabular Data

Explainable machine learning is concerned with the problem of providing explanations for complex machine learning models. Towards this goal, various streams of research follow different explainability paradigms which can roughly be categorized into feature highlighting and counterfactual explanations (Guidotti et al., 2018; Gade et al., 2019).

6.1. Feature Highlighting Explanations

Local input attribution techniques seek to explain the behaviour of machine learning models instance by instance. Those methods aim to understand how all inputs available to the model are being used to arrive at a certain prediction. Some popular approaches for model explanations aim at constructing classification models that are explainable by design (Lou et al., 2012; Alvarez-Melis and Jaakkola, 2018; Wang et al., 2019b). This is often achieved by enforcing the deep neural network model to be locally linear. Moreover, if the model's parameters are known and can be accessed, then the explanation technique can use these parameters to generate the model explanation. For such settings, relevance-propagation-based methods, e.g., Bach et al. (2015); Montavon et al. (2019), and gradient-based approaches, e.g., (Kasneji and Gottron, 2016; Sundararajan et al., 2017; Chattopadhyay et al., 2018), have been suggested. In cases where the parameters of the neural network cannot be accessed, model-agnostic approaches can prove useful. This group of approaches seeks to explain a model's behavior locally by applying surrogate models (Ribeiro et al., 2016; Lundberg and Lee, 2017; Ribeiro et al., 2018; Lundberg et al., 2020; Haug et al., 2021), which are interpretable by design and are used to explain individual predictions of black-box machine learning models. In order to test the performance of these black-box explanations techniques, Liu et al. (2021c) suggest a python based benchmarking library.

6.2. Counterfactual Explanations

From the perspective of algorithmic recourse, the main purpose of counterfactual explanations is to suggest constructive interventions to the input of a deep neural network so that the output changes to the advantage of an end user. By emphasizing both the feature importance and the recommendation aspect, counterfactual explanation methods can be further divided into two different groups: independence-based and dependence-based and approaches.

In the class of independence-based methods, where the input features of the predictive model are assumed to be independent, some approaches use combinatorial solvers to generate recourse in the presence of feasibility constraints (Ustun et al., 2019; Russell, 2019; Rawal and Lakkaraju, 2020; Karimi et al., 2020a). Another line of research deploys gradient-based optimization to find low-cost counterfactual

Method	Based upon	Application
medGAN Choi et al. (2017)	Autoencoder+GAN	Medical Records
TableGAN Park et al. (2018)	DCGAN	General
Mottini et al. (2018)	Cramér GAN	Passenger Records
Camino et al. (2018)	medGAN, ARAE	General
medBGAN, medWGAN Baowaly et al. (2019)	WGAN-GP, Boundary seeking GAN	Medical Records
ITS-GAN Chen et al. (2019)	GAN with AE for constraints	General
CTGAN, TVAE Xu et al. (2019)	Wasserstein GAN, VAE	General
actGAN Koivu et al. (2020)	WGAN-GP	Health Data
VAEM Ma et al. (2020)	VAE (Hierarchical)	General
OVAE Vardhan and Kok (2020)	Oblivious VAE	General
TAEI Darabi and Elor (2021)	AE+SMOTE (in multiple setups)	General
Causal-TGAN Zhao et al. (2021)	Causal-Model, WGAN-GP	General
Copula-Flow Kamthe et al. (2021)	Invertible Flows	General

Table 2

Generation of tabular data using deep neural network models (in chronological order).

explanations in the presence of feasibility and diversity constraints ([Dhurandhar et al., 2018](#); [Mittelstadt et al., 2019](#); [Mothilal et al., 2020](#)). The main problem with these approaches is that they abstract from input correlations.

To alleviate this problem, researchers have suggested building recourse suggestions on generative models ([Pawelczyk et al., 2020a](#); [Downs et al., 2020](#); [Joshi et al., 2019](#); [Mahajan et al., 2019](#); [Pawelczyk et al., 2020b](#); [Antorán et al., 2021](#)). The main idea is to change the geometry of the intervention space to a lower dimensional latent space, which encodes different factors of variation while capturing input dependencies. To this end, these methods primarily use (tabular data) variational autoencoders ([Kingma and Welling, 2014](#); [Nazabal et al., 2020](#)). In particular, [Mahajan et al. \(2019\)](#) demonstrate how to encode various feasibility constraints into such models.

For a more fine-grained overview over the literature on counterfactual explanations we refer the interested reader to the most recent surveys ([Karimi et al., 2020b](#); [Verma et al., 2020](#)). Finally, [Pawelczyk et al. \(2021\)](#) have implemented an open-source python library which provides support for many of the aforementioned counterfactual explanation models.

7. Discussion and Future Prospects

In this section, we summarize our findings and discuss current and future trends in deep learning approaches for tabular data (Section 7.1). Moreover, we identify several open research questions that could be tackled to advance the field of tabular deep neural networks (Section 7.2).

7.1. Summary and Trends

Tabular Data Preprocessing Many of the challenges for deep neural networks on tabular data are related to the heterogeneity of the data (e.g., categorical and sparse values). Therefore, some deep learning solutions transform them into a homogeneous representation more suitable to neural networks. While the additional overhead is small, such transforms can boost performance considerably and should thus be among the first strategies applied in real-world scenarios.

Architectures for Deep Learning on Tabular Data. Architecture-wise, there has been a clear trend towards transformer-based solutions (Section 4.2.2) in recent years. These approaches offer multiple advantages over standard

neural network architectures, for instance, learning with attention over both categorical and numerical features. Moreover, self-supervised or unsupervised pre-training that leverages unlabeled tabular data to train parts of the deep learning model is gaining popularity, not only among transformer-based approaches.

Performance-wise, multiple independent evaluations demonstrate that deep neural network methods from the hybrid (Sec. 4.2.1) and transformers-based (Sec. 4.2.2) groups exhibit superior predictive performance compared to plain deep neural networks on various data sets (Gorishniy et al., 2021; Ke et al., 2018, 2019; Somepalli et al., 2021). This underlines the importance of special-purpose architectures for tabular data.

Regularization Models for Tabular Data. It has also been shown that regularization reduces the hypersensitivity of deep neural network models and improves the overall performance (Shavitt and Segal, 2018; Kadra et al., 2021). We believe that regularization is one of the crucial aspects for a more robust and accurate performance of deep neural networks on tabular data and is gaining momentum.

Deep Generative Models for Tabular Data. Powerful tabular data generation is essential for the development of high-quality models, particularly in a privacy context. With suitable data generators at hand, developers can use large, synthetic, and yet realistic data sets to develop better models, while not being subject to privacy concerns (Jordon et al., 2018). Unfortunately, the generation task is as hard as inference in predictive models, so progress in both areas will likely go hand in hand.

Interpretable Deep Learning Models for Tabular Data. Interpretability is undoubtedly desirable, particularly for tabular data models frequently applied to personal data, e.g., in healthcare and finance. An increasing number of approaches offer it out-of-the-box, but most current deep neural network models are still mainly concerned with the optimization of a chosen error metric. Interpretable deep tabular learning is essential for understanding model decisions and results, especially for life-critical applications. Model explanations can be used to identify and mitigate potential bias or eliminate unfair discrimination against certain groups (Ntoutsis et al., 2020).

Learning From Evolving Data Streams. Many modern applications are subject to continuously evolving data streams, e.g., social media, online retail, or healthcare. Streaming data are usually heterogeneous and potentially unlimited. Therefore, observations must be processed in a single pass and cannot be stored. Indeed, online learning models can only access a fraction of the data at each time step. Furthermore, they have to deal with limited resources and shifting data distributions (i.e., concept drift). Hence, hyperparameter optimization and model selection, as typically involved in deep learning, are usually not feasible in a data stream. For this reason, despite the success of deep learning in other domains, less complex methods such as incremental decision trees (Domingos and Hulten, 2000; Manapragada et al., 2018) are often preferred in online learning applications.

7.2. Open Research Questions

Several open problems need to be addressed in future research. In this section, we will list those we deem fundamental to the domain.

Information-theoretic Analysis of Encodings. Encoding methods are highly popular when dealing with tabular data. However, the majority of data preprocessing approaches for deep neural networks are lossy in terms of information content. Therefore, it is challenging to achieve an efficient, almost lossless transformation of heterogeneous tabular data into homogeneous data. Nevertheless, the information-theoretic view on these transformations remains to be investigated in detail and could shed light on the underlying mechanisms.

Computational Efficiency in Hybrid-Models. The work by Shwartz-Ziv and Armon (2021) suggests that the combination of a gradient boosting decision tree and deep neural networks may improve the predictive performance of a machine learning system. However, it also leads to growing complexity. Training or inference times, which far exceed those of classical machine learning approaches, are a recurring problem developing hybrid models. We conclude that the integration of state-of-the-art approaches from classical machine learning and deep learning has not been conclusively resolved yet and future work should be conducted on how to mitigate the trade-off between predictive performance and computational complexity.

Spezialized Regularizations. We applaud recent research on regularization methods, in which we see a promising direction that necessitates further exploration. In particular, whether context- and architecture-specific regularizations for tabular data can be found, remains an open question. Additionally, it is relevant to explore the theoretical constraints that govern the success of regularization on tabular data more profoundly.

Novel Processes for Tabular Data Generation. For tabular data generation, modified Generative Adversarial Networks and Variational Autoencoders are prevalent. However, the modeling of dependencies and categorical distributions remains the key challenge. Novel architectures in this area, such as diffusion models, have not been adapted to the domain of tabular data. Furthermore, the definition of an entirely new generative process particularly focused on tabular data might be worth investigating.

Unified Benchmarking. There is no consensus in the machine learning community on how to do a fair and efficient comparison for deep neural networks on tabular data. Kadra et al. (2021) use about 40 different tabular data sets for assessing the predictive performance of machine learning algorithms. Shwartz-Ziv and Armon (2021) show that the choice of benchmarking data sets can have a non-negligible impact on the performance assessment. Because of the excessive number of data sets, there is a necessity for a standardized benchmarking procedure. *For tabular data generation tasks*, Xu et al. (2019) propose a sound evaluation framework with artificial and real-world data sets (Sec. 5.2), but researchers need to agree on common benchmarks in this subdomain as well.

Interpretability Going forward, counterfactual explanations for deep tabular learning can be used to improve the perceived fairness in human-AI interaction scenarios and to enable personalized decision-making (Verma et al., 2020). However, the heterogeneity of tabular data poses problems for counterfactual explanation methods to be reliably deployed in practice. Devising techniques aimed at effectively handling heterogeneous tabular data in the presence of feasibility constraints is still an unsolved task (Pawelczyk et al., 2021).

Transfer of Deep Learning Methods to Data Streams. Recent work shows that some of the limitations of neural networks in an evolving data stream can be overcome (Sahoo et al., 2017; Duda et al., 2020). Conversely, changes in the parameters of a neural network may be effectively used to weigh the importance of input features over time (Haug et al., 2020) or to detect concept drift (Haug and Kasneci, 2021). Accordingly, we argue that deep learning for streaming data – in particular strategies for dealing with evolving and heterogeneous tabular data – should receive more attention in the future.

Transfer Learning for Tabular Data. Reusing knowledge gained solving one problem and applying it to a different task is the research problem addressed by transfer learning. While transfer learning is successfully used in computer vision and natural language processing applications (Tan et al., 2018), there are no efficient and generally accepted ways to do transfer learning for tabular data. Hence, a general research question can be how to share knowledge between multiple (related) tabular data sets efficiently.

Data Augmentation for Tabular Data. Data augmentation has proven highly effective to prevent overfitting, especially in computer vision (Shorten and Khoshgoftaar, 2019). While some data augmentation techniques for tabular data exist, e.g., SMOTE-NC (Chawla et al., 2002), simple models fail to capture the dependency structure of the data. Therefore, generating additional samples in a continuous latent space is a promising direction. This was investigated by Darabi and Elor (2021) for minority oversampling. Nevertheless, the reported improvements are only marginal. Thus, future work is required to find simple, yet effective random transformations to enhance tabular training sets.

Self-supervised Learning. Large-scale labeled data are usually required to train deep neural networks, however, the data labeling is an expensive task. To avoid this expensive step, self-supervised methods propose to learn general feature representations from available unlabeled data. These methods have shown astonishing results in computer vision and natural language processing (Jing and Tian, 2020; Liu et al., 2021b). Only a few recent works in this direction (Yoon et al., 2020; Bahri et al., 2021) deal with heterogeneous data. Hence, novel self-supervised learning approaches dedicated to tabular data might be worth investigating.

8. Conclusion

This survey is the first work to systematically explore deep neural network approaches for heterogeneous tabular data. In

this context, we highlighted the main challenges and research advances in modeling, explaining, and generating aspects of tabular data. We also introduced a unified taxonomy that categorizes deep learning approaches for tabular data into three branches: data encoding methods, specialized architectures models, and regularization models. We believe our taxonomy will help catalog future research and better understand and address the remaining challenges in applying deep learning to tabular data. We hope it will help researchers and practitioners to find the most appropriate strategies and methods for their applications.

Due to the importance of tabular data to industry and academia, new ideas in this area are in high demand and can have a significant impact. With this review, we hope to provide interested readers with the references and insights they need to effectively address open challenges and advance the field.

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