Neural Databases

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ABSTRACT
In recent years, neural networks have shown impressive performance gains on long-standing AI problems, and in particular, answering queries from natural language text. These advances raise the question of whether they can be extended to a point where we can relax the fundamental assumption of database management, namely, that our data is represented as fields of a pre-defined schema.

This paper presents a first step in answering that question. We describe NeuralDB, a database system with no pre-defined schema, in which updates and queries are given in natural language. We develop query processing techniques that build on the primitives offered by the state of the art Natural Language Processing methods.

We begin by demonstrating that at the core, recent NLP transformers, powered by pre-trained language models, can answer select-project-join queries if they are given the exact set of relevant facts. However, they cannot scale to non-trivial databases and cannot perform aggregation queries. Based on these findings, we describe a NeuralDB architecture that runs multiple Neural SPJ operators in parallel, each with a set of database sentences that can produce one of the answers to the query. The result of these operators is fed to an aggregation operator if needed. We describe an algorithm that learns how to create the appropriate sets of facts to be fed into each of the Neural SPJ operators. Importantly, this algorithm can be trained by the Neural SPJ operator itself. We experimentally validate the accuracy of NeuralDB and its components, showing that we can answer queries over thousands of sentences with very high accuracy.

1 INTRODUCTION
In recent years, neural networks have shown impressive performance gains on long-standing AI problems, such as natural language understanding, speech recognition, and computer vision. Based on these successes, researchers have considered the application of neural nets to data management problems, including learning indices [21], query optimization and entity matching [25, 29]. In applying neural nets to data management, research has so far assumed that the data was modeled by a database schema.

The success of neural networks in processing unstructured data such as natural language and images raises the question of whether their use can be extended to a point where we can relax the fundamental assumption of database management, which is that the data we process is represented as fields of a pre-defined schema. What if, instead, data and queries can be represented as short natural language sentences, and queries can be answered from these sentences? This paper presents a first step in answering that question. We describe NeuralDB, a database system in which updates and queries are given in natural language. The query processor of a NeuralDB builds on the primitives that are offered by the state of the art Natural Language Processing (NLP) techniques. Figure 1 shows example facts and queries that NeuralDB can answer.

Realizing the vision of NeuralDB will offer several benefits that database systems have struggled to support for decades. The first, and most important benefit is that a NeuralDB, by definition, has no pre-defined schema. Therefore, the scope of the database does not need to be defined in advance and any data that becomes relevant as the application is used can be stored and queried. The second benefit is that updates and queries can be posed in a variety of natural language forms, as is convenient to any user. In contrast, a traditional database query needs to be based on the database schema. A third benefit comes from the fact that the NeuralDB is based on a pre-trained language model that already contains a lot of knowledge. For example, the fact that London is in the UK is already encoded in the language model. Hence, a query asking who lives in the UK can retrieve people who are known to live in London without having to explicitly specify an additional join. Furthermore, using the same paradigm, we can endow the NeuralDB with more domain knowledge by extending the pre-training corpus to that domain.

By nature, a NeuralDB is not meant to provide the same correctness guarantees of a traditional database system, i.e., that the answers returned for a query satisfy the precise binary semantics of the query language. Hence, NeuralDBs should not be considered...
as an alternative to traditional databases in applications where such guarantees are required.

Given its benefits, Neural Databases are well suited for emerging applications where the schema of the data cannot be determined in advance and data can be stated in a wide range of linguistic patterns. A family of such applications arise in the area of storing knowledge for personal assistants that currently available for home use and in the future will accompany Augmented Reality glasses. In these applications, users store data about their habits and experiences, their friends and their preferences, and designing a schema for such an application is impractical. Another class of applications is the modeling and querying of political claims [46] (with the goal of verifying their correctness). Here too, claims can be about a huge variety of topics and expressed in many ways.

Our first contribution is to show that state of the art transformer models [47] can be adapted to answer simple natural language queries. Specifically, the models can process facts that are relevant to a query independent of their specific linguistic form, and combine multiple facts to yield correct answers, effectively performing a join. However, we identify two major limitations of these models: (1) they do not perform well on aggregation queries (e.g., counting, max/min), and (2) since the input size to the transformer is bounded and the complexity of the transformer is quadratic in the size of its input, they only work on a relatively small collection of facts.

Our second contribution is to propose an architecture for neural databases that uses the power of transformers at its core, but puts in place several other components in order to address the scalability and aggregation issues. Our architecture runs multiple instances of a Neural SPJ operator in parallel. The results of the operator are either the answer to the query or the input to an aggregation operator, which is done in a traditional fashion. Underlying this architecture is a novel algorithm for generating the small sets of database sentences that are fed to each Neural SPJ operator.

Finally, we describe an experimental study that validates the different components of NeuralDBs, namely the ability of the Neural SPJ to answer queries or create results for a subsequent aggregation operator even with minimal supervision, and our ability to produce support sets that are fed into each of the Neural SPJ operators. Putting all the components together, our final result shows that we can accurately answer queries over thousands of sentences with very high accuracy. To run the experiments we had to create an experimental dataset with training data for NeuralDBs, which we make available for future research.

2 PROBLEM DEFINITION

The main goal of NeuralDB is to support data management applications where users do not need to pre-define a schema. Instead, they can express the facts in the database in any linguistic form they want, and queries can be posed in natural language. To that end, data and queries in a NeuralDB are represented as short sentences in natural language and the neural machinery of the NeuralDB is applied to these sentences.

Data: Users input data into an NeuralDB using simple natural language sentences. Intuitively, a sentence corresponds to a single fact, such as Sue is Mary’s mom, or Gustavo likes espresso. But in many situations, especially when updates to the database are spoken by users, it is more convenient for sentences to express multiple facts, such as Kiara is married to Kyrone and they have 3 kids. We refer to the latter sentences as composite and the former as atomic. To focus on the novel issues of NeuralDBs, we mostly consider atomic sentences in this paper, but we do demonstrate in Section 3 both atomic and composite sentences.

Formally, the data in an NeuralDB is a set of sentences, each with a time stamp, $D = \{(u_1, t_1), \ldots, (u_k, t_k)\}$. A NeuralDB allows updates, deletions and queries. The user does not need to distinguish between an update and a query because NLP technology can reliably make that distinction. We assume that deletions are explicitly marked and also refer to individual sentences.

Queries: Formally, a query $Q$ over a database, $D$, produces a set of answers: $Q(D) = \{a_1, \ldots, a_l\}$. While queries are formulated in natural language, we only consider queries that, if translated to SQL, would involve a select-project-join (SPJ) component followed by an aggregation. However, for our analysis we need to make some further distinctions between several classes of queries (outlined in Figure 1).

A lookup query is a query where each answer comes from a single fact in the database (e.g., Who is Susan’s husband?), whether there is a single answer or several. If the query returns True/False, we refer to it as a Boolean query. Note that in our context, lookup queries are non-trivial because facts in the database are expressed in a variety of linguistic forms.

A join query is one that requires combining two (or more) facts in the database in order to produce each answer. For example, the query ‘Who works in a company in France?’ could combine facts pertaining to a person’s country of residence, and others pertaining to people’s jobs. In some cases, the query may require a join even if one is not explicitly specified in the query. For example, the query

| Facts: (4 of 50 shown) |
|-----------------------|
| Nicholas lives in Washington D.C. with Sheryl. |
| Sheryl is Nicholas’s spouse. |
| Teuvo was born in 1912 in Ruskala. |
| In 1978, Sheryl’s mother gave birth to her in Huntsville. |

| Queries: |
|----------------|
| Does Nicholas’s spouse live in Washington D.C.? |
| (Boolean Join) $\rightarrow$ TRUE |
| Who is Sheryl’s husband? |
| (Lookup) $\rightarrow$ Nicholas |
| Who is the oldest person in the database? |
| (Max) $\rightarrow$ Teuvo |
| Who is Sheryl’s mother? |
| (Lookup) $\rightarrow$ NULL |

Figure 1: In NeuralDB, facts and queries are posed with short natural language sentences. The queries above are answered by our first prototype described in Section 3.
Who is John’s uncle? could involve combining a fact about John’s parents and about their brothers.

We also consider queries that require performing an aggregation (e.g., how many kids does Pat have?). In this paper, we focus on the count, min and max aggregation operators.

We note that while there is an intuitive mapping between natural language queries and SQL constructs, the mapping is not always precise in the context of NeuralDBs. For example, even though a query is a mere lookup, it may involve an implicit join. Consider the query does Susan live in the UK?, and a database that contains Susan lives in London. In this case, the query answering engine of the NeuralDB will benefit from a rich underlying language model in order to deduce that London is in the UK, and therefore answer that Susan lives in the UK. Finally, the selections in our queries are equality predicates on strings. Comparison predicates will be handled in future work.

**Unique names assumption:** In order to focus on the new issues that are raised by NeuralDBs, in this paper we assume that a given name refers to exactly one entity in the domain and each entity has a single name. We also assume that pronouns (e.g., she, they) are not used or have been resolved in advance. The application of the rich body of work on entity resolution to NeuralDBs will be reserved for future work.

### 2.1 NLP background

The field of natural language processing has made impressive progress in recent years by building on transformer architectures and pre-trained language models. Such models have led to major improvements on tasks such as question answering from text, text summarization, and machine translation. In NeuralDB, our goal is to represent the facts in a database as a set of simple natural language sentences. Hence, as a first step to realizing NeuralDBs, we consider whether techniques for question answering on text can be adapted to our context.

In this section we describe the relevant aspects of pre-trained language models and transformers that operate over them, and the challenges in adapting these techniques to our context.

**Pre-trained language models and transformers.** Pre-trained language models such as BERT [10], GPT-3 [8], RoBERTa [26], TS [35] are neural models trained on large corpora of text. The models are trained by randomly removing certain tokens from the corpus and training the neural net to predict the missing token, given its context (i.e., the words preceding and following the missing token). At an intuitive level, these models obtain two kinds of knowledge (1) the ability to make predictions independent of the exact linguistic form in which knowledge is stated [31, 45], and (2) some world knowledge that is mentioned frequently in text (e.g., London is the capital of the UK) [8, 33].

Pre-trained language models are usually fine-tuned to a given task. For example, for question answering from text, the system would be further trained with a pair of (question, answer) pairs in order to produce the final model. Importantly, since the pre-trained language models capture world knowledge [33] and act as an implicit regularizer [16, 34], fewer examples are needed for the fine-tuning compared to training a model from scratch.

The Transformer model [47] is the most common neural architecture to operate on pre-trained language models based on the high accuracy it produces on downstream tasks including question answering on text. In our prototype experiments, detailed in Section 3, we demonstrate that these reasoning abilities enable the transformer architecture to generate correct answers to a number of queries that we might pose to a NeuralDB.

**Training models.** We will train the parameters of our neural network of the NeuralDB with examples that includes (query, answer) pairs. In Section 3.1 we describe how we obtain training data by leveraging facts from Wikidata. The training data sets we use contain in the order of 10,000-100,000 examples. In a sense, one can view the need for training data as the cost we pay to support a database with no pre-defined schema. Indeed, we will show that without training data, the performance of NeuralDB degrades quite a bit. However, training is important not only for understanding new relations, but also to be able to handle the different linguistic variations in which facts are expressed. In contrast, a schema will always be brittle and allow only one way of expressing a given fact. Furthermore, training data is more easily transferred between different applications.

Along these lines, there is a question of whether the training data needs to cover all the relationships that are seen in the queries. For example, can a NeuralDB answer a query what are Ruth’s hobbies? if it has not been trained on examples that include mentions of hobbies. In Section 6 we show that while accuracy of answers drops for such out of domain queries, the number of additional training examples that need to be added to achieve reasonable performance is relatively small.

In more detail, training neural networks is an optimization problem: minimizing the expected loss over the instances in the training data through changes to the model parameters, weighted by their contribution to the error term over all instances in the training dataset. Formally, the loss is the cross-entropy between the model prediction and the reference: $L = -\sum_{c \in C} p(y_c) \log \hat{p}(y_c)$ which is non-negative and real-valued. For both sentence classification (assigning a single discrete label $c \in C$ for a sequence of tokens) and language generation tasks (decoding a sequence of tokens $(c_1, \ldots, c_n)$ from the vocabulary $C$ as output from the model) the model output is a probability distribution over labels $\hat{p}(y_c) \in C$.

**Evaluating accuracy of answers.** We measure the correctness of the answers generated by a NeuralDB by comparing them against reference data that contain the correct answers. The neural networks are trained with subset of the available data, leaving a portion of it held-out for evaluation, referred to as the test set.

For most queries, we measure correctness using Exact Match (EM), which is 1 if a binary the answer string generated by the NeuralDB is exactly equal to the reference answer and 0 otherwise. This metric is used to score outputs where either a Boolean, null answer, string or numeric answer is expected.

When a set of results is returned, we also consider the $F_1$ score that weighs the precision and recall of the answer generated by the NeuralDB as compared to the reference data. Precision and recall penalize false positives (denoted fp) and false negatives (denoted fp).
The transformer architecture. Transformers [47] take as input an
sequence of tokens \( x = (x_1, \ldots, x_N) \). They are typically trained
in one of two configurations: encoder only or encoder-decoder. In
the former, each token is encoded to a vector representation that is
used to predict a label. In the latter, used in sequence-to-sequence
applications (e.g., question answering or machine translation), the
decoder produces the output sequence.

In both configurations, the transformer works in two phases. In
the first phase, the transformer encodes the input into an interme-
diate representation \( z = (z_1, \ldots, z_N) \) where the dimension of the
vector is fixed, typically where \( d_{\text{model}} = 768 \). In the second phase,
the transformer decodes \( z \) to produce the output. For example, in
sequence-to-sequence generation the output would be a sequence
of tokens \( y = (y_1, \ldots, y_M) \), ending with a special token.

The model contains two stacks of repeating layers. The stacks
differ slightly in composition: one stack is for encoding an input
sequence, \( x \), to \( z \) and the other stack is for incrementally decoding
the output \( y \) from \( z \), using the partially generated \( y \) as context when
decoding. In each stack, the repeating layer contains a multi-head
attention mechanism, that weighs the importance of tokens given
the context it appears in, as well as fully connected network that
independently performs a transformation on the attended tokens.

A transformer model is composed of a fixed number of between
\( N = 6 \) and \( N = 12 \) layers.

It is important to note the complexity of transformers. During
encoding, self-attention considers the similarity between all tokens
in the input sequence, which has quadratic complexity with respect
to input sequence length. Similarly, during decoding, at step \( t \), the
attention mechanism scores the generated tokens \( y_{1:t-1} \) against
all of the encoded context \( z \), which is also quadratic. This complexity
is clearly of concern when inputs are large.

Scaling NLP to DB scale. The NLP problem of question answering
with external knowledge such as Wikipedia, (a.k.a. open-book QA)
forms a good starting point to explore the applicability of trans-
formers to NeuralDB. In the context of NeuralDBs, we use the
transformer in an encoder-decoder configuration, and the input
contains the query to the NeuralDB and all the relevant facts in
the database separated by a special delimiter symbol. The output is
a sequence of tokens that answers the query.

To scale neural reasoning to databases of non-trivial size, it
would not be feasible to encode the entire database as input to the
transformer for a given query, because transformers cannot accept
such large inputs, and even if they could, the latency would be
prohibitive. It is common to use a maximum input size of 512 or
1024 tokens. The typical approach in open-book QA is to comple-
ment the transformer reasoning with an information retriever that
extracts a small subset of the facts from the corpus. The informa-
tion retrieval component can either be a simple one (e.g., BM25)
trained jointly with the transformer to learn to extract relevant
parts of the corpus [14, 20, 22, 32, 46, 57]. However, the following
additional challenges arise in the context of NeuralDBs:

- Unlike open-book QA, which typically requires extracting a
  span from a single document or predicting a token as an
  answer, answering queries in a NeuralDB may require pro-
  cessing a large number of facts and in some cases performing
  aggregations over large sets.
- NeuralDBs do not enjoy the locality properties that usu-
  ally hold in open-book QA. In NeuralDBs, a query may be
  dependent on multiple facts that can be anywhere in the
database. In fact, by definition, the current facts in a data-
base can be reordered and the query answers should not
change. In contrast, in open-book QA, the fact needed to
answer a given question is typically located in a paragraph
or document with multiple sentences about the same subject
where this additional context may help information recall.
- When determining which facts to input to the transformer,
  NeuralDBs may require conditional retrieval from the data-
bases. For example, to answer the query Whose spouse is a
doctor? we’d first need to fetch spouses and then their
professions. In the NLP community this is known as multi-
hop query answering [6], which has recently become an
active area of research, but restricted to the case where we’re
looking for a single answer. In NeuralDBs, we may need to
perform multi-hops for sets of facts.

3 NEURAL QUERY PROCESSING

In this section we describe an initial experiment whose goal is to
better understand and quantify the applicability of transformers to
query processing in NeuralDBs. In particular, the goal of the experi-
ment is to answer the following question. Given a query and a small
number of facts from the database, can the transformer
accurately answer queries that are posed in natural language, whose
answer may require projection (i.e., extracting part of a sentence),
join and aggregation. Note that for the purpose of this experiment,
we are momentarily putting aside the issue that transformers can
only take a small number of facts as input. We’ll address that issue
with our full architecture in Section 4.

3.1 Data

Since NeuralDBs are a new kind of database, there are no existing
data sets that are directly applicable to evaluating them. Hence we
now describe a data set we developed to test NeuralDBs, and to
share with the community. While this dataset does not include data
in the wild, it has enough variety that it provides a good signal
about the validity of our techniques.

Training a NeuralDB requires supervision in the form of \((D, Q, A)\)
triples, where \(D\) is a set of facts, \(Q\) is a query and \(A\) is the correct
answer to \(Q\) over \(D\). We generate training data in a controlled
fashion using data from Wikidata [48] to express facts in natural
language. Because of the scale of Wikidata, it is possible to gen-
erate large numbers of training instances about a wide range of
relationships requiring very few templates. The data set we create
enables us to drill down our analysis by query type and relation
type to understand the performance limitations of NeuralDBs.
D1: Query and Answer dataset. Wikidata stores triples of the form (S,R,O), where R is a relationship between the subject S and the object O, e.g., (Bezos, employedBy, Amazon). For every relationship we consider, we construct multiple natural language templates, thereby providing different linguistic forms of stating the same fact. Each template has a placeholder for the subject and the object, e.g., SO is the place of birth of SS. We then generate different data instances by substituting entities from Wikidata for the placeholders in the templates.

We create databases with 7 different relationships and for each relationship we create between 5 and 14 templates which vary pronouns, temporal expressions and phrasing of the fact and query. We generate a training, validation and held-out test set containing 535, 50 and 50 databases respectively, each containing 50 facts. Each database has between 100–200 question and answer pairs yielding 60000 training, 5500 validation and 6000 test instances in total.

The facts that are generated from Wikipedia are consistent with real-world facts. Hence, there is a risk that the neuralDB is getting its answers from the pre-trained language model (trained on Wikipedia) and not by processing facts in the database itself. We mitigate this issue in two ways. First, we create some facts about fictional characters with simple traits (e.g. likes coffee or good at music). For these facts, we use relationships and entities that are not in Wikidata (the entities are referenced by first name only). Second, we attach a timestamp with each query, and only facts prior to this timestamp are used for inference. By purposefully setting the timestamp lower than the timestamp of the relevant facts, we verify that the model is returning the NULL answer when it’s supposed to and not relying on facts in the pre-trained language model.

The dataset contains both atomic and composite facts: composite facts combine more than one relation over the same subject, e.g., John [subject] is employed as a driver [object(employedAs)] in London [object(employedWhere)]. To generate queries that require joins we apply the same technique to combine two connected relations for the query rather than the fact. For example, we use "fatherOf" and "employedAs" to create the template for the query Does SS’s father work as a SO. To generate queries that require implicit language reasoning and test the knowledge captured by the language modelling task, we replace place names with a more general location. For example, for the fact: Mahesh’s mum gave birth to him in Mumbai, the questions generated would ask: Was Mahesh born in Europe? (with the answer No) and Was Mahesh born in India? (with the answer Yes).

3.2 Results

In our experiment, we use a T5 transformer model [35], a transformer variant that is designed for conditional language generation, as a neural query processor. To provide input to the transformer, we jointly encode relevant facts from the database by concatenating them with the query (separated by a special delimiter token), as illustrated in Figure 2. In what follows, we consider several variants on which input facts are encoded by the transformer which both provides an upper bound on performance (if all necessary facts were encoded), as well as evaluates the transformer’s resilience to noisy (low precision) or incomplete (low recall) information retrieval when performing neural query processing.

Figure 3: Exact match accuracy for different classes of queries. The results show that the transformer obtains high accuracy for lookup and join queries, but falls short for queries with aggregation or yielding set answers. Furthermore, adding information retrieval to scale to larger databases harms EM for queries outputting a set of results or requiring aggregations.

Varying the inputs to the transformer. We first investigate how resilient the transformer is to the number and relevance of its input facts. Figure 3 shows the exact match scores for several ways of retrieving/filtering facts before they enter the transformer, with respect to different query types. Examples of correctly answered queries for the Perfect IR model are shown in Figure 1.

Our first observation is that for queries which required either extracting information from the facts, or performing Boolean inference, the model attained near perfect scores, regardless of whether
the queries need to be answered from a single fact or by joining multiple facts. The fact that the model had high scores for queries that require the combination of multiple facts indicates that the transformer model is able to combine information from multiple sources when generating an answer to the user query. The different variants of our experiment provide further insights.

Perfect IR: This approach assumes that the information retrieval component of model can perfectly retrieve the set of facts needed to answer a query. This version assesses the model’s capability of performing the right computations when only the appropriate facts are given as input to the model. To implement it we select the appropriate facts using meta-data from construction of the controlled reference dataset.

Our results suggest that given the right facts, the model can be robust to multiple linguistic variations and generates the correct output. However, the model performs poorly for query types where an aggregation step is necessary or when the query result is a large set. This observation corroborates work by Hupkes et al. [17] that showed that neural models can’t generate long sequences well for certain sequence transduction tasks.

Whole DB: in this the approach we encode the whole database as input to the model. This would only work for small databases (it is prohibitive even for databases with 50 facts) because the self-attention mechanism in the transformer model has quadratic complexity \(^2\) with respect to input size. This method allows us to evaluate the model’s sensitivity to noise and whether having too much information (i.e. low precision with high recall) has an impact.

One positive takeaway is that the model is able to generate the correct answers despite the fact that it was exposed to irrelevant facts. Interestingly, this model also has a high \(F_1\) score for queries that generated sets as results (as opposed to a single fact) as well as for min/max queries. For count queries its performance is low.

TF-IDF IR: In this version we evaluate a simple baseline for the information retrieval component using TF-IDF which considers overlapping tokens between the query and fact. This evaluation would highlight whether the NEURALDB model adequately handles noise from the IR component as well as the difficulty of retrieving the necessary facts. We may fail to retrieve the relevant facts either due to the need for multi-hop reasoning or because facts are expressed with different linguistic expressions. Our experiment considers using both the top-5 and top-50 \(^3\) returned results from the TF-IDF component, and evaluating whether a small number of top results is sufficient for some query types.

Using TF-IDF for IR, the model still attains near-perfect accuracy for atomic queries. For queries where a join is required, the accuracy drops due to low recall. While the EM from Boolean QA is reduced from 99.2% (using the whole DB) to 91.6%, for queries that require extracting information the accuracy drop is more stark: from near perfect to 62.0%. From a modeling perspective, Boolean query answering is quite a simple simple task with low entropy (from near perfect to 62.0%). From a modeling perspective, Boolean query answering is quite a simple task with low entropy (i.e. low precision with high recall) has an impact.

DPR: To alleviate some of the limitations of TF-IDF, we experimented with dense passage retriever (DPR) [20], which scores the similarity of vector encodings of the query and the facts through computing the inner product assigned a non-zero score for all fact (meaning that all relevant facts could potentially be retrieved - even if there are no overlapping tokens). Our experiments, however, highlight a difficult precision-recall trade off. To retrieve facts for joins, many false positive facts must also be input into the model as we find that facts participating in joins are often ranked outside of the top 5 items returned from the information retrieval.

Independent encoding of facts with Fusion in Decoder. The following experiment provides an additional insight that is useful for developing the architecture for NEURALDBs. In the experiments so far, we concatenated all the facts before we fed it to the encoder of the transformer. All facts were encoded jointly with self-attention both considers intra- and inter-fact relations. Here we adapt the approach known as Fusion in Decoder (FID) [18] to our context. Specifically, each fact is fed separately to the encoder, but the fusion of the facts happens only in the decoder. Rather than one large self-attention operation over all facts, self-attention is computed independently for each fact, considering the relation between the fact and the query, but there is no attention between facts. This reduces the complexity of joint encoding of multiple concatenated facts from a single quadratic complexity operation (w.r.t. total input length) to a linear (w.r.t. number of facts) allowing this method to scale to larger numbers of facts.

\(^2\)While optimizations and linearizations have recently been introduced [42, 49] a single encoder would present a bottleneck. Furthermore aggregating large number of facts (such as with count) would still suffer from low accuracy.

\(^3\)The DB size is 50 facts. This evaluates whether the limitation in TF-IDF is the requirement for token overlap or whether the limitation in ranking or facts (i.e., it may be correct for the wrong reasons). The accuracy for queries that output sets, or require aggregation is much lower. For queries with min/max aggregation, the EM for TF-IDF was near zero, this is due to there being no token overlap between the query (such as Who is the oldest?) and the facts (such as John was born in 1962), yielding no results from the TF-IDF search engine.

![T5 Transformer answer accuracy by query type](image-url)

**Figure 4:** Fusing in the decoder, as opposed to concatenating the inputs (hence fusing in the encoder), reduces the transformer’s computational complexity, but accuracy drops significantly. This experiment suggests that NeuralDBs should only process small numbers of facts in every transformer while fusing facts in the encoder.
We compare FiD with the aforementioned perfect-IR version, where the only input to the models are the facts necessary to answer the query. The results in Figure 4 show that while the two models perform comparably for lookup queries, the FiD approach fails for queries that require join or aggregation. The implication of this experiment is that the self-attention in encoding is important to capture the inter-sentence dependencies between the facts. Therefore, trying to feed growing numbers of facts to a transformer is unlikely to scale.

**Summary.** We believe that the initial experiment suggests the following: (1) if there were a way to feed the transformer the relevant facts from the database, it can produce results with reasonable accuracy, (2) aggregation queries need to be performed outside of the neural machinery, and (3) in order to handle queries that result in sets of answers and in order to prepare sets for subsequent aggregation operators, we need to develop a neural operator that can process individual (or small sets of) facts in isolation and whose results outputted as the answer or fed into a traditional (i.e. non-neural) aggregation operator. The next section describes our first steps towards such an architecture.

4 THE ARCHITECTURE OF A NEURAL DATABASE

We now describe the architecture of a **NeuralDB** that addresses the challenges exposed in Section 3. The architecture is shown in Figure 5 and has the following key ideas:

**Running multiple transformers in parallel:** In Section 3, we demonstrated that if we provide our transformer model with the right facts needed to derive the query, and even in the presence of irrelevant facts, the transformer can produce correct answers for SPJ queries. The problem is that we can only feed a small number of facts to the transformer.

In our architecture we address this challenge by running multiple copies of a Neural SPJ operators in parallel. Each copy is a transformer similar to the one we used in Section 3. When queries don’t involve aggregation, the union of the outputs of the Neural SPJ operators are the answer to the query. When the query does involve aggregation, these machine-readable outputs are fed into the aggregation operator.

**Aggregation with a traditional operator:** Since the Neural SPJ operators were designed to output structured results, our architecture can use a separate traditional aggregation operator. Using a separate aggregation overcomes the limitation on transformers demonstrated in Section 3, and enables us to extend the system to new aggregation operators without retraining the basic models used in the system. The aggregation operator is selected through a classifier, which was trained to generate the final answers to the query, the Neural SPJ is trained to generate an intermediate result of the query. Figure 6 shows examples of the output of the Neural SPJ operator.

5 SUPPORT SET GENERATION

The Support set generator (SSG) is a module that given a query $Q$ and a database $D$, produces a set of support sets $SSG_Q(D)$, each of which is used to generate an answer with the SPJ module in parallel. Note that sets in $SSG_Q(D)$ may not be pairwise disjoint because some facts may be required for multiple answers (consider, for example, a one-to-many relation).

The outputs generated by SSG depend on the information need of the downstream SPJ, and whether the query requires joins or aggregation: (1) for queries that are answered by a single sentence, e.g., Who is Sheryl’s husband?, the support set containing a single fact should be generated, e.g., Sheryl is Nicholas’s spouse. (2) When the SPJ operator requires multiple facts to be joined, the support set would contain all participating facts. (3) For queries that require aggregation or whose answer is a set, multiple support sets must be generated, each containing enough information to generate the intermediate results that are aggregated. For example, for the query Who is the oldest person?, each of the support sets would contain a single fact that includes a person and their birth date. If joins are required to generate the intermediate result, the support sets would contain multiple facts.

Using information retrieval, such as TF-IDF in Section 3, could be considered a primitive SSG generating a single support set containing all relevant facts. As our experiments indicated, this method worked well for queries whose answer is generated from a single fact, but not for joins, aggregation queries or for queries outputting a set of answers. In what follows we describe a more robust algorithm for generating support sets.

**Incremental support set generation.** The output of the SSG is the set of all relevant support sets: $SSG_Q(D) \subset \mathcal{P}(D)$. It would be intractable to consider all possible support sets, as this would be akin to enumerating the powerset. We instead efficiently and incrementally construct support sets, starting from the empty set by modeling the task as multi-label structured prediction. At each step, a classifier, $C$, considers the partially generated support set $\hat{D}_k$ and the query and predicts which candidate facts $u_i \in D$ from the database should be added or whether to stop the iteration.

Incremental SSG is described in Algorithm 1 and illustrated in Figure 7. The action classifier predicts which facts $u_i \in D$ should be explored or whether to stop. If STOP is predicted, $\hat{D}_k$ is closed (i.e., it forms part of the output); otherwise, for each fact added, a new intermediate (i.e., open) support set is generated which is explored in the next iteration. For efficiency, to build the multi-label SSG action classifier, we use a bi-encoder architecture that independently encodes the facts in the database and the state (query and a partial support set) and computes the inner product between
Figure 5: Overview of NeuralDB architecture. The support set generator creates small sets of facts that are each fed into a separate Neural SPJ operator that runs a single transformer. The results of the individual Neural SPJ operators are either unioned to produce the result or passed on to a traditional aggregation operator.

Algorithm 1: Support Set Generator (SSG) modeled as multi-label classification: using maximum inner product search (MIPS) over vector encodings of facts $U$ and state $V$

**Input:** Bi-encoders $C$: $C_U$ (for actions), $C_V$ (for state), Database $D$, Query $Q$, Threshold $\tau$

**Output:** Set of support sets $(\hat{D}_1, \ldots, \hat{D}_k) \subset \mathcal{P}(D)$

Input: $\text{SSG} \leftarrow \text{null}$; $\text{closed} \leftarrow \text{null}$; $U := [C_U(u_1); \ldots; C_U(u_n); C_U(\text{STOP})]$ for $u_i \in D$;

while open $\neq \phi$

next := $\text{null}$;

for $\hat{D}_k$ in open do

$V := [C_V(Q, u_1 \ldots u_m)]$, for $u_i \in \hat{D}_k$;

$A := \text{MIPS}(U, V, \tau)$;

for $a_j$ in $A$ do

if $a_j$ == STOP then

$\text{closed} := \text{closed} \cup \{\hat{D}_k\}$;

else

$\text{next} := \text{next} \cup \{a_j \cup \hat{D}_k\}$;

end if

end for

end for

return closed;

Figure 6: Examples of the intermediate results that are produced by the Neural SPJ operator.

Figure 7: ISSG incrementally creates support sets. At each step, the classifier either decides to add another fact to the support set or to stop and output a completed support set.

The encoded representations to generate a score. The encoders are pre-trained transformers fine-tuned to yield a high inner product between the state’s encodings and relevant facts to be added to answer the query. The vectors encoding of the facts are static and

(1) Does Nicholas’s spouse live in Washington D.C.? (Nicholas lives in Washington D.C. with Sheryl, Sheryl is Nicholas’s spouse) $\rightarrow$ TRUE

(2) Who is the oldest person in the database? (Teuvo was born in 1912) $\rightarrow$ (Teuvo, 1912)

(3) Does Nicholas’s spouse live in Washington D.C.? (Teuvo was born in 1912) $\rightarrow$ NULL
methods for indexing (and/or clustering) the facts in the database so that only few facts need to be considered in each iteration of the inner loop of the algorithm, leading to significant speedups.

Training the action classifier: To train the action classifier, we need a supervision signal as to which facts the classifier must select at a given current state for a query. We generate such training data from the data set D1, where we have a set of queries, answers, and their corresponding support sets.

To alleviate the need for training data we describe a novel distant supervision approach for training the action classifier (see Algorithm 2). Instead of having perfect training data, we generate possibly noisy training data by taking advantage of the neural SPJ operator itself. Specifically, with a known (query, answer) pair and a pre-trained model, we can incrementally remove facts from the database until the answer predicted by the model changes from the correct answer to one which is incorrect. We know that for small databases, it is possible to encode the entire database as input to the SPJ operator, so we use the whole DB model we pre-trained from Section 3 for this purpose. The combination of facts removed from the DB that change the answer from the correct answer to an incorrect answer would be labeled as forming part of a support set. For example, removing the either the fact Sarah is a doctor or Sarah married John from the input to the model may change the output prediction for the how many people’s spouses are doctors? query from 1 to 0, and would be added to the support set. The training data may be noisy because the neural SPJ operator is not perfect: robustness to stochasticity could be introduced through reinforcement learning techniques such as Q-learning [50], but investigating that option is reserved for future work. Experimental results in Section 6.3 indicate that the models can be robust to this noise without explicitly mitigating the noise. Our method is a form of erasure-based black-box model explanation technique [24, 38]. However, we treat facts as features rather than individual tokens.

6 EXPERIMENTS

We begin in Section 6.1 by demonstrating the accuracy of the end-to-end NeuralDB, showing that queries can be answered with high accuracy over thousands of facts. We then validate the components of our architecture in isolation. In Section 6.2 we consider the basic architecture, consisting of Neural SPJ followed by aggregation (without the SSG). In section 6.3 we evaluate our SSG module. In Section 6.4 we discuss how the results depend on the amount of training data and how learning transfers to relations unseen in the training set.

Implementation. We use the HuggingFace [56] transformers library and its implementation of the t5-base transformer module [35] for SPJ. With the exception of one experiment, the parameters of the t5-base model have been pre-trained on the colossal Common Crawl (C4) dataset [35] by predicting tokens masked in sentences. For SSG, we use BERT which has a comparable architecture to T5. The learning-rate for fine-tuning and number of epochs were selected through maximizing the Exact-Match (EM) accuracy on a held-out validation set for the tasks. Fine-tuning is a stochastic process: for each experiment, we independently train 5 separate models with different random seeds and report mean accuracy.

### 6.1 End-to-end NeuralDB

Before validating the SSG and SPJ components independently, we first evaluate the full NeuralDB architecture end to end, reporting results in Table 1. At run time, the support sets generated by the SSG are input in to SPJ operators in parallel and then aggregated. Compared to state of the art transformer models (bottom 2 rows) with information retrieval, the NeuralDB achieves the highest EM accuracy on all types of queries. While these numbers cannot be directly compared (as the NeuralDB requires supervision to the intermediate results), the NeuralDB makes a substantial improvements over several query types, overcoming fundamental limitations in how the IR transformer models perform aggregations. It is expected that distantly supervising the SSG would decrease accuracy somewhat. However, given that the supervision signal is generated for free, this is encouraging, especially as the impact was negligible in some cases. The decrease in accuracy is most evident for joins because...
of the over sensitivity of the model used to distantly supervise the SSG, reflected in the low SSG recall in Table 3.

### 6.2 Neural SPJ + Aggregation

The experiments in Section 3 showed that the transformer model was capable of generating the correct answer to queries requiring lookups and joins with near perfect accuracy on our test set when provided with the right facts or small supersets thereof. We evaluate the Neural SPJ on two settings. In **Perfect IR**, we provide the Neural SPJ only the needed facts. Hence, Neural SPJ does not need to decide which facts to use to answer the query. In **Noisy IR**, we sample random facts and add them to the support set used to train the model. Hence, we’re also training the Neural SPJ to select the right set of facts to use for inference, thereby validating the resilience of the SPJ operator to extraneous facts that might be returned by a low-precision high-recall SSG. The noise was generated by sampling $1 \sim 3$ additional facts with uniform probability for $\frac{3}{4}$ of instances.

**Dataset D2.** Training and evaluating the Neural SPJ operator requires data that differs slightly from the data in D1. In D1, the training data for a given query $Q$ involved the answer, $Q(D)$. However, for the Neural SPJ training we need to provide the result of the SPJ component before the aggregation. In D1, the output to the question **How many countries use Euro?** would just be the number of countries, after aggregation. However, in D2, the training data consists of a pairs of facts and intermediate results. For the fact, Belgium’s currency is the Euro, the intermediate result is Belgium because the count operator needs the names of the countries that use the Euro. For the query **What is the most widely-used currency?**, the intermediate result for the same fact would include the pair (Euro, Belgium) because the aggregation operator first needs to group by currency before computing the max.

D2 includes queries for training the model to answer set and aggregation queries. We create a total of 632 templates: 115 for facts and 517 for the different query types over 27 relations, covering a variety of linguistic expressions. Using a sample of popular Wiki-data entities, we generate a single database of 8400 facts and 14000 queries over it. For training, we generate approximately 10,000 training instances per aggregation operation, preventing class imbalance by preserving the proportions of D1.

**Findings.** Table 2 shows the EM of the intermediate results produced by the Neural SPJ (projection EM), and the EM of the final answer (answer EM). In row 2 of Table 2 we observe a substantial drop of more than 20% in EM, both Projection, and Answer, when we add noise to the retrieved support set at test time. This suggests that adding noise from retrieval at training time (third row), makes the neural SPJ module more resilient to errors introduced by the SSG.

The Neural SPJ operator was also trained to predict the downstream aggregation function, which it did correctly with 99.97% accuracy. In 0.03% of cases, the wrong function name was selected. Answer EM reflects the accuracy of the end-to-end performance of the system. Furthermore, we inspected the error rate for each query type for the results reported in Table 2 and noted that there was no large deviation between queries with aggregation and those without. This validates our choice to postpone aggregation functions to happen after the Neural SPJ.

**Error Analysis.** For the Noisy IR model reported in Table 2 were no false positive or false negative errors (the model outputs a result when it should output NULL or vice versa). All errors were errors in the the content of the fact returned. Of the 253 errors, 166 were for symmetric relations (X borders Y) which introduced ambiguity in training. 80 errors were due to the model incorrectly applying implicit world knowledge when provided with insufficient facts to resolve geographical meronomy relations (e.g. incorrectly predicting Zeeland [sic] is in Asia). The remaining errors were differing punctuation (e.g. missing a period).

**Training data requirements.** To evaluate training data requirements for the Neural SPJ, we plot the learning curve for generating intermediate results using dataset D2 in Figure 8. For each point on this graph, 5 models are trained with different random initializations and we report the mean EM score. The model attains near perfect accuracy with approximately 80k training instances. It is interesting to note that the Neural SPJ struggled the most with learning what it doesn’t know. With little training data, the model often outputted a result even when it should have outputted NULL. This is a well known weakness of sequence-to-sequence models [36].

### 6.3 Support Set Generation

In this section we evaluate how well the SSG component (Section 5) retrieves facts to be fed to the Neural SPJ operators. It is tricky
Table 3: Precision and recall of distantly supervised SSG w.r.t. the reference set. Note that errors in training do not necessarily translate to wrong query answers because the Neural SPJ operator is somewhat robust to extra information.

| Query Type | Exact Match (%) | Soft Match (%) |
|------------|-----------------|----------------|
|            | Precision       | Recall         | Precision | Recall |
| Atomic (bool) | 81.45          | 98.92          | 95.02    | 99.90  |
| Atomic (extractive) | 80.44          | 88.47          | 94.00    | 99.61  |
| Join (bool)  | 62.28          | 83.13          | 62.28    | 83.13  |
| Join (extractive) | 72.22          | 85.95          | 72.22    | 85.95  |
| Set         | 29.97          | 89.14          | 33.13    | 89.14  |
| Count       | 56.42          | 92.80          | 59.68    | 92.80  |
| min/max     | 68.63          | 100.00         | 68.63    | 100.00 |
| Total       | 68.28          | 93.57          | 77.25    | 95.68  |

Figure 9: Even with relations omitted during training, Neural SPJ often generates correct intermediate results.

7 RELATED WORK

NLP and data management. Bridging the gap between unstructured natural language data and database-style querying has been a long-standing theme in database research [15]. The work on information extraction has developed techniques for translating segments of natural language text into triples that can be further processed by a database system. Wikidata [48] itself is a social experiment where additions to the knowledge graph are encouraged to use already existing relation names if possible, thereby alleviating the need for information extraction. There has been significant work on translating queries posed in natural language into SQL queries on a database whose schema is known [4, 23, 58], with extensions to semi-structured data and knowledge bases [7, 30]. More recently, systems such as BREAK [57] and ShARC [41] have trained models to translate a natural language query into a sequence of relational operators (or variants thereof).

NeuralDBs do not try to map data or queries into a pre-defined schema. At the core, we use neural techniques to process the facts in the database with the query given as context in natural language. However, NeuralDBs do some rudimentary analysis of the query when they decide whether it requires an aggregation operator, and one can imagine that NeuralDBs will need more sophisticated understanding of the structure of a query as they tackle more complex queries. Similarly, the processing performed by the Neural SPJ operator is reminiscent of information extraction in the sense that it produces a structured representation of facts that can be used by subsequent operators. However, a key difference is that the...
NeuralDB they couldn’t perform well; we hypothesize that encoding the query and facts together by a stack of self-attention in the encoder is necessary to answer database queries. There also have been considerable efforts in mixing traditional symbolic reasoning or data management algorithms with neural network architectures. For example, Rocktäschel et al. [40] have developed a differentiable version of the backward chaining algorithm that drives prolog. Most closely to our work, Minervini et al. [28] has showed how differentiable prolog interpreters can be used to support reasoning with facts in natural language. Instead of “neuralizing” existing symbolic reasoners, in our work we start off with a scalable neural architecture, and support it with symbolic computation only where necessary. This enables us to directly leverage the rapid progress made in retrieval augmented QA models and ensures scalability.

8 CONCLUSIONS AND FUTURE WORK

We described NeuralDB, a new kind of database system that uses neural reasoning, and is therefore able to answer queries from data expressed as natural language sentences that do not conform to a pre-defined schema. The design of the NeuralDB architecture was based on a careful examination of the strengths and weaknesses of current NLP transformer models. Our experimental results suggest that it is possible to attain very high accuracy for a class of queries that involve select, project, join, possibly followed by an aggregation.

To fully realize the promise of NeuralDBs, more research is needed on scaling up NeuralDBs to larger databases, supporting more complex queries and increasing the accuracy of the answers. In particular, an interesting area of research noted in Section 5 is developing novel indexing techniques that enable efficient support set generation. Another exciting area to investigate is to consider other media in the database. For example, a database can also contain a set of images and some queries can involve combining information from language and from images. Such an extension would benefit from recent progress on visual query answering systems [3, 5].

A possible downside of using neural techniques in a database system is the potential for bias that might be encoded in the underlying language model. As we discussed, the fact that London in the UK is encoded in the language model and is useful. However, suppose our database included facts saying that John and Jane work at a hospital, but when we asked what their profession is, the system would answer doctor for John and nurse for Jane. Currently, there is no good way of distinguishing biased from unbiased knowledge in a language model. A possible approach to this important issue is to design a separate module that attacks the database with queries in order to discover hidden biases. Then, we could devise safeguards within the database that ensure that we don’t use such biased knowledge in answering queries. Developing these components is an area for future research.

Finally, another interesting challenge concerns developing semantic knowledge that helps in identifying which updates should replace previous facts and which should not. For example, if the fact, Mariah is unemployed, was in the database and later the fact, Mariah works for Apple, was added, then the first fact should be removed (or at least, apply only to queries about the past). However, the same does not hold for the facts Kasper likes tea followed by the fact Kasper likes coffee.
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