ProvSQL: A General System for Keeping Track of the Provenance and Probability of Data

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ABSTRACT

We present the data model, design choices, and performance of ProvSQL, a general and easy-to-deploy provenance tracking and probabilistic database system implemented as a PostgreSQL extension. ProvSQL's data and query models closely reflect that of a large core of SQL, including multiset semantics, the full relational algebra, and terminal aggregation. A key part of its implementation relies on generic provenance circuits stored in memory-mapped files. We propose benchmarks to measure the overhead of provenance and probabilistic evaluation and demonstrate its scalability and competitiveness with respect to other state-of-the-art systems.

Artifact Availability:

ProvSQL is available at https://github.com/PierreSenellart/provsql while the benchmark is available at https://github.com/Aryak320/benchmark_suite.

1 INTRODUCTION

As data is increasingly used for decision making and training machine learning models, it is crucial to account for two of its main inherent challenges. The first is that *sources matter*. Indeed, more and more importance is given to being able to trace final results back to the original data, to ensure that the results being presented to final users represent the truth. Secondly, in many cases data itself is *uncertain*, be it from the data collection process or as a result of data processing, such as using machine learning. To successfully tackle these issues, it is important to have systems able to keep track of the *provenance* of data, but that are also capable to *reason probabilistically* about its uncertainty.

Data provenance – tracking data throughout a transformation process – has a long history in research, especially within relational data management. The main aims of data provenance are to keep track of *where* results come from, and to show *why* and *how* these results are computed. Early works on provenance [12, 13] reflected on the importance of determining the origin of query output, specifically in the form of *where* and *why* provenance. A related concept is that of data lineage [3], introduced in the Trio system for uncertain data management. A breakthrough was achieved through the *provenance semiring* framework [29] which concisely models many different forms of provenance, including why-provenance and Trio's lineage. In this framework, relations are *annotated* with elements of semirings and relational algebra operators are mapped to semiring operations. Extensions of this framework to more complex queries [6, 11, 27] have since been proposed.

Managing data uncertainty was another parallel line of research. Uncertainty was initially accounted for via concepts such as NULL values [17] and c-tables [34]. More recently, tuple-independent databases, where each tuple is independently annotated with a probability values, were introduced by [19], and extended to block-independent databases [18], as a simple probabilistic model of uncertainty. Even in these simple frameworks, *probabilistic query evaluation*, i.e., computing the probability of a query result, is a #P-hard problem [19]. Some tractable cases are however known: when queries have some specific properties (e.g., the *safe queries* of [20] over tuple-independent databases), or when data itself has a tree-like structure [4], captured by the notion of treewidth [40].

Though most of the works cited so far are theoretical in nature, various systems have been proposed that implement some form of provenance and probability evaluation or both: notable examples include Trio [3], Orchestra [30], Orion [48], MayBMS [33], Perm [28], and more recently GProM [8]. With the exception of GProM, these systems are unfortunately unmaintained, have become hard to deploy or are even defunct. None of these systems provide a generic tool able to both keep track of the probability and provenance of data, for a wide variety of provenance frameworks.

In this article, we explain how the rich literature on provenance and probabilistic query evaluation is a basis for the implementation of ProvSQL, a plugin for the PostgreSQL database management system. ProvSQL aims to provide a generic, easy-to-deploy, and scalable solution to store and evaluate data provenance and probabilities. The system was first demonstrated in [47]; since then it has become more mature and many features and optimizations were added. It was used as a provenance computation tool in several lines of research, by a variety of authors [9, 14, 22, 38, 44]. This paper is the first to provide a comprehensive presentation of its data model, query evaluation approach, and implementation aspects, as well as its real-world performance. Specifically, we provide the following contributions:

(i) We detail how the **theoretical results on provenance and probability can be applied to real-world systems** using the SQL data model, by using a generic representation of provenance and relying on a multiset semantics, and by evaluating the probability of Boolean provenance formulas to perform probabilistic query evaluation. We also discuss practical implementations of extension to the basic semiring model extended via the monus operator [27] and semimodules for aggregates [6].

(ii) We present **design choices in ProvSQL** for provenance and probability computation, such as rewriting SQL queries for provenance tracking, memory-mapped storage of provenance circuits, and knowledge compilation for probability computation.

(iii) To enable fair comparison with other systems and to quantitatively asses the performance of ProvSQL in real-world scenarios, we **propose publicly available benchmarks**, inspired from the TPC-H relational query benchmark, for both provenance and probabilistic query evaluation.

(iv) We **evaluate the performance of ProvSQL** on these benchmarks, both by itself (by measuring the provenance and probability overhead ProvSQL adds to PostgreSQL) and by comparing it to other systems that provide some of the features of ProvSQL. Specifically, we compare to GProM for provenance management and MayBMS for probabilistic query evaluation.

Our findings show that ProvSQL is able to handle provenance and probabilistic query evaluation at scale (on multi-gigabyte databases), with a reasonable overhead in most cases. Indeed, we find that in aggregate the overhead of provenance tracking is constant (around 2 to 3 times the cost of the query without provenance); variations exist for individual queries, suggesting potential for further optimization. In contrast with other similar systems, ProvSQL also captures a larger subset of SQL (notably including the full relational algebra with multiset semantics as well as aggregation), and readily allows for provenance computation in arbitrary semirings and extensions thereof. Thanks to the compact representation of provenance circuits, ProvSQL scales better than GProM for provenance tracking. When comparing probability computation, we find that MayBMS is competitive with ProvSQL *on those queries MayBMS support*; however, ProvSQL often performs similarly even though it does not use any query-based optimization as MayBMS does.

Section 2 reviews some of the most prominent systems for keeping track of the provenance of data and for managing probabilistic data. We provide the definition of the query language studied, an extension of the relational algebra with multiset semantics, in Section 3. In Section 4, we introduce annotated relations and how they are used for provenance tracking and probabilistic query evaluation. We then explain in Section 5 how these concepts are implemented in practice in ProvSQL. After illustrating in Section 6 how provenance is practically used in ProvSQL and some related systems, we present the result of our experimental evaluation in Section 7. The benchmark code is available at https://github.com/Aryak320/benchmark_suite.

2 RELATED SYSTEMS

Trio [3] was an early system for managing uncertain data, focusing on the representation on different forms of uncertainty, including probabilities. It does not support computation of arbitrary marginals, which is at the core of modern probabilistic databases. Though it adopts a mediator approach, it is tied to specific and obsolete versions of PostgreSQL (8.2 or 8.3).

Obsolescence is a common problem for systems of this era: the provenance tracking system Perm [28] and the probabilistic datbase system Orion [48] are respectively unmaintained forks of PostgreSQL 8.3 and 8.4; the distributed Orchestra system [30], which provides an early implementation of provenance semirings, cannot be compiled because some of its dependencies are on servers that have disappeared; MystiQ [10], implementing safe query plan evaluation, requires Java 5.0, which reached end-of-service in 2009.

MayBMS [33][1] is a probabilistic database system implementing the general and compact model of U-relations [7]. Its query evaluator, SPROUT [43] was designed for efficiency and is in particular able to exploit the structure of *safe* [20] queries. It was developed as a fork of PostgreSQL 8.3, which is unfortunately obsolete and hard to deploy. Some effort has been made in keeping the system compilable, however, though it requires using a virtual machine running an older operating system. It does not support provenance semirings. We use MayBMS in our experiments as a state-of-the-art system for probabilistic query evaluation.

GProM [8][2] serves as a middleware layer that adds provenance support to various database backends (in particular, Oracle and PostgreSQL). It translates declarative queries with provenance requirements into SQL code, which is subsequently executed by the backend database system. GProM supports the capture of provenance for SQL queries, as well as some Datalog queries. Some of its features that are not present in ProvSQL are support for transactions and PROV-JSON serialization [35]. On the other hand, in contrast with ProvSQL, it does not support probabilistic query evaluation, arbitrary semiring provenance, or provenance of aggregate or non-monotone queries. As it is modern, actively maintained, and feature-rich, we use it as a comparison point in Section 7.

ProbLog [26][3] is an actively maintained and easy-to-use probabilistic programming system, whose language is inspired from Prolog and Datalog. SQL queries and probabilistic databases can be encoded into ProbLog in a relatively straightforward way. Data for ProbLog programs can also be stored in a SQLite database and ProbLog uses knowledge compilation to compute probabilities of program outputs. However, our experiments showed it does not scale, as even though the data is stored in a database, it is loaded in main memory when needed by the query evaluator, and none of the usual query optimization infrastructure is used. Indeed, on the simplest query of our benchmark (query 1 of $\mathcal{Q}^{\text{cust}}$, see Section 7), ProbLog ran out-of-memory on the smallest database scale factor used in our experiments (1 GB). On a database 10 times smaller, it did not complete after 5 hours.

3 EXTENDED RELATIONAL ALGEBRA

We now present the query language underlying ProvSQL; it is an extension of the relational algebra with multiset (or *bag*) semantics, allowing for aggregation. We first give basic definitions and notation about multisets.

Definition 1. *A* multiset *m over a set V is a function $V \to \mathbb{N}^*$. It is is* finite *if it has finite domain. For $v \in V$, we note $v \in m$ if $m(v) > 0$ and $v \notin m$ otherwise. Given two multisets m_1 and m_2 over V, we define the* multiset union *of m_1 and m_2 as $m_1 \uplus m_2 : x \mapsto m_1(x) + m_2(x)$ and the* cross product *of m_1 and m_2 as the multiset over V^2 defined by $m_1 \times m_2 : (x_1, x_2) \mapsto m_1(x_1) \times m_2(x_2)$. Any set V can be seen as the multiset over V where $m(v) = 1$ for all $v \in V$.*

[1] https://maybms.sourceforge.net/

[2] https://github.com/IITDBGroup/gprom

[3] https://dtai.cs.kuleuven.be/problog/

A finite multiset with domain $\{a_1, \dots, a_n\}$ can be written in the form $\left\{\!\!\left\{ \underbrace{a_1, \dots, a_1}_{m(a_1)\text{ times}}, \dots, \underbrace{a_n, \dots, a_n}_{m(a_n)\text{ times}} \right\}\!\!\right\}$. *Finally, we also use the notation* $\{\!\{ f(x) \mid x \in m \}\!\}$ *or* $\biguplus_{x\in m} \{\!\{ f(x) \}\!\}$ *for a finite multiset m with domain $\{a_1, \dots, a_n\}$ and some function f over V to mean the multiset* $\left\{\!\!\left\{ \underbrace{f(a_1), \dots, f(a_1)}_{m(a_1)\text{ times}}, \dots, \underbrace{f(a_n), \dots, f(a_n)}_{m(a_n)\text{ times}} \right\}\!\!\right\}$.

We define an algebra for queries over relational databases under the multiset semantics which is as close as possible to a simple subset of SQL as dealt with by standard DBMSs. Our algebra is based on the relational algebra with set semantics typically used in database theory [2] but includes operators to explicitly control duplicate elimination as in [24, 32] and to express aggregation [39].

To simplify the presentation, we adopt an ordered, unnamed, and untyped perspective: attributes are referred to by their positions within the relation, do not have a name, and are assumed to be from a universal domain $\mathcal{V}$. In practical SQL implementations, attributes do have names and types, but it is straightforward to propagate them throughout query execution.

Let us fix a set $\mathcal{L}$ of relation labels and a set $\mathcal{V}$ of values. A database schema $\mathcal{D} : \mathcal{L} \to \mathbb{N}$ assigns arities to a *finite* set of relation labels. A *relation of arity* $k \in \mathbb{N}$ is a *finite multiset* of tuples over $\mathcal{V}^k$. An instance of a database schema $\mathcal{D}$, or a database over $\mathcal{D}$ for short, is a function mapping each relation name R in the domain of $\mathcal{D}$ to a relation of arity $\mathcal{D}(R)$.

A *positional index* is an expression of the form "$\#i$" for $i \in \mathbb{N}^*$. A *term* is any expression involving positional indices and values from $\mathcal{V}$, combined using arbitrary operators and functions over values in $\mathcal{V}$. The *max-index* of a term is the maximum of all i such that "$\#i$" appears in the term (or 0 if none appear). Given a tuple $u = (u_1, \dots, u_k)$ and a term t of max-index $\leqslant k$, we define $t(u)$ as the value of $\mathcal{V}$ obtained by replacing in t every positional index $\#i$ with u_i and evaluating the whole expression.

Given a database schema $\mathcal{D}$, we recursively define the language RA_k of relational algebra queries of arity $k \in \mathbb{N}$ as follows:

relation for any relation label R in the domain of $\mathcal{D}$, $R \in \mathsf{RA}_{\mathcal{D}(R)}$;
projection for $k \in \mathbb{N}$, $q \in \mathsf{RA}_k$, $t_1, \dots, t_n$ terms of max-index $\leqslant k$, $\Pi_{t_1,\dots,t_n}(q) \in \mathsf{RA}_n$;
selection for $k \in \mathbb{N}$, $q \in \mathsf{RA}_k$, and φ a Boolean combination of (in)equality comparisons between terms of max-index $\leqslant k$, $\sigma_\varphi(q) \in \mathsf{RA}_k$;
cross product for $k_1, k_2 \in \mathbb{N}$, $q_1 \in \mathsf{RA}_{k_1}$, $q_2 \in \mathsf{RA}_{k_2}$, $q_1 \times q_2 \in \mathsf{RA}_{k_1+k_2}$;
multiset sum for $k \in \mathbb{N}$, $q_1, q_2 \in \mathsf{RA}_k$, $q_1 \uplus q_2 \in \mathsf{RA}_k$;
duplicate elimination for $k \in \mathbb{N}$, $q \in \mathsf{RA}_k$, $\varepsilon(q) \in \mathsf{RA}_k$;
multiset difference for $k \in \mathbb{N}$, $q_1, q_2 \in \mathsf{RA}_k$, $q_1 - q_2 \in \mathsf{RA}_k$;
aggregation for $k \in \mathbb{N}$, $q \in \mathsf{RA}_k$, distinct $(i_j)_{1\leqslant j\leqslant k}$, terms $t_1, \dots t_n$ of max-index $\leqslant k$, functions $f_1, \dots, f_n$ from finite multisets of values to values, $\gamma_{i_1,\dots,i_m}[t_1 : f_1, \dots, t_n : f_n](q) \in \mathsf{RA}_{m+n}$.

Some other operators can be seen as syntactic sugar:

join $q_1 \bowtie_\varphi q_2 \stackrel{\text{def}}{=} \sigma_\varphi(q_1 \times q_2)$;
set union $q_1 \cup q_2 \stackrel{\text{def}}{=} \varepsilon(q_1 \uplus q_2)$;

We now define the semantics $[\![\cdot]\!]^I$ of relational algebra queries on an instance I over $\mathcal{D}$ by induction:

relation for any relation label R in the domain of $\mathcal{D}$, $[\![R]\!]^I \stackrel{\text{def}}{=} I(R)$;
projection for $k \in \mathbb{N}$, $q \in \mathsf{RA}_k$, $t_1, \dots, t_n$ terms of max-index $\leqslant k$, $[\![\Pi_{t_1,\dots,t_n}(q)]\!]^I \stackrel{\text{def}}{=} \left\{\!\!\left\{ (t_1(u), \dots, t_n(u)) \mid u \in [\![q]\!]^I \right\}\!\!\right\}$;
selection for $k \in \mathbb{N}$, $q \in \mathsf{RA}_k$, and φ a Boolean combination of (in)equality comparisons between terms of max-index $\leqslant k$, $[\![\sigma_\varphi(q)]\!]^I \stackrel{\text{def}}{=} \left\{\!\!\left\{ u \mid u \in [\![q]\!]^I, \varphi(u) \right\}\!\!\right\}$;
cross product for $k_1, k_2 \in \mathbb{N}$, $q_1 \in \mathsf{RA}_{k_1}$, $q_2 \in \mathsf{RA}_{k_2}$, $[\![q_1 \times q_2]\!]^I \stackrel{\text{def}}{=} [\![q_1]\!]^I \times [\![q_2]\!]^I$;
multiset sum for $k \in \mathbb{N}$, $q_1, q_2 \in \mathsf{RA}_k$, $[\![q_1 \uplus q_2]\!]^I \stackrel{\text{def}}{=} [\![q_1]\!]^I \uplus [\![q_2]\!]^I$;
duplicate elimination for $k \in \mathbb{N}$, $q \in \mathsf{RA}_k$, $[\![\varepsilon(q)]\!]^I$ maps t to 1 if $[\![q]\!]^I(t) > 0$ and to 0 otherwise;
multiset difference for $k \in \mathbb{N}$, $q_1, q_2 \in \mathsf{RA}_k$, $[\![q_1 - q_2]\!]^I$ maps t to 0 if $[\![q_2]\!]^I(t) > 0$ and to $[\![q_1]\!]^I(t)$ otherwise;
aggregation for $k \in \mathbb{N}$, $q \in \mathsf{RA}_k$, distinct $(i_j)_{1\leqslant j\leqslant k}$, terms $t_1, \dots t_n$ of max-index $\leqslant k$, functions $f_1, \dots, f_n$ from finite multiset of values to values, $[\![\gamma_{i_1,\dots,i_m}[t_1 : f_1, \dots, t_n : f_n](q)]\!]^I$ is:

$$\Big\{ \Big(v_1, \dots, v_m, f_1 \Big(\Big\{\!\!\Big\{ t_1(u) \mid u \in [\![q]\!]^I, (u_{i_1}, \dots, u_{i_m}) = (v_1, \dots, v_m) \Big\}\!\!\Big\} \Big), \dots, f_n \Big(\Big\{\!\!\Big\{ t_n(u) \mid u \in [\![q]\!]^I, (u_{i_1}, \dots, u_{i_m}) = (v_1, \dots, v_m) \Big\}\!\!\Big\} \Big) \Big) \Big| (v_1, \dots, v_m) \in [\![\varepsilon(\Pi_{\#i_1,\dots,\#i_m}(q))]\!]^I \Big\}.$$

Note that the definition of the multiset difference is not the usual one, and also not the one corresponding to the `EXCEPT ALL` operator of SQL, though it does correspond to the important `NOT IN` operator of SQL. This is mainly for practicality: the standard definition of multiset difference where $[\![q_1 - q_2]\!]^I(t) = \max(0, [\![q_1]\!]^I(t) - [\![q_2]\!]^I(t))$ leads to intractability of the provenance computation. The difference disappears in the set semantics: the semantics of $\varepsilon(q_1 - q_2)$ matches with that of `EXCEPT`.

Importantly, we assume that the aggregation operator, if it is used, is applied last (at the top-level operator), similarly to what is done in Section 3 of [6]; nested aggregation queries, discussed in Section 4 of [6], are out-of-scope of this work.

Example 2. *Consider the instance I of the relation Personnel given in Table 1, containing names of people, their position and their city (remember attribute names are not part of the model, they are just given here for ease of reading). Ignoring for now the t_i's, the relation has arity 4.*

Consider the following query: "What are the cities where at least two persons are working?". *This can be expressed (without using aggregation) as:*

$$q_{\text{city}} \stackrel{\text{def}}{=} \varepsilon\left(\Pi_{\#4}\left(\textit{Personnel} \bowtie_{\#4=\#8 \wedge \#1<\#5} \textit{Personnel}\right)\right).$$

Note the need for the duplicate elimination ε due to the multiset semantics. Then $[\![q_{\text{city}}]\!]^I = \{\!\{ (\text{New York}), (\text{Paris}), (\text{Berlin}) \}\!\}$.

4 QUERYING ANNOTATED RELATIONS

Now that our query language is fixed, we introduce the notion of annotated relations (Section 4.1) and the semantics of queries over such annotated relations in Section 4.2. This is based on annotated relations defined for provenance semirings as in [29], but with two key differences: we go beyond semirings for annotation,

Table 1: The *Personnel* relation (from [46])

id	name	position	city	
1	John	Director	New York	t_1
2	Paul	Janitor	New York	t_2
3	Dave	Analyst	Paris	t_3
4	Ellen	Field agent	Berlin	t_4
5	Magdalen	Double agent	Paris	t_5
6	Nancy	HR	Paris	t_6
7	Susan	Analyst	Berlin	t_7

namely using the m-semirings from [27] and the δ-semirings of [6], and, as in SQL, relations are multisets and not sets. We then show in Section 4.3 how the semantics of provenance over annotated relations can be captured by query rewriting. Finally, we define probabilistic query evaluation and show how it can be performed in an intensional way relying on provenance (Section 4.4).

4.1 Semirings and Beyond

Given some algebraic structure $\mathbb{K}$ for *annotations* (typically, a semiring or a generalization thereof) and some set $\mathcal{V}_\mathbb{K} \supseteq \mathcal{V}$ of *values* (typically, either $\mathcal{V}$ itself or an extension of $\mathcal{V}$ including $\mathbb{K}$-semimodules), a $\mathbb{K}$-*relation of arity* $k \in \mathbb{N}$ over $\mathcal{V}_\mathbb{K}$ is a *multiset* of tuples over $(\mathcal{V}_\mathbb{K})^k \times \mathbb{K}$, often written (u, α) with $u \in (\mathcal{V}_\mathbb{K})^k$ and $\alpha \in \mathbb{K}$. A $\mathbb{K}$-instance of a database schema $\mathcal{D}$, or $\mathbb{K}$-database over $\mathcal{D}$ for short, is a function mapping each relation name R in the domain of $\mathcal{D}$ to a $\mathbb{K}$-relation of arity $\mathcal{D}(R)$. Such $\mathbb{K}$-instances are typically denoted $\hat{I}$, and when we use such a notation I then means the relation projected on the first k columns, without the annotation.

We define in particular:

Definition 3. *A* semiring $(\mathbb{K}, \oplus, \otimes, \mathbb{0}, \mathbb{1})$ *is a set* $\mathbb{K}$ *of elements along with two binary operators over* $\mathbb{K}$ *(*$\oplus$ *and* $\otimes$*) and two distinguished elements of* $\mathbb{K}$ *(*$\mathbb{0}$ *and* $\mathbb{1}$*), such that:*
- *(i)* $(\mathbb{K}, \oplus, \mathbb{0})$ *is a commutative monoid;*
- *(ii)* $(\mathbb{K}, \otimes, \mathbb{1})$ *is a (non-necessarily commutative) monoid;*
- *(iii)* $\otimes$ *distributes over* $\oplus$*:* $\forall a, b, c \in \mathbb{K}$, $a \otimes (b \oplus c) = (a \otimes b) \oplus (a \otimes c)$ *and* $(a \oplus b) \otimes c = (a \otimes c) \oplus (b \otimes c)$*;*
- *(iv)* $\mathbb{0}$ *is annihilator for* $\otimes$*:* $\forall a\ \mathbb{0} \otimes a = a \otimes \mathbb{0} = \mathbb{0}$.

Example 4. *The following structures are semirings:*

Counting semiring $(\mathbb{N}, +, \times, 0, 1)$

Boolean function semiring *for a finite set X,* $(\mathcal{B}[X], \hat{\vee}, \hat{\wedge}, \hat{\bot}, \hat{\top})$ *where* $\mathcal{B}[X]$ *is the set of functions mapping valuations over X (i.e., functions from X to* $\{\bot, \top\}$*) to either* $\bot$ *(false) or* $\top$ *(true),* $f \hat{\vee} g$ *(resp.,* $f \hat{\wedge} g$*) is the function that maps a valuation* v *to* $f(v) \vee g(v)$ *(resp.,* $f(v) \wedge g(v)$*), and* $\hat{\bot}$ *(resp.,* $\hat{\top}$*) is the constant function returning always* $\bot$ *(resp.,* $\top$*)*

Why-provenance [13] *for a finite set X,* $(2^{2^X}, \varnothing, \{emptyset\}, \cup, \Cup)$ *where* $\Cup$ *is defined by* $A \Cup B \overset{\text{def}}{=} \{a \cup b \mid a \in A, b \in B\}$

Definition 5. *A* semiring with monus $\mathbb{K}$*, or* m-semiring *is a semiring along with an extra binary operation* $\ominus$ *such that for all* $a, b, c \in \mathbb{K}$*: (i)* $a \oplus (b \ominus a) = b \oplus (a \ominus b)$*; (ii)* $(a \ominus b) \ominus c = a \ominus (b \oplus c)$*; (iii)* $a \ominus a = \mathbb{0} \ominus a = \mathbb{0}$.

The semirings from Example 4 can be extended with a monus operator to form an m-semiring: this was noted in [27] for $\mathbb{N}$ (where $\ominus$ is the truncated difference ($a \ominus b \overset{\text{def}}{=} \max(a - b, 0)$) and in $\mathcal{B}[X]$ (where it is $(a, b) \mapsto a \wedge \neg b$). For Why-provenance:

Proposition 6. *For a set X,* $(2^{2^X}, \varnothing, \{\varnothing\}, \cup, \Cup, \setminus)$ *is an m-semiring.*

For computing the provenance of aggregate queries, [6] introduces an extra operator: a δ-*semiring* is a semiring along with a unary operation δ such that: (i) $\delta(\mathbb{0}) = \mathbb{0}$; (ii) $\delta(\mathbb{1} \oplus \cdots \oplus \mathbb{1}) = \mathbb{1}$ whatever the number of $\mathbb{1}$s as input to δ. For a discussion on choosing such a δ function, see [6]. A simple choice we will use for all semirings is the function that maps $\mathbb{0}$ to $\mathbb{0}$ and anything else to $\mathbb{1}$.

Finally, also to capture the provenance of aggregate queries, we will need to restrict which aggregate functions can be used:

Definition 7. *A* monoid aggregate function f *over values in a set V is a monoid homomorphism from the monoid of finite multisets of values of V (with multiset union as monoid operation) to some monoid over V. In other words,* $f : (V \to \mathbb{N}^*) \to V$ *is a monoid aggregate function if there exists a monoid* $(V, \cdot, e)$ *such that* $f(\{\!\{\ \}\!\}) = e$ *and* $f(S \uplus T) = f(S) \cdot f(T)$.

Example 8. *The function* count*, that turns a multiset m into the sum of all* $m(v)$ *for* v *in the domain of* m *is a monoid aggregate function from multisets of arbitrary values to* $(\mathbb{N}, +)$*. Similarly,* sum *is a monoid aggregate function from multisets over, say,* $\mathbb{Q}$ *to* $(\mathbb{Q}, +)$*, and* min *from multisets over* $\mathbb{Q}$ *to* $(\mathbb{Q}, \min)$.

4.2 Algebra over Annotated Relations

We define the semantics $\langle\!\langle \cdot \rangle\!\rangle^{\hat{I}}$ of extended relational algebra queries on a $\mathbb{K}$-instance $\hat{I}$ over $\mathcal{D}$ by induction; for the definition to be meaningful, $\mathbb{K}$ needs to be a semiring; a m-semiring for the multiset difference operator; and a δ-semiring for the aggregation operator. (We say that $\mathbb{K}$ is *appropriate* for q if this is the case.)

relation for any relation label R in the domain of $\mathcal{D}$, $\langle\!\langle R \rangle\!\rangle^{\hat{I}} \overset{\text{def}}{=} \hat{I}(R)$;

projection for $k \in \mathbb{N}$, $q \in \mathrm{RA}_k$, $t_1, \ldots, t_n$ of terms of max-index $\leqslant k$,
$$\langle\!\langle \Pi_{t_1,\ldots,t_n}(q) \rangle\!\rangle^{\hat{I}} \overset{\text{def}}{=} \left\{\!\!\left\{ (t_1(u), \ldots, t_n(u), \alpha) \mid (u, \alpha) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}} \right\}\!\!\right\};$$

selection for $k \in \mathbb{N}$, $q \in \mathrm{RA}_k$, and φ a Boolean combination of (in)equality comparisons between terms of max-index $\leqslant k$,
$$\langle\!\langle \sigma_\varphi(q) \rangle\!\rangle^{\hat{I}} \overset{\text{def}}{=} \left\{\!\!\left\{ (u, \alpha) \mid (u, \alpha) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}}, \varphi(u) \right\}\!\!\right\};$$

cross product for $k_1, k_2 \in \mathbb{N}$, $q_1 \in \mathrm{RA}_{k_1}$, $q_2 \in \mathrm{RA}_{k_2}$, $\langle\!\langle q_1 \times q_2 \rangle\!\rangle^{\hat{I}} \overset{\text{def}}{=}$
$$\left\{\!\!\left\{ (u, v, \alpha_1 \otimes \alpha_2) \mid (u, \alpha_1, v, \alpha_2) \in \langle\!\langle q_1 \rangle\!\rangle^{\hat{I}} \times \langle\!\langle q_2 \rangle\!\rangle^{\hat{I}} \right\}\!\!\right\};$$

multiset sum for $k \in \mathbb{N}$, $q_1, q_2 \in \mathrm{RA}_k$, $\langle\!\langle q_1 \uplus q_2 \rangle\!\rangle^{\hat{I}} \overset{\text{def}}{=} \langle\!\langle q_1 \rangle\!\rangle^{\hat{I}} \uplus \langle\!\langle q_2 \rangle\!\rangle^{\hat{I}}$;

duplicate elimination for $k \in \mathbb{N}$, $q \in \mathrm{RA}_k$,
$$\langle\!\langle \varepsilon(q) \rangle\!\rangle^{\hat{I}} \overset{\text{def}}{=} \bigcup_{u \mid \exists \alpha (u,\alpha) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}}} \left\{ \left(u, \bigoplus_{\alpha \mid (u,\alpha) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}}} \alpha \right) \right\};$$

multiset difference for $k \in \mathbb{N}$, $q_1, q_2 \in \mathrm{RA}_k$,
$$\langle\!\langle q_1 - q_2 \rangle\!\rangle^{\hat{I}} \overset{\text{def}}{=} \left\{\!\!\left\{ \left(u, \alpha \ominus \bigoplus_{\beta \mid (u,\beta) \in \langle\!\langle q_2 \rangle\!\rangle^{\hat{I}}} \beta \right) \middle| (u, \alpha) \in \langle\!\langle q_1 \rangle\!\rangle^{\hat{I}} \right\}\!\!\right\};$$

aggregation for $k \in \mathbb{N}$, $q \in \mathrm{RA}_k$, distinct $(i_j)_{1 \leqslant j \leqslant k}$, terms $t_1, \ldots t_n$ of max-index $\leqslant k$, monoid aggregate functions $f_1, \ldots, f_n$,
$$\langle\!\langle \gamma_{i_1,\ldots,i_m}[t_1 : f_1, \ldots, t_n : f_n](q) \rangle\!\rangle^{\hat{I}} \overset{\text{def}}{=}$$
$$\Big\{ (v_1,\ldots,v_m, \hat{f_1}\Big(\left\{\!\!\left\{ t_1(u) * \alpha \mid (u,\alpha) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}}, (u_{i_1},\ldots,u_{i_m}) = (v_1,\ldots,v_m) \right\}\!\!\right\} \Big),$$

$\ldots,\hat{f}_n\Big(\Big\{\!\!\Big\{ t_n(u)*\alpha \,\Big|\, (u,\alpha)\in\langle\!\langle q\rangle\!\rangle^{\hat{I}}, (u_{i_1},\ldots,u_{i_m})=(v_1,\ldots,v_m) \Big\}\!\!\Big\}\Big),$
$\delta(\beta))\,\Big|\,(v_1,\ldots,v_m,\beta)\in\langle\!\langle \varepsilon(\Pi_{\#i_1,\ldots,\#i_m}(q))\rangle\!\rangle^{\hat{I}}\Big\}$ where:

- "$*$" denotes a tensor product used to combine the data values of $\mathcal{V}$ with the δ-semiring annotations from $\mathbb{K}$ in a semimodule $\mathcal{V}_{\mathbb{K}}$;
- for any f_i, $\hat{f}_i$ is a new aggregate function lifted from values in $\mathcal{V}$ to values in $\mathcal{V}_{\mathbb{K}}$

See [6] for details about provenance semimodules.

Example 9. *We return to Example 2 and to the instance of the Personnel table of Table 1. The t_i's are now interpreted as tuple annotations in some semiring $\mathbb{K}$, resulting in a $\mathbb{K}$-relation $\hat{I}$. Following the semantics of q_{city} over annotated relations, we compute $\langle\!\langle q_{\text{city}}\rangle\!\rangle^{\hat{I}}$ as:*

New York	$t_1 \otimes t_2$
Paris	$(t_3 \otimes t_5) \oplus (t_5 \otimes t_6) \oplus (t_3 \otimes t_6)$
Berlin	$t_4 \otimes t_7$

If we choose for $\mathbb{K}$ the semiring $\mathcal{B}[X]$ where $X = \{ t_1, \ldots, t_7 \}$, the annotation for Paris *is the Boolean function given by the formula $(t_3 \wedge t_5) \vee (t_5 \wedge t_6) \vee (t_3 \wedge t_6)$. This is a form of* Boolean provenance *[46]:* Paris *is in the result iff either both tuples representing* Dave *and* Magdalen*, or* Magdalen *and* Nancy*, or* Dave *and* Nancy*, are present.*

4.3 Query Rewriting

The key way ProvSQL implements the semantics of the extended algebra over annotated relations is by *rewriting the query* over annotated relations to include in the query the necessary operations on provenance operations. The query can then be evaluated using the standard query evaluator of PostgreSQL. We employ the following 5 rewriting rules, which are applied inductively on an extended relational algebra formula:

(R1) for $k \in \mathbb{N}$, $q \in \mathsf{RA}_k$, $t_1, \ldots, t_n$ terms of max-index $\leqslant k$, $\Pi_{t_1,\ldots,t_n}(q)$ is rewitten to $\Pi_{t_1,\ldots,t_n,\#(k+1)}(q)$

(R2) For $k_1, k_2 \in \mathbb{N}$, $q_1 \in \mathsf{RA}_{k_1}$, $q_2 \in \mathsf{RA}_{k_2}$, $q_1 \times q_2$ is rewritten to: $\Pi_{\#1,\ldots,\#k_1,\#(k_1+2),\ldots,\#(k_1+k_2+1),\#(k_1+1)\otimes\#(k_1+k_2+2)}(q_1 \times q_2)$.

(R3) For $k \in \mathbb{N}$, $q \in \mathsf{RA}_k$, $\varepsilon(q)$ is rewritten to: $\gamma_{1,\ldots,k}[\#(k+1) : \bigoplus](q)$.

(R4) For $k \in \mathbb{N}$, $q_1, q_2 \in \mathsf{RA}_k$, $q_1 - q_2$ is rewritten to:

$$\Pi_{\#1,\ldots,\#(k+1)}\left(q_1 \bowtie_{\#1=\#(k+1)\wedge\cdots\wedge\#k=\#(2k)} \varepsilon(\Pi_{\#1,\ldots,\#k}(q_1) - \Pi_{\#1,\ldots,\#k}(q_2))\right)$$
$$\uplus\Pi_{\#1,\ldots,\#k,\#(k+1)\ominus\#(2k+2)}\left(q_1 \bowtie_{\#1=\#(k+2)\wedge\cdots\wedge\#k=\#(2k+1)} \gamma_{\#1,\ldots,\#k}[\#(k+1):\bigoplus](q_2)\right)$$

(R5) For $k \in \mathbb{N}$, $q \in \mathsf{RA}_k$, distinct $(i_j)_{1\leqslant j\leqslant k}$, terms $t_1, \ldots, t_n$ of max-index $\leqslant k$, monoid aggregate functions $f_1, \ldots, f_n$, $\gamma_{i_1,\ldots,i_m}[t_1 : f_1, \ldots, t_n : f_n](q)$ is rewritten to: $\gamma_{i_1,\ldots,i_m}[t_1{*}\#(k+1) : \hat{f}_1, \ldots, t_n{*}\#(k+1) : \hat{f}_n, \#(k+1) : \delta(\bigoplus)](q)$.

Note that relation names, selection, and multiset sum operators are not rewritten. We show that these rewriting rules allow us to recover the exact semantics of the extended relational algebra over annotated relations:

Theorem 10. *Let $\mathcal{D}$ be a database schema, q any extended relational algebra query over $\mathcal{D}$, $\mathbb{K}$ an appropriate algebraic structure, and $\hat{I}$ a $\mathbb{K}$-instance over $\mathcal{D}$. Let $\hat{q}$ be the query rewritten from q by applying the rewriting rules (R1)–(R5) recursively bottom up. Then $\langle\!\langle q\rangle\!\rangle^{\hat{I}} = [\![\hat{q}]\!]^{\hat{I}}$.*

Example 11. *Returning to query q_{city} from Example 2, let us trace the rewriting rules applied by ProvSQL bottom up (for space reasons, Personnel is abbreviated to P):*

$$\begin{aligned}
q_{\text{city}} &= \varepsilon(\Pi_{\#4}(P \bowtie_{\#4=\#8\wedge\#1<\#5} P))\\
&= \varepsilon(\Pi_{\#4}(\sigma_{\#4=\#8\wedge\#1<\#5}(P \times P)))\\
&\xrightarrow{(R2)} \varepsilon(\Pi_{\#4}(\sigma_{\#4=\#8\wedge\#1<\#5}(\Pi_{\#1,\ldots,\#4,\#6,\ldots\#9,\#5\otimes\#10}(P \times P))))\\
&\xrightarrow{(R1)} \varepsilon(\Pi_{\#4,\#9}(\sigma_{\#4=\#8\wedge\#1<\#5}(\Pi_{\#1,\ldots,\#4,\#6,\ldots\#9,\#5\otimes\#10}(P \times P))))\\
&\xrightarrow{(R3)} \gamma_1[\#2 : \textstyle\bigoplus](\\
&\qquad \Pi_{\#4,\#9}(\sigma_{\#4=\#8\wedge\#1<\#5}(\Pi_{\#1,\ldots,\#4,\#6,\ldots\#9,\#5\otimes\#10}(P \times P))))
\end{aligned}$$

If $\hat{q}_{\text{city}}$ is this rewritten query, one can check that $[\![\hat{q}_{\text{city}}]\!]^{\hat{I}} = \langle\!\langle q_{\text{city}}\rangle\!\rangle^{\hat{I}}$.

4.4 Probabilistic Query Evaluation

Annotated relations can be used for probabilistic query evaluation using the so-called intensional approach [49]. First, assume a finite set X of variables, each variable $x \in X$ being assigned a probability $\Pr(x)$. Pr can be extended to a probability distribution over valuations over X, assuming independence of variables: $\Pr(\nu) = \prod_{x\,|\,\nu(x)=\top} \nu(x) \times \prod_{x\,|\,\nu(x)=\bot}(1 - \nu(x))$. This in turns extends to a probability distribution over Boolean functions: if $f \in \mathcal{B}[X]$ is a Boolean function over variables in X, then $\Pr(f) = \sum_{\nu\,|\,f(\nu)=\top} \Pr(\nu)$.

Consider a $\mathcal{B}[X]$-relation $\hat{I}$ of arity k. For any subinstance $\hat{J}$ of $\hat{I}$, the characteristic Boolean function of $\hat{J}$ within $\hat{I}$ is: $\Phi_{\hat{I}}(\hat{J}) \overset{\text{def}}{=} \bigwedge_{(u,\alpha)\in\hat{J}} \alpha \wedge \bigwedge_{(u,\alpha)\in\hat{I},(u,\alpha)\notin J} \neg\alpha$. The probability of $\hat{J}$ is then $\Pr(\Phi_{\hat{I}}(\hat{J}))$. For a query q over $\hat{I}$ in RA_k, we define the marginal probability that a tuple t of arity k appears in the output of q as $\Pr(t \in q(\hat{I})) \overset{\text{def}}{=} \sum_{\hat{J}\subseteq\hat{I}, t\in[\![q]\!]^J} \Pr(\hat{J})$.

Our semantics for extended relational algebra over $\mathbb{K}$-relations is compatible with probabilistic query evaluation:

Theorem 12. *For any finite set of variables X, probability distribution* Pr *over X, $\mathcal{B}[X]$-relation $\hat{I}$ and relational algebra query q without aggregation, for any tuple t with same arity as q, $\Pr(t \in q(\hat{I})) = \Pr\left(\bigvee_{(t,\alpha)\in\langle\!\langle q\rangle\!\rangle^{\hat{I}}} \alpha\right)$.*

The reason why this theorem is about queries without aggregation is that the result of aggregate queries are tuples whose values include annotations; for a similar result, we would need to talk about the distribution of data values, or some summary thereof (such as the expected value). This is out of scope of this work.

Combining Theorems 10 and 12, we obtain:

Corollary 13. *For any finite set of variables X, probability distribution* Pr *over X, $\mathcal{B}[X]$-relation $\hat{I}$ and relational algebra query q without aggregation, for any tuple t with same arity as q, if $\hat{q}$ is the query rewritten from q by applying the rewritten rules (R1)–(R5) then $\Pr(t \in q(\hat{I})) = \Pr\left(\bigvee_{(t,\alpha)\in[\![\hat{q}]\!]^{\hat{I}}} \alpha\right)$.*

Example 14. *Returning again to Examples 2 and 9, assume we independently assign to each t_i in our Personnel $\mathcal{B}[\{t_1, \ldots, t_7\}]$-instance a probability $\Pr(t_i)$ as follows:*

	t_1	t_2	t_3	t_4	t_5	t_6	t_7
$\Pr(t_i)$	0.5	0.7	0.3	0.2	1.0	0.8	0.2

We can then compute the probability of q_{city} results as:

$$\begin{aligned}
\text{New York:}\quad & \Pr(t_1 \wedge t_2) = 0.5 \cdot 0.7 = 0.35\\
\text{Paris:}\quad & \Pr\left((t_3 \wedge t_5) \vee (t_5 \wedge t_6) \vee (t_3 \wedge t_6)\right)\\
& \quad = \Pr(t_3 \vee t_6 \vee (t_3 \wedge t_6))\\
& \quad = \Pr(t_3 \vee t_6)\\
& \quad = 1 - (1 - 0.3) \cdot (1 - 0.8) = 0.86\\
\text{Berlin:}\quad & \Pr(t_4 \wedge t_7) = 0.2 \cdot 0.2 = 0.04
\end{aligned}$$

Note that, in this case, we used the fact that $\Pr(t_5) = 1$ to simplify the computation for Paris. *This is not applicable in general.*

5 IMPLEMENTATION IN PROVSQL

Theorem 10 and Corollary 13 pave the way for a practical implementation of provenance management and probabilistic query evaluation in a SQL DBMS. We now explain how this is done in ProvSQL. ProvSQL uses PostgreSQL's extension mechanism to change the behavior of the DBMS. We can provide user-defined functions (UDFs) to implement provenance- and probability-related functionalities; and we can also add *hooks* at different phases of query evaluation.

Annotated relations. As in Section 4.1, ProvSQL adds to every relation for which provenance needs to be tracked (which can be specified with a UDF) an extra *provsql* attribute to store the annotation. Instead of choosing a specific algebraic structure for the annotation ahead of time, this annotation is a generic *universally unique identifier (UUID)* [23]. We explain further on how these generic annotations can be specialized to specific (m)-semirings. Annotations of *base tuples* are randomly generated using the UUIDv4 standard and can be interpreted as abstract tuple identifiers; the 128-bit address space makes the collision probability vanishingly small. Annotations are built from these base annotations by using the (m-)semiring operations; to store resulting annotations in the same attribute, they are also UUIDs, this time computed following UUIDv5 by computing a SHA-1 hash formed from a fixed namespace, and a normalized description of the operator and its UUID operands. This guarantees, in particular, that annotations are generated in a deterministic manner: the same query over the same data will result in the exact same result, annotations included.

Retaining opaque UUIDs is not enough: one also needs to be able to efficiently determine how they relate to each other. This is done by storing a *provenance circuit* (a compact DAG representation of provenance expressions, first introduced in [25]) where each UUIDv4 points to a leaf gate representing inputs of the circuit and each UUIDv5 to an inner gate labeled by the operator and with children the operand UUIDs. Similarly, data values that are results of aggregate queries are represented as gates in the same circuit (with UUIDv5 representation) encoding their semimodule construction.

Storage of this provenance circuit in the DBMS is a challenge:

(i) It is an append-only data structure; except in cases where one wants to perform some clean-up, there is never the need of removing gates from the circuit, and a gate never needs to be updated.

(ii) It is a data structure which is updated at the time a query is evaluated, following the query rewriting approach of Section 4.3.

(iii) The content of this circuit needs to be stored in a persistent manner: UUIDs become uninterpretable without the circuit.

(iv) The circuit can become very large, as it contains one gate per tuple, and one gate per operation performed in a query.

(v) Access to the circuit needs to be as fast as possible.

Initial implementations of ProvSQL stored this circuit as an extra table within the database, which solved (iii)–(iv). But PostgreSQL tables are not optimized for append-only operations (i) and, most importantly, (ii) caused concurrency control issues. We then experimented with shared-memory storage of the circuit, which solved most issues but did not scale (iv) and made persistence (iii) an issue in case of failure. Our final implementation provides a satisfactory solution to (i)–(v): The circuit is stored outside of the database, in *append-only files* that are properly indexed and *memory-mapped* so that the operating system can keep most often used fragments in RAM buffers. To avoid concurrency issues, access to these files is managed by a *single PostgreSQL worker process*, communicating with other backends through inter-process communication (with *pipes*). Finally, each backend process has a *small local cache* of most recently accessed circuit information.

Query rewriting. ProvSQL's main behavior is the query rewriting discussed in Section 4.3. To implement this within PostgreSQL, ProvSQL defines a custom hook at *query planning time* before the query is sent to PostgreSQL's planner. If the query involves annotated relations (i.e., tables with the special *provsql* attribute), the query is analyzed to determine if it is part of the supported language (the extended relational algebra described in Section 3, as represented in SQL). If not, an error message is displayed instead of performing inadequate provenance computation. If so, the query is rewritten as described in Section 4.3 and then sent to the regular planner for continued processing and evaluation.

Specialization to specific (m-)semirings. Annotations computed by ProvSQL are abstract UUIDs, with description in the circuit on how these are computed from base tuple UUIDs. One important point is that representation can be specialized to any arbitrary (m-)semiring and semimodule by applying homomorphisms: ProvSQL essentially works in the *universal* semiring (the how-semiring of integer polynomials, see [29]) and in the *universal* m-semiring (the free m-semiring, see [27]), from which there exist unique homomorphisms to any application (m-)semiring. At a user's request, given a *provenance mapping* from base UUIDs to values in some specific (m-)semiring, and a description of the operations ($\oplus$, $\otimes$, possibly $\ominus$ and δ), ProvSQL evaluates the circuit in a bottom-up manner to determine the actual semiring annotation of every tuple in the result of a query. This is currently done by a recursive PL/pgSQL function applied to a circuit.

Probability evaluation. Probabilistic query evaluation in ProvSQL relies on Corollary 13: provenance is computed in the same way as for provenance tracking, using query rewriting, and when a marginal probability computation is requested, we specialize the provenance to $\mathcal{B}[X]$ (given a mapping of base UUIDs to some Boolean function, e.g., one distinct variable per UUIDs to obtain a tuple-independent database) and then compute the probability of

Table 2: Provenance derivation for GProM on q_{city}

city	prov_personnel_id	prov_personnel_name	prov_personnel_position	prov_personnel_city	prov_personnel_1_id	prov_personnel_1_name	prov_personnel_1_position	prov_personnel_1_city
New York	1	John	Director	New York	2	Paul	Janitor	New York
Paris	3	Dave	Analyst	Paris	6	Nancy	HR	Paris
Paris	3	Dave	Analyst	Paris	5	Magdalen	Double agent	Paris
Berlin	4	Ellen	Field agent	Berlin	7	Susan	Analyst	Berlin
Paris	5	Magdalen	Double agent	Paris	6	Nancy	HR	Paris

Table 3: Provenance derivation for ProvSQL on q_{city}

city	why	provsql
New York	{"{John,Paul}"}	d1b22232-…
Paris	{"{Dave,Magdalen}","{Magdalen,Nancy}","{Dave,Nancy}"}	d82a769d-…
Berlin	{"{Ellen,Susan}"}	1a407bcb-…

the corresponding Boolean circuit. Note that the computation of Boolean provenance, as it is crucial for probabilistic query evaluation, is optimized and performed directly on the memory-mapped circuit, without the need for a PL/pgSQL recursive function.

ProvSQL implements different ways of computing the probability of a Boolean circuit (e.g., naïve enumeration of possible worlds, Monte-Carlo sampling, or some other approximation techniques such as WeightMC [15]). We focus here on its default computation method, which works in three steps:

(1) We determine whether the Boolean circuit is read-once [45], i.e., if every variable occurs only once; if so, its probability can be computed in linear-time.

(2) Otherwise, we use a heuristic algorithm [40] to quickly obtain a tree-decomposition of small width ($\leqslant 10$) of the circuit, if possible; if so, we use an algorithm from [5] to extract a deterministic and decomposable circuit from the Boolean circuit, on which the probability is computed in linear time.

(3) Otherwise, we encode the circuit in conjunctive normal form using Tseitin's transformation [50] and use an external knowledge compiler (by default d4 [37] but we also support c2d [21] and DSHARP [42]) as a black box to compile it into a deterministic and decomposable circuit, on which the probability is computed in linear time (but this new circuit may be exponential in size).

Recall that probabilistic query evaluation is intractable (#P-hard): the potential exponential blow-up of the last step is unavoidable.

Other features. At the time of writing, ProvSQL also implements other features, which are outside of the scope of this paper: it supports Shapley value computation and expected Shapley value computation as described in [36]; provenance of update operations as proposed in [11]; expected value computation for `COUNT`, `MIN`, `MAX`, `SUM`, following the algorithms in [1]; and where-provenance [13], which is a form of provenance not captured by semirings [16] and was a focus of an early demonstration of ProvSQL [47].

6 PROVENANCE AND PROBABILITY IN DIFFERENT SYSTEMS

We explain the query interface for provenance computation in GProM and ProvSQL, and for probabilistic query evaluation in MayBMS and ProvSQL. This helps understanding how these systems represent provenance and uncertain information, and how to produce a benchmark adapted to each system.

We consider again from Example 2 the *Personnel* instance introduced in Table 1 and the query q_{city}, which can be written in SQL as follows:

```
SELECT DISTINCT p1.city
FROM personnel p1 JOIN personnel p2
ON p1.city=p2.city AND p1.id<p2.id
```

Provenance computation. To find the provenance of this query in GProM we need to use the `PROVENANCE OF` construct in the query statement:

```
PROVENANCE OF (SELECT DISTINCT p1.city
  FROM personnel p1 JOIN personnel p2
  ON p1.city=p2.city AND p1.id<p2.id)
```

For this query, GProM produces the provenance derivation in Table 2. GProM attaches multiple additional attributes to the output tuples of a query. In GProM's result, "Paris" appears three times: once due to Dave and Magdalen, once due to Magdalen and Nancy, and once due to Dave and Nancy. Each occurrence of Paris in GProM's output is accompanied by the provenance attributes of the two input tuples that caused it to appear. We see in particular that GProM disregards the `DISTINCT` keyword: the output of the query would be the same without it.

To find similar provenance information for the same query using ProvSQL, we first make the table provenance-aware by using the `add_provenance` UDF and then specialize the generic provenance token, using a provenance mapping *personnel_name* where each tuple is represented by the *name* attribute, to why-provenance:

```
SELECT p1.city, why(provenance(), 'personnel_name')
FROM personnel p1 JOIN personnel p2
ON p1.city=p2.city AND p1.id<p2.id
GROUP BY p1.city
```

Provenance evaluation is seen as a form of aggregation, which explains why we transformed `DISTINCT` into a `GROUP BY`. This results in a more compact representation, as shown in Table 3. ProvSQL computes the why-provenance for each output tuple as sets of sets. Of course, in ProvSQL, any (m-)semiring can be used for the computation, not just why-provenance: ProvSQL defines a number of common examples, and a user can add new UDFs defining the operations of the semiring of choice.

Probability computation. We now consider the TID relation introduced in Example 14.

To compute probabilities in MayBMS, the following steps have to be followed. We first use `PICK TUPLES` to create a new TID table with probabilities given by some SQL expression. In this new table, named *Personnel_prob*, MayBMS adds three extra attribute: an event variable *_v0*, a decision value *_d0* and a probability *_p0*, as shown in Table 4. In short, each unique event variable translate to a set of mutually exclusive events, independent across event variables; the decision value specifies the event, and the probability is that of the

Table 4: The *Personnel_prob* table in MayBMS

id	name	position	city	_v0	_d0	_p0
1	John	Director	New York	1008	1	0.5
2	Paul	Janitor	New York	1009	1	0.7
3	Dave	Analyst	Paris	10010	1	0.3
4	Ellen	Field agent	Berlin	10011	1	0.2
5	Magdalen	Double agent	Paris	10012	1	1.0
6	Nancy	HR	Paris	10013	1	0.8
7	Susan	Analyst	Berlin	10014	1	0.2

Table 5: Result of probability computation in ProvSQL (right) and MaybMS (left)

city	conf
New York	0.35
Paris	0.86
Berlin	0.04

city	prob	provsql
New York	0.35	d1b22232-…
Paris	0.86	d82a769d-…
Berlin	0.04	1a407bcb-…

event value. This is an encoding of the compact U-relation model for probabilistic databases [7], itself very similar to that of probabilistic c-tables [31]. MayBMS offers two functions for probabilistic qurery evaluation: `conf()` and `tconf()` for computing the exact probabilities (along with some functions for computing approximations). The difference between these two functions is that `conf()` computes a probability of distinct results (along with a **GROUP BY** clause), while `tconf()` performs no duplicate elimination. We can then use the following query:

```
SELECT city, conf() FROM (
  SELECT p1.city
  FROM personnel_prob p1, personnel_prob p2
  WHERE p1.city=p2.city AND p1.id<p2.id) temp
GROUP BY city
```

whose result in MayBMS is given in Table 5 (left), matching what we computed in Example 14. Note that MayBMS does not support the **JOIN** keyword for queries with self-join, so the query needs to be rewritten with a subquery as shown.

In ProvSQL, we first attach a probability on Boolean variables using the `set_prob()` UDF then, at query time, we use the a UDF to perform probabilistic query evaluation:

```
SELECT p1.city, probability_evaluate(provenance())
FROM personnel p1 JOIN personnel p2
ON p1.city=p2.city AND p1.id<p2.id
GROUP BY p1.city
```

The result is shown in Table 5 (right) – we notice the result is still a provenance-aware table, with its *provsql* attribute.

7 EXPERIMENTAL EVALUATION

We start this section by presenting how the benchmark was built and what SQL queries are included. We then evaluate the performance of ProvSQL for provenance and probability computation, and compare it to GProM [8] and MayBMS [33].

7.1 Building the Benchmark

A natural candidate for benchmarking queries in database systems is the TPC benchmark suite[4]. We started with the TPC-H 3.0.1 database generator and its associated suite of queries. TPC-H is a standard benchmark for decision support systems, and includes 22 query templates that are typical of this kind of application, including some with high computational cost. The TPC-H schema is formed of 8 tables, 6 of which increase proportionally to a provided *scale factor* (`lineitem`, `orders`, `part`, `supplier`, `customer`, and `partsupp`) and 2 which are fixed (`nation` and `region`). The scale factor allows to control the total size of the database. A scale factor of k results in a database of roughly k GB.

None of the systems tested currently support the functionalities present in all TPC-H queries. In particular none of them support subqueries in the **WHERE** clause, nested aggregations, or **ORDER BY** on the result of aggregate queries. Only 6 queries of TPC-H work as is in at least one tested system (as it happens, ProvSQL); this query set is denoted as $\mathcal{Q}^{\mathrm{TPC}}$. As provenance tracking and probability evaluation can sometimes have high overhead (see further), we further simplify queries in $\mathcal{Q}^{\mathrm{TPC}}$ with the single addition of a **LIMIT** 1 clause on the main query. This query set is unfortunately not suitable for GProM and MayBMS as all queries include aggregation operators, which these systems do not support.[5]

MayBMS and its query evaluator SPROUT [43] were also evaluated on modified TPC-H queries, and MayBMS includes a benchmark of 4 such queries, modified to remove unsupported operations[6]. We include them in a second part of our benchmark, denoted $\mathcal{Q}^{\mathrm{TPC}^*}$, along with query 3 of TPC-H modified to remove its aggregation operator (which GProM and MayBMS do not support) – the unmodified version is in $\mathcal{Q}^{\mathrm{TPC}}$.

$\mathcal{Q}^{\mathrm{TPC}}$ and $\mathcal{Q}^{\mathrm{TPC}^*}$ are not representative, in that they do not cover the full range of SQL features as implemented by provenance systems. We thus created an additional set $\mathcal{Q}^{\mathrm{cust}}$ of 18 custom queries chosen to represent a wide variety of simple but query patterns. We relied on the DSQGEN query generator from the TPC-DS benchmark for generation, but the queries are on the TPC-H schema as well. These 18 queries include different SQL features such as joins, **EXCEPT**, **UNION**. Table 6 shows an overview of the features of all queries.

Table 7 provides a summary of which queries are supported on every system for the lowest scale factor (1 GB): a "Y" means the query runs correctly, a "N" is an error due to unsupported operators, a "O" an out-of-memory error, and a "T" a timeout at 3 000 seconds. For ProvSQL, we distinguish between computation of provenance and probability evaluation. We observe that ProvSQL is able to process all three query sets; for probabilistic query evaluation, all but three run to completion, and neither of those work in MayBMS. Other than that, a number of queries supported by ProvSQL are either unsupported (aggregation, difference, union operators) or

[4]https://www.tpc.org/information/benchmarks5.asp

[5]MayBMS supports limited forms of summaries for probabilistic query evaluation of aggregate queries, with the `ecount()` and `esum()` functions but not standard SQL aggregates.

[6]https://maybms.sourceforge.net/manual/index.html

Table 6: Benchmark query features

	$\mathcal{Q}^{\text{TPC}}$						$\mathcal{Q}^{\text{TPC}^*}$					$\mathcal{Q}^{\text{cust}}$																	
Query	1	6	7	9	12	19	1	3	4	12	15	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
# tables joined	1	1	6	6	2	2	1	3	2	2	2	1	2	5	2	2	1	1	2	8	4	3	2	2	5	3	4	3	1
# aggregates	8	1	1	1	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
UNION	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✓
EXCEPT	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✓	✗	✗

Table 7: System comparison: supported queries on the TPC-H 1GB dataset
(Y – successful execution, O – out of memory, N – query not supported, T – timeout $> 3000s$**)**

	$\mathcal{Q}^{\text{TPC}}$						$\mathcal{Q}^{\text{TPC}^*}$					$\mathcal{Q}^{\text{cust}}$																	
Query	1	6	7	9	12	19	1	3	4	12	15	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
ProvSQL (prov.)	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
ProvSQL (prob.)	O	Y	O	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	O	Y	Y	Y	Y	Y	Y	Y	Y	Y
GProM	N	N	N	N	N	N	Y	Y	O	Y	Y	O	Y	Y	Y	O	O	Y	O	T	Y	Y	O	Y	Y	Y	N	Y	N
MayBMS	N	N	N	N	N	N	Y	Y	Y	Y	Y	Y	Y	Y	T	O	Y	Y	Y	O	Y	Y	Y	Y	Y	Y	N	Y	N

fail using MayBMS or GProM. GProM in particular is particularly sensitive to running out of memory.

7.2 Experimental Setup

Benchmarks were run on an i9 16-core consumer computer running Debian 12 with 64GB RAM. ProvSQL and GProM used PostgreSQL 16. As MayBMS cannot be deployed on modern systems, we had to run it under a virtual machine run on the same machine, provided with 50 GB RAM and 8 CPU cores; the VM ran Ubuntu 10.

We perform the benchmarks on TPC-H 3.0.1 dataset for scale factors 1 to 10, i.e., with databases of size 1 to 10 GB. For experiments involving probability computation we modify the deterministic TPC-H database into a tuple-independent probabilistic database by assigning a probability of 0.5 to every tuple of the relations involved (note that algorithms used for exact probabilistic query evaluation in ProvSQL nor MayBMS do not depend on the actual probability values of uncertain tuples, so another probability valuation would have given the same results).

Each experiments was run 10 times, with the database server restarted each time, to avoid fluctuations independent on the system's performance. Results presented are the average over these 10 runs.

7.3 Benchmarking ProvSQL

We start with evaluating the provenance tracking of ProvSQL on our benchmark queries, for three scenarios: (i) the overhead of adding provenance tracking, (ii) the scalability of different semiring instantiations, and (iii) the scalability of adding probability evaluation.

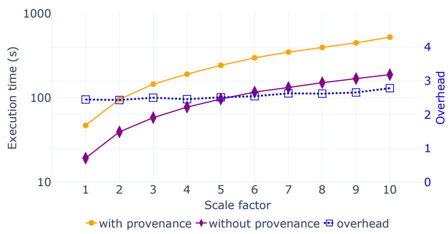
Scalability and provenance overhead. We compare running time of queries over PostgreSQL with running time under ProvSQL, with provenance tracking enabled, on TPC-H data of scale fators between 1 and 10. We are especially interested in the overhead ratio, computed as overhead $= \frac{t_{\text{provenance}}}{t_{\text{original}}}$. We run the experiment on the entire $\mathcal{Q}^{\text{cust}}$query set, and on individual queries from $\mathcal{Q}^{\text{TPC}}$. We show the results in Figure 1. Note that the blue curve corresponds to the overhead, on the right (linear) y-axis of each plot, while the other two curves use the left (logarithmic) y-axis.

On $\mathcal{Q}^{\text{cust}}$, Figure 1a shows that the overhead is constant with the dataset size, indicating that provenance tracking scales at a similar rate as regular query execution. This reflects the efficient implementation of provenance tracking by using provenance circuits, in ProvSQL.

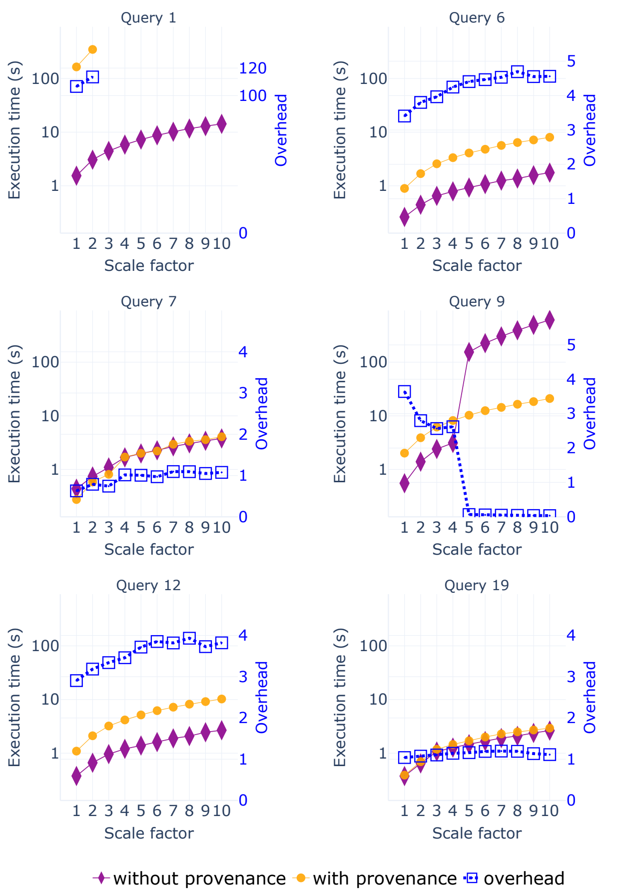
Results on $\mathcal{Q}^{\text{TPC}}$, Figure 1b, are of particular interest. Query 19 has a nearly constant overhead with little variation as the scale factor increases, characterizing efficient provenance tracking that scales independently of the database size.

For queries 7 and 9, we observe an anomalous *decrease* in computation time at certain scale factors due to PostgreSQL's query optimizer adopting different execution plans when provenance tracking is enabled, which happen to be better for that particular query. For instance on query 9, the execution time with provenance tracking is counter-intuitively lower than the baseline execution time, for scale factors 5 and above. In certain cases, provenance computation can accidentally lead to performance improvement by guiding the PostgreSQL optimizer to adopt a faster execution strategy. The size of the TPC-H dataset incrementally increases with each scale factor and can cause changes in join selectivity, indexing effectiveness and the optimizer's cost estimates. For example, in queries 7 and 9 which have complex joins, provenance tracking may force the optimizer to adopt a more efficient join order. Except for these optimizer-driven fluctuations, queries 7 and 9 have a constant overhead.

Queries 6 and 12 exhibit a high overhead that however remains under a factor of 4, indicating scalability challenges in comparison to other queries in this experiment. Query 6 does not involve any inner joins and operates exclusively on the largest table in the dataset, `lineitem`. The size of `lineitem` scales with the TPC-H scale factor and also contains attributes with skewed, uniform, and categorical distributions, making it a bottleneck for database optimizers in situations where provenance tracking involves queries with a high amount of filtering. For query 12, the high overhead

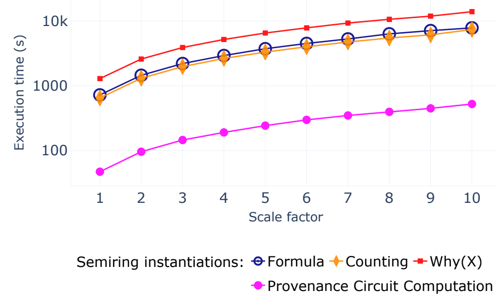


(a) On the entire $\mathcal{Q}^{\text{cust}}$ set.

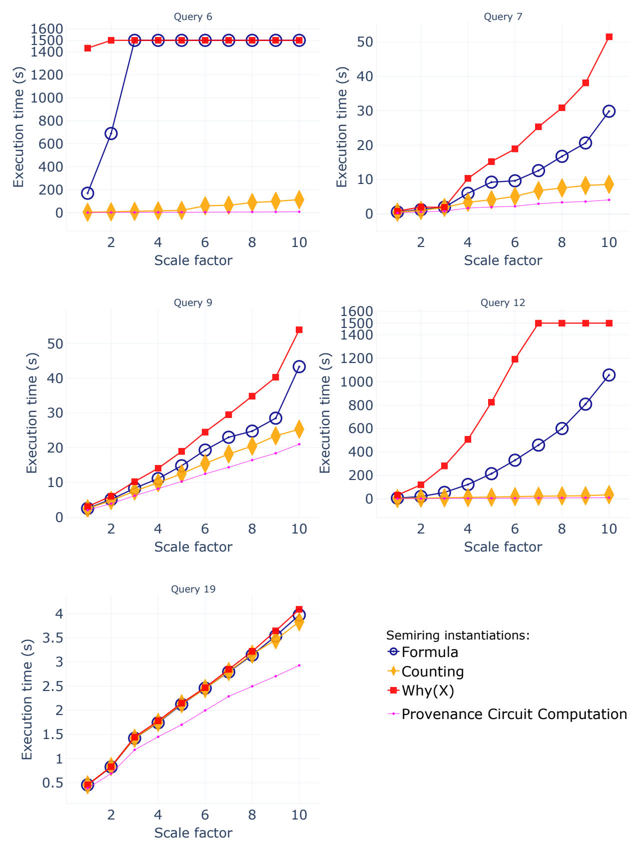


(b) On individual $\mathcal{Q}^{\text{TPC}}$ queries.

Figure 1: Scalability and provenance overhead: execution times (left y-axis, log-scale) and overhead (right y-axis, linear scale), at various scale factors (x-axis).



(a) On the entire $\mathcal{Q}^{\text{cust}}$ set (log scale)



(b) On individual $\mathcal{Q}^{\text{TPC}}$ queries (linear scale, execution times capped at 1 500 seconds).

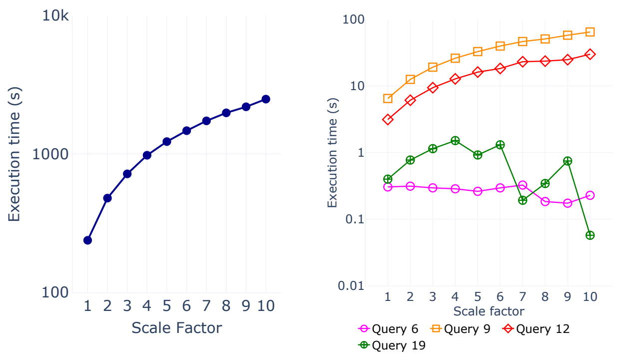
Figure 2: Scalability of different semiring instantiations in ProvSQL.

may be be because of the fact that it involves filtering conditions on tuples that it aggregates.

Finally, ProvSQL cannot scale beyond scale factor 2 for query 1 due to memory limitations; this query involves 8 aggregations on the `lineitem` table, leading to a considerable number of intermediate data structures when computing provenance annotations, thus limiting scalability and imposing unreasonable memory demands for higher scale factors.

This experiment provides us with an important insight: while computing provenance annotations generally adds overhead, it can sometime act as an implicit optimization guide in database systems.

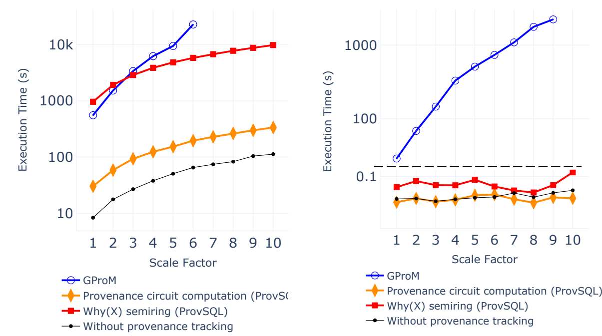
Semiring provenance evaluation. We evaluate in Figure 2 the overhead induced by evaluating the resulting provenance circuits on different semirings supported by ProvSQL (*counting*, *why-provenance*,



(a) On the entire $\mathcal{Q}^{\text{prob}}$ set (log scale)

(b) On individual $\mathcal{Q}^{\text{TPC}}$ queries (log scale)

Figure 3: Scalability of probability computation in ProvSQL



(a) On $\mathcal{Q}^{GProM}$ (log scale, execution times capped at 32 000 **seconds).**

(b) On query 3 from $\mathcal{Q}^{\text{TPC}^*}$ (log scale)

Figure 4: Scalability of GProM vs. ProvSQL

as well as a pseudo-semiring that just serializes in a *formula*-based representation the provenance circuit), on the TPC-H database across scale factors 1 to 10. On the queries in $\mathcal{Q}^{\text{cust}}$ (Figure 2a) we observe linear trends, with the semiring instantiations across TPC-H scale factors 1 to 10. Simple semirings, such as the formula and counting semiring introduce virtually the same overhead to provenance computation. In contrast why-provenance has a significantly higher overhead; this is due to the fact that this semiring operates on sets of sets and the corresponding $\oplus$ and $\otimes$ operators have costs that are linear in the number of tuples in the query. Nonetheless, the overheads observed are constant with the database size, as none of the queries in $\mathcal{Q}^{\text{cust}}$ have aggregates, allowing us to ignore the semantics of aggregation which would otherwise involve poly-sized overheads caused by the $K-$semimodule operations.

Figure 2b shows the overheads incurred for individual $\mathcal{Q}^{\text{TPC}}$ queries. We omit query 1 from $\mathcal{Q}^{\text{TPC}}$ in this experiment, as we just saw ProvSQL does not scale for query 1 even when we are only computing the provenance circuit. With execution time capped at 1 500 seconds for queries 6 and 12, it is clear that the overhead is not constant for both formula and why-provenance semirings. This is because both queries involve aggregates, joins and extensive filtering on tables including specifically the `lineitem` table. For queries 7 and 9, the performance is better, and for query 19 we observe minimal overheads.

Remember that specializations to specific semiring is currently performed by a recursive PL/pgSQL function on top of the provenance function, notoriously poorly optimized by PostgreSQL. Computation by the process directly in charge of managing the provenance circuit would considerably speed up the computation, but would make it more difficult to provide custom-defined semirings.

Probability evaluation. Query 9 in $\mathcal{Q}^{\text{cust}}$ has 8 joins and ProvSQL goes out of memory while computing probabilities for it (more precisely, the knowledge compiler d4 called by ProvSQL runs out of memory). We omit query 9 from $\mathcal{Q}^{\text{cust}}$ and denote this new query set as $\mathcal{Q}^{\text{prob}}$. Figure 3a shows that ProvSQL scales linearly with the dataset size, when computing probabilities on query set $\mathcal{Q}^{\text{prob}}$.

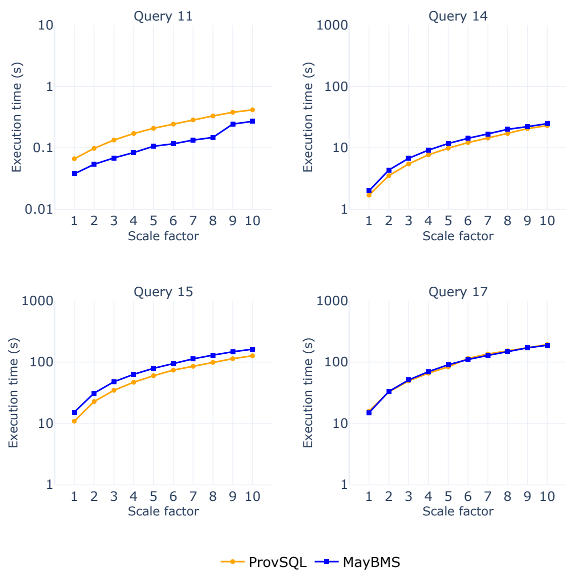
Figure 3b shows linear scalability trends typically across queries 6, 9, 12, 19 from $\mathcal{Q}^{\text{TPC}}$ with some optimizer driven fluctuations and erratic performance gains across certain scale factors for queries 6 and 19. For queries 1 and 7 ProvSQL goes out of memory when computing probabilities.

7.4 GProM vs ProvSQL for Provenance

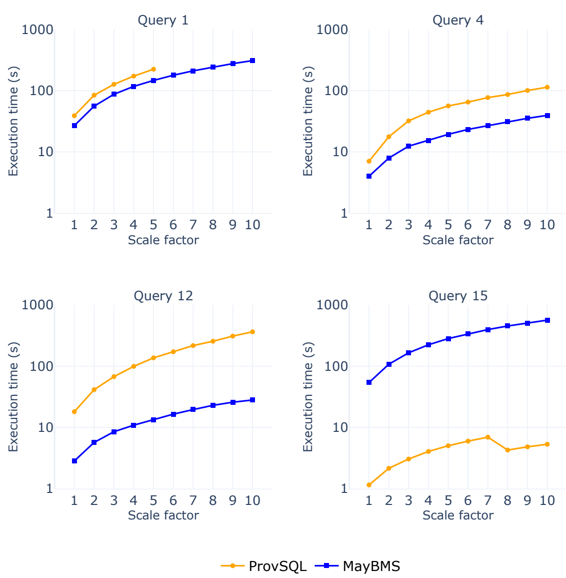
We compare the scalability of provenance tracking in GProM vs ProvSQL on $\mathcal{Q}^{\text{GProm}}$, consisting of all queries in $\mathcal{Q}^{\text{cust}}$ that GProM supports (see Table 7) in Figure 4a. We outline some scalability issues with GProM. For scale factors 8 and 9 GProM takes more than 32 000 seconds and for scale factor 10 it runs out of memory and crashes even before the timeout threshold. ProvSQL exhibits a significant overhead when it comes to provenance computation on the why-provenance semiring, but even then it scales linearly with TPC-H scale factors, unlike GProM which shows exponential growth in execution times.

We mirror this experiment for query 3 from $\mathcal{Q}^{\text{TPC}^*}$ as GProM does not support any of the original TPC-H queries. In Figure 4b (note the y-axis is cut in two parts for readability of both sets of plots), we see that GProM exhibits exponentially increasing execution times, indicating poor scalability. At scale factor 10, GProM crashes as it goes out of memory while running query 3.

GProM's provenance representation, as discussed in Section 6, may be the main reason for this scalability issue. The size of provenance expressions (represented by extra attributes) can considerably grow with the number of joins. While ProvSQL benefits from efficient provenance representations, GProM's explicit tuple-level provenance annotations, by means of appending duplicates of entire tuples with renamed schema features, results in poor scalability. Although ProvSQL shows a noticeable overhead when evaluating semirings on top of the provenance circuits, it still outperforms GProM by a large margin. Moreover, in Figure 4b it is obvious that ProvSQL, at certain scale factors, benefits from optimizer-driven performance improvements, as previously discussed.



(a) On queries 11, 14, 15 and 17 from $\mathcal{Q}^{MayBMS}$ (log scale)



(b) On queries 1, 4, 12 and 15 from $\mathcal{Q}^{\mathrm{TPC}^*}$ (log scale)

Figure 5: Scalability of MayBMS vs. ProvSQL.

7.5 MayBMS vs ProvSQL for Probability

We compare the scalability of ProvSQL and MayBMS when it comes to probability computation on uncertain tuple-independent databases, excluding queries involving set-operations and aggregations, that MayBMS does not support (see Table 7). The queries used in this experiment were rewritten for MayBMS to adhere to the syntax constraints of this system, in particular using `conf()` and `tconf()` were appropriate. This ensured ProvSQL and MayBMS computed the same probabilities.

MayBMS implements efficient query plans for *safe queries* [20], something ProvSQL does not. We first select 4 queries that are not safe (11, 14, 15 and 17), from our set of custom queries for which MayBMS can compute probabilities; this query set is denoted as $\mathcal{Q}^{\mathrm{MayBMS}}$. Figure 5a shows that both ProvSQL and MayBMS perform similarly on all 4 queries, exhibiting linear growth with TPC-H scale factors. ProvSQL performs slightly better on queries 14 and 15, and both ProvSQL and MayBMS have nearly the same execution times for query 17.

We also compared ProvSQL with MayBMS by carrying out probability computations on the modified TPC-H queries, which were used to benchmark MayBMS. These are the largest subqueries from the original TPC-H queries 1, 4, 12, and 15 but without aggregations and inequality joins. Figure 5b shows how MayBMS and ProvSQL scales against the TPC-H scale factors. For query 1, ProvSQL goes out of memory beyond scale factor 5. Both systems scale linearly with dataset size, but MayBMS performs noticeably better than ProvSQL on queries 1, 4 and 12. This difference in their performance is mainly because of the fact that MayBMS and ProvSQL have different approaches when it comes to probability evaluation. In this experiment all queries are safe and MayBMS employs safe query plans which often results in efficient probability evaluation. ProvSQL does not implement the safe query approach. It is designed to be a generic system that allows provenance tracking and also offers probability computation by means of Boolean provenance circuits. When provenance circuits exceed manageable limits it resorts to knowledge compilers, which sometimes are unable to exploit the structure of the provenance formula. In some queries, however, such as query 15, this fallback mechanism allows ProvSQL to compute probabilities faster than MayBMS.

8 CONCLUSION

ProvSQL's data model, architecture, and generic design makes it suitable to compute a large range of provenance annotations and to provide a generic solution for query evaluation in probabilistic databases. ProvSQL supports a larger subset of SQL than other existing systems and is actively maintained. Its performance is suitable for multi-GB databases; overhead of provenance computation is often constant (with the notable exception of aggregate queries) and, despite the #P-hardness of the problem, it is often possible to compute probabilities of query outputs in acceptable time.

Many perspectives for improvement exist. First, augmenting the support of SQL is a necessity for general applicability; this includes relatively simple cases such as subqueries in **`WHERE`** clauses or **`OUTER JOIN`** queries, and much more complex cases such as **`WITH RECURSIVE`** queries which may necessitate a dedicated query evaluator. Second, the performance of the specialization to a specific semiring is not fully satisfactory. Third, when evaluating safe queries over tuple-independent database, the intensional approach to probabilistic query evaluation is currently suboptimal. It is unknown whether the safe plan algorithm from [20] can be turned into an intensional approach, but first results in this direction [41] could suggest how to add safe query plan support in ProvSQL.

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A MATERIAL FOR SECTION 3 (EXTENDED RELATIONAL ALGEBRA)

We also give SQL translations of the operators defined in this section, assuming appropriate translations of unnamed positional indices to attribute names within terms (when it makes a difference, we use PostgreSQL syntax variants):

relation
`SELECT * FROM` R

projection
`SELECT` $t_1, t_2, \dots, t_n$ `FROM` (q)

selection
`SELECT * FROM` (q) `WHERE` φ

cross product
`SELECT * FROM` (q_1), (q_2)

multiset sum
q_1 `UNION ALL` q_2

duplicate elimination
`SELECT DISTINCT * FROM` (q)

multiset difference
`SELECT * FROM` (q_1) `AS temp WHERE ROW(temp.*) NOT IN` (q_2)

aggregation If $\#j$ stands for the name of the jth attribute returned by the query q:
`SELECT` $\#i_1, \dots, \#i_m, f_1(t_1), \dots, f_n(t_n)$ `FROM` (q)
`GROUP BY 1, ..., m`

join
`SELECT * FROM` (q_1) `JOIN` (q_2) `ON` φ
or simply
`SELECT * FROM` (q_1), (q_2) `WHERE` φ

set union
q_1 `UNION` q_2

In addition to relations being unlabeled and untyped, our query semantics slightly differs from SQL in the following way:

- As mentioned, our semantics for multiset difference follows `NOT IN`, not `EXCEPT ALL`.
- We do not consider `NULL` values in any way.
- We do not reproduce some quirks of SQL groupless aggregation: in SQL, `SELECT COUNT(x) FROM R` returns 0 on an empty relation of schema `R(x INT)` while `SELECT SUM(x) FROM R` returns `NULL`. In our semantics, $\gamma_{\#1}[\#1 : f](R)$ returns the empty relation, however f is defined, if evaluated on an instance where R is empty. This is more consistent with aggregation under grouping.

B MATERIAL FOR SECTION 4 (QUERYING ANNOTATED RELATIONS)

Proposition 6. *For a set X, $(2^{2^X}, \varnothing, \{\varnothing\}, \cup, \uplus, \setminus)$ is an m-semiring.*

Proof. For $R, S, T \in 2^{2^X}$:

(i) $S \cup (T \setminus S) = S \cup T = T \cup S = T \cup (S \setminus T)$.
(ii) $R \setminus (S \cup T) = \{x \in R \mid x \notin S, x \notin T\} = \{x \in R \setminus S \mid x \notin T\} = (R \setminus S) \setminus T$.
(iii) $S \setminus S = \varnothing \setminus S = \varnothing$. ◻

Theorem 10. *Let $\mathcal{D}$ be a database schema, q any extended relational algebra query over $\mathcal{D}$, $\mathbb{K}$ an appropriate algebraic structure, and $\hat{I}$ a $\mathbb{K}$-instance over $\mathcal{D}$. Let $\hat{q}$ be the query rewritten from q by applying the rewriting rules (R1)–(R5) recursively bottom up. Then $\langle\!\langle q \rangle\!\rangle^{\hat{I}} = [\![\hat{q}]\!]^{\hat{I}}$.*

Proof. We proceed by induction on the structure of q.

relation for any relation label R in the domain of $\mathcal{D}$, $[\![\hat{R}]\!]^{\hat{I}} = [\![R]\!]^{\hat{I}} = \hat{I}(R) = \langle\!\langle R \rangle\!\rangle^{\hat{I}}$.

projection for $k \in \mathbb{N}$, $q \in \mathrm{RA}_k$, $t_1, \dots, t_n$ of terms of max-index $\leqslant k$,

$$[\![\widehat{\Pi_{t_1,\dots,t_n}(q)}]\!]^{\hat{I}} = [\![\Pi_{t_1,\dots,t_n,\#(k+1)}(\hat{q})]\!]^{\hat{I}} = \left\{\!\!\left\{ (t_1(u), \dots, t_n(u), \alpha) \mid (u, \alpha) \in [\![\hat{q}]\!]^{\hat{I}} \right\}\!\!\right\} = \left\{\!\!\left\{ (t_1(u), \dots, t_n(u), \alpha) \mid (u, \alpha) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}} \right\}\!\!\right\} = \langle\!\langle \Pi_{t_1,\dots,t_n}(q) \rangle\!\rangle^{\hat{I}}.$$

selection for $k \in \mathbb{N}$, $q \in \mathrm{RA}_k$, and φ a Boolean combination of (in)equality comparisons involving terms of max-index $\leqslant k$,

$$[\![\widehat{\sigma_\varphi(q)}]\!]^{\hat{I}} = [\![\sigma(\varphi)(\hat{q})]\!]^{\hat{I}} = \left\{\!\!\left\{ u' \mid u' \in [\![\hat{q}]\!]^{\hat{I}}, \varphi(u') \right\}\!\!\right\} = \left\{\!\!\left\{ (u, \alpha) \mid (u, \alpha) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}}, \varphi(u) \right\}\!\!\right\} = \langle\!\langle \sigma_\varphi(q) \rangle\!\rangle^{\hat{I}}.$$

Indeed, since φ does not involve "$\#(k+1)$", $\varphi(u') = \varphi((u, \alpha)) = \varphi(u)$.

cross product for $k_1, k_2 \in \mathbb{N}$, $q_1 \in \mathsf{RA}_{k_1}$, $q_2 \in \mathsf{RA}_{k_2}$,

$$\begin{aligned}
\llbracket\widehat{q_1 \times q_2}\rrbracket^{\hat{I}} &= \llbracket\Pi_{\#1,\dots,\#k_1,\#(k_1+2),\dots,\#(k_1+k_2+1),\#(k_1+1)\otimes\#(k_1+k_2+2)}(\hat{q}_1 \times \hat{q}_2)\rrbracket^{\hat{I}} \\
&= \left\{\!\!\left\{ (u_1,\dots,u_{k_1},v_1,\dots,v_{k_2},\alpha\otimes\beta) \mid (u_1,\dots,u_{k_1},\alpha,v_1,\dots,v_{k_2},\beta) \in \llbracket\hat{q}_1 \times \hat{q}_2\rrbracket^{\hat{I}} \right\}\!\!\right\} \\
&= \left\{\!\!\left\{ (u_1,\dots,u_{k_1},v_1,\dots,v_{k_2},\alpha\otimes\beta) \mid (u_1,\dots,u_{k_1},\alpha,v_1,\dots,v_{k_2},\beta) \in \llbracket\hat{q}_1\rrbracket^{\hat{I}} \times \llbracket\hat{q}_2\rrbracket^{\hat{I}} \right\}\!\!\right\} \\
&= \left\{\!\!\left\{ (u_1,\dots,u_{k_1},v_1,\dots,v_{k_2},\alpha\otimes\beta) \mid (u_1,\dots,u_{k_1},\alpha,v_1,\dots,v_{k_2},\beta) \in \langle\!\langle q_1 \rangle\!\rangle^{\hat{I}} \times \langle\!\langle q_2 \rangle\!\rangle^{\hat{I}} \right\}\!\!\right\} \\
&= \langle\!\langle q_1 \times q_2 \rangle\!\rangle^{\hat{I}}.
\end{aligned}$$

multiset sum for $k \in \mathbb{N}$, $q_1, q_2 \in \mathsf{RA}_k$,

$$\llbracket\widehat{q_1 \uplus q_2}\rrbracket^{\hat{I}} = \llbracket\hat{q}_1 \uplus \hat{q}_2\rrbracket^{\hat{I}} = \llbracket\hat{q}_1\rrbracket^{\hat{I}} \uplus \llbracket\hat{q}_2\rrbracket^{\hat{I}} = \langle\!\langle q_1 \rangle\!\rangle^{\hat{I}} \uplus \langle\!\langle q_2 \rangle\!\rangle^{\hat{I}} = \langle\!\langle q_1 \uplus q_2 \rangle\!\rangle^{\hat{I}}.$$

duplicate elimination for $k \in \mathbb{N}$, $q \in \mathsf{RA}_k$,

$$\begin{aligned}
\llbracket\widehat{\varepsilon(q)}\rrbracket^{\hat{I}} &= \llbracket\gamma_{1,\dots,k}[\#(k+1) : \textstyle\bigoplus](\hat{q})\rrbracket^{\hat{I}} \\
&= \left\{ \left(v_1,\dots,v_k, \bigoplus \left\{\!\!\left\{ \alpha \mid u \in \llbracket\hat{q}\rrbracket^{\hat{I}}, u = (v_1,\dots,v_k,\alpha) \right\}\!\!\right\}\right) \,\middle|\, (v_1,\dots,v_k) \in \llbracket\varepsilon(\Pi_{1,\dots,k}(\hat{q}))\rrbracket^{\hat{I}} \right\} \\
&= \left\{ \left(v_1,\dots,v_k, \bigoplus \left\{\!\!\left\{ \alpha \mid u \in \llbracket\hat{q}\rrbracket^{\hat{I}}, u = (v_1,\dots,v_k,\alpha) \right\}\!\!\right\}\right) \,\middle|\, \llbracket\Pi_{1,\dots,k}(\hat{q})\rrbracket^{\hat{I}}(v_1,\dots,v_k) > 0 \right\} \\
&= \left\{ \left(v_1,\dots,v_k, \bigoplus \left\{\!\!\left\{ \alpha \mid u \in \llbracket\hat{q}\rrbracket^{\hat{I}}, u = (v_1,\dots,v_k,\alpha) \right\}\!\!\right\}\right) \,\middle|\, \exists\alpha\, \llbracket\hat{q}\rrbracket^{\hat{I}}(v_1,\dots,v_k,\alpha) > 0 \right\} \\
&= \left\{ \left(v_1,\dots,v_k, \bigoplus \left\{\!\!\left\{ \alpha \mid u \in \langle\!\langle q \rangle\!\rangle^{\hat{I}}, u = (v_1,\dots,v_k,\alpha) \right\}\!\!\right\}\right) \,\middle|\, \exists\alpha\, \langle\!\langle q \rangle\!\rangle^{\hat{I}}(v_1,\dots,v_k,\alpha) > 0 \right\} \\
&= \bigcup_{u \mid \exists\alpha (u,\alpha)(u,va) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}}} \left\{ \left(u, \bigoplus_{\alpha \mid (u,\alpha) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}}} \alpha \right) \right\} \\
&= \langle\!\langle \varepsilon(q) \rangle\!\rangle^{\hat{I}}.
\end{aligned}$$

multiset difference for $k \in \mathbb{N}$, $q_1, q_2 \in \mathsf{RA}_k$,

$$\begin{aligned}
\llbracket\widehat{q_1 - q_2}\rrbracket^{\hat{I}} = \llbracket \quad & \Pi_{\#1,\dots,\#(k+1)}(\hat{q}_1 \bowtie_{\#1=\#(k+1)\wedge\cdots\wedge\#k=\#(2k)} \varepsilon(\Pi_{\#1,\dots,\#k}(\hat{q}_1) - \Pi_{\#1,\dots,\#k}(\hat{q}_2))) \\
& \uplus \Pi_{\#1,\dots,\#k,\#(k+1)\ominus\#(2k+2)}(\hat{q}_1 \bowtie_{\#1=\#(k+2)\wedge\cdots\wedge\#k=\#(2k+1)} \gamma_{\#1,\dots,\#k}[\#(k+1) : \textstyle\bigoplus](\hat{q}_2))) \qquad \rrbracket^{\hat{I}} \\
= \quad & \llbracket\Pi_{\#1,\dots,\#(k+1)}(\hat{q}_1 \bowtie_{\#1=\#(k+1)\wedge\cdots\wedge\#k=\#(2k)} \varepsilon(\Pi_{\#1,\dots,\#k}(\hat{q}_1) - \Pi_{\#1,\dots,\#k}(\hat{q}_2)))\rrbracket^{\hat{I}} \\
& \uplus \llbracket\Pi_{\#1,\dots,\#k,\#(k+1)\ominus\#(2k+2)}(\hat{q}_1 \bowtie_{\#1=\#(k+2)\wedge\cdots\wedge\#k=\#(2k+1)} \gamma_{\#1,\dots,\#k}[\#(k+1) : \textstyle\bigoplus](\hat{q}_2))\rrbracket^{\hat{I}} \\
= \quad & \left\{\!\!\left\{ (u,\alpha) \mid (u,\alpha) \in \llbracket\hat{q}_1\rrbracket^{\hat{I}}, u \in \llbracket\Pi_{\#1,\dots,\#k}(\hat{q}_1) - \Pi_{\#1,\dots,\#k}(\hat{q}_2)\rrbracket^{\hat{I}} \right\}\!\!\right\} \\
& \uplus \left\{\!\!\left\{ (u,\alpha\ominus\beta) \mid (u,\alpha) \in \llbracket\hat{q}_1\rrbracket^{\hat{I}}, (u,\beta) \in \llbracket\gamma_{\#1,\dots,\#k}[\#(k+1) : \textstyle\bigoplus](\hat{q}_2))\rrbracket^{\hat{I}} \right\}\!\!\right\} \\
= \quad & \left\{\!\!\left\{ (u,\alpha) \mid (u,\alpha) \in \llbracket\hat{q}_1\rrbracket^{\hat{I}}, \nexists\, \beta\, (u,\beta) \in \llbracket\hat{q}_2\rrbracket^{\hat{I}} \right\}\!\!\right\} \uplus \left\{\!\!\left\{ \left(u, \alpha \ominus \bigoplus_{\beta \mid (u,\beta) \in \llbracket\hat{q}_2\rrbracket^{\hat{I}}} \beta \right) \mid (u,\alpha) \in \llbracket\hat{q}_1\rrbracket^{\hat{I}}, \exists\beta (u,\beta) \in \llbracket\hat{q}_2\rrbracket^{\hat{I}} \right\}\!\!\right\} \\
= \quad & \left\{\!\!\left\{ (u,\alpha) \mid (u,\alpha) \in \langle\!\langle q_1 \rangle\!\rangle^{\hat{I}}, \nexists\, \beta\, (u,\beta) \in \langle\!\langle q_2 \rangle\!\rangle^{\hat{I}} \right\}\!\!\right\} \uplus \left\{\!\!\left\{ \left(u, \alpha \ominus \bigoplus_{\beta \mid (u,\beta) \in \langle\!\langle q_2 \rangle\!\rangle^{\hat{I}}} \beta \right) \,\middle|\, (u,\alpha) \in \langle\!\langle q_1 \rangle\!\rangle^{\hat{I}}, \exists\beta (u,\beta) \in \langle\!\langle q_2 \rangle\!\rangle^{\hat{I}} \right\}\!\!\right\} \\
= \quad & \left\{\!\!\left\{ \left(u, \alpha \ominus \bigoplus_{\beta \mid (u,\beta) \in \langle\!\langle q_2 \rangle\!\rangle^{\hat{I}}} \beta \right) \,\middle|\, (u,\alpha) \in \langle\!\langle q_1 \rangle\!\rangle^{\hat{I}} \right\}\!\!\right\} = \langle\!\langle q_1 - q_2 \rangle\!\rangle^{\hat{I}}.
\end{aligned}$$

aggregation for $k \in \mathbb{N}$, $q \in \mathsf{RA}_k$, distinct $(i_j)_{1\leqslant j\leqslant k}$, terms $t_1, \dots t_n$ of max-index $\leqslant k$, monoid aggregate functions $f_1, \dots, f_n$,

$$\begin{aligned}
&\llbracket\gamma_{i_1,\dots,i_m}[t_1 : \widehat{f_1, \dots}, t_n : f_n](q)\rrbracket^{\hat{I}} \\
&= \llbracket\gamma_{i_1,\dots,i_m}[t_1 * \#(k+1) : \hat{f}_1, \dots, t_n * \#(k+1) : \hat{f}_n, \#(k+1) : \delta\left(\bigoplus\right)](\hat{q})\rrbracket^{\hat{I}} \\
&= \left\{ \left(v_1, \dots, v_m, \hat{f}_1\left(\left\{\!\!\left\{ t_1(u) * \alpha \,\middle|\, (u,\alpha) \in \llbracket\hat{q}\rrbracket^{\hat{I}}, (u_{i_1}, \dots, u_{i_m}) = (v_1, \dots, v_m) \right\}\!\!\right\} \right), \dots, \delta\left(\bigoplus_{\substack{(u,\beta) \in \llbracket\hat{q}\rrbracket^{\hat{I}} \\ (u_{i_1}, \dots, u_{i_m}) = (v_1, \dots, v_m)}} \beta \right) \right) \,\middle|\, (v_1, \dots, v_m) \in \llbracket\varepsilon(\Pi_{\#i_1,\dots,\#i_m}(\hat{q}))\rrbracket^{\hat{I}} \right\} \\
&= \left\{ \left(v_1, \dots, v_m, \hat{f}_1\left(\left\{\!\!\left\{ t_1(u) * \alpha \,\middle|\, (u,\alpha) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}}, (u_{i_1}, \dots, u_{i_m}) = (v_1, \dots, v_m) \right\}\!\!\right\} \right), \dots, \delta\left(\bigoplus_{\substack{(u,\beta) \in \llbracket\hat{q}\rrbracket^{\hat{I}} \\ (u_{i_1}, \dots, u_{i_m}) = (v_1, \dots, v_m)}} \beta \right) \right) \,\middle|\, (u,\beta) \in \llbracket\hat{q}\rrbracket^{\hat{I}}, (u_{i_1}, \dots, u_{i_m}) = (v_1, \dots, v_m) \right\} \\
&= \left\{ \left(v_1, \dots, v_m, \hat{f}_1\left(\left\{\!\!\left\{ t_1(u) * \alpha \,\middle|\, (u,\alpha) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}}, (u_{i_1}, \dots, u_{i_m}) = (v_1, \dots, v_m) \right\}\!\!\right\} \right), \dots, \delta\left(\bigoplus_{\substack{(u,\beta) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}} \\ (u_{i_1}, \dots, u_{i_m}) = (v_1, \dots, v_m)}} \beta \right) \right) \,\middle|\, (u,\beta) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}}, (u_{i_1}, \dots, u_{i_m}) = (v_1, \dots, v_m) \right\} \\
&= \left\{ \left(v_1, \dots, v_m, \hat{f}_1\left(\left\{\!\!\left\{ t_1(u) * \alpha \,\middle|\, (u,\alpha) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}}, (u_{i_1}, \dots, u_{i_m}) = (v_1, \dots, v_m) \right\}\!\!\right\} \right), \dots, \delta\left(\bigoplus_{(u,\beta) \in \langle\!\langle \Pi_{\#i_1,\dots,\#i_m}(q) \rangle\!\rangle^{\hat{I}}} \beta \right) \right) \,\middle|\, (u,\beta) \in \langle\!\langle \Pi_{\#i_1,\dots,\#i_m}(q) \rangle\!\rangle^{\hat{I}} \right\} \\
&= \left\{ \left(v_1, \dots, v_m, \hat{f}_1\left(\left\{\!\!\left\{ t_1(u) * \alpha \,\middle|\, (u,\alpha) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}}, (u_{i_1}, \dots, u_{i_m}) = (v_1, \dots, v_m) \right\}\!\!\right\} \right), \dots, \delta(\beta) \right) \,\middle|\, (u,\beta) \in \langle\!\langle \varepsilon(\Pi_{\#i_1,\dots,\#i_m}(q)) \rangle\!\rangle^{\hat{I}} \right\} \\
&= \langle\!\langle \gamma_{i_1,\dots,i_m}[t_1 : f_1, \dots, t_n : f_n](q) \rangle\!\rangle^{\hat{I}}.
\end{aligned}$$

□

Theorem 12. *For any finite set of variables X, probability distribution $\Pr$ over X, $\mathcal{B}[X]$-relation $\hat{I}$ and relational algebra query q without aggregation, for any tuple t with same arity as q,* $\Pr(t \in q(\hat{I})) = \Pr\left(\bigvee_{(t,\alpha) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}}} \alpha\right)$.

Proof. For a $\mathcal{B}[X]$-relation $\hat{I}$ and a valuation ν over X, we define $\nu(\hat{I})$ to be the (unannotated) relation J obtained from $\hat{I}$ by removing all tuples with annotation α such as $\alpha(\nu) = \bot$ and keeping all other tuples. In other words, $\nu(\hat{I}) = J \iff \Phi_{\hat{I}}(\hat{J})(\nu) = \top$.

For a $\mathcal{B}[X]$-relation $\hat{I}$, a query q without aggregation and a tuple t with same arity as q, we define $\mathrm{Prov}(t \in q(\hat{I}))$, the *Boolean provenance of t for q on $\hat{I}$*, to be the Boolean function that maps a valuation ν to $\top$ if $t \in \llbracket q\rrbracket^{\nu(\hat{I})}$ and to $\bot$ otherwise.

We first note that $\Pr(t \in q(\hat{I})) = \Pr(\mathrm{Prov}(t \in q(\hat{I})))$. Indeed:

$$\Pr(\mathrm{Prov}(t \in q(\hat{I}))) = \sum_{\nu \mid t \in \llbracket q\rrbracket^{v(\hat{I})}} \Pr(\nu) = \sum_{\hat{J} \subseteq \hat{I}, t \in \llbracket q\rrbracket^J} \sum_{\nu \mid \nu(\hat{I}) = J} \Pr(\nu) = \sum_{\hat{J} \subseteq \hat{I}, t \in \llbracket q\rrbracket^J} \sum_{\nu \mid \nu(\hat{I}) = J} \Pr(\nu)$$

while

$$\Pr(t \in q(\hat{I})) = \sum_{\hat{J} \subseteq \hat{I}, t \in \llbracket q\rrbracket^J} \Pr(\hat{J}) = \sum_{\hat{J} \subseteq \hat{I}, t \in \llbracket q\rrbracket^J} \Pr[\Phi_{\hat{I}}(\hat{J})] = \sum_{\hat{J} \subseteq \hat{I}, t \in \llbracket q\rrbracket^J} \sum_{\nu \mid \Phi_{\hat{I}}(\hat{J})(\nu) = \top} \Pr(\nu) = \sum_{\hat{J} \subseteq \hat{I}, t \in \llbracket q\rrbracket^J} \sum_{\nu \mid \nu(\hat{I}) = J} \Pr(\nu).$$

It then suffices to show that

$$\mathrm{Prov}(t \in q(\hat{I})) = \bigvee_{(t,\alpha) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}}} \alpha$$

or, in other terms, that

$$t \in \llbracket q\rrbracket^{\nu(\hat{I})} \quad \text{if and only if} \quad \exists (t,\alpha) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}}, \alpha(\nu) = \top.$$

We proceed by induction on the structure of q.

relation for any relation label R in the domain of $\mathcal{D}$, $t \in \llbracket R\rrbracket^{\nu(\hat{I})} \iff t \in \nu(\hat{I})(R) \iff \exists (t,\alpha) \in \hat{I}(R)\ \alpha(\nu) = \top \iff \exists (t,\alpha) \in \langle\!\langle R \rangle\!\rangle^{\hat{I}}, \alpha(\nu) = \top$.

projection for $k \in \mathbb{N}$, $q \in \mathsf{RA}_k$, $t_1, \ldots, t_n$ of terms of max-index $\leqslant k$,

$$\begin{aligned} t \in [\![\Pi_{t_1,\ldots,t_n}(q)]\!]^{\nu(\hat{I})} &\iff \exists u \in [\![q]\!]^{\nu(\hat{I})}, t = (t_1(u), \ldots, t_n(u)) \\ &\iff \exists (u, \alpha) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}}, \alpha(\nu) = \top \wedge t = (t_1(u), \ldots, t_n(u)) \\ &\iff \exists (t, \alpha) \in \langle\!\langle \Pi_{t_1,\ldots,t_n}(q) \rangle\!\rangle^{\hat{I}}, \alpha(\nu) = \top. \end{aligned}$$

selection for $k \in \mathbb{N}$, $q \in \mathsf{RA}_k$, and φ a Boolean combination of (in)equality comparisons involving terms of max-index $\leqslant k$,

$$\begin{aligned} t \in [\![\sigma_\varphi(q)]\!]^{\nu(\hat{I})} &\iff t \in [\![q]\!]^{\nu(\hat{I})}, \varphi(u) \\ &\iff \exists (t, \alpha) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}}, \alpha(\nu) = \top \wedge \varphi(u) \\ &\iff \exists (t, \alpha) \in \langle\!\langle \sigma_\varphi(q) \rangle\!\rangle^{\hat{I}}, \alpha(\nu) = \top. \end{aligned}$$

cross product for $k_1, k_2 \in \mathbb{N}$, $q_1 \in \mathsf{RA}_{k_1}$, $q_2 \in \mathsf{RA}_{k_2}$,

$$\begin{aligned} t \in [\![q_1 \times q_2]\!]^{\nu(\hat{I})} &\iff t = (t_1, t_2), t_1 \in [\![q_1]\!]^{\nu(\hat{I})} \wedge t_2 \in [\![q_2]\!]^{\nu(\hat{I})} \\ &\iff t = (t_1, t_2), \exists (t_1, \alpha) \in \langle\!\langle q_1 \rangle\!\rangle^{\hat{I}}, \alpha(\nu) = \top \wedge \exists (t_2, \beta) \in \langle\!\langle q_2 \rangle\!\rangle^{\hat{I}}, \beta(\nu) = \top \\ &\iff t = (t_1, t_2), \exists (t_1, \alpha, t_2, \beta) \in \langle\!\langle q_1 \rangle\!\rangle^{\hat{I}} \times \langle\!\langle q_2 \rangle\!\rangle^{\hat{I}}, (\alpha \hat{\wedge} \beta)(\nu) = \top \\ &\iff \exists (t, \gamma) \in \langle\!\langle q_1 \times q_2 \rangle\!\rangle^{\hat{I}}, \gamma(\nu) = \top. \end{aligned}$$

multiset sum for $k \in \mathbb{N}$, $q_1, q_2 \in \mathsf{RA}_k$,

$$\begin{aligned} t \in [\![q_1 \uplus q_2]\!]^{\nu(\hat{I})} &\iff t \in [\![q_1]\!]^{\nu(\hat{I})} \uplus [\![q_2]\!]^{\nu(\hat{I})} \\ &\iff (\exists (t, \alpha) \in \langle\!\langle q_1 \rangle\!\rangle^{\hat{I}} \alpha(\nu) = \top) \vee (\exists (t, \alpha) \in \langle\!\langle q_2 \rangle\!\rangle^{\hat{I}} \alpha(\nu) = \top) \\ &\iff \exists (t, \alpha) \in \langle\!\langle q_1 \rangle\!\rangle^{\hat{I}} \uplus \langle\!\langle q_2 \rangle\!\rangle^{\hat{I}} \alpha(\nu) = \top \\ &\iff \exists (t, \alpha) \in \langle\!\langle q_1 \uplus q_2 \rangle\!\rangle^{\hat{I}} \alpha(\nu) = \top. \end{aligned}$$

duplicate elimination for $k \in \mathbb{N}$, $q \in \mathsf{RA}_k$,

$$t \in [\![\varepsilon(q)]\!]^{\nu(\hat{I})} \iff t \in [\![q]\!]^{\nu(\hat{I})} \iff \exists (t, \alpha) \in \langle\!\langle q \rangle\!\rangle^{\hat{I}}, \alpha(\nu) = \top \iff \exists (t, \beta) \in \langle\!\langle \varepsilon(q) \rangle\!\rangle^{\hat{I}}, \beta(\nu) = \top$$

(the last equivalence comes from the fact that a disjunction is true if and only if one of the disjunct is true).

multiset difference for $k \in \mathbb{N}$, $q_1, q_2 \in \mathsf{RA}_k$,

$$\begin{aligned} t \in [\![q_1 - q_2]\!]^{\nu(\hat{I})} &\iff t \in [\![q_1]\!]^{\nu(\hat{I})} \wedge t \notin [\![q_2]\!]^{\nu(\hat{I})} \\ &\iff (\exists \alpha (t, \alpha) \in \langle\!\langle q_1 \rangle\!\rangle^{\hat{I}}, \alpha(\nu) = \top) \wedge \neg(\exists \beta (t, \beta) \in \langle\!\langle q_2 \rangle\!\rangle^{\hat{I}}, \beta(\nu) = \top) \\ &\iff (\exists \alpha (t, \alpha) \in \langle\!\langle q_1 \rangle\!\rangle^{\hat{I}}, \alpha(\nu) = \top) \wedge \neg \left(\bigvee_{\beta \mid (t, \beta) \in \langle\!\langle q_2 \rangle\!\rangle^{\hat{I}}} \beta(\nu) = \top \right) \\ &\iff (\exists \alpha (t, \alpha) \in \langle\!\langle q_1 \rangle\!\rangle^{\hat{I}}, \alpha(\nu) \wedge \neg \left(\bigvee_{\beta \mid (t, \beta) \in \langle\!\langle q_2 \rangle\!\rangle^{\hat{I}}} \beta(\nu) = \top \right) = \top \\ &\iff \exists (t, \alpha') \in \langle\!\langle q_1 - q_2 \rangle\!\rangle^{\hat{I}}, \alpha'(\nu) = \top. \end{aligned}$$

□

C GENERATING CUSTOM QUERIES USING DSQGEN

The TPC-DS 3.2.0 dataset comes with a query generator, DSQGEN. DSQGEN is more flexible than the query generator from the TPC-H dataset in the sense that the distributions for the scalars in the queries can be written directly in the query template syntax. This allows us to create our own query templates for querying the TPC-H dataset easily. We then use DSQGEN to generate the executable query files from our query templates.

For example let us consider a query to retrieve line items and their corresponding orders for a given ship date range on the TPC-H dataset. We will have to write the query template like below.

```
DEFINE SHIPDATE_MIN = RANDOM(1,121,uniform);
DEFINE SHIPDATE_MAX = RANDOM([SHIPDATE_MIN],121,uniform);
SELECT l.*, o.*
FROM lineitem l, orders o
WHERE l.l_orderkey = o.o_orderkey
AND l.l_shipdate >= date '1994-12-01'
- interval '[SHIPDATE_MIN]' day
AND l.l_shipdate < date '1995-12-01'
- interval '[SHIPDATE_MAX]' day;
```

We can then use DSQGEN to generate the following executable query file from the query template for a random seed(here, 3983237069).

```
SELECT l.*, o.*
FROM lineitem l, orders o
WHERE l.l_orderkey = o.o_orderkey
AND l.l_shipdate >= date '1994-12-01'
 - interval '98' day
AND l.l_shipdate < date '1995-12-01'
 - interval '117' day;
```

In this way we have written 18 different query templates following the DSQGEN query template syntax.

D DSQGEN QUERY TEMPLATES FOR QUERIES IN $\mathcal{Q}^{\mathbf{cust}}$

```
-- Query 1:
define QUANT=RANDOM(1,50,uniform);
define MODE=TEXT({"REG AIR",1},{"AIR",1},{"RAIL",1},
{"SHIP",1},{"TRUCK",1},{"MAIL",1},{"FOB",1});
define DISC=RANDOM(0,10,uniform);
SELECT l_orderkey, l_partkey, l_suppkey,
l_linenumber, l_linestatus
FROM lineitem
WHERE l_shipmode = '[MODE]'
AND l_quantity > [QUANT]
OR l_discount >= cast([DISC] as float)/100.0;

-- Query 2:
define NATION=RANDOM(0,24,uniform);
define PRICE=RANDOM(10000,100000,uniform);
SELECT DISTINCT o.o_orderdate, o.o_custkey
FROM orders o, customer c
WHERE o.o_custkey = c.c_custkey
AND o.o_totalprice > [PRICE]
AND c.c_nationkey = [NATION]
AND o.o_orderstatus IN ('P','F');

-- Query 3:
define REGION=RANDOM(0,4,uniform);
define COST=RANDOM(1,1000,uniform);
SELECT p.p_name, p.p_mfgr, p.p_partkey, p.p_retailprice
FROM part p
INNER JOIN partsupp ps ON p.p_partkey = ps.ps_partkey
INNER JOIN supplier s  ON ps.ps_suppkey = s.s_suppkey
INNER JOIN nation n    ON s.s_nationkey = n.n_nationkey
INNER JOIN region r    ON n.n_regionkey = r.r_regionkey
WHERE r.r_regionkey = [REGION]
AND ps.ps_supplycost < [COST];

-- Query 4:
define PRICE=RANDOM(10000,100000,uniform);
```

```sql
SELECT DISTINCT c.c_name, c.c_nationkey
FROM customer c, orders o
WHERE c.c_custkey = o.o_custkey
AND o.o_totalprice > [PRICE]
GROUP BY c.c_nationkey,c.c_name;

-- Query 5:
define COST=RANDOM(100,1000,uniform);
define AVAIL=RANDOM(1,8888,uniform);
SELECT s.s_name, s.s_address, s.s_phone
FROM supplier s INNER JOIN partsupp ps
ON s.s_suppkey = ps.ps_suppkey
WHERE ps.ps_supplycost > [COST]
OR (ps.ps_availqty > [AVAIL] AND
ps.ps_supplycost > cast([COST] as float)/2);

-- Query 6:
define A=TEXT({"STANDARD",1},{"SMALL",1},{"MEDIUM",1},
{"LARGE",1},{"ECONOMY",1},{"PROMO",1});
define B=TEXT({"ANODIZED",1},{"BURNISHED",1},{"PLATED",1},
{"POLISHED",1},{"BRUSHED",1});
define C=TEXT({"TIN",1},{"NICKEL",1},{"BRASS",1},
{"STEEL",1},{"COPPER",1});
define SIZE=RANDOM(1,50,uniform);
SELECT part.p_name, part.p_brand
FROM part
WHERE p_type = '[A] [B] [C]'
AND p_size = [SIZE]
GROUP BY part.p_brand, part.p_name;

-- Query 7:
define MODE=TEXT({"REG AIR",1},{"AIR",1},{"RAIL",1},
{"SHIP",1},{"TRUCK",1},{"MAIL",1},{"FOB",1});
define QUANT=RANDOM(1,50,uniform);
SELECT *
FROM lineitem
WHERE l_shipmode = '[MODE]'
AND l_quantity < [QUANT]
AND l_linestatus = 'F';

-- Query 8:
define OP=TEXT({"1-URGENT",1},{"2-HIGH",1},{"3-MEDIUM",1},
{"4-NOT SPECIFIED",1},{"5-LOW",1});
define CLERK=RANDOM(1,9,uniform);
SELECT c.c_name, o.o_orderdate
FROM orders o INNER JOIN customer c ON o_custkey= c_custkey
WHERE o_orderpriority = '[OP]'
AND o_clerk like 'Clerk#00000000[CLERK]%';

-- Query 9:
define NATION=RANDOM(0,24,uniform);
define BAL=RANDOM(1,10000,uniform);
SELECT c.c_name, o.o_orderstatus
FROM customer c, orders o, nation n, region r, part p,
supplier s, partsupp ps, lineitem l
WHERE c.c_custkey = o.o_custkey
AND o.o_orderkey = l.l_orderkey
```

```sql
AND l.l_partkey = ps.ps_partkey
AND ps.ps_suppkey= s.s_suppkey
AND ps.ps_partkey = p.p_partkey
AND s.s_nationkey = n.n_nationkey
AND n.n_regionkey = r.r_regionkey
AND c.c_nationkey = [NATION]
AND c_acctbal > [BAL]
GROUP BY o.o_orderstatus, c.c_name;

-- Query 10:
define NATION=RANDOM(0,24,uniform);
define BAL=RANDOM(1,10000,uniform);
SELECT c.c_name, o.o_orderstatus
FROM customer c, orders o, partsupp ps, lineitem l
WHERE c.c_custkey = o.o_custkey
AND o.o_orderkey = l.l_orderkey
AND l.l_partkey = ps.ps_partkey
AND c.c_nationkey = [NATION]
AND c_acctbal > [BAL]
GROUP BY o.o_orderstatus, c.c_name;

-- Query 11:
define REGION=RANDOM(0,4,uniform);
define BAL=RANDOM(1,10000,uniform);
SELECT s.*
FROM supplier s
INNER JOIN nation n ON  s.s_nationkey = n.n_nationkey
INNER JOIN region r ON  n.n_regionkey = r.r_regionkey
WHERE r.r_regionkey = [REGION]
AND s.s_acctbal < [BAL];

-- Query 12:
define DMIN = RANDOM(1,121,uniform);
define DMAX = RANDOM([DMIN],121,uniform);
define TAX_A = RANDOM(0,3,uniform);
define TAX_B = RANDOM(4,8,uniform);
SELECT l.*, o.o_clerk, o.o_orderdate, o.o_totalprice
FROM lineitem l INNER JOIN orders o
ON l.l_orderkey = o.o_orderkey
WHERE l.l_shipdate >= date '1994-12-01'
- interval '[DMIN]' day
AND l.l_shipdate < date '1996-12-01'
- interval '[DMAX]' day
AND (
l.l_tax <= cast([TAX_A] as float)/100.0
 OR
(l.l_tax > cast([TAX_B] as float)/100.0 AND o.o_orderstatus = 'O')
);

-- Query 13:
define NATION = RANDOM(0,24,uniform);
define P_MIN = RANDOM(10000,100000,uniform);
define P_MAX = RANDOM([P_MIN],200000,uniform);
SELECT c.c_name, o.o_orderstatus, c_nationkey, c.c_phone
FROM customer c, orders o
WHERE c.c_custkey = o.o_custkey
AND c.c_nationkey = [NATION]
```

```sql
AND o.o_totalprice >= [P_MIN]
AND o.o_totalprice <= [P_MAX];

-- Query 14:
define REGION=RANDOM(0,4,uniform);
define S_MIN=RANDOM(1,1000,uniform);
define S_MAX=RANDOM([S_MIN],2000,uniform);
SELECT s.s_name, p.p_brand, p.p_name
FROM supplier s, partsupp ps, part p, nation n, region r
WHERE s.s_suppkey = ps.ps_suppkey
AND ps.ps_partkey = p.p_partkey
AND s.s_nationkey = n.n_nationkey
AND n.n_regionkey = r.r_regionkey
AND r.r_regionkey = [REGION]
AND ps.ps_supplycost >= [S_MIN]
AND ps.ps_supplycost <= [S_MAX]
GROUP BY p.p_brand, p.p_name, s.s_name;

-- Query 15:
define P_MIN = RANDOM(10000,100000,uniform);
define P_MAX = RANDOM([P_MIN],200000,uniform);
SELECT DISTINCT c.c_name, o.o_orderkey, l.l_linenumber
FROM customer c, orders o, lineitem l
WHERE c.c_custkey = o.o_custkey
AND o.o_orderkey = l.l_orderkey
AND o.o_totalprice >= [P_MIN]
AND o.o_totalprice <= [P_MAX];

--Query 16:
define SIZE=RANDOM(1,50,uniform);
define M=RANDOM(1,5,uniform);
define N=RANDOM(1,5,uniform);
SELECT c.c_name AS name, 'Customer' AS type
FROM customer c, orders o, lineitem l, part p
WHERE c.c_custkey = o.o_custkey
AND o.o_orderkey = l.l_orderkey
AND l.l_partkey = p.p_partkey
AND p.p_size = [SIZE]
EXCEPT
SELECT c.c_name AS name, 'Customer' AS type
FROM customer c, orders o, lineitem l, part p
WHERE c.c_custkey = o.o_custkey
AND o.o_orderkey = l.l_orderkey
AND l.l_partkey = p.p_partkey
AND p.p_brand = 'BRAND#[M][N]';

-- Query 17:
define MIN = RANDOM(1,50,uniform);
define MAX = RANDOM([MIN],50,uniform);
SELECT p.p_type, p.p_name, s.s_name, ps.ps_supplycost
FROM part p, partsupp ps, supplier s
WHERE p.p_partkey = ps.ps_partkey
AND ps.ps_suppkey = s.s_suppkey
AND p.p_size >= [MIN]
AND p.p_size <= [MAX]
GROUP BY p.p_type, p.p_name, s.s_name, ps.ps_supplycost ;
```

```
-- Query 18:
define NATION = RANDOM(1,25,uniform);
SELECT c.c_name AS name, 'Customer' AS type
FROM customer c
WHERE c.c_nationkey = [NATION]
UNION
SELECT s.s_name AS name, 'Supplier' AS type
FROM supplier s
WHERE s.s_nationkey = [NATION];
```

E $\mathcal{Q}^{\mathrm{TPC}}$

```
    --Query 1:
    select
        l_returnflag,
        l_linestatus,
        sum(l_quantity) as sum_qty,
        sum(l_extendedprice) as sum_base_price,
        sum(l_extendedprice * (1 - l_discount)) as sum_disc_price,
        sum(l_extendedprice * (1 - l_discount) * (1 + l_tax)) as sum_charge,
        avg(l_quantity) as avg_qty,
        avg(l_extendedprice) as avg_price,
        avg(l_discount) as avg_disc,
        count(*) as count_order

from
        lineitem
where
        l_shipdate <= date '1998-12-01' - interval '117' day
group by
        l_returnflag,
        l_linestatus
order by
        l_returnflag,
        l_linestatus
limit 1;

--Query 6:
select
        sum(l_extendedprice * l_discount) as revenue
from
        lineitem
where
        l_shipdate >= date '1995-01-01'
        and l_shipdate < date '1995-01-01' + interval '1' year
        and l_discount between 0.09 - 0.01 and 0.09 + 0.01
        and l_quantity < 24
limit 1;

--Query 7:
select
        supp_nation,
        cust_nation,
        l_year,
        sum(volume) as revenue
from
        (
```

```
		select
			n1.n_name as supp_nation,
			n2.n_name as cust_nation,
			extract(year from l_shipdate) as l_year,
			l_extendedprice * (1 - l_discount) as volume
		from
			supplier,
			lineitem,
			orders,
			customer,
			nation n1,
			nation n2
		where
			s_suppkey = l_suppkey
			and o_orderkey = l_orderkey
			and c_custkey = o_custkey
			and s_nationkey = n1.n_nationkey
			and c_nationkey = n2.n_nationkey
			and (
				(n1.n_name = 'RUSSIA' and n2.n_name = 'INDIA')
				or (n1.n_name = 'INDIA' and n2.n_name = 'RUSSIA')
			)
			and l_shipdate between date '1995-01-01' and date '1996-12-31'
	) as shipping
group by
	supp_nation,
	cust_nation,
	l_year
order by
	supp_nation,
	cust_nation,
	l_year
limit 1;

--Query 9:

select
	nation,
	o_year,
	sum(amount) as sum_profit
from
	(
		select
			n_name as nation,
			extract(year from o_orderdate) as o_year,
			l_extendedprice * (1 - l_discount) - ps_supplycost * l_quantity as amount
		from
			part,
			supplier,
			lineitem,
			partsupp,
			orders,
			nation
		where
			s_suppkey = l_suppkey
			and ps_suppkey = l_suppkey
			and ps_partkey = l_partkey
```

```
                        and p_partkey = l_partkey
                        and o_orderkey = l_orderkey
                        and s_nationkey = n_nationkey
                        and p_name like '%orchid%'
        ) as profit
group by
        nation,
        o_year
order by
        nation,
        o_year desc
limit 1 ;


--Query 12:
select
        l_shipmode,
        sum(case
                when o_orderpriority = '1-URGENT'
                        or o_orderpriority = '2-HIGH'
                        then 1
                else 0
        end) as high_line_count,
        sum(case
                when o_orderpriority <> '1-URGENT'
                        and o_orderpriority <> '2-HIGH'
                        then 1
                else 0
        end) as low_line_count
from
        orders,
        lineitem
where
        o_orderkey = l_orderkey
        and l_shipmode in ('TRUCK', 'AIR')
        and l_commitdate < l_receiptdate
        and l_shipdate < l_commitdate
        and l_receiptdate >= date '1997-01-01'
        and l_receiptdate < date '1997-01-01' + interval '1' year
group by
        l_shipmode
order by
        l_shipmode
limit 1;

--Query 19:
select
        sum(l_extendedprice* (1 - l_discount)) as revenue
from
        lineitem,
        part
where
        (
                p_partkey = l_partkey
                and p_brand = 'Brand#54'
                and p_container in ('SM CASE', 'SM BOX', 'SM PACK', 'SM PKG')
                and l_quantity >= 4 and l_quantity <= 4 + 10
```

```
            and p_size between 1 and 5
            and l_shipmode in ('AIR', 'AIR REG')
            and l_shipinstruct = 'DELIVER IN PERSON'
    )
    or
    (
            p_partkey = l_partkey
            and p_brand = 'Brand#51'
            and p_container in ('MED BAG', 'MED BOX', 'MED PKG', 'MED PACK')
            and l_quantity >= 11 and l_quantity <= 11 + 10
            and p_size between 1 and 10
            and l_shipmode in ('AIR', 'AIR REG')
            and l_shipinstruct = 'DELIVER IN PERSON'
    )
    or
    (
            p_partkey = l_partkey
            and p_brand = 'Brand#21'
            and p_container in ('LG CASE', 'LG BOX', 'LG PACK', 'LG PKG')
            and l_quantity >= 28 and l_quantity <= 28 + 10
            and p_size between 1 and 15
            and l_shipmode in ('AIR', 'AIR REG')
            and l_shipinstruct = 'DELIVER IN PERSON'
    )
limit 1;
```

F $\mathcal{Q}^{\text{TPC}^*}$

ID	Query
1	`SELECT *, probability_evaluate (provenance ()) FROM ( SELECT DISTINCT l_returnflag, l_linestatus FROM lineitem WHERE l_shipdate<=date '1998-09-01' GROUP BY l_returnflag, l_linestatus ) t;`
3	`SELECT l_orderkey FROM customer, orders, lineitem WHERE c_mktsegment='BUILDING' AND c_custkey=o_custkey AND l_orderkey=o_orderkey AND o_orderdate<date '1995-03-15' AND l_shipdate>date '1995-05-15' GROUP BY l_orderkey, o_orderdate, o_shippriority LIMIT 20;`
4	`SELECT *, probability_evaluate (provenance ()) FROM ( SELECT DISTINCT o_orderpriority FROM orders, lineitem WHERE o_orderdate>=date '1993-07-01' AND o_orderdate<date '1993-10-01' AND l_orderkey=o_orderkey AND l_commitdate<l_receiptdate GROUP BY o_orderpriority ) t;`
12	`SELECT *, probability_evaluate (provenance ()) FROM (SELECT DISTINCT l_shipmode FROM orders, lineitem WHERE o_orderkey=l_orderkey AND (l_shipmode='MAIL' OR l_shipmode='SHIP') AND l_commitdate<l_receiptdate AND l_shipdate<l_commitdate AND l_receiptdate>='1992-01-01' AND l_receiptdate<'1999-01-01' GROUP BY l_shipmode) t;`
15	`SELECT *, probability_evaluate (provenance ()) FROM ( SELECT DISTINCT s_suppkey, s_name, s_address, s_phone FROM supplier, lineitem WHERE s_suppkey=l_suppkey AND l_shipdate>=date '1991-10-10' AND l_shipdate<date '1992-01-10' GROUP BY s_suppkey, s_name, s_address, s_phone ) t;`