A Unified Deep Model of Learning from both Data and Queries for Cardinality Estimation

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ABSTRACT
Cardinality estimation is a fundamental problem in database systems. To capture the rich joint data distributions of a relational table, most of the existing work either uses data as unsupervised information or uses query workload as supervised information. Very little work has been done to use both types of information, and cannot fully make use of both types of information to learn the joint data distribution. In this work, we aim to close the gap between data-driven and query-driven methods by proposing a new unified deep autoregressive model, UAE, that learns the joint data distribution from both the data and the query workload. First, to enable using the supervised query information in the deep autoregressive model, we develop differentiable progressive sampling using the Gumbel-Softmax trick. Second, UAE is able to utilize both types of information to learn the joint data distribution in a single model. Comprehensive experimental results demonstrate that UAE achieves single-digit multiplicative error at tail, better accuracies over state-of-the-art methods, and is both space and time efficient.

1 INTRODUCTION
Cardinality estimation — estimating the result size for a SQL predicate — is a critical component in query optimization, which aims to identify a good execution plan based on cardinality estimation [5, 7, 32]. In spite of the importance of cardinality estimation, modern DBMS systems may still produce large estimation errors on complex queries and datasets with strong correlations [43]. Additionally, cardinality estimation can also be used for approximate query processing [31].

The fundamental difficulty of cardinality estimation is to construct or learn an accurate and compact representation to estimate the joint data distribution of a relational table (the frequency of each unique tuple normalized by the table’s cardinality). Most of the existing work on cardinality estimation can be broadly categorized into two classes: data-driven and query-driven cardinality estimation. Data-driven methods aim to summarize the joint data distribution for cardinality estimation. Traditional data-driven methods include data-driven histograms, sampling, and sketching. However, they usually make independence and uniformity assumptions that do not hold in complex real-world datasets. Learning-based methods have been proposed for data-driven cardinality estimation by formulating cardinality estimation as a machine learning problem. Traditional machine learning methods still have their shortcomings. For example, kernel density estimation [30, 37] is vulnerable to high-dimensional data and probabilistic graphical models [14, 22, 66, 72] are inefficient in estimation.

Recent advances in deep learning have offered promising tools in this regard. Recently, the Sum-Product Networks-based model [31] has been applied for approximating the joint distribution. However, it will not handle well strong attribute correlations in real-world datasets. A promising recent advance in this direction would be applying deep autoregressive models [20, 53, 63] for cardinality estimation [28, 78], which can capture attribute correlations and have reasonable estimation efficiency. However, the optimization target (loss function) of deep autoregressive models is to minimize the ordinary average error over the overall data, and could neglect tricky (e.g., long tail) data regions, because the model may be largely dominated by those few head data regions, but degraded for many other tail data regions. Alternatively, query-driven cardinality estimation utilizes query workload (from either query log or generated workload) to perform cardinality estimation without seeing the data, and it is expected to have more focused information on workload queries than data-driven methods [12]. Traditional query-driven histograms [8, 9, 12, 46, 67] also suffer from the same problems of histogram-based methods. Recently, deep learning (DL)-based estimators can estimate complex joins without independence assumptions, based on the powerful representation ability of deep neural networks [64]. However, query-driven models assume that test queries share similar properties with training queries: they are drawn from the same distribution. This may not be the case due to workload shifts. In other words, test and training workloads may focus on different data regions. Moreover, it would be expensive to generate workload queries that sufficiently cover all data areas to train a model.

It would be a natural idea of utilizing both data and query workload for cardinality estimation. In fact, a few proposals (e.g., DeepDB) consider the combination as an interesting avenue for future work. Moreover, towards this direction several solutions [19, 30, 37, 39] have been proposed to utilize both data and workload.
However, the combination methods of the two types of information in these pioneering studies are simple, and they are not sufficient in capturing both types of information to learn the joint data distribution for cardinality estimation. As to be discussed in related work in more details, these solutions simply use one side of data and queries as auxiliary information to enhance the model of the other side. Consequently, these pioneering solutions cannot model the data as unsupervised information and query workload as supervised information in a unified model to learn the joint data distribution for cardinality estimation.

Goals To solve the aforementioned problems, we conclude four design goals as follows:

- G1. Capturing data correlations without independence or uniformity assumption;
- G2. Utilizing both data and query workload for model training;
- G3. Incrementally ingesting new data and query workload;
- G4. Time and space efficient estimation.

Our Solution To achieve the four goals, in this paper we propose a new unified deep autoregressive estimator UAE to utilize data as unsupervised information and query workload as supervised information for learning the joint data distribution. Deep autoregressive models have demonstrated superior performance for their effectiveness and efficiency in the pioneering work [28, 78] of training autoregressive models for cardinality estimation. However, no existing deep autoregressive model in the literature is able to incorporate the query workload as supervised information for learning joint data distribution, much less support both data as unsupervised information and query workload as supervised information in the same model. To enable incorporating query workload as supervised information in the deep autoregressive model to learn the joint data distribution, we propose a novel idea — we utilize the Gumbel-Softmax trick [36, 50] to differentiate the categorically sampled variables so that the deep autoregressive model can learn joint data distribution directly from queries. Furthermore, we propose to combine the unsupervised and supervised losses produced from data and queries, respectively, with a trade-off hyper-parameter, and thus we are able to train the deep autoregressive model to learn the joint data distribution with a single set of model parameters. Moreover, since UAE is trained with both data and queries, it is naturally capable of incorporating incremental data and query workload.

Contributions This work makes the following contributions:

- We conduct comprehensive experiments to compare UAE with 9 baseline methods on three real-life datasets. The 9 baseline methods cover data-driven methods, query-driven methods, and hybrid methods, including the recent deep learning based methods. The experimental results show that UAE achieves single-digit multiplicative error at tail, better accuracies over other state-of-the-art estimators, and is both space and time efficient. The results demonstrate that our method can well achieve the four aforementioned goals. Interestingly, the experimental results also show that UAE-Q, which is trained on queries only, outperforms the state-of-the-art query-driven method.

2 RELATED WORK

Selectivity or cardinality estimation has been an active area of research for decades [16]. We present the previous solutions in three categories: data-driven estimators, query-driven estimators, and hybrid estimators as summarized in Table 1.

Data-driven Cardinality Estimation Data-driven cardinality estimation methods construct estimation models based on the underlying data. First, sampling-based methods [27, 47, 60] estimate cardinalities by scanning a sample of data, which has space overhead and can be expensive. Histograms [17, 34, 35, 49, 52, 58, 69, 70, 73] construct histograms to approximate the data distribution. However, most of these methods make partial or conditional independence and uniformity assumptions, i.e., the data is uniformly distributed in a bucket. A host of unsupervised machine learning based methods have been developed for data-driven cardinality estimation. Probabilistic graphical models (PGM) [14, 22, 66, 72] use Bayesian networks to model the joint data distribution, which also relies on conditional independence assumptions. Kernel density estimation (KDE)-based methods [25, 26] do not need the independence assumptions, but their accuracy is not very competitive due to the difficulty in adjusting the bandwidth parameter. Recently, Naru [78] and MADE [28] utilize unsupervised deep autoregressive models for learning the conditional probability distribution and use it for answering point queries. Naru uses progressive sampling and MADE uses adaptive importance sampling algorithm for answering range queries and they achieve comparative results. Both Naru and MADE do not make any independence assumption.

Query-driven Cardinality Estimation Supervised query-driven cardinality estimation approaches build models by leveraging the query workload. As opposed to data-driven histograms, query-driven histograms [8, 9, 12, 46, 67] build histogram buckets from query workload, without seeing the underlying data. Recently, QuickSel [56] uses uniform mixture model to fit the data distribution using every query in the query workload, which avoids the overhead of multi-dimensional histograms. QuickSel also relies on uniformity assumptions. Deep Learning models have recently been employed for query-driven cardinality estimation. Ortiz et al. [54] evaluate the performance of using multi-layer perceptron neural networks and recurrent neural networks on encoded queries for cardinality estimation. Sup [28] encodes queries as a set of features and learns weights for these features utilizing a fully connected neural network to estimate the selectivity. In addition, Wu et al. [76] consider a relevant but different problem, which is to estimate the cardinality for each point of a query plan graph by training a traditional machine learning model. Sun et al. [68] consider estimating
both the execution cost of a query plan and cardinality together using a multi-task learning framework.

**Hybrid Cardinality Estimation** A few proposals leverage both query workload and the underlying data to predict the cardinalities. Query-enhanced KDE approaches [30, 37] leverage query workload to further adjust the bandwidth parameter of KDE to numerically optimize a KDE model for better accuracy. However, KDE-based models do not work well for high-dimensional data [30, 37]. Recently, selectivity estimation results from data-driven models are used together with encoded queries as input features to machine learning models [19, 39]. Dutt et al. include the cardinality estimates of histograms as extra features in addition to query features, and use neural network and tree-based ensemble machine learning models for cardinality estimation. Kipf et al. [39] include estimator results from sampling as extra features in addition to query features and use convolutional neural networks for cardinality estimation. However, the two approaches have the following problems: (1) They cannot be trained on data directly and do not fully capture the benefits of the two types of information; (2) Their combination methods significantly increase the model budgets (for storing samples or histograms) and negatively affect the training and estimating efficiencies of the model; (3) They cannot directly ingest incremental data because they have to be trained with new queries whose cardinalities are obtained on the updated data.

**Autoregressive Models** Autoregressive models capture the joint data distribution $P(x)$ by decomposing it into a product of conditional distributions. Recent deep autoregressive models include Masked Autoencoder [21], Masked Autoregressive Flow [55] and Autoregressive Energy Machines [53].

**Remark** Our UAE belongs to the hybrid family and is based on deep autoregressive models. To our knowledge, no existing work on deep autoregressive models in the machine learning literature is able to support using query workload as supervised information to train the model, much less supporting both data as unsupervised information and query workload as supervised information in one model. In UAE, we propose a novel solution to enable using query workload as supervised information, as well as a unified model to utilize both data as unsupervised information and query workload as supervised information w.r.t. deep autoregressive models.

### Table 1: A summary of existing cardinality estimation methods.

| Category         | Method                                      | Without Assumptions | Learning from Data | Learning from Queries | Incorporating Incremental Data | Incorporating Incremental Query Workload | Efficient Estimation |
|------------------|---------------------------------------------|---------------------|--------------------|-----------------------|--------------------------------|---------------------------------------|---------------------|
| Data-driven      | Sampling [27, 47, 60]                        | ✓                   | ✓                  | ✓                     |                                |                                       |                     |
|                  | Histograms [17, 34, 35, 49, 52, 58, 69, 70, 75] | ✓                   | ✓                  | ✓                     |                                |                                       |                     |
|                  | KDE [25, 26]                                | ✓                   | ✓                  | ✓                     | ✓                              |                                       |                     |
|                  | PGM [14, 22, 66, 72]                        | ✓                   | ✓                  | ✓                     | ✓                              | ✓                                     |                     |
|                  | RSPN model [31]                             | ✓                   | ✓                  | ✓                     | ✓                              | ✓                                     |                     |
|                  | DL models [28, 78]                          | ✓                   | ✓                  | ✓                     | ✓                              | ✓                                     |                     |
| Query-driven     | Histograms [8, 9, 12, 46, 67]               | ✓                   | ✓                  | ✓                     | ✓                              | ✓                                     | ✓                   |
|                  | Mixture models [56]                         | ✓                   | ✓                  | ✓                     | ✓                              | ✓                                     | ✓                   |
|                  | DL models [28, 39, 54, 68, 76]              | ✓                   | ✓                  | ✓                     | ✓                              | ✓                                     | ✓                   |
| Hybrid           | Sampling-enhanced ML models [39]            | ✓                   | ✓                  | ✓                     | ✓                              | ✓                                     | ✓                   |
|                  | Histogram-enhanced ML models [19]           | ✓                   | ✓                  | ✓                     | ✓                              | ✓                                     | ✓                   |
|                  | Query-enhanced KDE [30, 37]                 | ✓                   | ✓                  | ✓                     | ✓                              | ✓                                     | ✓                   |
|                  | UAE (Ours)                                  | ✓                   | ✓                  | ✓                     | ✓                              | ✓                                     | ✓                   |

3 PROBLEM STATEMENT

Consider a relation $T$ that consists of $n$ columns (or attributes) $\{A_1, A_2, ..., A_n\}$. A tuple (or data point) $x \in T$ is an $n$-dimensional vector. The row count of $T$ is defined as $|T|$. The domain region of attribute $A_i$ is given by $R_i$, which represents the set of distinct values in $A_i$.  

**Predicates** A query is a conjunction of predicates, each of which contains an attribute, an operator and a value. A predicate indicates a constraint on an attribute (e.g., equality constraint $A_2 = 6$, or range constraint $A_1 > 1$).  

**Cardinality** The cardinality of a query $q$, $\text{Card}(q)$, is defined as the number of tuples of $T$ that satisfy the query. Another related term, selectivity, is defined as the fraction of the rows of $T$ that satisfy the query, i.e., $\text{Sel}(q) = \frac{\text{Card}(q)}{|T|}$.

**Supported Queries** Our proposed estimator supports cardinality estimation for queries with conjunctions of predicates. Each predicate contains a range constraint ($\neq$, $>$, $\geq$, $<$, $\leq$), equality constraint ($=$) or IN clause on a numeric or categorical column. For a numerical column, we make the assumption that the domain region is finite and use the values present in that column as the attribute domain. Moreover, the estimator can also support disjunctions via the inclusion-exclusion principle. Note that our formulation follows a large amount of previous work on cardinality estimation [22, 28, 56, 78]. For joins, UAE supports multi-way and multi-key equi-joins, as is it in [77]. Moreover, group-by queries could be supported by learning query containment rates [29].

**Problem** Consider (1) the underlying tabular data $T = \{x\}$ and (2) a set of queries $Q = \{q\}$ with their cardinalities $C = \{c\}$. Then, this work aims to build a model that leverages the set of queries and their cardinalities $(Q, C)$ and the underlying data $T$ to predict the cardinalities for incoming queries. Furthermore, after training the model, it is also desirable that the model can ingest new data and query workload in an incremental fashion, rather than retraining. Note that such labeled queries can be collected as feedback from prior query executions (query log).
We present the proposed unified deep autoregressive estimator, called UAE, that is capable of learning from both data and query workload to support cardinality estimation. We first present an overview of UAE (Section 4.1). Then we introduce how to use a trained autoregressive model for cardinality estimation (Section 4.2). We then present our idea on differentiating progressive sampling to enable the deep autoregressive models to be trained with query workload (Section 4.3). Next, a hybrid training procedure (Section 4.4) is proposed to use data as unsupervised information and queries as supervised information to jointly train UAE. We present the approaches to incorporating incremental data and query workload in Section 4.5. Finally, we discuss several miscellaneous issues (Section 4.6), and make several remarks (Section 4.7).

4 PROPOSED MODEL

Formulation as Distribution Estimation. Consider a set of attributes \( \{A_1, ..., A_n\} \) of a relation \( T \) and an indicator function \( I(a_1, ..., a_n) \) for a query \( q \), which produces 1 if the tuple \((a_1, ..., a_n) \in A_1 \times ... \times A_n\) satisfies the predicate of \( q \) and 0 otherwise. The joint data distribution of \( T \) is given by \( P(a_1, ..., a_n) = \frac{\text{number of occurrences of } (a_1, ..., a_n) \text{ in } T}{|T|} \) which is a valid distribution. Next, we can form the selectivity as: \( \text{Sel}(q) = \sum_{x=(a_1, ..., a_n) \in A_1 \times ... \times A_n} I(x) \cdot P(x) \). Thus, the key problem of selectivity estimation is obtaining the joint data distribution \( P(x) \) under the formulation.

4.1 Overview

Motivations On the one hand, data-driven methods have been claimed to be more general and robust to workload shifts than query driven methods [31, 78]. On the other hand, query workload with true selectivities provides additional information of the workload [12]. Therefore, it would be a natural idea of combining data-driven and query-driven models. As discussed before, the existing proposals leveraging both data and query workload [19, 30, 37, 39] are insufficient towards this direction.

An idea to overcome the problem of data-driven methods suffering the tail of the distribution due to their averaging optimization target would be using ensemble methods with each component targeting a different part of the distribution. However, 1) it is not easy to define a good partition. 2) It is nontrivial to integrate the results of different ensembles since queries may span multiple ensembles. For example, [31] uses an SPN to combine different ensembles and consequently independence assumptions are made. 3) Using ensembles is orthogonal to UAE. We can integrate UAE with ensemble methods if good ensemble methods could be designed.

Challenges In this work, to achieve the four goals in Introduction, we resort to deep autoregressive models since they [28, 78] have demonstrated superior performance for their expressiveness in capturing attribute correlations and efficiency. This is however challenging in two aspects: 1) Off-the-shelf deep autoregressive models in the machine learning literature are not able to incorporate the query workload information as supervised information for training the model. (2) As the naive combination of data-driven and query-driven models is not desirable, we aim to develop a unified autoregressive model with a single set of model parameters to use both data as unsupervised information and query workload as supervised information to learn the joint data distribution.

Overview of High-level Idea Both challenges call for designing new deep autoregressive models. First, deep autoregressive models rely on sampling techniques to answer range queries [78]. However, it cannot be trained with queries because the sampled categorical variables are not differentiable (to be explained in detail in Section 4.3). Therefore, to enable the deep autoregressive model to incorporate query workload as supervised information to learn the joint data distribution, we propose a novel idea that we utilize the Gumbel-Softmax trick to differentiate the sampled variables so that the deep autoregressive model can learn the joint data distribution directly from queries. In this way, our proposed model can also incorporate incremental query workload as discussed later.

Second, to fully leverage data as unsupervised information and queries as supervised information in the hybrid training setting, we combine the unsupervised and supervised losses produced from data and queries, respectively, with a trade-off hyper-parameter. This enables UAE to jointly train the deep autoregressive model to learn the joint data distribution by minimizing the combined loss. Therefore, the deep autoregressive model can learn from both data and queries simultaneously using the same set of model parameters.

Figure 1 shows the workflow of our proposed estimator UAE. We can train UAE with data only, and batches of random tuples are fetched from the table \( T \) for learning the joint data distribution. We can also train UAE with query as supervised information only and batches of random (query, cardinality) pairs are read from the query workload log to learn the joint data distribution. UAE is able to learn the joint data distribution with a single autoregressive model from both data and queries.

4.2 Preliminary: Deep Autoregressive Models for Cardinality Estimation

Autoregressive Decomposition Naively, one could store the point distribution of all tuples \((a_1, ..., a_n) \in A_1 \times ... \times A_n\) in a table for exact selectivity estimation. However, the number of entries in the table will grow exponentially in the number of attributes and is not feasible. Many previous methods have attempted to use Bayesian Networks (BN) for approximating the joint distribution \( P(x) \) via factorization [22, 71]. However, (1) they still make some conditional independence assumptions and (2) the expense of learning and inferring from BN is often prohibitive (we empirically found that the estimation time of a BN could be 110-120s on the DMV dataset).

To achieve a better trade-off between the ability to capture attribute correlations and space budgets while keeping the tractability and efficiency in model training and inference, we utilize the autoregressive decomposition mechanism which factorizes the joint distribution \( P(x) \) in an autoregressive manner without any independence assumption:
We thus use binary encoding, which encodes the same attribute values into integers in range \([0, |A_i| - 1]\) in a natural order. For instance, consider a string attribute \(A_i = \{\text{James, Tim, Paul}\}\), the encoded dictionary would be: \(\{\text{James} \rightarrow 0, \text{Tim} \rightarrow 2, \text{Paul} \rightarrow 1\}\). It is a bijection transformation without any information loss.

After the integer transformation, for each attribute, a specific encoder further encodes these integers into vectors for training the neural networks. The simplest method would be one-hot encoding. Specifically, consider the encoded integers of an attribute \(A_i\) with three distinct values: \(\{0, 1, 2\}\), one-hot encoding represents them as \((1, 0, 0), (0, 1, 0), (0, 0, 1)\). However, this naive method is not efficient in storage because the encoded vector is \(|A_i|\)-dimensional. We thus use binary encoding, which encodes the same attribute into \(\{(00), (01), (10)\}\), a \(\log_2 |A_i|\) dimensional vector.

**Model Architectures** We use ResMADE [53], a multi-layer perceptron with information masking technique which masks out the influence of \(x_{<i}\) on \(P(x_i|x_{<i})\). Exploring advanced architectures of deep autoregressive models [21, 55] is orthogonal to our work.

**Model Training** In a nutshell, the input to deep autoregressive estimators is each data tuple and its output is the corresponding predicted density estimation. In the training phase, the weights (or parameters) of deep autoregressive estimators are learned from data tuples by minimizing the cross-entropy between real and estimated data distributions [20].

\[
L^{data} = - \sum_{x \in D} P_\theta(x) \log \hat{P}_\theta(x)
\]

where \(\theta\) are the model weights. Normally, gradient updates for neural networks are performed by stochastic gradient descent (SGD) [11] using backpropagation [23, 62] as a gradient computing technique. Backpropagation is an efficient method for computing gradients in directed graphs of computations, such as neural networks, using chain rule [61]. It is a simple implementation of chain rule of derivatives, which computes all required partial derivatives in linear time in terms of the graph size, as shown in (1) of Figure 2.

**Answering Range Queries with Sampling** After being trained, deep autoregressive models can be directly used to answer point queries (e.g., \(A_1 = 2\) AND \(A_2 = 5\) for a relation with two attributes), because a deep autoregressive model is essentially a point distribution estimator. However, it is not easy to use the point estimator to answer range queries. Estimating the selectivity of a range query is equivalent to estimating the sum of selectivities for the set of data points the query contains. Suppose the region of a query \(q\) is: \(R^q = R^q_1 \times \cdots \times R^q_n\), where \(n\) denotes the number of attributes.

A naive approach for estimating the range query \(q\) is exhaustive enumeration:

\[
\hat{S}_\text{el}(q) = \sum_{x^q \in R^q} \hat{P}_\theta(x^q),
\]

where \(\{x^q | x \in R^q\}\) represents the list of distinct tuples contained in \(R^q\) and \(S_\text{el}(q)\) is the estimated selectivity of query \(q\). However, this method is computationally prohibitive because in the worst case, the number of estimated tuples would grow exponentially in the number of attributes. We thus resort to sampling techniques to efficiently compute the approximate selectivity result as follows.

- **Uniform Sampling** method samples \(S\) tuples at random and then computes the estimated selectivity as

\[
\hat{S}_\text{el}(q) = \frac{|R^q|}{S} \sum_{s=1}^{\frac{|R^q|}{S}} \hat{P}_\theta(x^q),
\]

where \(x^q \sim \text{Uniform}(\cdot)\). However, uniform sampling could produce large variances if the data distribution is skewed.

- **Progressive Sampling** is a Monte Carlo integration approach [78], which sequentially samples each tuple in order of its attributes by concentrating on the regions of high probability. Specifically, to sample a tuple \(x \in R^n\), we sequentially sample its attributes \(\{x_i\}\) from distributions \(P_\theta(x_i|x_{<i})\), respectively, where the categorical distribution \(P_\theta(x_i|x_{<i})\) is the distribution of \(x_i\) given attributes \(x_{<i}\) predicted by the deep autoregressive model. Therefore, the tuple having higher probabilities in \(P_\theta(x_i|x_{<i})\), \((i \in [1, N])\) could be more likely sampled. The selectivity estimate made by a sampled tuple is given by \(\hat{P}_\theta(x_i|x_{<i})\). The estimation result from multiple sampled tuples can be easily obtained by averaging the estimate of each single tuple. It is easy to verify that progressive sampling estimates are unbiased. This method is more robust to skewed data distribution than uniform sampling. We thus adopt progressive sampling in our work.

### 4.3 Training Deep Autoregressive Models with Queries

We proceed to present our idea of empowering the autoregressive model with the ability of learning from queries. Nevertheless, the existing autoregressive models cannot learn from queries via backpropagation in an end-to-end manner, because in principle gradients cannot flow through the sampled discrete random variables, and hence the process of progressive sampling is not differentiable, which is a prerequisite of backpropagation as explained earlier.

Specifically, consider a set of queries \(Q = \{q\}\), we define the query loss for autoregressive models as:

\[
L^{query} = \sum_{q \in Q} \text{Discrepancy}(\hat{S}_\text{el}(q), S_\text{el}(q)),
\]

where \(S_\text{el}(q)\) is the predicted selectivity of \(q\). There are many choices to define the function \(\text{Discrepancy}(\cdot, \cdot)\), e.g., root mean square error (RMSE) and Q-error [51]:

\[
\text{Q-error} = \max \left(1, \frac{S_\text{el}(q)}{\hat{S}_\text{el}(q)} \frac{\hat{S}_\text{el}(q)}{S_\text{el}(q)}\right).
\]

Next, let us focus on (2) in Figure 2, which illustrates the gradient flow of a deep autoregressive model with progressive sampling using \(S = 1\) sample, trained with queries. In each forward pass, the autoregressive model utilizes progressive sampling to successively sample one-hot vectors \(z_1, z_2, ..., z_{n-1}\) for each attribute. In practice, the result of sampling from \(P_\theta(x_i|x_{<i})\) in deep autoregressive models. \]
Figure 2: Gradient estimation in stochastic computation graphs for different models. We denote $L_{\text{data}}$ and $L_{\text{query}}$ by $L^d$ and $L^q$. (1) The autoregressive model trained with data. All nodes are deterministic so gradients can easily flow from $L^d$ to $ \theta$. (2) The original autoregressive model fed by queries. The presence of stochastic, non-differentiable nodes $z_1, ..., z_{n-1}$ prevents backpropagation because the categorically sampled variables do not have a well-defined gradient. (3) Our UA trained with queries. UA allows gradients to flow from $L^q$ to $ \theta$ by using a continuous variable to approximate $z$. The stochastic variable $g$ for each attribute is not involved in the gradient flow from $L^q$ to $ \theta$.

models is an one-hot vector $z_i$ that represents $x_i$, we thus denote $P_\theta(X_i|x_{<i})$ as $P_\theta(Z_i|\cdot)$ thereafter for clarity) and use them to compute $\mathcal{S}\ell(q)$. $L_{\text{query}}$ can be obtained after this. However, we observe that during backpropagation, gradients cannot completely flow from $L_{\text{query}}$ to $ \theta$. This is because that gradients cannot flow from $z_1, ..., z_{n-1}$ to $P_\theta(Z_1), ..., P_\theta(Z_{n-1}|\cdot)$, respectively, since the stochastic variables $z_1, ..., z_{n-1}$ do not have a well-defined gradient w.r.t. $P_\theta(Z_1), ..., P_\theta(Z_{n-1}|\cdot)$. One can easily generalize the case for $S > 1$ as only an averaging operation is needed to combine the estimate of each sample and it does not change the non-differentiable property of progressive sampling. Consequently, the model weights $\theta$ cannot be trained using query workload with the current techniques.

Our key insight is that if we can find a method making the process of progressive sampling differentiable, the deep autoregressive models can be trained directly from queries by minimizing the discrepancy between the actual selectivities and the estimated selectivities through progressive sampling via back-propagation.

The key challenge of differentiating progressive sampling is differentiating the non-differentiable sample $z_i$ from the categorical distribution $P_\theta(Z_i|\cdot)$. To this end, we consider two ideas: score function estimators and the Gumbel-Softmax trick, and analyze which is more suitable for our work.

Score Function Estimators. The score function estimator (SF), also known as REINFORCE [75], derives the gradient of query loss for autoregressive models w.r.t. the model weights $\theta$ by:

\[
\nabla_\theta \mathbb{E}_z [L_{\text{query}}] = \mathbb{E}_z [L_{\text{query}} \nabla_\theta \log P_\theta(Z) + \nabla_\theta L_{\text{query}}],
\]

where $z$ is sampled from $P_\theta(Z)$, and $L_{\text{query}}$ is a function of $\theta$ and $z$. With SF, we only need $P_\theta(Z)$ and $L_{\text{query}}$ being continuous in $\theta$ (which is valid), without requiring back-propagating through the sampled tuple $z$.

However, SF often suffers from high variance, even if it is improved with variance reducing techniques [24]. Also, SF is not scalable if used for categorical distribution because the variance will grow linearly in the number of dimensions in categorical distribution [59]. Consequently, a better method is needed.

The Gumbel-Softmax Trick. The Gumbel-Softmax trick [36, 50], which was originally used to differentiate discrete latent variables in variational auto-encoders [38] and is summarized in Algorithm 1.

Algorithm 1 The Gumbel-Softmax Trick (GS-Sampling)

**Input:** Temperature $\tau$; Categorical distribution $\pi$ with $k$ items;

**Output:** A differentiable one-hot vector $e$ from $\pi$;

1. Sample $u \sim \text{Uniform}(0,1)$ for $j = 1, ..., k$;
2. Compute $g_j = -\log(-\log(u))$ for $j = 1, ..., k$;
3. Sample $e$ according to Eq. 10;
4. return Sampled differentiable one-hot vector $e$;

Consider a categorical distribution with $k$-dimensional class probability $\pi$, to sample a one-hot vector $e$ from $\pi$, the key idea of the Gumbel-Softmax trick is:

\[
e = \text{onehot}(\text{argmax} \{g_j + \log \pi_j\}), \quad j = 1, ..., k.
\]

where $g_1, ..., g_n$ are independent and identically distributed samples drawn from a Gumbel$(0,1)$ distribution, which can be sampled by:

\[
g_j = -\log(-\log(u)), u \sim \text{Uniform}(0,1).
\]

Since argmax is non-differentiable, we can use differentiable Softmax as a continuous and approximate distribution to sample $e$:

\[
e \approx \text{softmax}(\log \pi + g)/\tau.
\]
where $\tau$ is an adjustable hyper-parameter, referred as temperature. When the temperature $\tau$ approaches 0, sampling from the Gumbel-Softmax distribution becomes one-hot. Hence, the temperature $\tau$ is a trade-off between the gradient variance and the degree of approximation to a one-hot vector. Essentially, $e$ sampled by the Gumbel-Softmax trick is differentiable and has been proven to have lower variance and be more scalable than SF. Therefore, in this work we use the Gumbel-Softmax trick as the core technique for differentiating progressive sampling. Note that $\pi$ can be any categorical distribution, including $P_\theta(Z_i|\cdot)$.

Based on the procedure of the Gumbel-Softmax trick, we introduce in detail how to use the Gumbel-Softmax trick to differentiate progressive sampling. As shown in (3) of Figure 2, the key idea of differentiable progressive sampling is using deterministic, continuous variables $y_1, ..., y_{n-1}$ to approximate stochastic discrete variables $z_1, ..., z_{n-1}$ so that gradient can flow from $L^{\text{query}}$ to $\theta$ completely. Specifically, for each attribute $i$, in a forward pass, a stochastic vector $g$ is first generated from Eq. 9. Next, we define $h_i = (\log P_\theta(Z_i|\cdot)+g_i)/\tau$ and sample $y_i$ from softmax ($h_i$), according to Eq. 10. Note here the categorical distribution $\pi$ in Eq. 10 is set to $P_\theta(Z_i|\cdot)$. Then we can use the sampled $y_1, ..., y_{n-1}$ to continue the forward pass. In doing so, we surprisingly find that gradients from $L^{\text{query}}$ to $\theta$ can be computed completely, because the stochastic nodes $\{g\}$ are dis-encountered from the entire gradient flows.

### Algorithm 2 Differentiable Progressive Sampling (DPS)

**Input:**
- Temperature $\tau$; Number of samples $S$;
- Query region $R^d$; Model density estimation $P_\theta(\cdot)$;

**Output:** Estimated selectivity $\bar{S}(q)$;

```plaintext
1: $\hat{p} = 0$; // Initialize the ultimate density estimate
2: for $s = 1$ to $S$ do
3:   $\hat{p}^s = 1$; // Initialize the $s$-th sample’s density estimate
4:   for $i = 1$ to $n$ do
5:     Forward pass the model and obtain $P_\theta(Z_i|z_{<i})$;
6:     $\hat{p}^s = \hat{p}^s \cdot P_\theta(z_i \in R^d_{|z_{<i}})$;
7:     Zero-out probabilities outside $R^d_{|z_{<i}}$ for $P_\theta(Z_i|z_{<i})$;
8:     Normalize $P_\theta(Z_i|z_{<i})$ and obtain $P_\theta(Z_i|z_{<i}, z_i \in R^d_{|z_{<i}})$;
9:     Sample differentiable $z_i$ via the Gumbel-Softmax trick:
10:    $z_i = \text{GS-Sampling}(\tau, P_\theta(Z_i|z_{<i}, z_i \in R^d_{|z_{<i}}))$; // Alg. 1
11: end for
12: end for
13: Average the density estimates of $S$ samples: $\hat{p} = \hat{p}/S$;
14: return $\bar{S}(q) = \hat{p}$
```

We present the flow of differentiable progressive sampling (DPS) in Algorithm 2. Note that in practice we can perform DPS with $S > 1$ samples in batch. Note that in line 7 of Algorithm 2, we can simply musk out the probabilities of $z_i \notin R^d_{|z_{<i}}$ by setting the corresponding values in $\log P_\theta(Z_i|z_{<i})$ to negative infinity (-inf). This does not change the categorical property of $P_\theta(Z_i|z_{<i})$ and does not affect GS-Sampling.

### Algorithm 3 Hybrid Training of UAE

**Input:**
- Temperature $\tau$; Number of samples $S$; // Used in DPS
- $\lambda$: The underlying data $D$; Query workload $(Q, C)$;

**Output:** Trained model weights $\theta$;

```plaintext
1: Randomly initialize model weights $\theta$;
2: while JointTraining() do
3:   $D_b \leftarrow \text{RandomBatch}(D)$;
4:   $(Q_b, C_b) \leftarrow \text{RandomBatch}((Q, C))$;
5:   Obtain $L^{\text{data}}$ for $D_b$;
6:   Obtain $L^{\text{query}}$ for $(Q_b, C_b)$ through Alg. 2 using $\tau, S$;
7:   Perform SGD via backpropagation for $L$ (Eq. 11);
8: end while
9: return $\theta$
```

### 4.4 Hybrid Training

Now, UAE is able to learn from either data or queries. To achieve our ultimate goal, which is to take both data as unsupervised information and queries as supervised information into the training of UAE, we propose a hybrid training method, which trains the model of UAE by minimizing an overall loss function $L$ combining $L^{\text{data}}$ (Eq. 2) and $L^{\text{query}}$ (Eq. 5) by a hyper-parameter $\lambda$:

$$L = L^{\text{data}} + \lambda L^{\text{query}}.$$  

The adjustable hyper-parameter $\lambda$ rescales the relative values of $L^{\text{data}}$ and $L^{\text{query}}$. In doing so, UAE learns to capture both the data and query workload information simultaneously to learn the joint data distribution. We summarize the workflow of the hybrid training of UAE in Algorithm 3.

### 4.5 Incorporating Incremental Data and Query Workload

We introduce the superiorities of UAE in efficiently and effectively ingesting incremental data or query workload.

**Incremental Data** denotes the tuples newly added to the database after the model is trained. UAE can perform incremental training on the incremental data by minimizing the unsupervised loss $L^{\text{data}}$ produced from the new data.

**Incremental Query Workload** is a set of queries drawn from a different distribution compared to the training workload (i.e., they focus on different data regions). For example, on IMDB dataset, a workload might focus on the data area where title.production_year $>$ 1975 but another workload might focus on title.production_year $<$ 1954. To adapt to the new query workload after being trained, UAE only need to minimize the supervised loss offered from $L^{\text{query}}$ for incrementally ingesting these new queries. In our experiments, we find a smaller value of training epochs (10-20) is enough to prevent UAE from catastrophic forgetting.

### 4.6 Miscellaneous Issues

**Supporting Join Queries.** A natural idea of supporting multi-table joins for UAE is to train UAE on join results offered by join samplers [33, 42]. We follow the idea [31, 77] to handle join queries, which adds virtual indicator and fanout columns into the model architecture of UAE. Then we train UAE on tuples sampled by the Exact Weight algorithm [80] and queries with fanout scaling. Interested readers may refer to [31, 77] for details.
Handling Columns with Large NDVs. A problem of the autoregressive architecture UAE is when the number of distinct values (NDVs) in a column is very large, storing the model parameters would consume large space. Hence, for columns with large NDVs, we leverage 1) embedding method (which embeds one-hot column vectors by learnable embedding matrices) for tuple encoding and decoding; 2) column factorization which slice a value into groups of bits and then transforms them into base-10 integers [77].

Handling Unqueried Columns (Wildcards). We use wildcard skipping [45, 78] which randomly masks tuples and replaces them with special tokens as the inputs to UAE’s data part during training. This could improve the efficiency of training UAE and query inference, because for omitted columns we can skip DPS during training and skip progressive sampling during query inference.

4.7 Remarks

We call the UAE trained with data and queries as UAE-D and UAE-Q, respectively. We make several remarks as follows:

- UAE can accurately capture complex attribute correlations without independence or uniformity assumptions because of its deep autoregressive model architecture;
- By learning from both data and query workload, UAE is further forced to produce more accurate estimates in the data regions accessed by the workload. Meanwhile, UAE can maintain the knowledge of overall data distribution;
- In fact, UAE-D is equivalent to Naru [78]. We thus claim that UAE generalizes Naru;
- We opt for Q-error as the Discrepancy(.) for UAE-Q because it is consistent with our evaluation metric.
- A distinct feature of UAE-Q is that, different from other supervised methods [28, 54, 68, 76] or sampling enhanced ML model [39] for cardinality estimation which are all discriminative, deep autoregressive model-based UAE-Q is a generative model. To the best of our knowledge, UAE-Q is the first supervised deep generative model for cardinality estimation.
- When being used to estimate the cardinality of a query, UAE only uses its model weights, without scanning the data. Thus the estimation process is convenient and efficient, especially if accelerated by advanced GPU architectures.
- By switching between UAE-D and UAE-Q, UAE can learn from new data or query workload in an incremental manner, without being retrained. To the best of our knowledge, there is no single deep learning-based model for cardinality estimation can achieve the two goals of incremental learning, although it is a consequent advantage of UAE’s construction strategy.

5 EXPERIMENTAL RESULTS

We conduct comprehensive experiments to answer the following research questions.

- **RQ1:** Compared to state-of-the-art cardinality estimation models, how does UAE perform in accuracy (Section 5.2)?
- **RQ2:** How different hyper-parameters (e.g., temperature \( \tau \), trade-off parameter \( \lambda \)) affect the results of UAE (Section 5.3)?
- **RQ3:** How well can UAE incrementally incorporate new data and query workload (Section 5.4)?
- **RQ4:** How long does it take to train UAE and how efficient does it produce a cardinality estimate (Section 5.5)?
- **RQ5:** How does UAE impact on a query optimizer (Section 5.6)?

5.1 Experimental Settings

5.1.1 Datasets. We use three real-world datasets with different characteristics for single-table experiments as follows:

1. **DMV** [79]. This dataset consists of vehicle registration information in New York. We follow the preprocessing strategy in previous work [78], and get 11.6M tuples and 11 columns after preprocessing. The 11 columns has widely different data types and domain sizes ranging from 2 to 2101. We also use **DMV-large** which includes columns with very large NDVs (e.g., 100% unique VIN column and 31K unique CITY column) and has 16 columns. This dataset is used to evaluate the sensitivities of compared methods to very large NDVs. We find that the results provide similar clues as those on DMV, and thus we do not report them here due to the space limit.

2. **Census** [6]. This dataset was extracted from the 1994 Census database, consisting of person income information. It contains 48K tuples and 14 columns. The 14 columns contain a mix of categorical columns and numerical columns with domain sizes ranging from 2 to 123.

3. **Kddcup98** [6]. This dataset was used in the KDD Cup 98 Challenge. We use 100 columns for experiments and use this dataset to evaluate the sensitivities of various methods to very high-dimensional data. It contains 95K tuples with domain sizes ranging from 2 to 43.

We use two statistics in probability theory to measure the skewness and correlation of datasets: Fisher–Pearson standardized moment coefficient [18] for skewness and Nonlinear Correlation Information Entropy (NCIE) [74] for correlation. Smaller values of the two measures indicate weaker skewness or correlation. The skewness measures are 4.9, 2.1, 4.7 and the correlation measures are 0.23, 0.15, 0.32 for DMV, Census and Kddcup98, respectively. Therefore, DMV and Kddcup98 have relatively stronger skewness and attribute correlation while Census has weaker skewness and attribute correlation. In addition, we use the real-world IMDB dataset for experiments on join queries. IMDB was reported to have strong attribute correlation [41].

5.1.2 Query Workload.

Training Queries. We follow the previous work [12, 39] to generate query workload as there is no real query log available for the datasets we use. Specifically, we first choose an attribute with a relatively large domain size as the bounded attribute. The bounded attribute is specified by a distribution for the centers and a target measure is chosen uniformly within a specific range and the target measure is a target volume of 1% of the distinct values. We have also varied the selection method for the centers (e.g., following
data distribution) and the target measure (e.g., target selectivity) and the experimental results turned out to be qualitatively similar. We thus do not report these results due to the page limit. Next, for other attributes (i.e., random attributes), we follow the method [39, 78] to generate queries. We draw the number of filters ($n_f \geq 5$) at random. Then we uniformly sample $n_f$ columns and the corresponding filter operators. Finally, the filter literals are set from the values of a randomly sampled tuple. We generate 20K training queries for each dataset. For join experiments, we use one template (a join table subset) out of 18 templates in JOB-light, a 70-query benchmark used by a number of previous work, to generate 10K training queries. This template includes 3 tables, title, movie_companies, movie_info. We set title.production_year as the bounded attribute and then choose 2-5 filters on other content columns as discussed above. This generation procedure follows [77] which produces more diversified queries than job-light, using the same join template. We term this benchmark as JOB-light-ranges-focused.

**Test Queries.** Apart from the performance on the training workload (i.e., in-workload queries), we also evaluate whether the estimators are robust to out-of-workload queries. Therefore, we generate two kinds of test queries to thoroughly evaluate the performance of estimators: (1) In-workload Queries: 2K test queries are generated in the same procedure of training query workload. For joins experiments we generate 1K test queries from JOB-light-ranges-focused; (2) Random Queries: We also generate 2K test queries without bounded attributes, i.e., all attribute filters are generated randomly, to evaluate the robustness of different models to workload shifts. For join experiments we use JOB-light as it contains no focused information.

**Workload Characteristics.** Figure 3 plots the selectivity distributions of 2K in-workload and random queries on all datasets. We observe: 1) the selectivities of generated workloads are widely spaced. 2) Random queries have much wider selectivity spectrums than in-workload queries because in-workload queries have an additional bounded column. Note that though training and test in-workload queries share the same generation procedure, we manually ensure that each training query is different from each test query.

5.1.3 **Performance Metric.** Following the previous work [28, 39, 78], we evaluate all models by the popular metric for cardinality estimation, $\epsilon$-error, which is defined in Eq. 6.

5.1.4 **Baseline Methods.** We compare UAE 1 to 9 cardinality estimation methods, including state-of-the-art and the newest methods.

**Query-driven Models:**

1. **MSCN-base [39].** This query-driven deep learning (DL)-based method uses a multi-set convolutional neural network for answering correlated joins. For each predicate, it features the attribute and operator using one-hot vectors and normalizes the value. It then concatenates the average results over the predicate set as the query encoding. We use two layers (256 hidden units) of multilayer perceptrons, the default setting of [39], on the query encoding. We apply the code from [3]. Note that the original MSCN was proposed to handle join queries. We adapt MSCN to single-table queries by dropping the join module. We also evaluate another query-driven DL method Sup [28] and find that it shares the similar performance with MSCN.

2. **LR [40].** This method first represents a query as the concatenation of the domain range of each predicate (following [19]), and trains a linear regression model on the query representation. We use this method as a non-DL query-driven counterpart to demonstrate the effectiveness of DL-based query-driven methods (MSCN-base).

**Data-driven Models:**

3. **Sampling.** This method keeps a portion ($p$) of tuples uniformly from the dataset and scans them to estimate query cardinalities.

4. **BayesNet [14].** We follow the same setting [78] for this method for a fair comparison.

5. **KDE [26].** This method leverages the kernel density estimator for estimating the data distribution. Gaussian kernels are adopted in the experiments and the bandwidth is calculated from data by Scott’s rule [65].

6. **DeepDB [31].** This method models joint data distribution by learning relational sum-product networks, which is based on the structure of Sum Product Networks (SPN) [57]. The number of samples per SPN for learning the ensemble is set to 1M. We use its open-sourced code [1]. DeepDB is a deep model but non-neural, which is a proxy to compare neural deep models (Naru, UAE) against the effectiveness of non-neural deep models.

7. **Naru [78].** Naru is equivalent to UAE-D. We extend the open-sourced code from [4] because the original code does not support two-sided queries. We also compare with MADE [28], which also uses deep autoregressive models and its performance is close to Naru [78]. For join queries, we compare UAE with NeuroCard [77], a concurrent work that extends Naru for join.

**Hybrid Models:**

8. **MSCN+Sampling [39].** This method uses estimates on materialized sampled tuples as additional inputs to MSCN-base. We use this method to demonstrate the advantages of leveraging both data and workload information.

9. **Feedback-KDE [30].** This method further utilizes query feedback to adjust the bandwidth in KDE [26]. We apply the code from the authors [2] and modify it to run it with more than 10 columns. SquaredQ loss function and Batch variant are adopted for bandwidth optimization.

We also compared with STHoles [12], Postgres [5] and MHIST [58]. The performances are worse than the 9 methods, and thus we do not report them here. The numbers of sample tuples in two KDE-based methods (KDE and Feedback-KDE) and two sampling-based methods (Sampling and MSCN+sampling) are set to match the memory budget of our model for a fair comparison. For Sampling method, the sample ratios are 0.2%, 9%, 4.6% for DMV, Census and Kddcup98, respectively. We also test two sampling budgets, one smaller (0.75$p$) and one larger (1.25$p$) than $p$. The results do not change the conclusions in this paper, and thus we do not report them here. Additionally, for a fair comparison, two autoregressive based models (UAED and Naru) share the same model architecture, which is 2 hidden layers (2x128 units). We also turn on column factorization on IMDB due to its high-cardinality columns. Afterward, the space consumption of the autoregressive model is 2.0MB, 0.5MB, 3.45MB and 4.1MB on DMV, Census, Kddcup98 and IMDB, respectively. In addition, the two deep autoregressive based methods, Naru and

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1. The source code is available at https://github.com/pagegitss/UAE.
UAE, rely on progressive sampling for answering range queries. For fair comparison, the number of estimate samples is set to 200 on DMV in-workload queries, Census and 1K on DMV random queries, Kddcup98, IMDB for both of them, because we empirically found by this setting, they can strike a better balance between the estimation accuracy and overheads, e.g., further increasing the estimate number will not result in a significantly improvement in accuracy but will increase the estimation overhead. In UAE, the temperature \( r \) and the number of samples \( S \) in DPS are set to 1 and 200, respectively, on all the datasets. The trade-off parameter \( \lambda \) is set to \( 1e^{-4} \) on three single-table datasets and 10 on IMDB dataset. All the experiments were run on a machine with a Tesla V100 GPU and a 20 cores E5-2698 v4 @ 2.20GHz CPU.

### 5.2 Performance Comparison

Tables 2 ~ 5 show the experimental results of all models on both in-workload queries and random (out-of-workload) queries. The results show that UAE matches or significantly exceeds the best estimator across the board, not only in terms of mean and median, but also in terms of max, which demonstrates the robustness of UAE in handling tail of difficult queries. From these experimental results, we conclude several major findings as follows.

1. **UAE-Q outperforms other supervised methods in most cases and they are vulnerable to workload shifts.** We observe that the proposed UAE-Q outperforms LR and MSCN-base in most of the cases. We also observe that for all the supervised methods, the accuracy on random queries is much worse than that on in-workload queries. This indicates that supervised models may learn the data distribution on the data regions the training workload focuses on, but are vulnerable to workload shifts. For example, on DMV, when moving from in-workload queries to random queries, MSCN-base degrades by \( 46\times \) in mean error and \( 27\times \) in max error.

2. **Unsupervised methods are more robust to workload shifts but still produce large error at tail.** The performance gap of unsupervised methods between in-workload and random queries is much smaller than those of supervised methods. Nevertheless, these unsupervised models still have large worst-case errors likely due to their optimization target of minimizing the average error. For instance, on DMV dataset, Naru produces 108 for max error.

3. **DL-based methods outperform non-DL methods, especially at tail.** For supervised methods, deep learning (DL) models MSCN-base preforms significantly better than traditional machine learning method LR. Also, for unsupervised methods, deep learning method Naru and DeepDB usually perform better than non-DL methods (e.g., BayesNet), especially in mean and max errors. These results demonstrate that DL can better capture complex data correlation than non-DL models.

4. **KDE-based methods suffer from large domain sizes.** KDE-based methods (KDE and Feedback-KDE) perform poorly on two datasets with large domain sizes (DMV). Moreover, We find that Feedback-KDE can not enhance the performance of KDE significantly. It is likely because KDE-based methods suffer on these datasets inherently or the bandwidths computed by Feedback-KDE are not optimal on these datasets.

5. **DeepDB preforms relatively well on datasets with weak attribute correlation but degrades largely on datasets with strong attribute correlation.** On the dataset with weaker attribute correlation (i.e., Census), DeepDB offers accurate estimates across all error quantiles. Nevertheless, on DMV that has strong attribute correlations, DeepDB’s performance drops quickly especially at tail, since the independence assumption in sum-product networks of DeepDB does not hold for this dataset.

6. **Deep autoregressive models suffer from high dimensional data and SPNs might suffer from high NDVs.** We draw interesting conclusions in the comparison between deep autoregressive model-based methods (Naru, UAE) and SPNs-based method (DeepDB). On two datasets with relatively high domain sizes (2K for DMV, 100% unique for DMV-large), DeepDB may suffer at tail (e.g., max error \( 3 \cdot 10^4 \) on DMV random queries) while deep autoregressive model-based methods achieve much more stable accuracy. This is likely because that the histograms used in the leaf nodes of DeepDB cannot accurately model the distributions of attributes with high NDVs while deep autoregressive models can well capture them because they consider the probability of each distinct value at the output layer. On the contrary, on Kddcup98 with 100 attributes, deep autoregressive models may degrade at tail (e.g., Naru makes max error 690 on random queries. Although UAE improves Naru by \( 2\times \), it still makes max error 345), but DeepDB can achieve very low max error. This is likely because a higher dimensional dataset would contain more independent attributes. In this case, the autoregressive decomposition of autoregressive models might introduce noises to the model learning since it “forces” the model to learn the correlation between independent attributes. However, DeepDB would not have this problem as SPNs successfully separate those independent attributes into different groups for this dataset. The result indicates that a promising future work would be to combine the best of deep autoregressive models and SPNs for high-dimensional datasets with high NDVs.

7. **Additional data information boosts supervised methods by a large margin.** Compared to MSCN-base, MSCN+sampling achieves much better performance on all datasets. The improvements become more obvious on random queries. The results demonstrate that including the estimates from sampling as extra features together with query features improve the accuracy of neural networks in MSCN. We also note that integrating query as supervised information in KDE does not help on the three datasets.

8. **UAE outperforms both of its two modules.** For example, on DMV both UAE-D and UAE-Q have a max error 108. However, UAE is able to achieve max error 5.0, which greatly improves the tail behaviour. This demonstrates the effectiveness of the unified modeling and training in UAE for cardinality estimation.

9. **UAE achieves the best performance on in-workload queries while maintaining the robustness on random queries.** UAE achieves the best overall results (in mean and max errors) on in-workload queries on all single-table datasets. For instance, on DMV, UAE outperforms the second best method Naru by \( 21\times \) at tail. Also, UAE produces the lowest median errors on in-workload queries on most datasets. Additionally, UAE also achieves the best or comparable overall performance for join queries. As shown in Table 5, on JOB-light-ranges-focused, UAE produces the lowest median error and beats two newest data-driven models (DeepDB, NeuroCard) by a large margin across all error quantiles. Although MSCN+sampling outperforms UAE at tail on this workload, its performance drops on
Impact of Temperature

Temperature parameter $\tau$ is used in the Gumbel-Softmax algorithm which works for the supervised part of UAE (i.e., UAE-Q). We have to isolate the influence from UAE’s unsupervised part (i.e., UAE-D) when training with UAE-Q. To this end, we first train UAE only with UAE-D to obtain the overall data knowledge. Next UAE is refined by UAE-Q with various settings of $\tau$. Specifically, 10k training queries are generated following the procedure described in Section 5.1.2 and the evaluation is conducted on 2K in-workload queries since we are interested in the effect of $\tau$ on the performance of UAE’s supervised part. As discussed in [36], fixed $\tau$ between 0.5 and 1.0 yields good results empirically. We thus evaluate candidate values $\{0.5, 0.75, 1.0, 1.25\}$ for $\tau$. In addition, we use 2K samples for estimation because we are interested in the limits of UAE influenced by $\tau$ and lower numbers of estimation samples also share the same trend. We empirically find that at $\tau = 1.0$, UAE achieves the lowest estimation errors.

Impact of Trade-off Parameter $\lambda$

Trade-off parameter $\lambda$ rescales the losses produced by two parts of UAE, UAE-D and UAE-Q. We thus use the same query workload in Section 5.1.3. The candidate values of $\lambda$ are $\{1e^{-6}, 1e^{-5}, 1e^{-4}, 1e^{-3}, 1e^{-2}\}$. Figure 4 (b) shows the performance of UAE on both in-workload and random queries as $\lambda$ is varied, from which we conclude $\lambda$’s best setting is $1e^{-4}$. Moreover, when $\lambda$ is larger than $1e^{-3}$, the performance drops quickly on both kinds of queries, indicating that putting too much emphasis on...
Table 6: Effectiveness of incorporating incremental query workload. Stale Naru vs. Refined UAE.

| Ingested Partitions | 1     | 2     | 3     | 4     | 5     |
|---------------------|-------|-------|-------|-------|-------|
| Naru: mean          | 1.035 | 1.047 | 1.152 | 1.197 | 2.903 |
| UAE: mean           | 1.031 | 1.039 | 1.095 | 1.132 | 1.073 |

UAE-Q will negatively affect model training and is not encouraged.

5.4 Incremental Data and Query Workload

This experiment is to study the incremental learning ability of UAE. Since the ability of autoregressive models to incorporate incremental data has been demonstrated in previous work [28, 78], UAE, based on autoregressive model, can inherently handle incremental data. Consequently, we will not repeat the experiment in this paper. Beyond the previous work, we aim to show that UAE is also able to incorporate incremental query workload while previous work [28, 78] cannot. To this end, using the same procedure in Section 5.1.3, we generate 5 parts of query workload with different query center for the bounded column, i.e., different query workload focuses on different data region. Each part consists of 4K training queries and 200 in-workload test queries since we our goal is to demonstrate UAE’s effectiveness of incorporating new query workload. After training UAE with the underlying data, we ingest each partition of query workload in order, following the experimental setting of incremental data in [78]. Evaluations are conducted after each ingest using the test queries in that partition. We compare refined UAE to the model only trained with the underlying data (i.e., Naru), which cannot further ingest incremental query workload, on DMV. Table 6 shows the mean errors of both methods, which are estimated by 200 samples. From the table, we observe:

1. due to the incapability of leveraging query workload, the performance of Naru is not stable on queries of various workloads.
2. UAE can offer consistently accurate estimates after being refined by each query workload, which demonstrates the ability of UAE in effectively ingesting incremental query workload.

5.5 Training Time & Estimation Efficiency

An epoch of UAE takes about 363 seconds, 62 seconds, and 657 seconds on DMV, Census, and Kddcup98, respectively. We report the changing process of max error estimated by 200 samples as training progresses on Census in-workload queries in Figure 5 (1). We observe that about 13 epochs for UAE yields the performance of single-digit max error, which is 9.0.

On all datasets, UAE can produce estimates in around 10ms on a V100 GPU. Figure 5 (2) shows the estimation latencies of different estimators on DMV. As shown in the figure, UAE can produce estimates in reasonable efficiency, much faster than sampling-based methods (MSCN+sampling, Sampling).

5.6 Impact on Query Optimization

We proceed to evaluate the impact of UAE on query optimization, compared to PostgreSQL and NeuroCard. We follow the procedure [15] and we modify the source code of PostgreSQL to allow it accept external cardinality estimates. Then, for each query we collect the cardinality estimates of its subqueries returned by different estimators and inject them into the modified PostgreSQL. We use the JOB-M [41] benchmark as the testbed for this case because it has a more complex join schema, which is more challenging for query optimization. We generate 50 test queries using a template of JOB-M (including 6 tables and multi-way joins), following the generation procedure of JOB-light-ranges-focused. For training UAE, we use the same template to randomly generate 10k subqueries (including 2~5 tables). Figure 6 shows the impact of cardinality estimates from NeuroCard and UAE on query performance compared to PostgreSQL. We have two major findings. First, more accurate cardinality estimates from deep autoregressive model-based estimators could translate into better query plans in query optimization of PostgreSQL. Second, for in-workload queries, UAE could result in equivalent or better query plans to improve the quality of query optimization without any significant slowdown compared with PostgreSQL and NeuroCard.

6 CONCLUSIONS AND FUTURE WORK

We propose a novel unified deep autoregressive model that is able to utilize both data as unsupervised information and query workload as supervised information for cardinality estimation. Experiments demonstrate that UAE achieves the four goals in Section 1.

We see this work as the first step toward a unified deep learning model that is able to train a single model exploiting both data information and workload information for cardinality estimation. We expect that our unified model for cardinality estimation would be inspirational to future developments of cardinality estimation models that fuse data information and query workload. We believe that our model will open interesting and promising future research directions. For example, exploring the power of UAE-Q on database generation is a very promising direction. The generative characteristic of UAE-Q allows us to efficiently sample tuples from the model. This is not the case in other supervised models because it is hard to obtain the normalizing constant [15] of the data probability for these models. This characteristic makes UAE-Q suitable for database generation for DBMS testing and benchmarking [10, 44, 48], another important task for big data management.

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