

# Autoencoder-based cleaning in probabilistic databases

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## Abstract

In the field of data integration, data quality problems are often encountered when extracting, combining, and merging data. The probabilistic data integration approach represents information about such problems as uncertainties in a probabilistic database. In this paper, we propose a data-cleaning autoencoder capable of near-automatic data quality improvement. It learns the structure and dependencies in the data to identify and correct doubtful values. A theoretical framework is provided, and experiments show that it can remove significant amounts of noise from categorical and numeric probabilistic data. Our method does not require clean data. We do, however, show that manually cleaning a small fraction of the data significantly improves performance.

**Keywords**— data cleaning, probabilistic databases, autoencoders

## I. INTRODUCTION

Data quality problems are a large threat in data science. Specifically, in the field of *data-integration*, i.e., combining several data sources into a single and unified view [1], often uncertainties are encountered when extracting, combining, and merging data. These uncertainties can result from the nature of data (such as noise in measurements), but can also be a result of the integration process itself. Information about these uncertainties is considered an important result of the integration process [2]. In *probabilistic data integration* (PDI), the integration result as well as information on uncertainty is stored in a *probabilistic database* (PDB) [3]. The PDB maintains possible alternatives for values and records, their likelihoods, and the dependencies among them.

The PDI process (see Figure 1) consists of two main phases. The *integration* phase constructs a partial integration containing unresolved issues as alternative integration results. This phase is followed by the *improvement* phase, which gathers evidence while the data is being used for the purpose of gradually improving its quality. An example of obtaining evidence is when users provide feedback on the correctness of query answers, which can be used to rule out certain alternatives, hence reducing uncertainty and improving data quality. Evidence, however, need not always come from users. Also, patterns in the data itself can be used as evidence for a higher or lower likelihood of particular data values. In this paper, we propose a machine learning technique for automatically improving data quality. In particular, our approach is based on an *autoencoder* (see, for instance, [4]), a machine learning technique that can learn the structure and dependencies in data. Autoencoders are traditionally used for dimensionality reduction and denoising [4]. In this paper, we demonstrate that autoencoders also have great potential for improving data quality in probabilistic databases. In particular, we present a method that i) reduces overall uncertainty in records, but also ii) identifies and corrects records in which there is little uncertainty, but whose values are doubtful because they are not in line with the other records in the database. We refer to our proposed solution as a *data-cleaning autoencoder* (DCAE).

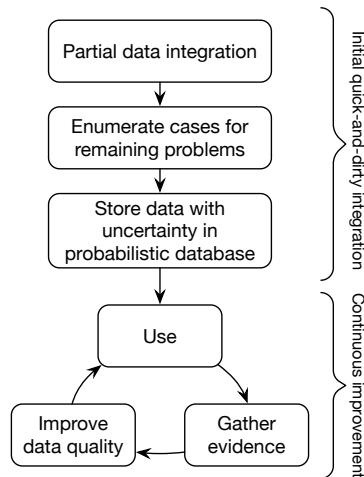


Fig. 1: Probabilistic Data Integration [3].

*a) Contributions:*

- An autoencoder-based approach for cleaning of data with categorical and numeric attributes. The basic approach is unsupervised, meaning that it does not require clean data (i.e. correct without uncertainty) for training.
- An extension of the basic approach in which a small fraction of the records is manually cleaned. A semi-supervised approach is used in which the clean records are used as labelled data.
- A method for generating synthetic test data with embedded dependencies for the purpose of evaluating our cleaning approach.
- Experimental evaluation of the cleaning performance under many varying circumstances: levels and kinds of uncertainty and errors, different architectures, and several data parameters and architecture hyperparameters.

*b) Outlook:* Section II provides related work on probabilistic databases and autoencoders, introduces notation, and describes the intuition behind applying autoencoders for the purpose of data cleaning. Section III describes the proposed solution by formalizing its core as a machine learning problem. Section IV introduces our evaluation framework and experimental setup. Section V presents the experimental results and we conclude with Section VI containing conclusions and future work.

## II. PRELIMINARIES AND RELATED WORK

### A. Probabilistic databases

Various probabilistic databases have been proposed. Examples include MayBMS [5], Trio [6], and MCDB [7] for uncertain relational data, and IMPrECISE [8, 9] and others [10] for uncertain XML. Also, probabilistic logics have been defined to capture and reason with uncertain information [11, 12, 13]. There is much variety in how the uncertainty is modelled in these systems. For example, MayBMS’s U-relations [14] focus on tuple-level uncertainty where probabilities are attached to tuples, while MCDB focuses on attribute-level uncertainty where a probabilistic value generator function captures the possible values for the attribute. These uncertainty models vary in expressiveness [10]. In models that only attach probabilities to tuples, the uncertainty of the tuples is inherently independent of each other. In contrast, the world set descriptors of MayBMS and the descriptive sentences of JudgeD [12] also allow them to express complex dependencies

	Eye colour		Hair colour	
	<i>Blue</i>	<i>Brown</i>	<i>Light</i>	<i>Dark</i>
<b>1</b>	0.7	0.3	1.0	0.0
<b>2</b>	0.8	0.2	0.9	0.1
<b>3</b>	0.0	1.0	0.5	0.5

TABLE I: Example Probabilistic database (PDB).

involving full dependence and mutual exclusion [15] necessary for faithfully capturing the possible outcomes of a data integration process.

### B. Uncertainty model and assumptions

In this paper, we focus on attribute-level uncertainty in categorical attributes of relational data. Uncertainty of an attribute value is modelled as a probability distribution over all possible values for that attribute, i.e., with a probability for each possible value summing up to 1. To illustrate, the uncertainty that the colour of a car is green or blue, but not red, is modelled as assigning probabilities 0.5, 0.5, and 0 to the possible values “green”, “blue”, and “red”, respectively.

We use the following notation for our uncertainty model:

- Without loss of generality, we restrict our attention to a single table with  $N$  attributes and  $M$  records.
- Let  $\mathcal{A}$ ,  $|\mathcal{A}| = N$ , be the set of names of the attributes. If not stated otherwise, we assume  $\mathcal{A} = \{1, 2, \dots, N\}$ .
- All attributes are categorical. Attribute  $j \in \mathcal{A}$  takes values in  $\mathcal{K}_j$ . Let  $K_j = |\mathcal{K}_j|$ , i.e., attribute  $j$  can take  $K_j$  different categories. If not stated otherwise, we assume  $\mathcal{K}_j = \{1, 2, \dots, K_j\}$ .
- The likelihood of the value of attribute  $j$  in record  $i$  is represented as a probability mass function  $p_{ij}$  over  $\mathcal{K}_j$ , where  $p_{ij}(k)$  is the probability that the attribute has value  $k \in \mathcal{K}_j$ .
- Let  $x_i$  denote the  $i$ -th record. In the remainder it will be useful to represent  $x_i$  as the concatenation of all probability mass functions, i.e., if  $\mathcal{A} = \{1, 2, \dots, N\}$  and  $\mathcal{K}_j = \{1, 2, \dots, K_j\}$  for all  $j \in \mathcal{A}$  we obtain

$$x_i = (p_{i1}(1), p_{i1}(2), \dots, p_{i1}(K_1), p_{i2}(1), \dots, p_{i2}(K_2), p_{i3}(1), \dots, p_{iN}(K_N)). \quad (1)$$

We illustrate our notation through the example database that is depicted in Table I. In this database we have:

$$\mathcal{A} = \{\text{eye colour}, \text{hair colour}\}, \quad (2)$$

$$\mathcal{K}_{\text{eye colour}} = \{\text{blue}, \text{brown}\}, \quad \mathcal{K}_{\text{hair colour}} = \{\text{light}, \text{dark}\}, \quad (3)$$

and, for instance

$$x_1 = (0.7, 0.3, 1.0, 0.0), \quad (4)$$

$$p_{1,\text{eye colour}} = (0.7, 0.3), \quad (5)$$

$$p_{1,\text{eye colour}}(\text{blue}) = 0.7. \quad (6)$$

The above model covers only categorical attributes. For probabilistic databases, extensions to the discrete categorical distribution model exist, allowing for the use of probabilities with a continuous distribution [16]. In Section III-E we explain how we deal with continuous attributes.

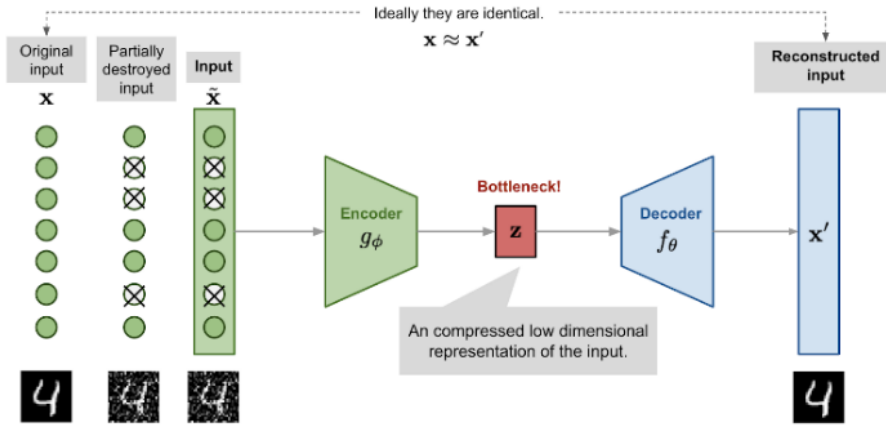


Fig. 2: An example of how a denoising autoencoder can remove artificial noise from data [18].

### C. Autoencoders

The *autoencoder* (AE) dealt with in this paper is a feedforward, non-recurrent neural network having an input layer, several hidden layers and an output layer with the same number of nodes as the input layer. An AE is meant to learn the structure and patterns in the input data to reproduce its input according to this structure and these patterns. To achieve this, constraints (such as a reduced dimensionality of the middle layer) are added to force the network to learn a representation of the training data with a reduced feature space. An AE is usually an *unsupervised* learning method, as no other prior knowledge about the data (i.e., in terms of targets) is required for this process [17]. A typical use of an AE is for noise-cancelling in images: given an input image, it can learn to reproduce the image in the output without the noise. This can be achieved using only unsupervised learning, but performance can be improved by using semi-supervised or supervised learning, where the intended output of the AE is used during training.

An AE consists of an encoder  $g_\phi(\cdot) : \mathcal{X} \rightarrow \mathcal{H}$  and decoder  $f_\theta(\cdot) : \mathcal{H} \rightarrow \mathcal{X}$ , parameters  $\phi$  and  $\theta$  are the weights and biases of the encoder and decoder, respectively. These parameters are trained via minimizing the loss function  $\mathcal{L}$  which is a measure for reconstruction error:

$$\phi, \theta = \arg \min_{\phi, \theta} \mathcal{L}(Y, f_\theta(g_\phi(X))), \quad (7)$$

where  $Y$  represents the desired output,  $X$  represents the set of training data and  $f_\theta(g_\phi(X))$  represents the output to the AE based on input  $X$ . In the case of unsupervised learning (the standard use case for AE's), the desired output is taken as  $Y = X$ . In a supervised setting, for instance, in image denoising  $X$  represents noisy image and the corresponding noise-free version.

As mentioned, an AE is well known for its dimensionality reduction and noise-cancelling ability. Other uses for AEs include anomaly (outlier) detection, where the input is determined to be an anomaly if the network is unable to reconstruct the input [19]. Note that nothing in Equation (7) prevents the AE from not learning the identity function, which is an extreme case of overfitting. Several types of AEs exist with designs that mitigate this problem. These types of AEs are not mutually exclusive, and they may (and in fact, we do so in our DCAE) be combined [20]:

- An *undercomplete autoencoder* has a hidden middle layer with a lower dimensionality than the input or output spaces. This implicit regularization ensures that the AE has to learn to capture the most important features from the data for it to be able to reconstruct its input well.

- A *denoising autoencoder* has noise added to the input data before being fed to the network. The AE then is forced to learn how to remove this noise because the loss function compares the output with the original, clean input data. This prevents overfitting and enhances its noise-cancelling capabilities [17]. An example of such an AE can be found in Figure 2.
- A *sparse autoencoder* adds a sparsity penalty to the training criterion. The AE is now also penalized on the number of active neurons in the code (middle) layer. This constraint encourages the AE to retain a more meaningful representation of the data in the code layer.
- A *variational autoencoder* (VAE) consists of an encoder section that passes both a tensor of means and a tensor of standard deviations to the decoder section, instead of deterministic variables as is usually the case. A term consisting of the Kullback-Leibler divergence [21] between this distribution, and a standard normal distribution is added to the loss function. A sample is taken from this distribution and fed to the decoder section [22]. The VAE ensures that the learned latent space representation is continuous (meaning that neighbouring data points should lead to similar outputs) and complete (all inputs should lead to a sensible output). Moreover, the attributes in the latent space are orthogonal, a property that is known as disentanglement.

#### D. Application of AEs to data cleaning

Our application of an AE is data cleaning. We argue that data cleaning can be seen as *noise-cancelling in records*. Whereas in images, noise is formed by pattern-less deviations in the colour of pixels, data quality problems in relational data can be regarded as pattern-less deviations in the values of attributes. The AE in our approach is meant to learn the structure and patterns in the relational data for the purpose of reproducing its records, suggesting adjustments to its attribute values for them to be more in line with the structure and patterns in the data set. This also motivates our use of probabilistic data as it allows the AE to indicate with probabilities weak and strong recommendations for adjustments to the attribute values.

Our DCAE can be used in various scenarios. Given a data set with suspected data quality problems, an AE can be used to identify suspicious attribute values for manual inspection. Note that it is in principle an unsupervised approach, so no laborious labelling is necessary beforehand, although we have extended our approach such that it can exploit labelled data. We show that labelling a small fraction of the significantly improves the performance.

The approach can also be used as a data cleaning step in the aforementioned PDI process (see Figure 1). About the latter, it should be remarked that the AE in our approach abstracts from the dependencies stored in a probabilistic database (see Section II-B). It takes as input probabilities derived from the world set descriptors [14] or descriptive sentences [15] and produces ‘new’ probabilities. It may seem that the dependencies necessary for expressing things like mutual exclusion are lost in the process. However, the dependencies can be retained by regarding the output of the AE as *soft evidence* with which the probabilistic database is conditioned [23]. For the output of the AE, a soft rule can be constructed with a trust level of  $\alpha$ , and then we incorporate this evidence by conditioning the probabilistic database. In a sense, the original data is trusted with a level of  $1 - \alpha$ .

Note that the overall effect of only training an AE on the noisy data is that the structure of the data as learned by the AE includes the uncertainty and errors of this data. As long as the amount of noise is limited, the AE will suggest corrections on how to remove that uncertainty from records affected by noise. Also, there may be records for which the PDI process indicated no uncertainty, but that are wrong. The corrections on these records will perturb them towards the general structure that has been learned. Effectively, the AE introduces uncertainty on these records, indicating a doubt on the correctness of these records. Finally, because all records will be

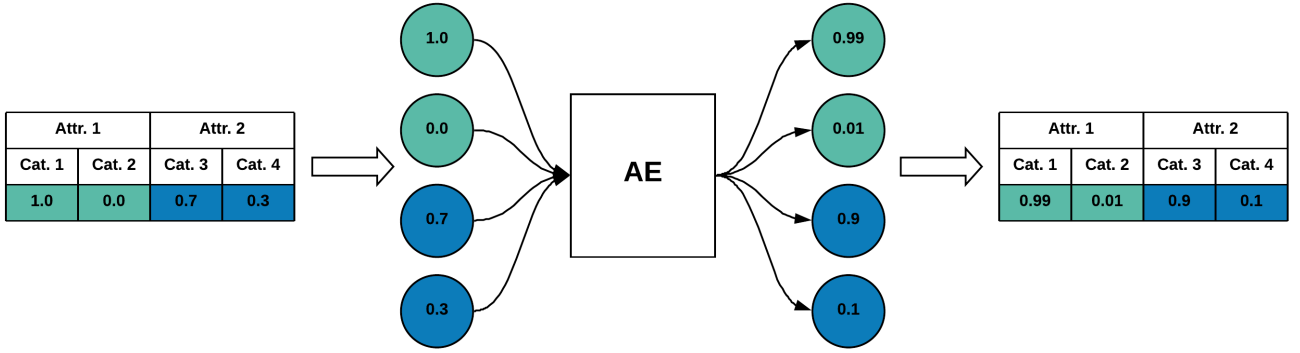


Fig. 3: DCAE: Input and output representation.

perturbed towards the general structure, correct records without uncertainty will also be affected by introducing small amounts of uncertainty. This effect is expected to be limited; we verify this through numerical experiments in Section V.

### III. PROBLEM FORMULATION & PROPOSED SOLUTION

As explained in Section I, our goal is to improve the data quality in a PDB by means of an AE that learns the structure of the data and is able to identify and correct outliers. We refer to such an autoencoder as a data-cleaning autoencoder (DCAE). Our idea is to use records of the probabilistic database  $\mathcal{D}_{\text{PDB}}$  as input to the DCAE so that the DCAE learns the structure of this probabilistic data. The DCAE operates on a per-record basis, providing a cleaned record at its output. This is illustrated in Figure 3. More details are provided in the remainder of this section.

#### A. Input and output representation

Vectors  $x_i$  of the form of Equation (1) are used as input for our AE. As a result, each attribute  $j \in \mathcal{A}$  has  $K_j$  corresponding nodes in the input layer of the model, one for each possible category from  $\mathcal{K}_j$ . In total, the model then has  $\sum_{j=1}^N K_j$  of input nodes.

We denote by  $y_i$  the output corresponding to input  $x_i$ . The number of output nodes (i.e., dimension of  $y_i$ ) is equal to the number of input nodes (i.e., dimension of  $x_i$ ). Similar to Equation (1) we denote  $y_i$  as

$$y_i = (q_{i1}(1), q_{i1}(2), \dots, q_{i1}(K_1), q_{i2}(1), \dots, q_{i2}(K_2), q_{i3}(1), \dots, q_{iN}(K_N)), \quad (8)$$

where  $q_{ij}$  is the output probability distribution for attribute  $j \in \mathcal{A}$ , i.e.,  $q_{ij}$  is the cleaned version of  $p_{ij}$ .

In order to ensure that  $q_{ij}$  is a probability distribution over  $\mathcal{K}_j$ , the last layer in our network is a per-attribute softmax [4, Section 6.2.2.3], as illustrated in Figure 4. More specifically, we let

$$q_{ij}(k) = \frac{e^{\bar{q}_{ij}(k)}}{\sum_{k=1}^{K_j} e^{\bar{q}_{ij}(k)}}, \quad \forall k \in \mathcal{K}_j, j \in \mathcal{A}, \quad (9)$$

where

$$(\bar{q}_{i1}(1), \bar{q}_{i1}(2), \dots, \bar{q}_{i1}(K_1), \bar{q}_{i2}(1), \dots, \bar{q}_{i2}(K_2), \bar{q}_{i3}(1), \dots, \bar{q}_{iN}(K_N)) \quad (10)$$

is the input to this softmax layer.

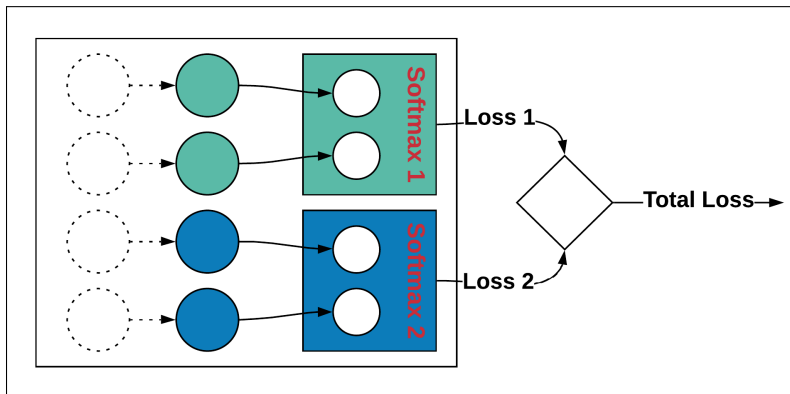


Fig. 4: Per-attribute softmax function in the output layer and overall loss function.

### B. Autoencoder architecture

The standard AE architecture that we use for our DCAE model is given in Figure 5. The AE consists of an input layer consisting of  $\sum_{j=1}^N K_j$  nodes (see Section III-A). In (and only in) the training process, Gaussian noise is added so that the AE becomes a denoising AE that has to learn to remove the Gaussian noise, see Section II-C. In Section V, we explore various parameter settings to justify our choice for the amount of Gaussian noise that we add to this layer. This layer is then fully connected to the input layers of each of five sub-channels, having the same number of nodes. Each channel uses a different and fixed activation function (sin, cos, linear, ReLU and Swish). The idea behind this is that each channel can capture a different non-linearity in the input data, which mostly linear activation functions like ReLU would not capture. This is similar to a convolutional layer leading to multiple channels capturing different structures. Then, for each sub-channel, the input layer is fully connected to the hidden layer of each sub-channel. Each hidden layer has  $N$  nodes. This approach encourages the encoder section to produce one "best guess" for each of the  $N$  PDB attributes as its output, like in a regression network. As a result, the decoder section is meant to learn to produce a one-hot encoding of this number. Each hidden layer from a sub-channel is again fully connected to the output layer of each sub-channel. Those five output layers are in turn fully connected to a single output layer having again  $\sum_{j=1}^N K_j$  nodes that uses a softmax as activation function (see Section III-A).

We tried various modifications of this architecture in an attempt to increase performance, none of which succeeded. Turning the DCAE into a VAE (see Section II-C by doubling the size of the encoder section's output to form the parameters  $\mu_{\text{latent}}$  and  $\sigma_{\text{latent}}$  which are used to sample from a normal  $N(\mu_{\text{latent}}, \sigma_{\text{latent}})$ , and adding a penalty to the loss function based on this distribution's deviation from  $N(0, 1)$  did not lead to a reliable performance increase. Using 1D convolutional layers [4] led to the best performance with only one convolutional layer, which had 64 output channels and a kernel size of 3 and a stride of 1. However, its performance was always worse than the architecture without convolutional layers. Another attempt to increase performance incorporated the use of an RBF [24] kernel to imitate a support-vector machine. The best performance using this modification was seen when using 100 landmarks, but its performance was always worse than without the RBF kernel. The details of these experiments are provided in [25].

### C. Loss function

As the data is of probabilistic nature and more specifically consists of records that are themselves ensembles of categorical probability distributions (see Equation (1)), it makes sense to use a loss

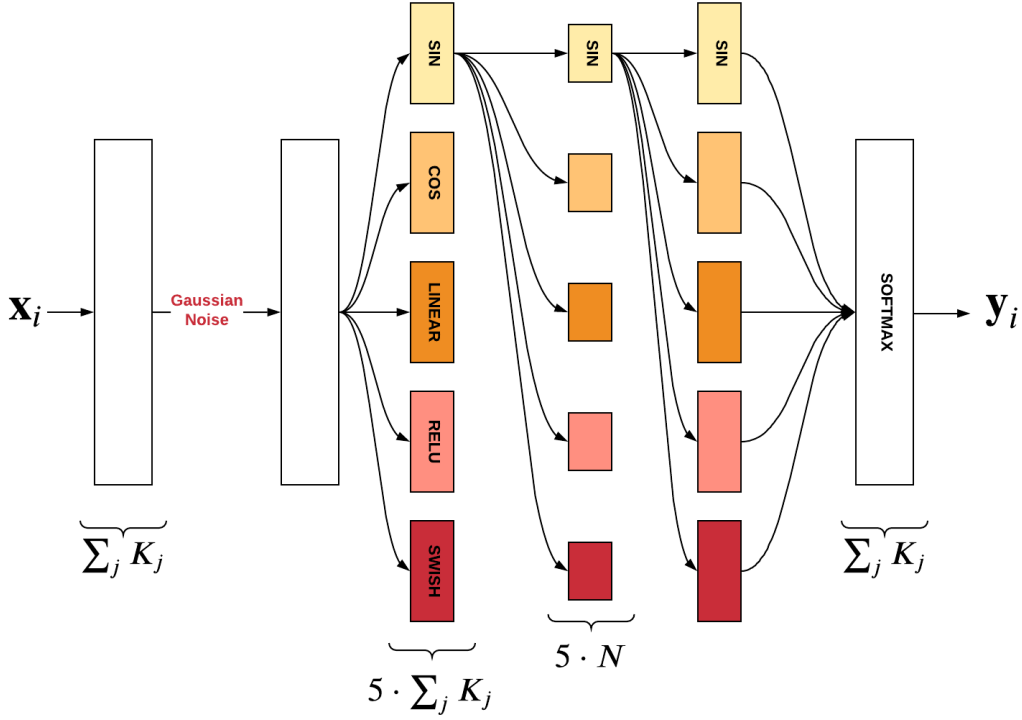


Fig. 5: Default architecture of the AE. Gaussian noise is only added during the training process.

function that can measure the distance between probability distributions. We denote by  $\mathcal{L}(x_i, y_i)$  the loss function of the DCAE, i.e., the loss at input record  $x_i$  and output record  $y_i$ . Our loss function is a summation of loss per attribute, i.e.,

$$\mathcal{L}(x_i, y_i) = \sum_{j \in \mathcal{A}} \mathcal{L}_j(p_{ij}, q_{ij}), \quad (11)$$

where  $\mathcal{L}_j(p_{ij}, q_{ij})$  denotes the loss for attribute  $j$ . This is illustrated in Figure 4. The most commonly used probabilistic loss function is the categorical cross-entropy loss, often called the “log loss” [26, Chapter 4.3.2], defined by:

$$\mathcal{L}_j(p_{ij}, q_{ij}) = - \sum_{k \in \mathcal{K}_j} p_{ij}(k) \log q_{ij}(k). \quad (12)$$

Because this loss function is so common, we sometimes use it in our experiments as a baseline.

Intimately related, and in fact, identical up to a constant [4] to the log loss, is the Kullback–Leibler divergence[21], defined as

$$D_{KL}(p_{ij} \parallel q_{ij}) = \sum_{k \in \mathcal{K}_j} p_{ij}(k) \log \frac{p_{ij}(k)}{q_{ij}(k)}. \quad (13)$$

For the case that one of  $q_{ij}(k)$  is zero, these functions are defined as  $\infty$ . For our application in a DCAE, this is troublesome because  $q_{ij}(k) = 0$  corresponds to the often encountered situation of no uncertainty for attribute  $j$  in record  $x_i$ . Having extremely large (or  $\infty$ ) values for our loss function hampers learning. Therefore, we often use

the Jensen-Shannon divergence (JSD)[27], which circumvents this problem. It is defined as

$$JSD(p_{ij} \parallel q_{ij}) = \frac{1}{2} D_{KL}(p_{ij} \parallel r_{ij}) + \frac{1}{2} D_{KL}(q_{ij} \parallel r_{ij}), \quad (14)$$



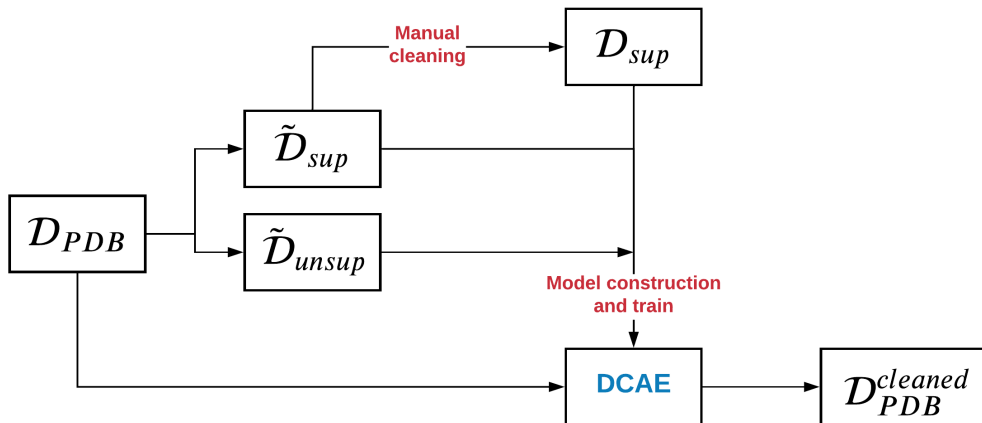


Fig. 6: Semi-supervised training.

where  $r_{ij}(k) = (p_{ij}(k) + q_{ij}(k)) / 2$ . The JSD measures how different probability distributions are; a larger JSD means a larger difference. By using this JSD as loss function, the AE learns to minimize the difference between the probability distributions  $p_{ij}$  and  $q_{ij} \forall j \in \mathcal{A}$ .

When evaluating the performance of our approach we calculate the loss between two probabilistic databases  $X$  and  $Y$ . This is defined as the sum of the loss value over the individual records, i.e.,

$$\mathcal{L}(X, Y) = \sum_{i=1}^M \mathcal{L}(x_i, y_i), \quad (15)$$

where the loss for one record,  $\mathcal{L}(x_i, y_i)$ , is defined in Equation (11).

#### D. Semi-supervised approach

As mentioned in the introduction, the improvement phase of a PDI process often involves manual data cleaning via, e.g. user feedback or inspection by domain experts. Our basic approach does not require such manual cleaning, and the corresponding machine learning problem is unsupervised.

In addition to this unsupervised approach, we also investigate the performance of including a small fraction of manually cleaned records. Besides learning the DCAE model to improve the data quality in an unsupervised setting, we thus also investigate the performance of the DCAE model in a semi-supervised setting. This means that the DCAE is trained on and applied to a PDB for which we know for a (small) subset what the outcome should be. In other words, given the probabilistic data  $\mathcal{D}_{PDB}$ , we partition it into a set  $\tilde{\mathcal{D}}_{unsup}$  for which we do not know the ground truth, and a set  $\tilde{\mathcal{D}}_{sup}$  for which we do know the ground truth. These ground truth labels are denoted with  $\mathcal{D}_{sup}$ . This is a semi-supervised setting: the DCAE is given  $\tilde{\mathcal{D}}_{unsup}$  and  $\tilde{\mathcal{D}}_{sup}$  as input and is trained to return  $\tilde{\mathcal{D}}_{unsup}$  and  $\mathcal{D}_{sup}$ , respectively. This is depicted in Figure 6.

#### E. Extension to continuous attributes

So far, both the PDB model in Section II-B and the description of the input and output representation from Section III-A require the data to be categorical. In order to use this framework for continuous data we quantize the continuous attributes, resulting in discrete, categorical data. More precisely, for each continuous attribute  $j \in \mathcal{A}$ , the sample space is partitioned into  $K_j$  bins, resulting in a histogram representation of the uncertainty.

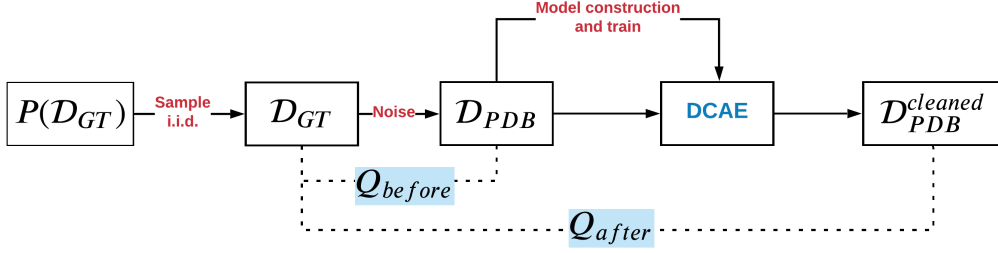


Fig. 7: Evaluation process for the unsupervised setting.

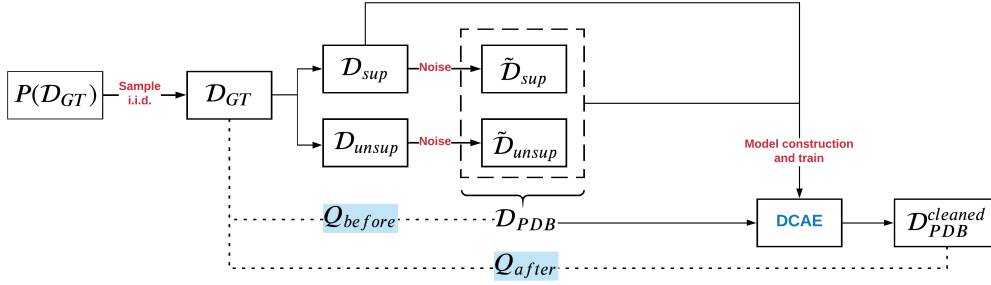


Fig. 8: Evaluation process for the semi-supervised setting.

More precisely, suppose attribute  $j$  is taking values in the interval  $[a, b]$ . We perform binning based on  $K_j + 1$  thresholds  $L_k$ ,  $k = 0, 1, \dots, K_j$  that satisfy

$$a = L_0 < L_1 < \dots < L_{K_j} = b. \quad (16)$$

In our experiments we work with  $L_k = a + k \cdot \frac{b-a}{K_j}$ ,  $k = 0, 1, \dots, K_j$ .

Now, if the value in record  $i$  is represented as a random variable with cumulative distribution function (CDF)  $F_{ij}(x)$ , the resulting categorical probability distribution is

$$p_{ij}(k) = F_{ij}(L_k) - F_{ij}(L_{k-1}), \quad k = 1, 2, \dots, K_j. \quad (17)$$

In this setting, we refer to  $K_j$  as the *sampling density* for attribute  $j$ .

## IV. METHODOLOGY

### A. Overview of performance evaluation framework

To get insight into the behaviour of our proposed solution and the impact of various design choices, we perform experiments in a well-controlled setting with synthetic data. We use a different performance valuation framework for the unsupervised and semi-supervised setting. An overview of these frameworks is given in Figure 7 and Figure 8. The details are provided below.

The elements of these frameworks are as follows:

- 1) We start from a synthetic database in which there is no uncertainty and no errors. We refer to this data as our ground truth  $\mathcal{D}_{GT}$  data, which can be seen as a data set that is sampled i.i.d. from an underlying ground truth data generating distribution  $P(\mathcal{D}_{GT})$ . We provide more details in Section IV-B.
- 2) We split  $\mathcal{D}_{GT}$  into a labeled set and an unlabeled set, denoted as  $\mathcal{D}_{sup}$  and  $\mathcal{D}_{unsup}$ , respectively. For unsupervised learning,  $\mathcal{D}_{unsup} = \mathcal{D}_{GT}$  and  $\mathcal{D}_{sup} = \emptyset$ .

- 3) Both  $\mathcal{D}_{\text{sup}}$  and  $\mathcal{D}_{\text{unsup}}$  are corrupted through the same noise process that yields  $\tilde{\mathcal{D}}_{\text{sup}}$  and  $\tilde{\mathcal{D}}_{\text{unsup}}$ , respectively. This noise represents the uncertainty in the PDB. Together, they form  $\mathcal{D}_{\text{PDB}}$ , a corrupted version of the ground truth, similar to real-world probabilistic databases. In Section IV-C we provide more details on this noise and how it is added.
- 4) The DCAE model is trained using  $\tilde{\mathcal{D}}_{\text{unsup}}$  and  $\tilde{\mathcal{D}}_{\text{sup}}$ . Note, that  $\mathcal{D}_{\text{sup}}$  corresponds to the manually cleaned version of  $\tilde{\mathcal{D}}_{\text{sup}}$ . Therefore, we additionally use  $\mathcal{D}_{\text{sup}}$  in the supervised setting. Note that in the unsupervised setting we train only on data *with* noise, because this is what is typically available in practice. In the semi-supervised setting we include ground truth knowledge  $\mathcal{D}_{\text{sup}}$  for part of the database.
- 5) The performance of the DCAE model is tested by applying the trained DCAE to  $\mathcal{D}_{\text{PDB}}$  so that we obtain  $\mathcal{D}_{\text{PDB}}^{\text{cleaned}}$ . We evaluate the improvement in data quality by comparing two values; on the one hand we measure the difference between  $\mathcal{D}_{\text{GT}}$  and the original PDB data  $\mathcal{D}_{\text{PDB}}$ . We refer to this values as  $\mathcal{Q}_{\text{before}}$ . On the other hand we measure the difference between  $\mathcal{D}_{\text{GT}}$  and the cleaned PDB data  $\mathcal{D}_{\text{PDB}}^{\text{cleaned}}$ . We refer to this value as  $\mathcal{Q}_{\text{after}}$ . By comparing  $\mathcal{Q}_{\text{before}}$  and  $\mathcal{Q}_{\text{after}}$ , we can measure the performance of the DCAE. For more details on this performance measure, we refer to Section IV-D.

Note that for evaluation, we do not use a test-train split. The method is intended to learn from a given real-world data set in order to clean 100% of this same data set, instead of learning a model for evaluation on *unseen data*. Note also that a DCAE can easily and should be retrained on different datasets, as the underlying distributions and the size of the AE's (corresponding to the number of columns in the database) are probably different. Furthermore, we want to emphasize that ground truth knowledge (i.e., labelled data  $\mathcal{D}_{\text{sup}}$ ) is only used for training in the semi-supervised setting. In the unsupervised setting, the ground truth database  $\mathcal{D}_{\text{GT}}$ , and its partitions  $\mathcal{D}_{\text{unsup}}$  and  $\mathcal{D}_{\text{sup}}$ , are not used in any way to train the DCAE, but only to measure the DCAE performance and for synthetic generation of data of lesser quality. Using the loss functions of Section III-C,

we can choose hyperparameters that maximize the DCAE's performance regardless of the underlying databases or distributions.

## B. Generating $\mathcal{D}_{\text{GT}}$

We use Bayesian networks (BN) [26, Chapter 8.1] to represent the data generating distribution  $P(\mathcal{D}_{\text{GT}})$  which is used to generate the synthetic data for the experiments. Such a network represents a set of variables (PDB attributes in our situation) and their conditional dependencies by means of a directed acyclic graph. The variables in the BN can be categorical as well as numerical. While categorical variables and their realizations can be directly used in our PDB framework (Section II-B), we first need to quantize our numerical variables to categorical variables (Section III-E).

For most of our experiments, we use the BN  $A \rightarrow B \rightarrow C$ , but in some cases, we extend this chain to more than three variables. In all cases, the BN's that are used have the following properties:

- The first variable,  $A$ , is binary categorical, with  $P(A = 0) = 0.4$  and  $P(A = 1) = 0.6$ .
- Variable  $B$  is based on a continuous distribution. In particular, conditioned on  $A = 0$  and  $A = 1$  it is created by quantizing a truncated standard normal random variable on intervals  $[-10, 3]$  and  $[-2, 6]$ , respectively. The resulting probability mass functions are illustrated in Figure 9a. Note that these conditional distributions  $P(B|A)$  are skewed.
- Variable  $C$  is a truncated and quantized Gamma distributed random variable. Conditioned on  $B = b$ , we use the Gamma distribution with parameters  $\frac{30b}{K_C} + 1$  and 1 for shape and scale, respectively. We truncate to the interval  $[4, 5 + \frac{30b}{K_C}]$ . The resulting probability distribution is illustrated in Figure 9b.

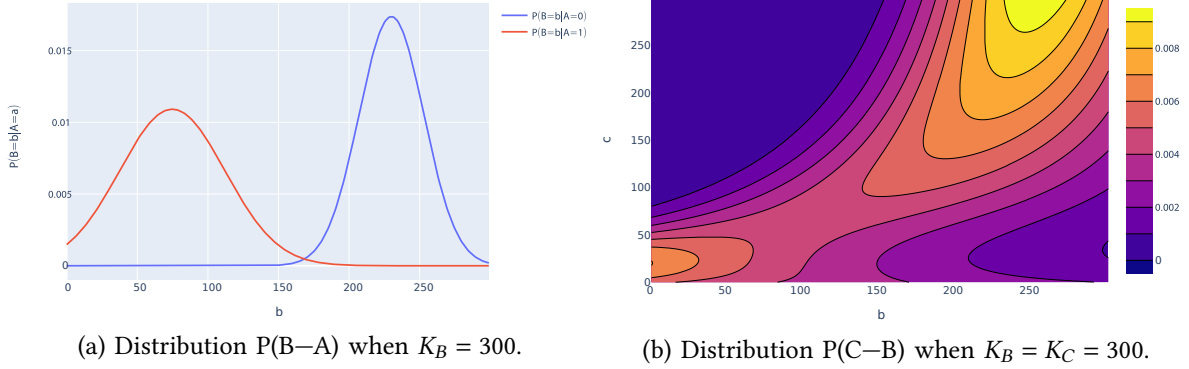


Fig. 9: The probability distributions used in the Bayesian network

	A	B	C
0	1	1	0
...	...	...	...
48	0	2	2
49	1	0	3
50	1	0	1
...	...	...	...
9999	1	1	0

(a) Example database sampled from a Bayesian Network.

Attribute	A		B			C				
Category	0	1	0	1	2	3	0	1	2	3
0	0	1	0	1	0	0	1	0	0	0
...	...	...	...	...	...	...	...	...	...	...
48	1	0	0	0	1	0	0	0	1	0
49	0	1	1	0	0	0	0	0	0	1
50	0	1	1	0	0	0	0	1	0	0
...	...	...	...	...	...	...	...	...	...	...
9999	0	1	0	1	0	0	1	0	0	0

(b) The certain data of Table IIa transformed to a probabilistic representation.

TABLE II: From sampled data to PDB.

When running an experiment with more than three BN variables, we append a new variable  $D$  to the bottom of the network, such as  $D$ , where  $P(D|C) = P(C|B)$ . We repeat this process for the next variables, i.e.:  $P(E|D) = P(C|B)$ , etc. Samples are taken from the joint probability distribution represented by this BN to generate  $\mathcal{D}_{GT}$ . An example is given in Table IIa. The input representation for the AE is generated by transforming this to a ‘one-hot encoding’, because certain data is a special case of probabilistic data, where one value takes all the probability mass. See Table IIb for an example.

### C. Corrupting our data with noise and errors

We model the data  $\mathcal{D}_{PDB}$  residing in a PDB as a noisy version of the underlying ground truth data  $\mathcal{D}_{GT}$ , where noisy means that uncertainty (noise) is added to the ground truth data representative for data quality problems or imperfections in the data integration process. We start with ‘clean’ records  $x_i^{GT} \in \mathcal{D}_{GT}$  in the form of Table IIb and corrupt it producing noisy data as illustrated in Table III. We investigate two types of noise:

**Gaussian noise** We add Gaussian noise to  $\mathcal{D}_{GT}$  by drawing and adding  $\epsilon \sim N(0, \sigma)$  to each cell in  $\mathcal{D}_{GT}$ , where we set negative entries to 0 and entries above 1 to 1. The probabilities are then normalized to sum to 1.

**Missing entry** Missing entry noise represents the realistic situation where a record contains missing entries. In a PDB with categorical data, this means that for a certain record  $i$  and attribute  $j$ , we make the  $K_j$  elements from  $p_{ij}$  equal to each other, that is  $p_{ij} = (\frac{1}{K_j}, \frac{1}{K_j}, \dots, \frac{1}{K_j})$ , so that  $p_{ij}$  contains zero knowledge about what category was observed.

Gaussian noise is used in most experiments, as we expect that to be more prevalent than missing entries. In the last experiments shown in Section V, we try to clean missing entries instead of removing Gaussian noise.

The data in Table III is an example of the data with the aforementioned noise, which we clean with our DCAE. An example of a result of cleaning Table III can be found in Table V.

#### D. Performance measure

The notion of a ground truth allows us to define what it means to improve the data quality of data residing in the PDB. ‘Improving data quality’ in essence means that given a corrupted record  $x_i \in \mathcal{D}_{\text{PDB}}$ , we incorporate evidence into it - where the evidence is the collection of data dependencies defined by  $P(\mathcal{D}_{\text{GT}})$ , being indirectly present in  $\mathcal{D}_{\text{PDB}}$  - so that its corresponding updated record  $x_i^n$  is closer to its corresponding ground-truth record  $x_i^{\text{GT}}$ . In order to quantify the ‘closeness’ as mentioned above, we need to use an appropriate distance measure. In order to determine the data quality improvement between the old and newly updated probabilistic data  $\mathcal{D}_{\text{PDB}}$  and  $\mathcal{D}_{\text{PDB}}^{\text{cleaned}}$ , respectively, we use the following measure:

$$\text{Noise reduction in \%} = 100 - \left( \frac{Q_{\text{before}}}{Q_{\text{after}}} \cdot 100 \right), \quad (18)$$

where  $Q_{\text{before}}$  and  $Q_{\text{after}}$  are as defined in Section IV-A. For both quality measures, we use the JSD applied to the entire data sets, taking the sum over all the attributes and records as described in Equation (11), Equation (14) and Equation (15). This measure should compensate for the size of the dataset and the amount of noise added, showing the relative improvement of the DCAE. The higher this value is, the better the network performed, with a maximum of 100% (meaning that all the noise was removed). If this value is below 0, the network was unable to remove noise and added noise to the dataset instead.

#### E. Experimental setup and hyperparameters

For the experiments, we used TensorFlow and Keras to train the DCAE model, pyAgrum [29] for modelling BN’s, and Pandas for operating on databases. We used a batch size of 32, with training split into 100 mini-batches, as these values led to the best trade-off between speed and performance. Each row  $x_i$  in a PDB is one data point for training

, where it is converted to a 1D input tensor compatible with the DCAE. Its length is equal to the amount of columns  $\sum_{j=1}^N K_j$  in the PDB. However, as in most cases, we use a PDB with 10000 records and a batch size of 32 for training, the actual inputs used during training are 2D tensors with dimensions  $\left( 32, \sum_{j=1}^N K_j \right)$ , as the first dimension in Keras/TensorFlow is the batch dimension. For training we use the Adam optimizer [28] to perform gradient descent.

In most experiments, except those where we explicitly vary the sampling density, we use  $K_j = 4$  and  $K_j = 100$  as sampling densities for categorical and continuous attributes, respectively. Note that each attribute  $j$  adds  $K_j$  neurons to the input and output layers. Hence, more attributes or higher sampling densities increase the size of the network, which has a negative impact on training

Attribute Category	A		B				C			
	0	1	0	1	2	3	0	1	2	3
0	0.320	0.680	0.000	0.806	0.000	0.194	1.000	0.000	0.000	0.000
...	...	...	...	...	...	...	...	...	...	...
48	0.911	0.089	0.000	0.000	1.000	0.000	0.000	0.000	0.391	0.609
49	0.459	0.541	0.250	0.250	0.250	0.250	0.500	0.000	0.000	0.500
50	0.104	0.896	0.606	0.000	0.394	0.000	0.000	0.492	0.000	0.508
...	...	...	...	...	...	...	...	...	...	...
9999	0.000	1.000	0.055	0.766	0.145	0.034	1.000	0.000	0.000	0.000

TABLE III: The data from Table IIb with Gaussian noise added, and some missing entries by making all their probabilities equal.

Hyperparameter	Value
Epochs	100
Batch size	32
Optimizer	Adam [28]
Training method	Either semi-supervised (100 epochs unsupervised followed by 100 epochs supervised) or fully unsupervised
Activation types	Sin, cos, linear, ReLU, Swish
Hidden layers	3
Latent space dimensions	Equal to BN size ( $N$ )
Loss function	JSD
Activity regularizer	L2, ( $\lambda = 10^{-4}$ )
Input layer type	Gaussian noise
$\sigma_{\text{Gaussian noise layer}}$	$0.01 \cdot (100/K_j)$
VAE	Disabled
Conv1D layers	0 (sometimes 1)
Conv1D output channels	64 (when layers > 0)
Conv1D kernel size	3 (when layers > 0)
Conv1D stride	3 (when layers > 0)
RBF kernel	Disabled
RBF kernel landmarks	100 (when enabled)
Output layer	softmax

(a) DCAE hyperparameters.

Database parameter	Value
BN size ( $N$ )	3
Sampling density ( $K_j$ )	4 ("categorical") or 100 ("continuous")
Records	10000
Gaussian noise	Enabled
$\sigma_{\text{PDB}}$	$0.02 \cdot (100/K_j)$
Missing entry noise	Disabled
Labeled data amount	2%

(b) PDB hyperparameters.

TABLE IV: Default yperparameters for experiments.

time and cleaning performance. Therefore, there is a trade-off for continuous attributes between a close approximation of the value, which calls for a high  $K_j$  and a DCAE that is still small enough to train quickly and clean well.

Unless stated otherwise, we use a variance of  $\sigma_{\text{PDB}} = 0.02 \cdot (100/K_j)$  for the Gaussian noise, which is a data corruption ratio that often leads to the true value not being recognizable anymore by the naked eye and keeps the amount of noise added to the database independent of the sampling density.

In all experiments, we investigate the difference in behaviour for categorical and continuous attributes as well as the influence of the loss function. We use categorical cross-entropy (log loss) and the Jensen-Shannon divergence (JSD loss).

Other loss functions, such as the mean square error (MSE) and Kullback-Leibler (KL) divergence, were omitted for presentation reasons and their mediocre performance.

1) *Experimental setup of DCAE architectural and hyperparameter experiments:* The goal of this set of experiments is to make a design choice or to establish a best setting for a (hyper)parameter. Our approach is to keep and mention the best choice/setting as established by the results given in Section V for all other experiments.

- *Experiment 1: Training methods*

For semi-supervised training, we explore several possible approaches: unsupervised training followed by supervised training, supervised training followed by unsupervised training, or switching between the two after every epoch. We use fully supervised, fully unsupervised, and training with only the supervised data as baselines. The approach with the best performance is used for all other experiments (unlabelled data first).

- *Experiment 2: Varying the amount of labelled data for semi-supervised training*  
We vary the amount of labelled data for semi-supervised learning from 0% to 100%. Unless stated otherwise, we use a labelled data set with a size of 2% of the data (i.e., 200 rows) for the other experiments, as this seemed like a realistic amount of data that could be labelled in real-world situations.
- *Experiment 3: Activation functions*  
We experimented with several combinations of the activation functions sin, cos, linear, ReLU, Swish, and sigmoid to establish the best configuration on this aspect.
- *Experiment 4: Regularization methods*  
We investigated the influence of an activity regularizer (which updates the cost function based on each layer’s activity to induce sparsity). We compared the performance between no regularization, L2 with  $\lambda = 0.01$ , L2 with  $\lambda = 10^{-4}$ , L1 with  $\lambda = 0.01$ , and L1 with  $\lambda = 10^{-4}$ . We chose an L2 regularizer with  $\lambda = 10^{-4}$  for all other experiments, as this increased performance at high sampling densities while not affecting performance at lower sampling densities.
- *Experiment 5: Input layer modifications*  
Our base configuration for the input layer is a dense layer with ReLU activation. We investigate several architectural modifications: following the denoising AE approach (see Section II-C), we add Gaussian noise to the input (note that this is different from and independent of what is described in Section IV-C); adding 1D convolutional layers (often used to capture structures in high-dimensional data such as images); applying a square root followed by a softmax to the input layer to make the input layer neurons’ outputs closer to each other but still ensuring they are a proper probabilistic distribution, and turning the DCAE into a VAE (which modifies not only the input layer but also the middle layer). It turns out that the denoising AE method is the only one with a significant positive influence, so we only kept this one for the other experiments.
- *Experiment 6: Changing  $\sigma_{\text{Gaussian noise layer}}$*   
The denoising AE method introduces a hyperparameter  $\sigma_{\text{Gaussian noise layer}}$ . We vary it between 0.01 and 0.2, as well as relative to sampling density  $K_j$  between  $0.01 \cdot (100/K_j)$  and  $0.1 \cdot (100/K_j)$ . We establish a best setting of  $0.01(100/K_j)$ .
- *Experiment 7: Latent space dimensionality*  
Another important hyperparameter is the latent space dimensionality, i.e., the size of the middle ‘bottleneck’ layer of the AE (see Figure 2). Note that because of the 5 sub-channels, the middle layer contains  $5 \cdot N$  neurons. We vary latent space dimensionality between 2 and 6, effectively producing a hidden layer of 10 to 30 neurons. Theoretically, a hidden layer of 3 neurons should provide the necessary latent space for the information of 3 variables, but we expect that a somewhat larger middle layer is needed in practice, especially due to our sub-channels. We established a best setting of 3 for each channel.
- *Experiment 8: Hidden layers*  
We investigate the influence of the depth of the neural network by varying the number of hidden layers between 3 and 30. We found that the best configuration is a shallow network with 3 layers.

2) *Experimental setup of DCAE architectural and hyperparameter experiments:* The goal of this set of experiments is to measure the cleaning behaviour of the DCAE under varying data quality

Attribute Category	A		B				C			
	0	1	0	1	2	3	0	1	2	3
0	0.000	1.000	0.010	0.990	0.000	0.000	0.990	0.001	0.007	0.002
...	...	...	...	...	...	...	...	...	...	...
48	1.000	0.000	0.000	0.000	1.000	0.000	0.000	0.001	0.328	0.670
49	0.016	0.984	0.403	0.488	0.050	0.059	0.227	0.003	0.023	0.747
50	0.000	1.000	0.992	0.007	0.002	0.000	0.049	0.504	0.008	0.439
...	...	...	...	...	...	...	...	...	...	...
9999	0.000	1.000	0.048	0.952	0.000	0.000	0.992	0.001	0.005	0.002

TABLE V: The result of training and evaluating the DCAE on the data from Table III.

and database parameters.

- *Experiment 9: Changing  $\sigma_{PDB}$*

We vary the amount of Gaussian noise  $\sigma_{PDB}$  added to the source data between  $0.01 \cdot (100/K_j)$  and  $0.2 \cdot (100/K_j)$ .

- *Experiment 10: Adding missing entry noise*

As mentioned in Section IV-C, besides adding Gaussian noise, we also introduce and experiment with missing values. We vary the number of missing values between 0.1% and 40%.

- *Experiment 11: Missing entry noise without Gaussian noise*

To also investigate the two types of noise individually, we conduct the previous experiment also without the presence of Gaussian noise.

- *Experiment 12: Changing the number of records in the database*

To see how well the DCAE solution scales to larger datasets, we investigate the effect of varying the number of records in the database that we train and evaluate the DCAE on.

- *Experiment 13: Changing the sampling density  $K_j$*

We investigate the effect of the sampling density  $K_j$  for continuous variables and the number of possible values for a categorical variable by varying  $K_j$  between 4 and 300.

- *Experiment 14: Changing the BN size  $N$*

Finally, we experiment with the size of the database in terms of the number of attributes  $N$ . Note that the number of attributes is the same as the BN size. We vary  $N$  between 2 and 30. We expect to see similar effects as in Experiment 13 because the main consequence of a larger  $N$  is similar to the main consequence of a larger sampling density  $K_j$ : a larger input and output layer.

An overview of the hyperparameters used in our experiments can be found in Table IV. The source code and data used for this research, including the complete experimental setup, are open-source and can be found at [30].

## V. EXPERIMENTS AND RESULTS

### A. Example results

In Table V we show the result of evaluating the DCAE (with the default hyperparameters as described in Section IV-E) on a database with both Gaussian noise ( $\sigma_{PDB} = 0.02 \cdot \frac{100}{K_j}$ ) and missing entry noise (with the probability of entries missing at 0.01%).

When comparing this table and Table III to Table IIb, we see that the DCAE manages to drastically improve the data quality of most rows (such as row 9999, which now has practically the same values as that same row in  $\mathcal{D}_{GT}$  although it does have some unneeded uncertainty added to attribute C).

It appears that the DCAE can often recover the ground truth (leading to distributions where the original value has a probability of  $\geq 0.9$ ), but this is not always the case. Sometimes, we wrongly introduce uncertainty (such as for row 9999, attribute C), or that we remove uncertainty for the



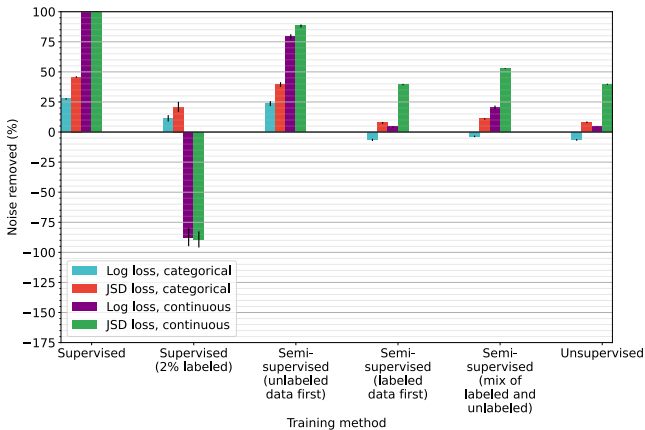


Fig. 10: Effect of training methods on performance. (Section V-B1)

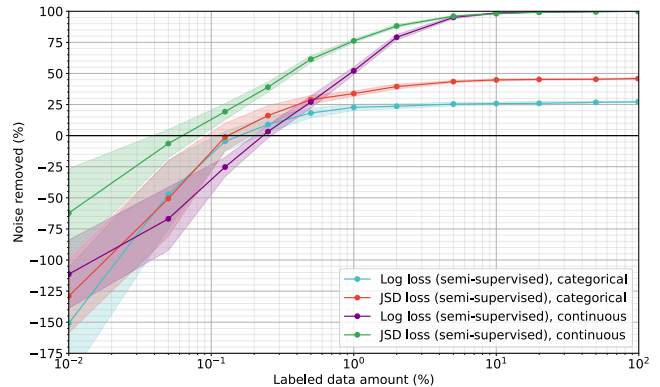


Fig. 11: Effect of the amount of labeled data on semi-supervised training performance. (Section V-B2)

wrong variable (such as for row 48, attribute C, where the wrong bin is increased by the DCAE), or that the DCAE barely removes any noise (such as in row 50, attribute C). If the DCAE could always perfectly remove noise and never make any errors, we would see performance scores of near 100%, so these errors are expected.

To show some more interesting properties of the DCAE, we look at row 49. In row 49 of  $\mathcal{D}_{GT}$ , attribute  $A = 1$ , but this is corrupted to  $P(A = 0) = 0.459$ ,  $P(A = 1) = 0.541$ . However, the DCAE seems to accurately reproduce the original value after cleaning, with  $P(A = 1) = 0.984$ . The true value  $B = 0$  is corrupted to a missing entry, with all probabilities equal to 0.25. Instead of reproducing  $P(B = 0)$  with a high probability as we would hope the DCAE would do, it outputs the following distribution:  $[0.403, 0.488, 0.050, 0.059]$ . This is very similar to the distribution of  $P(B|A = 1)$  as seen in Figure 9a. Indeed, checking what this distribution would look like when discretized using  $K_j = 4$  gives us  $[0.488, 0.488, 0.023, 0]$ . It seems that the DCAE does truly learn the underlying distributions.

In the remainder of this section, we demonstrate through numerical experiments the influence of various design options and choice of hyperparameters. Additional results are available in [31, 25].

### B. DCAE hyperparameter modifications

In this subsection, we perform experiments that change the hyperparameters of the DCAE and show their influence on the performance measure introduced in Section IV-D. All plots shown have at least  $n = 10$  measurements for every measurement so that we can show the mean and standard deviation of all measurements with these configurations, allowing us to make assumptions about their reliability.

1) *Experiment 1: Training methods*: In Figure 10, we show the effect of various training methods on the performance of the DCAE. The fully supervised baseline shows that almost perfect cleaning for continuous variables is possible with DCAE, but categorical variables cannot be perfectly reconstructed even with labels for all records. This is due to our rather high corruption rate of  $\sigma_{PDB} = 0.02 \cdot \frac{100}{K_j}$ , which leads to high amounts of noise per bin at low sampling densities and possibly even to probability distributions that represent missing entries. The performance of labelling 2% of the data for semi-supervised learning (when training on the unsupervised data first) is very high, reliably removing over 80% of noise for continuous data (when using the JSD loss function) and around 40% of noise at low sampling densities. We can see that a large part of this high

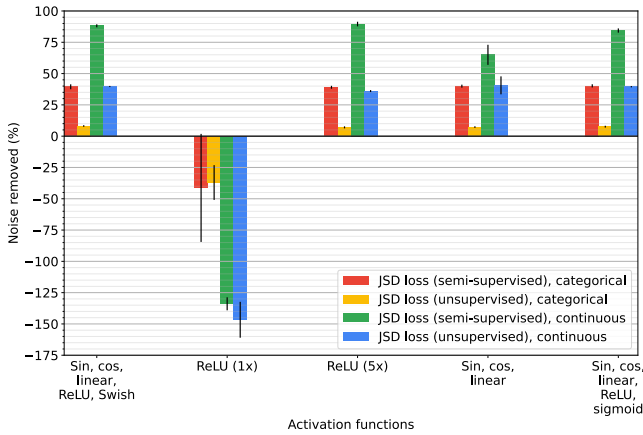


Fig. 12: Effect of different activation functions on performance. (Section V-B3)

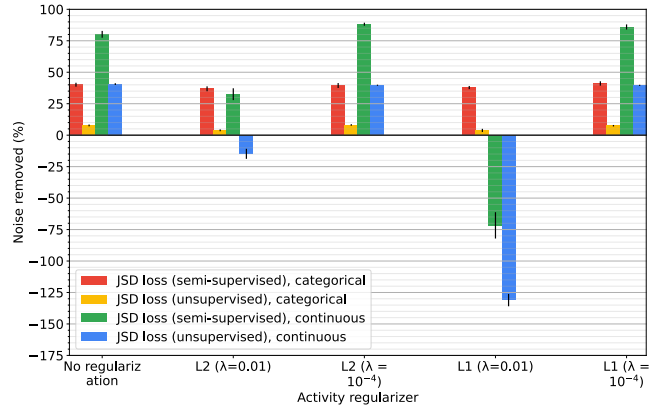


Fig. 13: Effect of activity regularization on performance. (Section V-B4)

performance is caused by the unsupervised training; when we remove the unsupervised training and only do supervised training on the 2% of data that we labelled, performance is much lower. Interestingly, for categorical data the performance when training on only the 2% labelled data is higher than when using purely unsupervised training. However, for continuous data, unsupervised training performs much better. Again, this is likely due to the missing entries introduced by the high amounts of noise at low sampling densities. These are more well-suited to removal with (semi-)supervised training, and they are not affected by adding noise during training (as we do with the Gaussian noise layer). As using unsupervised training followed by supervised training leads to the highest performance, this is the configuration we use for semi-supervised training.

2) *Experiment 2: Varying the amount of labeled data for semi-supervised training:* In Figure 11, we show a similar experiment, but with a varying amount of labelled data for semi-supervised training. Here, 100% labelled data should be the same as supervised learning, while 0% labelled data should theoretically be the same as unsupervised learning. (The Keras/TensorFlow implementation we used did not allow us to set values of 0% and 100%, so we used 0.01% and 99% instead).

Performance at high amounts of labelled data seems to match the performance seen during supervised training (shown in Figure 10). However, we witness diminishing returns for the amount of labelled data we provide: labelling more than 10% of the data does not seem to affect the performance at all; at 5%, it is not much worse. Thus, it seems that this solution does not require a lot of labelled data for good performance. Choosing 2% for the other experiments appears not only to be a realistic setting, but also one that still achieves good cleaning performance.

Interestingly, performance at very low amounts of labelled data does not at all match the performance of unsupervised learning in Figure 10. We suspect that this is caused by overfitting, as in the most extreme case, we perform unsupervised training on 99.9% of the data for 100 epochs, followed by 100 epochs of supervised training on 0.01% of the data. In a database of 10000 rows, this is merely one row, which could explain the drop in performance.

As we could see in Figure 10 and Figure 11, the performance seen when using the JSD loss function is much higher than when using the categorical cross-entropy loss. This was the case for almost any modification we made during the later experiments as well. To improve the legibility of the figures, we no longer show the log loss performance for the subsequent experiments, as using the JSD loss function is the better alternative.

3) *Experiment 3: Activation functions:* In Figure 12 we can see that the combination of activation sections that we mentioned in Section III-B (sin, cos, linear, ReLU and Swish) leads to the best per-

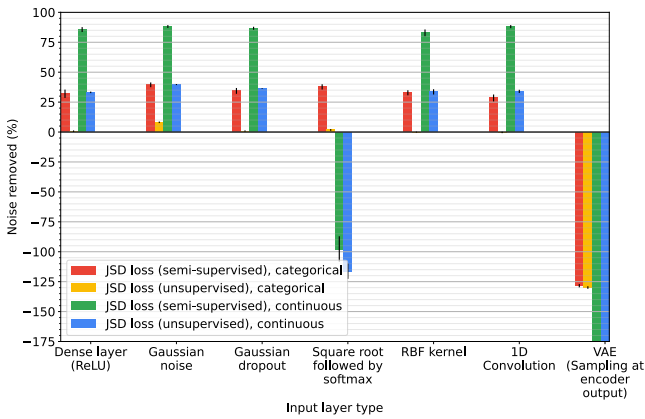


Fig. 14: Effect of different input layer types on performance. (Section V-B5)

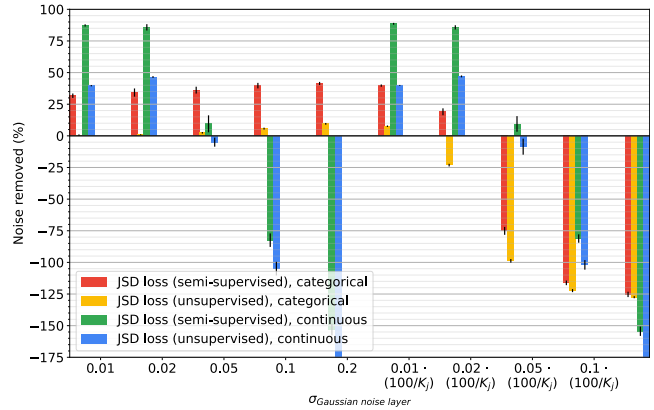


Fig. 15: Effect of  $\sigma_{\text{Gaussian noise layer}}$  on performance. (Section V-B6)

formance, although using 5 concatenated ReLU layers performs only slightly worse (and has equal performance for semi-supervised training on continuous data). The configuration that replaces the Swish activation function with a sigmoid activation function leads to equal performance in most cases, but a 5% reduction in performance for semi-supervised training on continuous data. Merely using sin, cos and linear activation functions lead to worse performance for continuous data but equal performance for categorical data. Using only 1 ReLU layer has the worst performance out of all, adding large amounts of noise.

These observations allow us to obtain some meaningful insights about which of the DCAE’s features contribute to its ability to clean noise from the data. The activation functions themselves seem to not matter much, as using 5 ReLU layers leads to performance that is only slightly worse than using a combination of 5 non-linear activation functions. It appears that using this concatenation of different layers (as explained in Section III-B) is what increases performance, not the activation function themselves.

4) *Experiment 4: Regularization methods:* Figure 13 shows that using L2 activity regularization on every layer (with  $\lambda = 10^{-4}$ ) increases performance from 80% to 88% for semi-supervised learning on continuous data, while not affecting performance for other training methods or categorical data. Using L1 activity regularization with  $\lambda = 10^{-4}$  also lead to a slight increase in performance, but this increase was not as significant. For both L1 and L2 regularization, using  $\lambda = 0.01$  either did not affect performance or made the performance of the DCAE worse. The reduced dimensionality of the latent space of the DCAE and the addition of Gaussian noise during training are both expected to have a similar effect as regularization constraints. Hence, we did not expect a large improvement by applying an activity regularizer. The performance improvement witnessed during semi-supervised training on continuous data can be explained as follows. The regularization constraint encourages the outputs of layers in the DCAE to be more sparse, thus making the output more similar to a one-hot encoding, which is the format of the labelled data we are trying to reproduce during semi-supervised training. The penalties for having many activated neuron outputs becomes more relevant for continuous data, as there are more neurons that can be activated.

5) *Experiment 5: Input layer modifications:* In Figure 14, we show that out of the many possible modifications to the network topology, adding Gaussian noise at the input layer during training is the only one to have a significant positive effect on the performance when comparing to a densely connected input layer with ReLU activation function, especially for unsupervised learning. In that case, the DCAE is truly a denoising AE (as described in Section II-C). Interestingly, 1D convo-

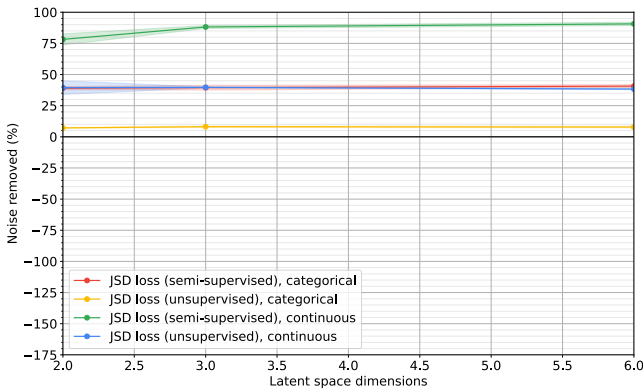


Fig. 16: Effect of latent space dimensionality on performance. (Section V-B7)

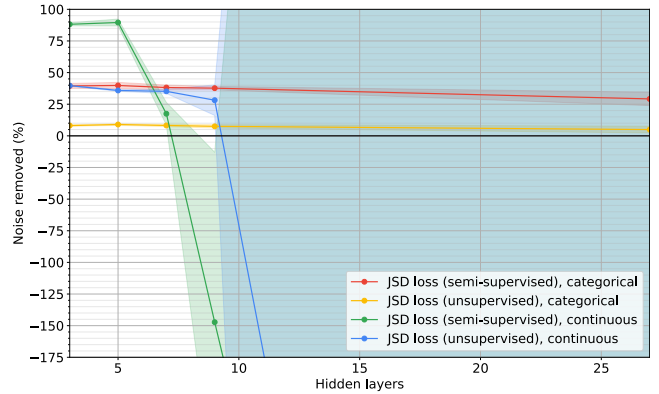


Fig. 17: Effect of the amount of hidden layers on performance. (Section V-B8)

lutional layers slightly raise performance for continuous data during semi-supervised learning, while lowering performance for semi-supervised learning on categorical data, and not affecting unsupervised learning performance. Convolutional layers are often used to capture structures in high-dimensional data (such as images). Thus, a high performance on the larger rows induced by a high  $K_j$  in continuous data could be expected. Applying a square root followed by a softmax to the input layer slightly raised performance for categorical data when using semi-supervised learning. Turning the DCAE into a VAE severely decreased performance, perhaps due to the inaccuracy added by the resampling of the data necessary for the variational method.

6) *Experiment 6: Changing  $\sigma_{\text{Gaussian noise layer}}$* : From Figure 15, we can see that our default choice for  $\sigma_{\text{Gaussian noise layer}}$  has the best performance out of all possibilities that we tested. It is clear from this figure that training on continuous data appears to benefit most from low amounts of noise, while categorical data is easier to clean when adding higher amounts of noise. As we add higher amounts of noise to each bin in  $\mathcal{D}_{\text{PDB}}$  when the sampling density  $K_j$  is low (to ensure the same amount of noise is added to the database), it can be expected that more noise needs to be added during training to compensate for this. A good compromise was found by scaling  $\sigma_{\text{Gaussian noise layer}}$  with  $K_j$  as well, with the highest performance seen at  $\sigma_{\text{Gaussian noise layer}} = 0.01 \cdot \frac{100}{K_j}$ . This means that to each bin, the Gaussian noise layer adds half of the noise that we added to  $\mathcal{D}_{\text{PDB}}$  (as  $\sigma_{\text{PDB}} = 0.02 \cdot \frac{100}{K_j}$ ).

7) *Experiment 7: Latent space dimensionality*: In Figure 16 one can see that the DCAE performance is largely unaffected by the various parameters for the latent space dimensions in each channel. Performance seems slightly lower at a dimensionality of 2 in some cases. Thus, using a dimensionality of 3 (the default when the BN size  $N = 3$ ) offers the best performance. Increasing the dimensionality will only make training slower due to the increased amount of neurons and trainable weights. Furthermore, using a total dimensionality of 3 makes the most sense in this case, as it should encourage the DCAE to learn a representation for each BN variable in each neuron. However, our use of 5 sub-channels of this size already allows the network to learn a more complex representation. This also explains why performance is largely unaffected by this experiment: even when setting the latent space dimensionality for each channel to 1, the encoder output already has a dimensionality of 5.

8) *Experiment 8: Hidden layers*: From Figure 17, we can see that shallow networks offer the best performance. While using 5 hidden layers leads to a small performance increase for semi-supervised training on continuous data, using 3 hidden layers is the best option in all other cases. Increasing the number of hidden layers makes training much, much slower (due to the vast increase

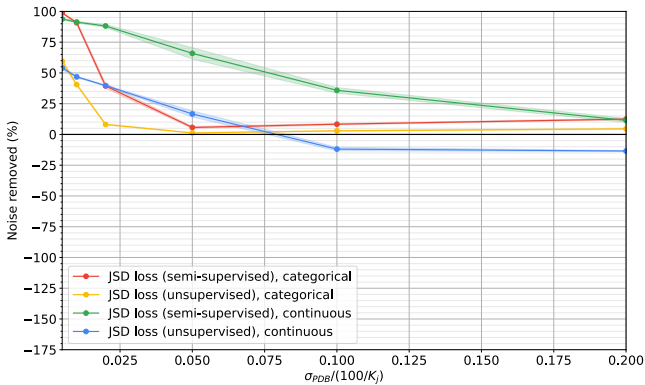


Fig. 18: Effect of changing  $\sigma_{\text{PDB}}$  on performance. (Section V-C1)

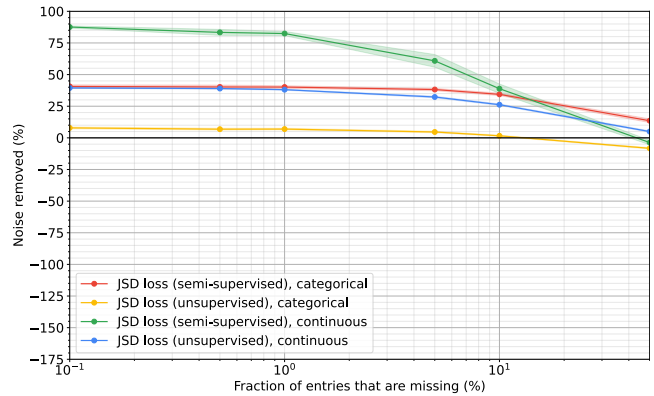


Fig. 19: Effect of missing entries on performance, when  $\sigma_{\text{PDB}} = 0.02 \cdot (100/K_j)$ . (Section V-C2)

in trainable weights) and makes the performance not only worse, but more unreliable. This might be due to the vanishing gradient problem [4]. DCAEs trained on categorical data do not suffer from this problem as much, perhaps due to their comparably low amount of trainable weights. The large confidence interval for the performance at 30 hidden layers for unsupervised training on continuous data seems to be caused by the introduction of NaN values into the cleaned data, possibly caused by overflow or underflow errors that are sometimes seen in deep neural networks.

### C. Database parameter modifications

1) *Experiment 9: Changing  $\sigma_{\text{PDB}}$* : It can be seen from Figure 18 that the DCAE removes noise quite well, regardless of the amount. Only when there are high amounts of noise on continuous data does the performance of unsupervised learning drop substantially (above  $\sigma_{\text{PDB}} = 0.05 \cdot \frac{100}{K_j}$ ). It can be seen from Table III that the noise added at  $\sigma_{\text{PDB}} = 0.02 \cdot \frac{100}{K_j}$  is already a quite substantial. The fact that performance for semi-supervised training on high sampling densities remains quite high when adding even larger amounts of noise is quite remarkable. The performance seems to decrease linearly when more noise is added.

For categorical data, this solution removes noise very well at low values of  $\sigma_{\text{PDB}}$ , but the performance drops off sharply at values of  $0.02 \cdot \frac{100}{K_j}$  and higher. This is probably because the noise leads to missing entries at low sampling densities (this can also be seen in Experiment 13). In either case, the DCAE seems quite robust to small amounts of noise, but more significant amounts of noise are only removable with semi-supervised training.

2) *Experiment 10: Adding missing entry noise when  $\sigma_{\text{PDB}} = 0.02 \cdot (100/K_j)$* : We can see in Figure 19 that adding missing entry noise to a  $\mathcal{D}_{\text{PDB}}$  that already has Gaussian noise ( $\sigma_{\text{PDB}} = 0.02 \cdot (100/K_j)$ ) does not seem to affect performance much until 5% of entries or more are missing. This is a very high amount of missing data. Even then, the performance is still quite good. Performance starts sharply decreasing for all cases except semi-supervised learning on categorical data when 10% or more of the entries are missing. Even then, the performance in most cases is still relatively high. It was to be expected that semi-supervised training on categorical data would lead to the best performance, as this solution already learns to remove missing entries even when we do not manually add them, as they are introduced by high values of  $\sigma_{\text{PDB}}$ .

3) *Experiment 11: Missing entry noise without Gaussian noise*: In Figure 20 we show what happens when we stop adding Gaussian noise to  $\mathcal{D}_{\text{PDB}}$  and only add missing entries. Strangely, the high performance that we witnessed in Experiment 10 can no longer be seen here. The DCAE is unable



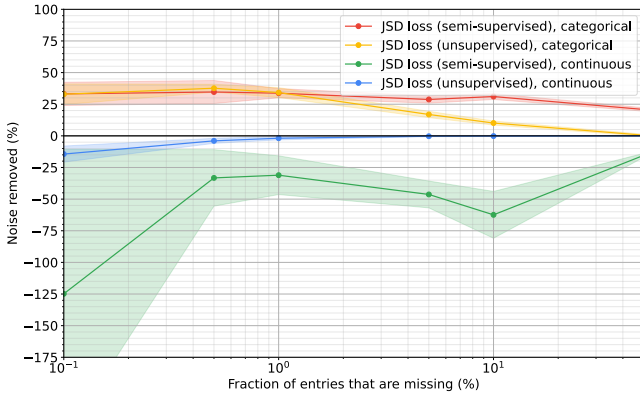


Fig. 20: Effect of the likelihood of missing entry noise on performance, when  $\sigma_{\text{PDB}} = 0$ . (Section V-C3)

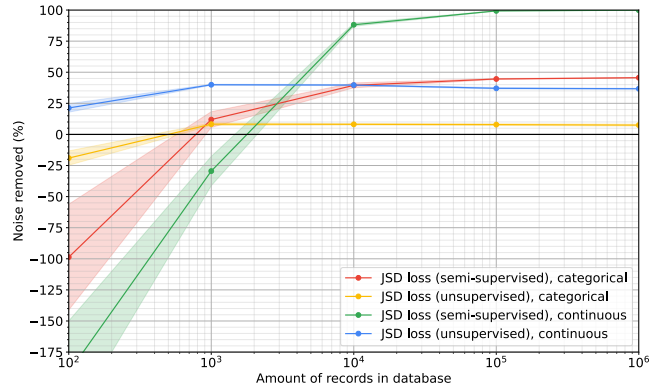


Fig. 21: Effect of the amount of rows in the database on performance. (Section V-C4)

to compensate for missing entries in continuous data. Performance for categorical data is quite good, removing 20% to 30% of missing entry noise when using semi-supervised learning even when 50% of entries are missing. This high performance is also seen in unsupervised training on categorical data, but only when a small percentage of entries are missing. Thus, it seems the DCAE is not feasible for purely removing missing entries in continuous data, while it has no problems with categorical data.

One of our interpretations of this experiment was that the low performance seen was caused by the fact that we were still using a Gaussian noise layer, even though there is no Gaussian noise in the data we were trying to clean. However, some further testing showed us the performance seen in Figure 20 always decreased when setting  $\sigma_{\text{Gaussian noise layer}}$  to 0.

4) *Experiment 12: Changing the amount of records in the database:* Figure 21 shows us that the performance of the DCAE scales very well with the number of records when semi-supervised training is used. For continuous data, data cleaning performance reaches almost 100% when the amount of records is high. Performance seems to be barely affected by the number of records when unsupervised training is used. This is what we expected: machine learning solutions generally perform better when there is a larger amount of data available.

5) *Experiment 13: Changing the sampling density  $K_j$ :* In Figure 22, we see once more that the JSD loss function outperforms the log loss function in most situations. There is one case where the log loss leads to better performance: at very high sampling densities ( $K_j = 300$ ), but performance is quite reduced there in all cases. Still, the fact that this configuration is able to reduce 25% of noise with the log loss function at such a high sampling density is remarkable, as this has an input layer of 602 neurons ( $2 \cdot 300 + 2$ ;  $A$  can only take two possible values) and is also representative of a probabilistic database with about 150 categorical attributes with 4 possible values ( $602/4$ ).

Performance seems to be highest at  $K_j = 15$ . The fact that the performance decreases as the sampling density increases makes sense, as the dimensionality of the data increases and as a result, there are more trainable weights. The decrease in performance at very low sampling densities can also be explained by the fact that missing entries are introduced by the relatively large amounts of Gaussian noise per bin.

We also observed that at low sampling densities ( $K_j = 4$ ), it is much faster to train the network with a consumer-grade quad-core CPU than a consumer-grade GPU. This is probably caused by the overhead introduced by moving data to the GPU, which offers no speed-up due to the lack of large matrix multiplications for small neural networks. At higher sampling densities ( $K_j \geq 100$ ),

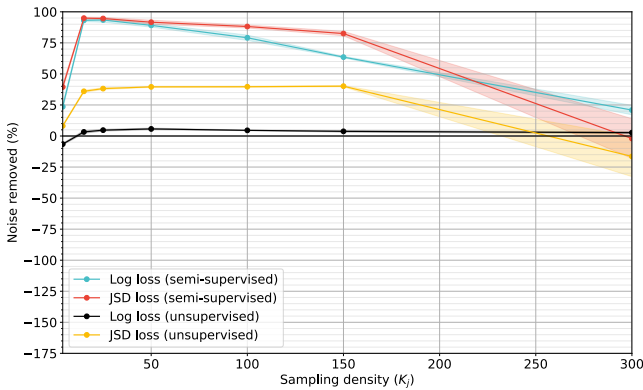


Fig. 22: Effect of sampling density ( $K_j$ ) on performance. (Section V-C5)

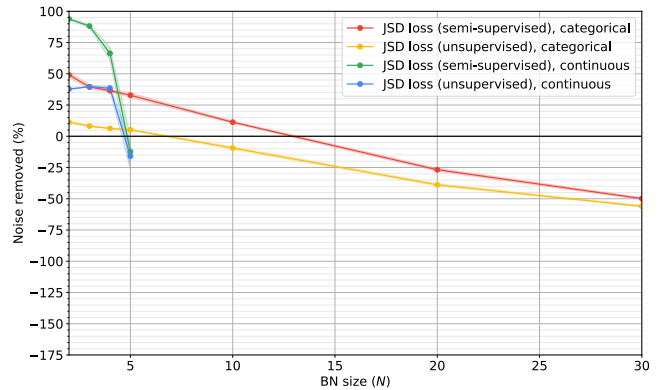


Fig. 23: Effect of BN size ( $N$ ) on performance. (Section V-C6)

this difference was not observed.

6) *Experiment 14: Changing the BN size ( $N$ ):* The same trends that could be observed in Experiment 13 can also be seen in Figure 23. The performance of the DCAE seems to decrease as the amount of neurons in the DCAE increases, hence also when the number of attributes in  $\mathcal{D}_{\text{PDB}}$  increases. The drop-off is much sharper at high sampling densities, as at  $N = 5$ , there are already  $4 \cdot 100 + 2 = 402$  neurons, while for low sampling densities at  $N = 5$ , there are  $4 \cdot 4 + 2 = 18$  neurons. Higher values of  $N$  for continuous data would have taken several days to train, which was aborted due to low performance.

Thus, while our current solution seems to work well for complex databases of categorical data (as long as  $N \leq 10$ ), it does not work so well for complex databases of continuous data.

## VI. CONCLUSIONS

In this paper, we propose an autoencoder-based data cleaning approach, referred to as DCAE, capable of near-automatic data quality improvement. The intuition behind the approach is that an autoencoder can learn structure and dependencies hidden in data, which can be used to identify and correct doubtful values. The approach uses a probabilistic data representation to express weak and strong doubts. It can be used for cleaning both ordinary ‘crisp’ data sets as well as probabilistic data resulting from a probabilistic data integration process. We also introduce a Bayesian Network-based approach for generating synthetic test data with embedded dependencies to evaluate our cleaning approach.

In our experiments, we varied the level of noise and missing values, number of attributes, the number of records, sampling density for continuous attributes, and several other hyper-parameters. We also experimented with several alternatives for the autoencoder architecture. Results show that fully automatic cleaning in an unsupervised manner is possible, but that a semi-supervised setting with a mix of unlabeled data and only little reference data (2% in our experiments) produced significantly better results: for data sets with up to 4 attributes, 30%-50% removal of artificially introduced noise in categorical attributes and 70%-90% in continuous attributes. The performance increases further when more records are added to the database. Apparently, an autoencoder is able to learn structure and dependencies hidden in data sets, and we can exploit this for the purpose of data cleaning. The DCAE managed to restore missing entries in categorical data reasonably well (when they make up to 10% of the data), but was unable to do so for continuous data. When Gaussian noise is present and up to 10% of entries are missing, performance is good for continuous and categorical data. Best results were obtained with an architecture with a Gaussian noise layer,

limited (up to 5) hidden layers, JSD loss function, a combination of sin, cos, linear, ReLU and Swish activation functions, and L2 activity regularization with  $\lambda = 10^{-4}$ .

For future work, more experimentation is desired. First, it would be interesting to experiment with more complex dependencies by sampling data from Bayesian Networks  $P(\mathcal{D}_{GT})$  with different non-linear structures. Second, it seems logical that longer training (we trained for 100 epochs) and more effective labelling approaches for semi-supervised learning (such as scaling the number of epochs for supervised training with the amount of labelled data), will improve performance. However, such expectations need to be validated before they can be used as recommendations. Third, the performance of the approach seems to degrade when the input and output layers grow beyond about 500 neurons. Architectural changes may counteract this disadvantageous behaviour. Furthermore, the context of cleaning data integration results makes an investigation of applying approaches for distributed or federated learning interesting.

Finally, the largest challenge when applying the DCAE solution on real-world databases is that it is impossible to know whether the data cleaning was a success, as there is no ground truth data  $\mathcal{D}_{GT}$  to compare to. Whether the DCAE successfully learned to improve data quality is not apparent from its output. A possible solution would be to incorporate techniques that also output confidence intervals, such as those used in Gaussian Process classifiers [32]. Then, the user can see whether the DCAE was able to learn the underlying structures of the data. When the confidence intervals of the output are small, the output is likely to be correct, while when confidence intervals are large, the output is more likely to be wrong (as the DCAE is "unsure" about the underlying distribution).

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