Incremental Knowledge Base Construction Using DeepDive

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ABSTRACT
Populating a database with unstructured information is a long-standing problem in industry and research that encompasses problems of extraction, cleaning, and integration. A recent name used to characterize this problem is knowledge base construction (KBC). In this work, we describe DeepDive, a system that combines database and machine learning ideas to help develop KBC systems, and we present techniques to make the KBC process more efficient. We observe that the KBC process is iterative, and we develop techniques to incrementally produce inference results for KBC systems. We propose two methods for incremental inference, based respectively on sampling and variational techniques. We also study the tradeoff space of these methods and develop a simple rule-based optimizer. DeepDive includes all of these contributions, and we evaluate DeepDive on five KBC systems, showing that it can speed up KBC inference tasks by up to two orders of magnitude with negligible impact on quality.

1. INTRODUCTION
The process of populating a structured relational database from unstructured sources has received renewed interest in the database community through high-profile start-up companies (e.g., Tamr and Trifacta), established companies like IBM's Watson [8,19], and a variety of research efforts [12,30,33,41,45]. At the same time, communities such as natural language processing and machine learning are attacking similar problems under the name knowledge base construction (KBC) [6,17,27]. While different communities place differing emphasis on the extraction, cleaning, and integration phases, all communities seem to be converging toward a common set of techniques that include a mix of data processing, machine learning, and engineers-in-the-loop.

The ultimate goal of KBC is to obtain high-quality structured data from unstructured information. These databases are richly structured with tens of different entity types in complex relationships. Typically, quality is assessed using two complementary measures: precision (how often a claimed tuple is correct) and recall (of the possible tuples to extract, how many are actually extracted). These systems can ingest massive numbers of documents—far outstripping the document counts of even well-funded human curation efforts. Industrially, KBC systems are constructed by skilled engineers in a months-long (or longer) process—not a one-shot algorithmic task. Arguably, the most important question in such systems is how to best use skilled engineers’ time to rapidly improve data quality. In its full generality, this question spans a number of areas in computer science, including programming languages, systems, and HCI. We focus on a narrower question, with the axiom that the more rapid the programmer moves through the KBC construction loop, the more quickly she obtains high-quality data.

This paper presents DeepDive, our open-source engine for knowledge base construction.† DeepDive’s language and execution model are similar to other KBC systems: DeepDive uses a high-level declarative language [12,33,35]. From a database perspective, DeepDive’s language is based on SQL. From a machine learning perspective, DeepDive’s language is based on Markov Logic [16,35]: DeepDive’s language inherits Markov Logic Networks’ (MLN’s) formal semantics. Moreover, it uses a standard execution model for such systems [12,33,35] in which programs go through two main phases: grounding, in which one evaluates a sequence of SQL queries to produce a data structure called a factor graph that describes a set of random variables and how they are correlated. Essentially, every tuple in the database or result of a query is a random variable (node) in this factor graph. The inference phase takes the factor graph from grounding and performs statistical inference using standard techniques, e.g., Gibbs sampling [46,49]. The output of inference is the marginal probability of every tuple in the database. As with Google’s Knowledge Vault [17] and others [36], DeepDive also produces marginal probabilities that are calibrated: if one examined all facts with probability 0.9, we would expect that approximately 90% of these facts would be correct. To calibrate these probabilities, DeepDive estimates (i.e., learns) parameters of the statistical model from data. Inference is a subroutine of the learning procedure and is the critical loop. Inference and learning are computationally intense (hours on 1TB RAM/48-core machines).

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‡DeepDive has some technical differences from Markov Logic that we have found useful in building applications. We discuss these differences in Section 2.3.
In our experience with DeepDive, we found that KBC is an iterative process. In the past few years, DeepDive has been used to build dozens of high-quality KBC systems by a handful of technology companies, a number of defense contractors, and scientists in fields such as paleobiology, drug repurposing, and genomics. Recently, we compared a DeepDive system’s extractions to the quality of extractions provided by human volunteers over the last ten years for a paleobiology database, and we found that the DeepDive system had higher quality (both precision and recall) on many entities and relationships. Moreover, on all of the extracted entities and relationships, DeepDive had no worse quality [37]. Additionally, the winning entry of the 2014 TAC-KBC competition was built on DeepDive [4]. In all cases, we have seen the process of developing KBC systems is iterative: quality requirements change, new data sources arrive, and new concepts are needed in the application. This led us to develop techniques to make the entire pipeline incremental in the face of changes both to the data and to the DeepDive program. Our primary technical contributions are to make the grounding and inference phases more incremental.

Incremental Grounding. Grounding and feature extraction are performed by a series of SQL queries. To make this phase incremental, we adapt the algorithm of Gupta, Mumick, and Subrahmanian [21]. In particular, DeepDive allows one to specify “delta rules” that describe how the output will change as a result of changes to the input. Although straightforward, this optimization has not been applied systematically in such systems and can yield up to 360× speedup in KBC systems.

Incremental Inference. Due to our choice of incremental grounding, the input to DeepDive’s inference phase is a factor graph along with a set of changed data and rules. The goal is to compute the output probabilities computed by the system. Our approach is to frame the incremental maintenance problem as one of approximate inference. Previous work in the database community has looked at how machine learning data products change in response to both to new labels [28] and to new data [10, 11]. In KBC, both the program and data change on each iteration. Our proposed approach can cope with both types of change simultaneously.

The technical question is which approximate inference algorithms to use in KBC applications. We choose to study two popular classes of approximate inference techniques: sampling-based materialization (inspired by sampling-based probabilistic databases such as MCDB [24]) and variational-based materialization (inspired by techniques for approximating graphical models [43]). Applying these techniques to incremental maintenance for KBC is novel, and it is not theoretically clear how the techniques compare. Thus, we conducted an experimental evaluation of these two approaches on a diverse set of DeepDive programs.

We found that these two approaches are sensitive to changes along three largely orthogonal axes: the size of the factor graph, the sparsity of correlations, and the anticipated number of future changes. The performance varies by up to two orders of magnitude in different points of the space. Our study of the tradeoff space highlights that neither materialization strategy dominates the other. To automatically choose the materialization strategy, we develop a simple rule-based optimizer.

Experimental Evaluation Highlights. We used DeepDive programs developed by our group and DeepDive users to understand whether the improvements we describe can speed up the iterative development process of DeepDive programs. To understand the extent to which DeepDive’s techniques improve development time, we took a sequence of six snapshots of a KBC system and ran them with our incremental techniques and completely from scratch. In these snapshots, our incremental techniques are 22× faster. The results for each snapshot differ at most by 1% for high-quality facts (90%+ accuracy); fewer than 4% of facts differ by more than 0.05 in probability between approaches. Thus, essentially the same facts were given to the developer throughout execution using the two techniques, but the incremental techniques delivered them more quickly.

Related Work

Knowledge Base Construction (KBC) KBC has been an area of intense study over the last decade, moving from pattern matching, rule-based systems to systems that use machine learning for KBC [6, 9, 17, 18, 33]. Many groups have studied how to improve the quality of specific components of KBC systems [22, 45]. We build on this line of work. We formalized the development process and built DeepDive to ease and accelerate the KBC process, which we hope is of interest to many of these systems as well. DeepDive has many common features to Chen and Wang [12], Google’s Knowledge Vault [17], and a forerunner of DeepDive, Tuffy [35]. We focus on the incremental evaluation from feature extraction to inference.

Declarative Information Extraction The database community has proposed declarative languages for information extraction, a task with similar goals to knowledge base construction, by extending relational operations [20, 30, 41], or rule-based approaches [33]. These approaches can take advantage of classic view maintenance techniques to make the execution incremental, but they do not study how to incrementally maintain the result of statistical inference and learning, which is the focus of our work.

Incremental Maintenance of Statistical Inference and Learning Related work has focused on incremental inference for specific classes of graphs (tree-structured graphical models). We deal instead with the class of factor graphs that arise from the KBC process, which is much more general than the ones examined in previous approaches. Nath and Domingos [34] studied how to extend belief propagation on factor graphs with new evidence, but without any modification to the structure of the graph.
Wick and McCallum [17] proposed a “query-aware MCMC” method. They designed a proposal scheme so that query variables tend to be sampled more frequently than other variables. We frame our problem as approximate inference, which allows us to handle changes to the program and the data in a single approach.

2. KBC USING DEEPDIVE

We describe DeepDive, an end-to-end framework for building KBC systems with a declarative language. We first recall standard definitions, and then introduce the essentials of the framework by example, compare our framework with Markov Logic, and describe DeepDive’s formal semantics.

2.1 Definitions for KBC Systems

The input to a KBC system is a heterogeneous collection of unstructured, semi-structured, and structured data, ranging from text documents to existing but incomplete KBs. The output of the system is a relational database containing facts extracted from the input and put into the appropriate schema. Creating the knowledge base may involve extraction, cleaning, and integration.

**Example 2.1.** Figure 1 illustrates our running example: a knowledge base with pairs of individuals that are married to each other. The input to the system is a collection of news articles and an incomplete set of married persons; the output is a KB containing pairs of person that are married. A KBC system extracts linguistic patterns, e.g., “... and his wife ...” between a pair of mentions of individuals (e.g., “Barack Obama” and “M. Obama”). Roughly, these patterns are then used as features in a classifier deciding whether this pair of mentions indicates that they are married (in the HasSpouse relation).

We adopt standard terminology from KBC, e.g., ACE[4]. There are four types of objects that a KBC system seeks to extract from input documents, namely entities, relations, mentions, and relation mentions. An entity is a real-world person, place, or thing. For example, “Michelle_Obama_1” represents the actual entity for a person whose name is “Michelle Obama”; another individual with the same name would have another number. A relation associates two (or more) entities, and represents the fact that there exists a relationship between the participating entities. For example, “Barack_Obama_1” and “Michelle_Obama_1” participate in the HasSpouse relation, which indicates that they are married. These real-world entities and relationships are described in text; a mention is a span of text in an input document that refers to an entity or relationship: “Michelle” may be a mention of the entity “Michelle_Obama_1.” A relation mention is a phrase that connects two mentions that participate in a relation such as “(Barack Obama, M. Obama)”. The process of mapping mentions to entities is called entity linking.

2.2 The DeepDive Framework

DeepDive is an end-to-end framework for building KBC systems, as shown in Figure 1. We walk through each phase. We use datalog syntax for exposition, but DeepDive is SQL based. The rules we described in this section are manually created by the user of DeepDive and the process of creating these rules is application-specific.

**Candidate Generation and Feature Extraction.** All data in DeepDive is stored in a relational database. The first phase populates the database using a set of SQL queries and user-defined functions (UDFs) that we call feature extractors. By default, DeepDive stores all documents in the database in one sentence per row with markup produced by standard NLP pre-processing tools, including HTML stripping, part-of-speech tagging, and linguistic parsing. After this loading step, DeepDive executes two types of queries: (1) candidate mappings, which are SQL queries that produce possible mentions, entities, and relations, and (2) feature extractors that associate features to candidates, e.g., “... and his wife ...” in Example 2.1.

**Example 2.2.** Candidate mappings are usually simple. Here, we create a relation mention for every pair of candidate persons in the same sentence (s):

\[
\text{(R1) MarriedCandidate(m1,m2):} \rightarrow \text{PersonCandidate(s,m1),PersonCandidate(s,m2)}
\]

Candidate mappings are simply SQL queries with UDFs that look like low-precision but high-recall ETL scripts. Such rules must be high recall: if the union of candidate mappings misses a fact, DeepDive has no chance to extract it.

We also need to extract features, and we extend classical Markov Logic in two ways: (1) user-defined functions and (2) weight tying, which we illustrate by example.

**Example 2.3.** Suppose that phrase(m1, m2, sent) returns the phrase between two mentions in the sentence, e.g., “... and his wife” in the above example. The phrase between two

For more information, including examples, please see [http://deepdive.stanford.edu](http://deepdive.stanford.edu).

Note that our engine is built on Postgres and Greenplum for all SQL processing and UDFs. There is also a port to MySQL.
mentions may indicate whether two people are married. We would write this as:

\[
\text{(FE1)} \quad \text{MarriedMentions}(m_1, m_2) : - \\
\quad \text{MarriedCandidate}(m_1, m_2), \text{Mention}(s, m_1), \text{Mention}(s, m_2), \text{Sentence}(s, \text{sent}); \\
\quad \text{weight} = \text{phrase}(m_1, m_2, \text{sent})
\]

One can think about this like a classifier: This rule says that whether the text indicates that the mentions \( m_1 \) and \( m_2 \) are married is influenced by the phrase between those mention pairs. The system will infer based on training data its confidence (by estimating the weight) that two mentions are indeed indicated to be married.

Technically, \text{phrase} returns an identifier that determines which weights should be used for a given relation mention in a sentence. If \text{phrase} returns the same result for two relation mentions, they receive the same weight. We explain weight tying in more detail in Section 2.3. In general, \text{phrase} could be an arbitrary UDF that operates in a per-tuple fashion. This allows DeepDive to support common examples of features such as “bag-of-words” to context-aware NLP features to highly domain-specific dictionaries and ontologies. In addition to specifying sets of classifiers, DeepDive inherits Markov Logic’s ability to specify rich correlations between entities via weighted rules. Such rules are particularly helpful for data cleaning and data integration.

**Supervision.** Just as in Markov Logic, DeepDive can use training data or evidence about any relation; in particular, each user relation is associated with an evidence relation with the same schema and an additional field that indicates whether the entry is true or false. Continuing our example, the evidence relation \text{MarriedMentions}_Ev could contain mention pairs with positive and negative labels. Operationally, two standard techniques generate training data: (1) hand-labeling, and (2) distant supervision, which we illustrate below.

**Example 2.4.** Distant supervision \([23, 72]\) is a popular technique to create evidence in KBC systems. The idea is to use an incomplete KB of married entity pairs to heuristically label (as True evidence) all relation mentions that link to a pair of married entities:

\[
\text{(S1)} \quad \text{MarriedMentions}_Ev(m_1, m_2, \text{true}) : - \\
\quad \text{MarriedCandidates}(m_1, m_2), \text{EL}(m_1, e_1), \text{EL}(m_2, e_2), \text{Married}(e_1, e_2)
\]

Here, Married is an (incomplete) list of married real-world persons that we wish to extend. The relation EL is for “entity linking” that maps mentions to their candidate entities. At first blush, this rule seems incorrect. However, it generates noisy, imperfect examples of sentences that indicate two people are married. Machine learning techniques are able to exploit redundancy to cope with the noise and learn the relevant phrases (e.g., “and his wife”). Negative examples are generated by relations that are largely disjoint (e.g., siblings). Similar to DIPRE \([7]\) and Hearst patterns \([22]\), distant supervision exploits the “duality” \([7, 22]\) between patterns and relation instances; furthermore, it allows us to integrate this idea into DeepDive’s unified probabilistic framework.

**Learning and Inference.** In the learning and inference phase, DeepDive generates a factor graph, similar to Markov Logic, and uses techniques from Tuffy \([35]\). The inference and learning are done using standard techniques (Gibbs Sampling) that we describe below after introducing the formal semantics.

**Error Analysis.** DeepDive runs the above three phases in sequence, and at the end of the learning and inference, it obtains a marginal probability \( p \) for each candidate fact. To produce the final KB, the user often selects facts in which we are highly confident, e.g., \( p > 0.95 \). Typically, the user needs to inspect errors and repeat, a process that we call error analysis. Error analysis is the process of understanding the most common mistakes (incorrect extractions, too-specific features, candidate mistakes, etc.) and deciding how to correct them \([39]\). To facilitate error analysis, users write standard SQL queries.

**2.3 Discussion of Design Choices.**

We have found three related aspects of the DeepDive approach that we believe enable non-computer scientists to write DeepDive programs: (1) there is no reference in a DeepDive program to the underlying machine learning algorithms. Thus, DeepDive programs are declarative in a
strong sense. Probabilistic semantics provide a way to debug the system independently of any algorithm. (2) DeepDive allows users to write feature extraction code in familiar languages (Python, SQL, and Scala). (3) DeepDive fits into the familiar SQL stack, which allows standard tools to inspect and visualize the data. A second key property is that the user constructs an end-to-end system and then refines the quality of the system in a pay-as-you-go way [31]. In contrast, traditional pipeline-based ETL scripts may lead to end-to-end application quality. Anecdotally, pay-as-you-go leads to more informed decisions about how to improve quality.

Comparison with Markov Logic. Our language is based on Markov Logic [16][35], and our current language inherits Markov Logic’s formal semantics. However, there are three differences in how we implement DeepDive’s language:

Weight Tying. As shown in rule FE1, DeepDive allows factors to share weights across rules, which is used in every DeepDive system. As we will see in Section 2.4, DeepDive’s factor graph on which inference takes place.

User Relations

| R | x | y | S | y | Q | x |
|---|---|---|---|---|---|---|
|   | a | 0 |   | 0 |   | a |
|   | a | 1 |   | 10|   |   |
|   | a | 2 |   |   |   |   |

Grounding

| User Relations |
|----------------|
| R(x,y) = (x,y) |
| S(y)           |

q(x) :- R(x,y)  F1
q(x) :- R(x,y), S(y)  F2

Factor Graph

Factors F

Variables V

N

Semantics

\( g(n) \)

Linear

\( n \)

Ratio

\( \log(1+n) \)

Logical

\( 1 \) for \( n > 0 \)

We denote the body predicates of \( q \) as \( \text{body}(\mathcal{Z}) \) where \( \mathcal{Z} \) are all variables in the body of \( q \), e.g., \( \mathcal{Z} = \{ x, y \} \) in the example above. Given a rule \( \gamma = (q, w) \) and a possible world \( I \), we define the sign of \( q \) on \( I \) as \( \text{sign}(\gamma, I) = 1 \) if \( q(I) \in I \) and \( -1 \) otherwise.

Given \( \mathcal{C} \in \mathbb{D}^{\mathcal{Z}} \), a grounding of \( q \) w.r.t. \( \mathcal{C} \) is a substitution \( \text{body}(\mathcal{Z}/\mathcal{C}) \), where the variables in \( \mathcal{Z} \) are replaced with the values in \( \mathcal{C} \). For example, for \( q \) above with \( \mathcal{C} = (a, b) \) then \( \text{body}(\mathcal{Z}/(a, b)) \) yields the grounding \( R(a, b), S(b) \), which is a conjunction of facts. The support \( n(\gamma, I) \) of a rule \( \gamma \) in a possible world \( I \) is the number of groundings \( \mathcal{C} \) for which \( \text{body}(\mathcal{Z}/\mathcal{C}) \) is satisfied in \( I \):

\[
 n(\gamma, I) = |\{ \mathcal{C} \in \mathbb{D}^{\mathcal{Z}} : I \models \text{body}(\mathcal{Z}/\mathcal{C}) \}|
\]

The weight of \( \gamma \) in \( I \) is the product of three terms:

\[
 w(\gamma, I) = w \ \text{sign}(\gamma, I) \ g(n(\gamma, I))
\]

Figure 3: Schematic illustration of grounding. Each tuple corresponds to a Boolean random variable and node in the factor graph. We create one factor for every set of groundings.

Figure 4: Semantics for \( g \) in Equation 1

5Our system Tuffy introduced this feature to MLNs, but its semantics had not been described in the literature.
where $g$ is a real-valued function defined on the natural numbers. For intuition, if $w(y, I) > 0$, it adds a weight that indicates that the world is more likely. If $w(y, I) < 0$, it indicates that the world is less likely. As motivated above, we introduce $g$ to support multiple semantics. Figure 4 shows choices for $g$ that are supported by DeepDive, which we compare in an example below.

Let $\Gamma$ be a set of Boolean rules, the weight of $\Gamma$ on a possible world $I$ is defined as

$$W(\Gamma, I) = \sum_{\gamma \in \Gamma} w(\gamma, I).$$

This function allows us to define a probability distribution over the set $J$ of possible worlds:

$$Pr[I] = Z^{-1} \exp(W(\Gamma, I)) \text{ where } Z = \sum_{\Gamma} \exp(W(\Gamma, I)),$$

and $Z$ is called the partition function. This framework is able to compactly specify much more sophisticated distributions than traditional probabilistic databases.

**Example 2.5.** We illustrate the semantics by example. From the Web, we could extract a set of relation mentions that supports “Barack Obama is born in Hawaii” and another set of relation mentions that support “Barack Obama is born in Kenya.” These relation mentions provide conflicting information, and one common approach is to “vote.” We abstract this as up or down votes about a fact $q$.

- $q()$: Up(x) weight = 1
- $q()$: Down(x) weight = -1

We can think of this as a having a single random variable $q()$ in which the size of Up (resp. Down) is an evidence relation that indicates the number of “Up” (resp. “Down”) votes. There are only two possible worlds: one in which $q() \in I$ (is true) and not. Let $|\text{Up}|$ and $|\text{Down}|$ be the sizes of Up and Down. Following Equation 2 we have

$$W = \text{sign}(q) \cdot (g(|\text{Up}|) - g(|\text{Down}|)),$$

and then the probability of $Q$ is

$$Pr[q() | I] = \frac{e^w}{e^w + e^{-w}}.$$

Consider the case when $|\text{Up}| = 10^6$ and $|\text{Down}| = 10^6 - 100$. In some scenarios, this small number of differing votes could be due to random noise in the data collection processes. One would expect a probability for $q()$ close to 0.5. In the linear semantics $g(n) = n$, the probability of $q$ is $(1 + e^{-200})^{-1} \approx 1 - e^{-200}$, which is extremely close to 1. In contrast, if we set $g(n) = \log(1 + n)$, then $Pr[q] \approx 0.5$. Intuitively, the probability depends on their ratio of these votes. The logical semantics $g(n) = \mathbb{1}_{n \neq 0}$ gives exactly $Pr[q] = 0.5$. However, it would do the same if $|\text{Down}| = 1$. Thus, logical semantics may ignore the strength of the voting information. At a high level, ratio semantics can learn weights from examples with different raw counts but similar ratios. In contrast, linear is appropriate when the raw counts themselves are meaningful.

No semantic subsumes the other, and each is appropriate in some application. We have found that in many cases the ratio semantics is more suitable for the application that the user wants to model. We show in the full version that these semantics also affect efficiency empirically and theoretically—even for the above simple example. Intuitively, sampling converges faster in the logical or ratio semantics because the distribution is less sharply peaked, which means that the sampler is less likely to get stuck in local minima.

**Extension to General Rules.** Consider a general inference rule $\gamma = (q, w)$, written as:

$$q(g) : \text{body}(z), \text{weight} = w(x)$$

where $x \subseteq z$ and $y \subseteq z$. This extension allows weight tying. Given $b \in \mathbb{D}^{w(g)}$ where $b_1$ (resp. $b_2$) are the values of $b$ in $x$ (resp. $y$), we expand $\gamma$ to a set $\Gamma$ of Boolean rules by substituting $x \cup y$ with values with $\mathbb{D}$ in all possible ways.

$$\Gamma = \{(q_{b_1} w_{b_2}) | q_{b_1}() : \text{body}(z/b) \text{ and } w_{b_2} = w(x/b_1)\}$$

where each $q_{b_1}()$ is a fresh symbol for distinct values of $b_1$, and $w_{b_2}$ is a real number. Rules created this way may have free variables in their bodies, e.g., $q(x) : -R(x, y, z)$ with $w(y)$ create $|\mathbb{D}|^2$ different rules of the form $q_{a_1}() : -R(a, b, z_1)$, one for each $(a, b, z_1) \in \mathbb{D}^2$, and rules created with the same value of $b$ share the same weight. Tying weights allows one to create models succinctly.

**Example 2.6.** We use the following as an example:

$$\text{Class}(x) : -R(x, f) \text{ weight} = w(f)$$

This declares a binary classifier as follows. Each binding for $x$ is an object to classify as in Class or not. The relation $R$ associates each object to its features. E.g., $R(a,f)$ indicates that object $a$ has a feature $f$. weight $= w(f)$ indicates that weights are functions of feature $f$; thus, the same weights are tied across values for $a$. This rule declares a logistic regression classifier.

It is straightforward formal extension to let weights be functions of the return values of UDFs as we do in DeepDive.

### 2.5 Inference on Factor Graphs

As in Figure 3, DeepDive explicitly constructs a factor graph for inference and learning using a set of SQL queries. Recall that a factor graph is a triple $(V, F, w)$ in which $V$ is a set of nodes that correspond to Boolean random variables, $F$ is a set of hyperedges (for $f \in F$, $f \subseteq V$, and $w : F \times \{0, 1\}^V \rightarrow \mathbb{R}$ is a weight function. We can identify possible worlds with assignments since each node corresponds to a tuple; moreover, in DeepDive, each hyperedge $f$ corresponds to the set of groundings for a rule $\gamma$. In DeepDive, $V$ and $F$ are explicitly created using a set of SQL queries. These data structures are then passed to the sampler, which runs outside the database, to estimate the marginal probability of each node or tuple in the database. Each tuple is then reloaded into the database with its marginal probability.

**Example 2.7.** Take the database instances and rules in Figure 3 as an example, each tuple in relation $R$, $S$, and $Q$ is a random variable, and $V$ contains all random variables. The inference rules $F_1$ and $F_2$ ground factors with the same name in the factor graph as illustrated in Figure 4. Both $F_1$ and $F_2$ are implemented as SQL in DeepDive.

To define the semantics, we use Equation 1 to define $w(f, I) = w(\gamma, I)$, in which $\gamma$ is the rule corresponding to
f. As before, we define \( W(F, I) = \sum_{t \in T} \hat{w}(f, I) \), and then the probability of a possible world is the following function:

\[
Pr[I] = Z^{-1} \exp \left\{ W(F, I) \right\} \text{ where } Z = \sum_{I \in \mathcal{I}} \exp(W(F, I))
\]

The main task that DeepDive conducts on factor graphs is statistical inference, i.e., for a given node, what is the marginal probability that this node takes the value 1? Since a node takes value 1 when a tuple is in the output, this process computes the marginal probability values returned to users. In general, computing these marginal probabilities is #P-hard [44]. Like many other systems, DeepDive uses Gibbs sampling [40] to estimate the marginal probability of every tuple in the database.

### 3. Incremental KBC

To help the KBC system developer be more efficient, we developed techniques to incrementally perform the grounding and inference step of KBC execution.

**Problem Setting.** Our approach to incrementally maintaining a KBC system runs in two phases. (1) **Incremental Grounding.** The goal of the incremental grounding phase is to evaluate an update of the DeepDive program to produce the “delta” of the modified factor graph, i.e., the modified variables \( \Delta V \) and factors \( \Delta F \). This phase consists of relational operations, and we apply classic incremental view maintenance techniques. (2) **Incremental Inference.** The goal of incremental inference is given \( (\Delta V, \Delta F) \) run statistical inference on the changed factor graph.

#### 3.1 Standard Techniques: Delta Rules

Because DeepDive is based on SQL, we are able to take advantage of decades of work on incremental view maintenance. The input to this phase is the same as the input to the grounding phase, a set of SQL queries and the user schema. The output of this phase is how the output of grounding changes, i.e., a set of modified variables \( \Delta V \) and their factors \( \Delta F \). Since \( V \) and \( F \) are simply views over the database, any view maintenance techniques can be applied to incremental grounding. DeepDive uses DRED algorithm [21] that handles both additions and deletions. Recall that in DRED, for each relation \( R_i \) in the user’s schema, we create a *delta relation*, \( R_i^\delta \), with the same schema as \( R_i \) and an additional column 

#### 3.2 Novel Techniques for Incremental Maintenance of Inference

We present three techniques for the incremental inference phase on factor graphs: given the set of modified variables \( \Delta V \) and modified factors \( \Delta F \) produced in the incremental grounding phase, our goal is to compute the new distribution. We split the problem into two phases. In the *materialization phase*, we are given access to the entire DeepDive program, and we attempt to store information about the original distribution, denoted \( Pr^{(0)} \). Each approach will store different information to use in the next phase, called the *inference phase*. The input to the inference phase is the materialized data from the preceding phase and the changes made to the factor graph, the modified variables \( \Delta V \) and factors \( \Delta F \). Our goal is to perform inference with respect to the changed distribution, denoted \( Pr^{(A)} \). For each approach, we study its space and time costs for materialization and the time cost for inference. We also analyze the empirical trade-off between the approaches in Section 3.2.4.

#### 3.2.1 Strawman: Complete Materialization

The strawman approach, complete materialization, is computationally expensive and often infeasible. We use it to set a baseline for other approaches.

**Materialization Phase** We explicitly store the value of the probability \( Pr[I] \) for every possible world \( I \). This approach has perfect fidelity, but storing all possible worlds takes an exponential amount of space and time in the number of variables in the original factor graph. Thus, the strawman approach is often infeasible on even moderate-sized graphs.

**Inference Phase** We use Gibbs sampling: even if the distribution has changed to \( Pr^{(A)} \), we only need access to the new factors in \( \Delta F \) and to \( Pr[I] \) to perform the Gibbs update. The speed improvement arises from the fact that we do not need to access all factors from the original graph and perform a computation with them, since we can look them up in \( Pr[I] \).

#### 3.2.2 Sampling Approach

The sampling approach is a standard technique to improve over the strawman approach by storing a set of possible worlds sampled from the original distribution instead of storing all possible worlds. However, as the updated distribution \( Pr^{(A)} \) is different from the distribution used to draw the stored samples, we cannot reuse them directly. We use a (standard) Metropolis-Hastings scheme to ensure convergence to the updated distribution.

**Materialization Phase** In the materialization phase, we store a set of possible worlds drawn from the original distribution. For each variable, we store the set of samples as a *tuple bundle*, as in MCDB [24]. A single sample for one random variable only requires 1 bit of storage. Therefore, the sampling approach can be efficient in terms of materialization space. In the KBC systems we evaluated, 100 samples require less than 5% of the space of the original factor graph.

**Inference Phase** We use the samples to generate proposals and adapt them to estimate the up-to-date distribution. This idea of using samples from similar distributions as proposals is standard in statistics, e.g., importance sampling, rejection sampling, and different variants of Metropolis-Hastings methods. After investigating these approaches, in DeepDive, we use the independent Metropolis-Hastings approach.

\[\text{Compared with running inference from scratch, the strawman approach does not materialize any factors. Therefore, it is necessary for strawman to enumerate each possible world and save their probability because we do not know a priori which possible world will be used in the inference phase.}\]
Algorithm 1 Variational Approach (Materialization)

Input: Factor graph $FG = (V, F)$, regularization parameter $\lambda$, number of samples $N$ for approximation.
Output: An approximated factor graph $FG' = (V, F')$.

1: $I_1, ..., I_N \leftarrow N$ samples drawn from $FG$.
2: $NZ \leftarrow \{(v_i, v_j) \mid v_i$ and $v_j$ are in some factor in $FG\}$.
3: $M \leftarrow$ covariance matrix estimated using $I_1, ..., I_N$, such that $M_{ij}$ is the covariance between variable $i$ and variable $j$. Set $M_{ij} = 0$ if $(v_i, v_j) \notin NZ$.
4: Solve the following optimization problem using gradient descent and let the result be $X$:
   $$\arg \max X \log det X$$
   s.t.,
   $$X_{kk} = M_{kk} + 1/3, \quad |X_{ij} - M_{ij}| \leq \lambda$$
   $$X_{ij} = 0 \text{ if } (v_i, v_j) \notin NZ$$
5: for all $i, j$ s.t. $X_{ij} \neq 0$ do
6:   Add in $F'$ a factor from $(v_i, v_j)$ with weight $X_{ij}$.
7: end for
8: return $FG' = (V, F')$.

which generates proposal samples and accepts these samples with an acceptance test. We choose this method only because the acceptance test can be evaluated using the sample, $\Delta V$, and $\Delta F$ without the entire factor graph. Thus, we may fetch many fewer factors than in the original graph, but we still converge to the correct answer.

The fraction of accepted samples is called the acceptance rate, and it is a key parameter in the efficiency of this approach. The approach may exhaust the stored samples, in which case the method resorts to another evaluation method or generates fresh samples.

3.2.3 Variational Approach

The intuition behind our variational approach is as follows: rather than storing the exact original distribution, we store a factor graph with fewer factors that approximates the original distribution. On the smaller graph, running inference and learning is often faster.

Materialization Phase The key idea of the variational approach is to approximate the distribution using simpler or sparser correlations. To learn a sparser model, we use Algorithm 1 which is a log-determinant relaxation \[43\] with a $t_1$ penalty term \[6\]. We want to understand its strengths and limitations on KBC problems, which is novel. This approach uses standard techniques for learning that are already implemented in DeepDive \[50\].

The input is the original factor graph and two parameters: the number of samples $N$ to use for approximating the covariance matrix, and the regularization parameter $\lambda$, which controls the sparsity of the approximation. The output is a new factor graph that has only binary potentials.

The intuition for this procedure comes from graphical model structure learning: an entry $(i, j)$ is present in the inverse covariance matrix only if variables $i$ and $j$ are connected in the factor graph. Given these inputs, the algorithm first draws a set of $N$ possible worlds by running Gibbs sampling on the original factor graph. It then estimates the covariance matrix based on these samples (Lines 1-3). Using the estimated covariance matrix, our algorithms solves the optimization problem in Line 4 to estimate the inverse covariance matrix $X$. Then, the algorithm creates one factor for each pair of variables such that the corresponding entry in $X$ is non-zero, using the value in $X$ as the new weight (Line 5-7). These are all the factors of the approximated factor graph (Line 8).

Inference Phase Given an update to the factor graph (e.g., new variables or new factors), we simply apply this update to the approximated graph, and run inference and learning directly on the resulting factor graph. As shown in Figure 5(c), the execution time of the variational approach is roughly linear in the sparsity of the approximated factor graph. Indeed, the execution time of running statistical inference using Gibbs sampling is dominated by the time needed to fetch the factors for each random variable, which is an expensive operation requiring random access. Therefore, as the approximated graph becomes sparser, the number of factors decreases and so does the running time.

Parameter Tuning We are among the first to use these methods in KBC applications, and there is little literature about tuning $\lambda$. Intuitively, the smaller $\lambda$ is, the better the approximation is—but the less sparse the approximation is. To understand the impact of $\lambda$ on quality, we show in Figure 6 the quality F1 score of a DeepDive program called News (see Section 4) as we vary the regularization parameter. As long as the regularization parameter $\lambda$ is small (e.g., less than 0.1), the quality does not change significantly. In all of our applications we observe that there is a relatively large “safe” region from which to choose $\lambda$. In fact, for all five systems in Section 4 even if we set $\lambda$ at 0.1 or 0.01, the impact on quality is minimal (within 1%), while the impact on speed is significant (up to an order of magnitude). Based on Figure 6 DeepDive supports a simple search protocol to set $\lambda$. We start with a small $\lambda$, e.g., 0.001, and increase it by 10x until the KL-divergence is larger than a user-specified threshold, specified as a parameter in DeepDive.

3.2.4 Tradeoffs

We studied the tradeoff between different approaches and summarize the empirical results of our study in Figure 5. The performance of different approaches may differ by more than two orders of magnitude, and neither of them dominates the other. We use a synthetic factor graph with pairwise factors and control the following axes:

1. Number of variables in the factor graph. In our experiments, we set the number of variables to values in \{2, 10, 17, 100, 1000, 10000\}.
2. Amount of change. How much the distribution changes affects efficiency, which manifests itself in the acceptance rate: the smaller the acceptance rate is, the more difference there will be in the distribution.
3. Sparsity of correlations. This is the ratio between the number of non-zero weights and the total weight. We set the sparsity to values in \{0.1, 0.2, 0.3, 0.4, 0.5, 1.0\} by selecting uniformly at random a subset of factors and set their weight to zero.

We now discuss the results of our exploration of the tradeoff space, presented in Figure 5(a-c).

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\[40\] In Figure 5 the numbers are reported for a factor graph whose factor weights are sampled at random from $[-0.5, 0.5]$. We also experimented with different intervals $([-0.1, 0.1], [-1, 1], [-10, 10])$, but these had no impact on the tradeoff.
Figure 5: A Summary of the tradeoffs. Left: An analytical cost model for different approaches; Right: Empirical examples that illustrate the tradeoff space. All converge to <0.1% loss, and thus, have comparable quality.

**Size of the Factor Graph** Since the materialization cost of the strawman is exponential in the size of the factor graph, we observe that, for graphs with more than 20 variables, the strawman is significantly slower than either the sampling approach or the variational approach. Factor graphs arising from KBC systems usually contain a much larger number of variables; therefore, from now on, we focus on the tradeoff between sampling and variational approaches.

**Amount of Change** As shown in Figure 5(b), when the acceptance rate is high, the sampling approach could outperform the variational one by more than two orders of magnitude. When the acceptance rate is high, the sampling approach requires no computation and is much faster than Gibbs sampling. In contrast, when the acceptance rate is low, e.g., 0.1%, the variational approach could be more than $5 \times$ faster than the sampling approach. An acceptance rate lower than 0.1% occurs for KBC operations when one updates the training data, adds many new features, or concept drift happens during the development of KBC systems.

**Sparsity of Correlations** As shown in Figure 5(c), when the original factor graph is sparse, the variational approach can be $11 \times$ faster than the sampling approach. This is because the approximate factor graph contains less than 10% of the factors than the original graph, and it is therefore much faster to run inference on the approximate graph. On the other hand, if the original factor graph is too dense, the variational approach could be more than $7 \times$ slower than the sampling one, as it is essentially performing inference on a factor graph with a size similar to that of the original graph.

**Discussion: Theoretical Guarantees** We discuss the theoretical guarantee that each materialization strategy provides. Each materialization method inherits the guarantee of that inference technique. The strawman approach retains the same guarantees as Gibbs sampling; For the sampling approach we use standard Metropolis-Hasting scheme. Given enough time, this approach will converge to the true distribution. For the variational approach, the guarantees are more subtle and we point the reader to the consistency of structure estimation of Gaussian Markov random field \cite{38} and log-determinate relaxation \cite{43}. These results are theoretically incomparable, motivating our empirical study.

3.3 Choosing Between Different Approaches

From the study of the tradeoff space, neither the sampling approach nor the variational approach dominates the other, and their relative performance depends on how they are being used in KBC. We propose to materialize the factor graph using both the sampling approach and the variational approach, and defer the decision to the inference phase when we can observe the workload.

**Materialization Phase** Both approaches need samples from the original factor graph, and this is the dominant cost during materialization. A key question is “*How many samples should we collect?*” We experimented with several heuristic methods to estimate the number of samples that are needed, which requires understanding how likely future changes are, statistical considerations, etc. These approaches were difficult for users to understand, so DeepDive takes a best-effort approach: it generates as many samples as possible when idle or within a user-specified time interval.

**Inference Phase** Based on the tradeoffs analysis, we developed a *rule-based optimizer* with the following set of rules:

- If an update does not change the structure of the graph, choose the sampling approach.
- If an update modifies the evidence, choose the variational approach.
- If an update introduces new features, choose the sampling approach.
- Finally, if we run out of samples, use the variational approach.
## 4. EXPERIMENTS

We conducted an experimental evaluation of DeepDive for incremental maintenance of KBC systems.

### 4.1 Experimental Settings

To evaluate DeepDive, we used DeepDive programs developed by our users over the last three years from paleontologists, geologists, biologists, a defense contractor, and a KBC competition. These are high-quality KBC systems: two of our KBC systems for natural sciences achieved quality comparable to (and sometimes better than) human experts, as assessed by double-blind experiments, and our KBC system for a KBC competition is the top system among all 45 submissions from 18 teams as assessed by professional annotators. To simulate the development process, we took snapshots of DeepDive programs at the end of every development iteration, and we use this dataset of snapshots in the experiments to understand our hypothesis that incremental techniques can be used to improve development speed.

### Datasets and Workloads

To study the efficiency of DeepDive, we selected five KBC systems, namely (1) News, (2) Genomics, (3) Adversarial, (4) Pharmacogenomics, and (5) Paleontology. Their names refer to the specific domains on which they focus. Figure 7 illustrates the statistics of these KBC systems and of their input datasets. We group all rules in each system into six rule templates with four workload categories. We focus on the News system below.

The News system builds a knowledge base between persons, locations, and organizations, and contains 34 different relations, e.g., HasSpouse or MemberOf. The input to the KBC system is a corpus that contains 1.8 million news articles and Web pages. We use four types of rules in News in our experiments, as shown in Figure 8, error analysis (rule A1), candidate generation and feature extraction (FE1, FE2), supervision (S1, S2), and inference (I1), corresponding to the steps where these rules are used.

Other applications are different in terms of the quality of the text. We choose these systems as they span a large range in the spectrum of quality: Adversarial contains advertisements collected from websites where each document may have only 1-2 sentences with grammatical errors; in contrast, Paleontology contains well-curated journal articles with precise, unambiguous writing and simple relationships. Genomics and Pharma have precise texts, but the goal is to extract relationships that are more linguistically ambiguous compared to the Paleontology text. News has slightly degraded writing and ambiguous relationships, e.g., “member of.” Rules with the same prefix, e.g., FE1 and FE2, belong to the same category, e.g., feature extraction.

### DeepDive Details

DeepDive is implemented in Scala and C++, and we use Greenplum to handle all SQL. All feature extractors are written in Python. The statistical inference and learning and the incremental maintenance component are all written in C++. All experiments are run on a machine with four CPUs (each CPU is a 12-core 2.40 GHz Xeon E5-4657L), 1 TB RAM, and 12×1TB hard drives and running Ubuntu 12.04. For these experiments, we compiled DeepDive with Scala 2.11.2, g++-4.9.0 with -O3 optimization, and Python 2.7.3. In Genomics and Adversarial, Python 3.4.0 is used for feature extractors.

### 4.2 End-to-end Performance and Quality

We built a modified version of DeepDive called RE_RUN, which gives an update on the KBC system, runs the DeepDive program from scratch. DeepDive, which uses all techniques, is called INCREMENTAL. The results of our evaluation show that DeepDive is able to speed up the development of high-quality KBC systems through incremental maintenance with little impact on quality. We set the number of samples to collect during execution to {10, 100, 1000} and the number of samples to collect during materialization to {1000, 2000}. We report results for (1000, 2000), as results for other combinations of parameters are similar.

#### Quality Over Time

We first compare RE_RUN and INCREMENTAL in terms of the wait time that developers experience to improve the quality of a KBC system. We focus on News because it is a well-known benchmark competition. We run all six rules sequentially for both RE_RUN and INCREMENTAL, and after executing each rule, we report the quality of the system measured by the F1 score and the cumulative execution time. Materialization in the INCREMENTAL system is performed only once. Figure 10(a) shows the results. Using INCREMENTAL takes significantly less time than RE_RUN to achieve the same quality. To achieve an F1 score of 0.36 (a competition-winning score), INCREMENTAL is 22× faster than RE_RUN. Indeed, each run of RE_RUN takes 6 hours, while a run of INCREMENTAL takes at most 30 minutes.

We further compare the facts extracted by INCREMENTAL and RE_RUN and find that these two systems not only have similar end-to-end quality, but are also similar enough to
support common debugging tasks. We examine the facts with high-confidence in Rerun (> 0.9 probability), 99% of them also appear in Incremental, and vice versa. High confidence extractions are used by the developer to debug precision issues. Among all facts, we find that at most 4% of them have a probability that differs by more than 0.05. The similarity between snapshots suggests, our incremental maintenance techniques can be used for debugging.

Efficiency of Evaluating Updates We now compare Rerun and Incremental in terms of their speed in evaluating a given update to the KBC System. To better understand the impact of our technical contribution, we divide the total execution time into parts: (1) the time used for feature extraction and grounding; and (2) the time used for statistical inference and learning. We implemented classical incremental materialization techniques for feature extraction and grounding, which achieves up to a 360× speedup for rule FE1 in News. We get this speedup for free using standard RDBMS techniques, a key design decision in DeepDive.

Figure 9 shows the execution time of statistical inference and learning for each update on different systems. We see that with the ability to choose between the sampling approach and variational approach even when the distribution for a group of variables does not change. For supervision rules, disabling the variational approach is 36× slower because the distribution does not change. For feature extraction rules, disabling the sampling approach slows down the execution compared to the “full” system. For analysis rule A1, disabling the sampling approach leads to a more than 11× slow down, because the sampling approach has, for this rule, a 100% acceptance rate because the distribution does not change. For analysis rule A1, disabling the sampling approach slows down the execution compared to the “full” system. For analysis rule A1, disabling the sampling approach slows down the execution compared to the “full” system. For analysis rule A1, disabling the sampling approach slows down the execution compared to the “full” system. For analysis rule A1, disabling the sampling approach slows down the execution compared to the “full” system.

4.3 Lesion Studies

We conducted lesion studies to verify the effect of the tradeoff space on the performance of DeepDive. In each lesion study, we disable a component of DeepDive, and leave all other components untouched. We report the execution time for statistical inference and learning.

We evaluate the impact of each materialization strategy on the final end-to-end performance. We disabled either the sampling approach or the variational approach and left all other components untouched. Figure 11 shows the results for News. Disabling either the sampling approach or the variational approach slows down the execution compared to the “full” system. For analysis rule A1, disabling the sampling approach slows down the execution by 5× because it forces the use of the variational approach even when the distribution for a group of variables does not change. For supervision rules, disabling the variational approach is 36× slower because the introduction of training examples decreases the acceptance rate of the sampling approach.

Optimizer Using different materialization strategies for different groups of variables positively affects the performance of DeepDive. We compare Incremental with a strong baseline NoWorkloadInfo which, for each group, first runs the sampling approach. After all samples have been used, we switch to the variational approach. Note that this baseline is stronger than the strategy that fixes the same strategy for all groups. Figure 11 shows the results of the experiment. We see that with the ability to choose between the sampling ap-
proach and variational approach according to the workload, DeepDive can be up to $2 \times$ faster than NoWorkLoadInfo.

5. CONCLUSION

We described the DeepDive approach to KBC and our experience building KBC systems over the last few years. To improve quality, we argued that a key challenge is to accelerate the development loop. We described the semantic choices that we made in our language. By building on SQL, DeepDive is able to use classical techniques to provide incremental processing for the SQL components. However, these classical techniques do not help with statistical inference, and we described a novel tradeoff space for approximate inference techniques. We used these approximate inference techniques to improve end-to-end execution time in the face of changes both to the program and the data; they improved system performance by two orders of magnitude in five real KBC scenarios while keeping the quality high enough to aid in the development process.

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APPENDIX

A. ADDITIONAL THEORETICAL DETAILS

We find that the three semantics that we defined, namely, Linear, Logical, and Ratio, have impact to the convergence speed of the sampling procedure. We describe these results in Section A.1 and provide proof in Section A.2.

A.1 Convergence Results

We describe our results on convergence rates, which are summarized in Figure 12. We first describe the Voting program from Example 2.5 and summarize those results in a theorem. We now introduce the standard metric of convergence in Markov Chain theory [26].

Definition A.1. The total variation distance between two probability measures \( \mathbb{P} \) and \( \mathbb{P}' \) over the same sample space \( \Omega \) is defined as

\[
\| \mathbb{P} - \mathbb{P}' \|_{tv} = \sup_{A \in \Omega} |\mathbb{P}(A) - \mathbb{P}'(A)|,
\]

that is, it represents the largest difference in the probabilities that \( \mathbb{P} \) and \( \mathbb{P}' \) assign to the same event.

In Gibbs sampling, the total variation distance is a metric of comparison between the actual distribution \( \mathbb{P}_n \) achieved at some timestep \( k \) and the equilibrium distribution \( \pi \).

Types of Programs. We consider two families of programs motivated by our work in KBC: voting programs and hierarchical programs. The voting program is used to continue the example, but some KBC programs are hierarchical (13/14 KBC systems from the literature). We consider some enhancements that make our programs more realistic. We allow every tuple (DB or EDB) to have its own weight, i.e., we allow every ground atom \( R(a) \) to have a rule \( w_a : R(a) \). Moreover, we allow any atom to be marked as evidence (or not), which means its value is fixed. We assume that all weights are not functions of the number of variables (and so are \( O(1) \)). Finally, we consider two types of programs.

The first we call voting programs, which are a generalization of Example 2.5, in which any subset of variables may be evidence and the weights may be distinct.

Proposition A.2. Let \( \epsilon > 0 \). Consider Gibbs sampling running on a particular factor graph with \( n \) variables, there exists a \( \tau(n) \) that satisfies the upper bounds in Figure 12 and such that \( |\mathbb{P}_k - \pi|_{tv} \leq \epsilon \) after \( \tau(n) \log(1 + \epsilon^{-1}) \) steps. Furthermore, for each of the classes, we can construct a graph on which the minimum time to achieve total variation distance \( \epsilon \) is at least the lower bound in Figure 12.

For example, for the voting example with logical semantics, \( \tau(n) = O(n \log n) \). The lower bounds are demonstrated with explicit examples and analysis. The upper bounds use the special form of Gibbs sampling on these factor graphs, and then use a standard argument based on coupling [15] and an analysis very similar to a generalized coupon collector process. This argument is sufficient to analyze the voting program in all three semantics.

We consider a generalization of the voting program in which each tuple is a random variable (possibly with a weight); specifically, the program consists of a variable \( Q \), a set of “Up” variables \( U \), and a set of “Down” variables \( D \). Experimentally, we compute how different semantics converges on the voting program as illustrated in Figure 13.

Evaluation of hierarchical programs is \#P-hard, e.g., any Boolean query is hierarchical, but there are \#P-hard Boolean queries [42]. Using a similar argument, we show that any set of hierarchical rules that have non-overlapping bodies converges in time \( O(N \log N \log(1 + \epsilon^{-1})^3) \) for either Logical or Ratio semantics, where \( N \) is the number of factors. This statement is not trivial, as we show that Gibbs sampling on the simplest non-hierarchical programs may take exponential time to converge. Our definition is more general than the typical notions of safety [13]: we consider multiple rules with rich correlations rather than a single query over a tuple independent database. However, we only provide guarantees about sampling (not exact evaluation) and have no dichotomy theorem.

We also analyze an asymptotic setting, in which the domain size grows, and we show that hierarchical programs also converge in polynomial time in the Logical semantics. This result is a theoretical example that suggests that the more data we have, the better Gibbs sampling will behave. The key technical idea is that for the hierarchical programs no variable has unbounded influence on the final result, i.e., no variable contributes an amount depending on \( N \) to the final joint probability.

A.2 Proofs of Convergence Rates

Here, we prove the convergence rates stated in Proposition A.2. The strategy for the upper bound proofs involves...
constructing a coupling between the Gibbs sampler and another process that attains the equilibrium distribution at each step. First, we define a coupling \cite{15,29}.

**Definition A.4 (Coupling).** A coupling of two random variables \(X\) and \(X'\) defined on some separate probability spaces \(P\) and \(P'\) is any new probability space \(\hat{P}\) over which there are two random variables \(\hat{X}\) and \(\hat{X}'\) such that \(X\) has the same distribution as \(\hat{X}\) and \(X'\) has the same distribution as \(\hat{X}'\).

Given a coupling of two sequences of random variables \(X_k\) and \(X'_k\), the coupling time is defined as the first time \(T\) when \(X_k = \hat{X}'_k\). The following theorem lets us bound the total variance distance in terms of the coupling time.

**Theorem A.5.** For any coupling \((\hat{X}_k, \hat{X}'_k)\) with coupling time \(T\),

\[
\|P(X_k \in \cdot) - P'(X'_k \in \cdot)\|_{tv} \leq 2\hat{P}(T > k).
\]

All of the coupling examples in this section use a correlated flip coupler, which consists of two Gibbs samplers \(X\) and \(X'\), each of which is running with the same random inputs. Specifically, both samplers choose to sample the same variable at each timestep. Then, if we define \(p\) as the probability of sampling 1 for \(X\), and \(p'\) similarly, it assigns both variables to 1 with probability \(\min(p, p')\), both variables to 0 with probability \(\min(1 - p, 1 - p')\), and assigns different values with probability \(|p - p'|\). If we initialize \(\hat{X}\) with an arbitrary distribution and \(X'\) with the stationary distribution \(\pi\), it is trivial to check that \(\hat{X}_k\) has distribution \(\hat{P}_k\), and \(\hat{X}'_k\) always has distribution \(\pi\). Applying Theorem A.5 results in

\[
\|\hat{P}_k - \pi\|_{tv} \leq 2\hat{P}(T > k).
\]

Now, we prove the bounds in Figure 12.

**Theorem A.6 (UB for Voting: Logical and Ratio).**

For the voting example, if all the weights on the variables are bounded independently of the number of variables \(n\), and \(|U| = O(n)\), and \(|D| = O(n)\), then for either the logical or ratio projection semantics, there exists a \(\tau(n) = O(n \log n)\) such that for any \(\epsilon > 0\), \(\|\hat{P}_k - \pi\|_{tv} \leq \epsilon\) for any \(k \geq \tau(n) \log(e^{-\epsilon})\).

**Proof.** For the voting problem, if we let \(f\) denote the projection semantic we are using, then for any possible world \(I\) the weight can be written as

\[
W = \sum_{u \in \hat{U}} w_u + \sum_{d \in \hat{D}} w_d + w\sigma([U \cap I]) - w\sigma([D \cap I]),
\]

where \(\sigma = \text{sign}(Q, I)\). Let \(I\) denote the world at the current timestep, \(I'\) be the world at the next timestep, and \(\hat{I}\) be \(I\) with the variable we choose to sample removed. Then if we sample a variable \(u \in \hat{U}\), and let \(m_u = \min(U \cap I, U \cap I')\), then

\[
P(u \in I') = \frac{\exp(w_u + w\sigma(m_u + 1))}{\exp(w_u + w\sigma(m_u + 1)) + \exp(w\sigma(m_u))}
= \left(1 + \exp(-w_u - w\sigma(m_u + 1) - f(m_u)))\right)^{-1}.
\]

Since \(f(x + 1) - f(x) < 1\) for any \(x\), it follows that \(\sigma(f(m_u + 1) - f(m_u))) < -1\). Furthermore, since \(w_u\) is bounded independently of \(n\), we know that \(w_u \geq w_{\text{min}}\) for some constant \(w_{\text{min}}\). Substituting this result in

\[
P(u \in I') \geq \frac{1}{1 + \exp(-w_{\text{min}} + w)} = p_{\text{min}},
\]

for some constant \(p_{\text{min}}\) independent of \(n\). The same argument will show that, if we sample \(d \in D\),

\[
P(d \in I') \geq p_{\text{min}}.
\]

Now, if \(|U \cap I| > \min(|U|)\), it follows that, for both the logical and ratio semantics, \(f(m_u + 1) - f(m_u) \leq 2\min(|U|)\). Under these conditions, then if we sample \(u\), we will have

\[
\frac{1}{1 + \exp(-w_u + 2\min(|U|))} \leq \frac{1}{1 + \exp(-w_u + 2\min(|U|))},
\]

The same argument applies to sampling \(d\).

Next, consider the situation if we sample \(Q\).

\[
P(Q \in I') = (1 + \exp(-2w(|U \cap I|) + 2w(|D \cap I|)))^{-1}.
\]

Under the condition that \(|U \cap I| > \min(|U|)\), and similarly for \(D\), this is bounded by

\[
\left(1 + \exp\left(-2w\left(\frac{\min(|U|)}{2} + 2w(|D|)\right)\right)^{-1} \leq P(Q \in I') \leq \left(1 + \exp\left(-2w\right)^{-1}\right)\right.
\]

But, for both logical and ratio semantics, we have that \(f(cn) - f(n) = O(1)\), and so for some \(q_u\) and \(q_d\) independent of \(n\),

\[
q_u \leq P(Q \in I') \leq q_d.
\]

Now, consider a correlated-flip coupler running for \(4n \log n\) steps on the Gibbs sampler. Let \(E_1\) be the event that, after the first \(2n \log n\) steps, each of the variables has been sampled at least once. (This will have probability at least \(\frac{1}{2}\) by the coupon collector’s problem.) Let \(E_2\) be the event that, after the first \(2n \log n\) steps, \(|U \cap I| > \min(|U|)\) for the next \(2n \log n\) steps for both samplers, and similarly for \(E_D\). After all the entries have been sampled, \(|U \cap I|\) and \(|D \cap I|\) will each be bounded from below by a binomial random variable with parameter \(p_{\text{min}}\) at each timestep, so from Hoeffding’s inequality, the probability that this constraint will be violated by a sampler at any particular step is less than \(\exp(-\frac{1}{2}p_{\text{min}}(|U|))\). Therefore,

\[
\hat{P}(E_2|E_1) \geq \left(1 - \exp\left(-\frac{1}{2}p_{\text{min}}(|U|)\right)\right)^{4n \log n} = \Omega(1).
\]

The same argument shows that \(E_0 = \Omega(1)\). Let \(E_2\) be the event that all the variables are resampled at least once between time \(2n \log n\) and \(4n \log n\). Again this event has probability at least \(\frac{1}{2}\). Finally, let \(C\) be the event that the coupling occurs at time \(4n \log n\). Given \(E_1, E_2, E_U, \) and \(E_D\), this probability is equal to the probability that each variable coupled individually the last time it was sampled. For \(u\), this probability is

\[
1 - \frac{1}{1 + \exp\left(-w_u + \frac{2}{p_{\text{min}}(|U|)}\right)} + \frac{1}{1 + \exp\left(-w_u + \frac{2}{p_{\text{min}}(|U|)}\right)}.
\]
and similarly for $d$. We know this probability is $1 - O(\frac{1}{n})$ by Taylor’s theorem. Meanwhile, for $Q$, the probability of coupling is $1 - q_+ + q_-$, which is always $\Omega(1)$. Therefore,

$$\hat{P}(C|E_1, E_2, E_U, E_D) \geq \Omega(1) \left(1 - O\left(\frac{1}{n}\right)\right)^{n-1} = \Omega(1),$$

and since

$$\hat{P}(C) = \hat{P}(C|E_1, E_2, E_U, E_D)\hat{P}(E_U|E_1)\hat{P}(E_D|E_1)\hat{P}(E_2|E_1)\hat{P}(E_1),$$

we can conclude that $\hat{P}(C) = \Omega(1)$.

Therefore, this process couples with at least some constant probability $p_c$ after $4n\log n$ steps. Since we can run this coupling argument independently an arbitrary number of times, it follows that, after $4n\log n$ steps, the probability of coupling will be at least $1 - (1 - p_c)^k$. Therefore,

$$\|P_{4n\log n} - \pi|_{tv} \leq \hat{P}(T > 4n\log n) \leq (1 - p_c)^k.$$

This will be less than $\epsilon$ when $L \geq \frac{\log(\epsilon)}{\log(1 - p_c)}$, which occurs when $k \geq 4n\log n \frac{\log(\epsilon)}{\log(1 - p_c)}$. Letting $\tau(n) = \frac{4n\log n}{\log(1 - p_c)}$ proves the theorem. $\square$

**Theorem A.7** (LB for Voting: Logical and Ratio) For the voting example, using either the logical or ratio projection semantics, the minimum time to achieve total variation distance $\epsilon$ is $O(n \log n)$.

**Proof.** At a minimum, in order to converge, we must sample all the variables. From the coupon collector’s problem, this requires $O(n \log n)$ time. $\square$

**Theorem A.8** (UB for Voting: Linear) For the voting example, if all the weights on the variables are bounded independently of $n$, then for linear projection semantics, there exists a $\tau(n) = 2^{O(n)}$ such that for any $\epsilon > 0$, $\|P_k - \pi|_{tv} \leq \epsilon$ for any $k \geq \tau(n) \log(e^{-\epsilon})$.

If at some timestep we choose to sample variable $u$, $u$ is active, we have

$$P_u = \frac{\exp(w_u + wq)}{\exp(w_u + wq) + \exp(0)} = \Omega(1),$$

where $q = \text{sign}(Q, I)$. The same is true for sampling $d$. If we choose to sample $Q$,

$$P_Q = \frac{\exp(w|U \cap I| - w|D \cap I|)}{\exp(w|U \cap I| - w|D \cap I|) + \exp(-w|U \cap I| + w|D \cap I|)} = (1 + \exp(-2w|U \cap I| - |D \cap I|))^{-1} = \exp(-O(n)).$$

Therefore, if we run a correlated-flip coupler for $2n\log n$ timesteps, the probability that coupling will have occurred is greater than the probability that all variables have been sampled (which is $\Omega(1)$) times the probability that all variables were sampled as 1 in both samplers. Thus if $p_c$ is the probability of coupling,

$$p_c \geq \Omega(1) \left(\exp(-O(n))\right)^2 = \Omega(1)^{2^O(n)} = \exp(-O(n)).$$

Therefore, if we run for some $\tau(n) = 2^{O(n)}$ timesteps, coupling will have occurred at least once with high probability. The statements in terms of total variance distance follow via the same argument used in the previous lower bound proof. $\square$

**Theorem A.9** (LB for Voting: Linear). For the voting example using linear projection semantics, the minimum time to achieve total variation distance $\epsilon$ is $2^{O(n)}$.

**Proof.** Consider a sampler with unary weights all zero that starts in the state $I = Q \cup U$. We will show that it takes an exponential amount of time until $Q \not\in I$. From above, the probability of flipping $Q$ will be

$$P(Q \not\in I') = (1 + \exp(2w(|U \cup I| - |D \cap I|)))^{-1}.$$

Meanwhile, the probability to flip any $u$ while $Q \in I$ is

$$P(u \not\in I') = \frac{\exp(|0|)}{\exp(w) + \exp(0)} = \exp(w + 1)^{-1} = p,$$

for some $p$, and the probability of flipping $d$ is similarly

$$P(d \in I') = \frac{\exp(-w)}{\exp(-w) + \exp(0)} = p.$$

Now, consider the following events which could happen at any timestep. While $Q \in I$, let $E_U$ be the event that $|U \cap I| \leq (1 - 2p)n$, and let $E_D$ be the event that $|D \cap I| \geq 2pn$. Since $|U \cap I|$ and $|D \cap I|$ are both bounded by binomial random variables with parameters $1 - p$ and $p$ respectively, Hoeffding’s inequality states that, at any timestep,

$$P(|U \cap I| \leq (1 - 2p)n) \leq \exp(-2p^2n),$$

and similarly

$$P(|D \cap I| \geq 2pn) \leq \exp(-2p^2n).$$

Now, while these bounds are satisfied, let $E_Q$ be the event that $Q \not\in I'$. This will be bounded by

$$P(E_Q) = (1 + \exp(2w(1 - 4p)n))^{-1} \leq \exp(-2w(1 - 4p)n).$$

It follows that at any timestep, $P(E_U \lor E_D \lor E_Q) = \exp(-O(n))$. So, at any timestep $k$, $P(Q \in I) = k\exp(-\Omega(n))$. However, by symmetry the stationary distribution $\pi$ must have $\pi(Q \in I) = \frac{1}{2}$. Therefore, the total variation distance is bounded by

$$\|P_k - \pi|_{tv} \geq \frac{1}{2} - k\exp(-\Omega(n)).$$

So, for convergence to less than $\epsilon$, we must require at least $2^{O(n)}$ steps. $\square$

**B. ADDITIONAL SYSTEM DETAILS**

**B.1 Decomposition with Inactive Variables**

Our system also uses the following heuristic. The intuition behind this heuristic is that, the fewer variables we materialize, the faster all approaches are. DeepDive allows the user to specify a set of rules (the “interest area”) that identify a set of relations that she will focus on in the next iteration of the development. Given the set of rules, we use the standard dependency graph to find relations that could be changed by the rules. We call variables in the relations that the developer wants to improve active variables, and we call inactive variables those that are not needed in the next KBC iteration. Our previous discussion assumes that all the variables are active. The intuition is that we only require the active variables, but we first need to marginalize out the inactive variables to create a new factor graph. If done naïvely, this new factor graph can be excessively large. The observation that serves as the basis of our optimization
Inference Time

Figure 14: The Lesion Study of Decomposition.

| # Samples | Adv. News | Gen. Pharma | Paleo. |
|-----------|----------|-------------|--------|
| 2083      | 2083     | 2083        | 2083   |
| 3007      | 3007     | 3007        | 3007   |
| 22162     | 22162    | 22162       | 22162  |
| 1852      | 1852     | 1852        | 1852   |
| 2375      | 2375     | 2375        | 2375   |

Figure 15: Number of Samples We can Materialize in 8 Hours.

is as follows: conditioning on all active variables, we can partition all inactive variables into sets that are conditionally independent from each other. Then, by appropriately grouping together some of the sets, we can create a more succinct factor graph to materialize.

**Procedure.** We now describe in detail our procedure to decompose a graph in the presence of inactive variables, as illustrated in Algorithm 2. Let \( \mathcal{V}'_{(i)} \) be the collection of all the sets of inactive variables that are conditionally independent for all other inactive variables, given the active variables. This is effectively a partitioning of all the inactive variables (Line 1). For each set \( \mathcal{V}'_{(i)} \), let \( \mathcal{V}'_{(a)} \) be the minimal set of active variables on which the variables in \( \mathcal{V}'_{(i)} \) are independent of all other inactive variables (Line 2). Consider now the set \( \mathcal{G} \) of pairs \( \{\mathcal{V}'_{(i)}, \mathcal{V}'_{(a)}\} \). It is easy to see that we can materialize each pair separately from other pairs. Following this approach to the letter, some active random variables may be materialized multiple times, once for each pair they belong to, with an impact on performance. This can be avoided by grouping some pairs together, with the goal of minimizing the runtime of inference on the materialized graph. Finding the optimal grouping is actually NP-hard, even if we make the simplification that each group \( g = \{\mathcal{V}'_{(i)}, \mathcal{V}'_{(a)}\} \) has a cost function \( c(g) \) that specifies the inference time, and the total inference time is the sum of the cost of all groups. The key observation concerning the NP-hardness is that two arbitrary groups \( g_1 = \{\mathcal{V}'_{(1)}, \mathcal{V}'_{(a)}\} \) and \( g_2 = \{\mathcal{V}'_{(2)}, \mathcal{V}'_{(a)}\} \) can be materialized together to form a new group \( g_3 = \{\mathcal{V}'_{(1)} \cup \mathcal{V}'_{(2)}, \mathcal{V}'_{(a)} \cup \mathcal{V}'_{(a)}\} \), and \( c(g_3) \) could be smaller than \( c(g_1) + c(g_2) \) when \( g_1 \) and \( g_2 \) share most of the active variables. This allows us to reduce the problem to WEIGHTEDSETCOVER. Therefore, we use a greedy heuristic that starts with groups, each containing one inactive variable, and iteratively merges two groups \( \{\mathcal{V}'_{(1)}, \mathcal{V}'_{(a)}\} \) and \( \{\mathcal{V}'_{(2)}, \mathcal{V}'_{(a)}\} \) if \( |\mathcal{V}'_{(a)}| \leq \max(|\mathcal{V}'_{(a)}|, |\mathcal{V}'_{(a)}|) \) (Line 4-6). The intuition behind this heuristic is that, according to our study of the tradeoff between different materialization approaches, the fewer variables we materialize, the greater the speedup for all materialization approaches will be.

**Experimental Validation.** We also verified that using the decomposition technique has a positive impact on the performance of the system. We built NODECOMPOSITION that does not decompose the factor graph and select either the sampling approach or the variational approach for the whole factor graph. We report the best of these two strategies as the performance of NODECOMPOSITION in Figure 14. We found that, for A1, removing structural decomposition does not slow down compared with DeepDive, and it is actually 2% faster because it involves less computation for determining sample acceptance. However, for both feature extraction and supervision rules, NODECOMPOSITION is at least 6× slower. For both types of rules, the NODECOMPOSITION costs corresponds to the cost of the variational approach. In contrast, the sampling approach has near-zero acceptance rate because of a large change in the distribution.

### B.2 Materialization Time

We show how materialization time changes across different systems. In the following experiment, we set the total materialization time to 8 hours, a common time budget that our users often used for overnight runs. We execute the whole materialization phase of DeepDive for all systems, which will materialize both the sampling approach and the variational approach, and we require the whole process to finish in 8 hours. Figure 15 shows how many samples we can collect given this 8-hour budget: for all five systems, in 8 hours, we can store more than 2000 samples, from which to generate 1000 samples during inference if the acceptance rate for the sampling approach is 0.5.

### B.3 Incremental Learning

Relearning learning happens when one labels new documents (typically an analyst in the loop), so one would like this to be an efficient procedure. One interesting observation is that a popular technique called distant supervision (used in DeepDive) is able to label new documents heuristically using rules, so that new labeled data is created without human intervention. Thus, we study how to incrementally perform learning. This is well studied in the online learning community, and here we adapt essentially standard techniques. We essentially get this for free because we choose to adapt standard online methods, such as stochastic gradient descent with warmstart, for our training system. Here, warmstart means that DeepDive uses the learned model in the last run as the starting point instead of initializing the model to start randomly.
Experimental Validation. We validate that, by adapting standard online learning methods, DeepDive is able to outperform baseline approaches. We compare DeepDive with two baseline approaches, namely (1) stochastic gradient descent without warmstart and (2) gradient descent with warmstart. We run on the dataset News with rules F2 and S2, introduces both new features and new training examples with labels. We obtain a proxy for the optimal loss by running both stochastic gradient descent and gradient descent separately for 24 hours and picking the lowest loss. For each learning approach, we grid search its step size in \{1.0, 0.1, 0.01, 0.001, 0.0001\}, run for 1 hour, and pick the fastest one to reach a loss that is within 10% of the optimal loss. We estimate the loss after each learning epoch and report the percentage within the optimal loss in Figure 17.

As shown in Figure 17, the loss of all learning approaches decrease, with more learning epochs. However, DeepDive’s SGD+Warmstart approach reaches a loss that achieves a loss within 10% optimal loss faster than other approaches. Compared with SGD-Warmstart, SGD+Warmstart is 2× faster in reaching a loss that is within 10% of the optimal loss because it starts with a model that has lower loss because of warmstart. Compared with gradient descent, SGD+Warmstart is about 10× faster. Although SGD+Warmstart and gradient descent with warmstart have the same initial loss, SGD converges faster than gradient descent in our example.

B.4 Discussion of Concept Drift

Concept drift [58,63] refers to the scenario that arises in online learning when the training examples become available as a stream, and the distribution from which these examples are generated keeps changing overtime. Therefore, the key technique in how to resolve the problem of concept drift is primarily in how to design a machine learning system to automatically detect and adapt to the changes. The design needs to consider how to not only update the model incrementally, but also “forget the old information” [58]. Although we have not observed quality issues caused by concept drift in our KBC applications, it is possible for DeepDive to encounter this issue in other applications. Thus, we study the impact of concept drift to our incremental inference and learning approach.

Impact on Performance. In this work, we solely focus on the efficiency of updating the model incrementally. When concept drift happens, the new distribution and new target model would be significantly different from the materialized distribution as well as the learned model from last iteration. From our analysis in Section B.3, we hypothesize there are two impacts of concept drift that require consideration in DeepDive. First, the difference between materialized distribution and the target distribution is modeled as the amount of change in Section B.3 and therefore, in the case of concept drift, we expect our system favors variational approach more than sampling approach. Second, because the difference between the learned model and target model is large, it is not clear whether the warmstart scheme we discussed in Section B.3 will work.

Experimental Validation. As our workloads do not have concept drift, we follow prior art [63], we use its dataset that contains 9,324 emails ordered chronologically, and predict exactly the same task that for each email predict whether it is spam or not. We implement a logistic regression classifier in DeepDive with a rule similar to Example 2.6. We use the first 10% emails and first 30% emails as training sets, respectively, and use the remaining 70% as the testing set. We construct two systems in a similar way as Section 4: Re-run that trains directly on 30% emails, and INCREMENTAL that materialize using 10% emails and incrementally train on 30% emails. We run both systems and measure the test set loss after each learning epoch.

Figure 17 shows the result. We see that even with concept drift, both systems converge to the same loss. INCREMENTAL converges faster than RERUN, and it is because even with concept drift, warmstart still allows INCREMENTAL to start from a lower loss at the first iteration. In terms of the time used for each iteration, INCREMENTAL and RERUN uses roughly the same amount of time for each iteration. This is expected because INCREMENTAL rejects almost all samples due to the large difference between distributions and switch to variational approach, which, for a logistic regression model where all variables are active and all weights have been changed, is very similar to the original model. From these results we see that, even with concept drifts, INCREMENTAL still provides benefits over re-running the system from scratch due to warmstart; however, as expected, the benefit from incremental inference is smaller.

C. ADDITIONAL RELATED WORK

We provide additional related work, especially those work that impacts the current design of DeepDive’s language component.

More Related KBC Systems. DeepDive’s model of KBC is motivated by the recent attempts of using machine learning-based technique for KBC [51,52,62,72,76,81,84] and the line
of research that aims to improve the quality of a specific component of KBC system \[32, 48, 53, 56, 57, 60, 65–68, 70, 73, 74, 77, 78, 82, 83\]. When designing DeepDive, we used these systems as test cases to justify the generality of our framework. In fact, we find that DeepDive is able to model 13 of these popular KBC systems \[32, 48, 57, 61, 65–68, 70, 73, 74, 82, 83\].

Other Incremental Algorithms. We build on decades of study of incremental view maintenance \[55, 59\]: we rely on the classic incremental maintenance techniques to handle relational operations. Recently, others have proposed different approaches for incremental maintenance for individual analytic workflows like iterative linear algebra problems \[71\], classification as new training data arrived \[28\], or segmentation as new data arrives \[10\].

Factor graphs have been used by some probabilistic databases as the underlying representation \[16, 75\], but they did not study how to reuse computation across different, but similar, factor graphs.

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