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REGULAR PAPER

Query reverse engineering

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Abstract In this paper, we introduce a new problem termed *query reverse engineering* (QRE). Given a database D and a result table T—the output of some *known* or *unknown* query Q on D—the goal of QRE is to reverse-engineer a query Q' such that the output of query Q' on database D (denoted by $Q'(D)$) is equal to T (i.e., $Q(D)$). The QRE problem has useful applications in database usability, data analysis, and data security. In this work, we propose a data-driven approach, TALOS for **T**ree-based classifier with **A**t **L**east **O**ne **S**emantics, that is based on a novel dynamic data classification formulation and extend the approach to efficiently support the three key dimensions of the QRE problem: whether the input query is known/unknown, supporting different query fragments, and supporting multiple database versions.

Keywords Query reverse engineering · Instance-equivalent queries · At-least-one semantics

1 Introduction

This paper introduces a new problem, termed *query reverse engineering* (QRE), that aims to reverse-engineer a query given its output from a database. Formally, given a database D and a result table T, which is the output of some *known* or *unknown* query Q on D; the goal of QRE is to reverse-engineer a query Q' such that the output of query Q' on database D (denoted by $Q'(D)$) is equal to T (i.e., $Q(D)$). We say that two queries Q and Q' are *instance-equivalent queries (IEQs)* w.r.t. a database D if their results (w.r.t. D) are equal, i.e., $Q \equiv_D Q'$.

In the following, we highlight several use cases of QRE.

Database usability The most obvious application of QRE is in database usability. Consider the situation when a user wants to evaluate a query Q on a database D. Instead of simply returning the query result $Q(D)$ to the user, the database system can also apply QRE to derive instance-equivalent queries Q' of Q that describe alternative characterizations of tuples in the query result of Q.

Example 1 Suppose a user issues a query Q_1 to a movie database to search for movies that are directed by "James Cameron" since 1997. The query result $Q_1(D)$ consists of two movies: "Avatar" and "Titanic." By applying QRE, the database system could also have augmented the result the following instance-equivalent query Q'_1 (w.r.t. D) "select movies that have gross revenue greater than $2 billion." The query Q'_1 provides a different and insightful characterization of the query result to the user.

As the above example illustrates, the ability to return instance-equivalent queries for a given query Q can reveal interesting properties of the query result $Q(D)$. In addition, unusual or surprising IEQs can be useful for uncovering hidden relationships among the data. In several instances, simpler or easier to understand relationships may be uncovered, which can again aid in the understanding of the data contained within the complex database. As another example,

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consider a skyline query Q_2 to search for people with maximal capital gain and minimal age in the U.S. Census Income data set.[1] An instance-equivalent query Q'_2 of Q_2 provides a simpler characterization of Q_2 as "find people who are very young ($age \leq 17$) and have low capital gain (<5,000) or who have very high capital gain (>27,828), work in the protective service and whose race is not classified as others."

Besides providing alternative characterizations of the query results, IEQs can also help users to better understand the database schema. Since many enterprise data schema are very complex and large, the part of the database schema that is referenced by the user's query may be quite different from that referenced by an IEQ. The discovery of this alternative "part" in the schema to generate an instance-equivalent query can aid the user's understanding of the database schema or potentially help refine the user's initial query.

Example 2 Consider the baseball data set[2] and a query Q_3 that finds managers of "Cincinnati Reds" team during the years from 1982 to 1988. This query involves the join between two relations *Manager* and *Team*. An instance-equivalent query Q'_3 of Q_3 reveals that some of these managers were also the *players* of "Cincinnati Reds" team at the same time they managed the team. The IEQ Q'_3 has revealed the alternative schema part that involves the joins among *Manager*, *Team*, *Master*, and *Batting* relations and provided users useful information about these player-managers.

Explaining why-not questions QRE can also be applied to provide an explanation capability that allows users to seek clarifications on unexpected query results. For example, consider the scenario where a user has issued a query and is surprised to find that the returned query result does not contain certain expected tuples. It would be very useful to have some functionality that enables the user to ask a follow-up query on why those expected tuples are missing from the query result. The idea of QRE can be applied to automatically generate one or more *refined query*, whose result includes both the original query's result as well as the missing tuple(s). The refined queries would serve as a form of explanation for the missing tuples: They not only could help identify the original query predicates that are responsible for the missing tuples, but also suggest alternative means to "fix" the missing tuple(s). Essentially, QRE treats the query's result $Q(D)$ together with the missing tuples as the output result of some query Q' and derives IEQs for Q' as refined queries [28].

Data exploration & analysis Another important class of QRE applications is in scenarios where the input query Q is unknown.

Consider a view V (defined on a database D) which may have been derived manually (e.g., a user selected some tuples of the database of interest to her) or by an application program that is no longer available (e.g., the program is no longer maintained or is lost). Therefore, given only the view result V on the database D, it will be very useful to be able to derive instance-equivalent queries Q' of the unknown query for V (i.e., $V = Q'(D)$) that describe the characteristics of such tuples in V. In data exploration, such scenarios arise when the documentation and meta-data for the data sets being analyzed are incomplete, inaccurate, or missing. As an example, in the AT&T's Bellman project [12], the data set made available to data analysts is often in the form of a delimited ASCII text file representing the output result of some query, where the query is not available for various reasons. Clearly, it will be useful to reverse-engineer the queries to help make sense of the data before performing further analysis tasks (e.g., data mining).

Database security QRE may also have interesting applications in database security where attackers who have some prior domain knowledge of the data may attempt to derive sensitive information. For example, if an attacker is aware of the existing correlation structure in the data, they can easily use this information to formulate two or more separate queries that on paper look very different (e.g., using different selection criteria), but in reality may be targeting the same set of tuples in the database. Such sets or groups of queries can potentially be used to reverse-engineer the privacy preserving protocol in use. Subsequently, sensitive information can be gleaned. As a specific example, consider a protocol such as ϵ-diversity [32], which relies on detecting how similar the current query is with a previous set of queries answered by the database, to determine whether the current query can be answered without violating the privacy constraints. By generating IEQs for the historical queries, the collection of historical queries is enlarged thereby strengthening the protection against such kinds of attacks.

1.1 Contributions

Despite its usefulness, there is very little work on the QRE problem. An early version of this paper [29] introduces the *query by output (QBO)* problem where the focus is on deriving select-project-join instance-equivalent queries (SPJ-IEQs) given an input query Q, database D, and the query's result $Q(D)$. This paper is a significant extension that generalizes QBO along three key dimensions of the problem space: (1) The original query Q is unknown; (2) the derived query Q' belongs to a more expressive query fragment beyond the simple select-project-join (SPJ) query fragment; and (3) the database D has multiple versions.

Unknown query First, unlike the QBO problem where the original query Q is given as a part of the input (along with

[1] http://archive.ics.uci.edu/ml/datasets/Adult.

[2] http://baseball1.com/statistics/.

the database D), Q is unknown in the QRE problem, and the absence of Q makes it more challenging to identify the relations to be included in the reverse-engineered query Q' to generate the given result table T (i.e., $T \equiv Q'(D)$).

Supporting more expressive IEQs Second, for QRE to be more practical, QRE should support more expressive IEQs beyond the SPJ fragment (referred to as *SPJ-IEQs*) such as SPJ-IEQs with union operators (referred to as *SPJU-IEQs*) and SPJ-IEQs with group-by aggregation operators (referred to as *SPJA-IEQs*). With this enhanced expressiveness, QRE becomes useful in more application domains such as data integration, where SPJU-IEQs are predominant. In data integration systems, the goal is to combine data residing at different sources to provide users with a unified view of these data [13]. The *global-as-view* integration approach requires that the global schema be expressed in terms of the data sources, which necessitates a query over the global schema to be reformulated in terms of a set of queries over the data sources. Thus, the QRE problem in this context requires deriving an IEQ that is a union of sub-queries over the data sources given a result table T that is generated by the integration system. Another application domain that is supported by the enhanced expressiveness of IEQs is in data analysis, where SPJA-IEQs are very common due to aggregation computations (e.g., group-by aggregation queries in OLAP applications).

Multiple database versions Third, in contrast to the QBO problem where the specific database D is known and given as part of the input, the setting of the QRE problem is often more general where there could be multiple database versions. We consider two specific scenarios of this generalization and the additional challenges introduced by them.

The first scenarios occur in exploratory/analysis applications: It is typically the case that the time when a user needs to reverse-engineer a query Q' for a result table T occurs much later than the time when T was actually produced. Thus, it may not be meaningful or possible to derive Q' from the current version of the database, as this could be very different from the version that T was generated from. Specifically, given a result table T and a sequence of database versions $< D_1, D_2, \cdots, D_\ell >$, a specific goal may be to determine the most recent database version D_i, $i \in [1, \ell]$ and query Q' such that $Q'(D_i) = T$. Depending on the applications, other variations of the problem (e.g., finding the earliest database version or all versions) are also possible. The performance challenge is how to efficiently determine both D_i as well as Q' for a given result T.

In the second scenario, the input to the QRE problem is a sequence of database versions and result pairs (D_1, T_1), (D_2, T_2), $\ldots$ (D_ℓ, T_ℓ), where each T_i is the result of the *same* unknown query Q on database version D_i (i.e., $T_i = Q(D_i)$). For example, the T_i's could correspond to weekly reports generated by the same query on weekly versions of the database, or Q could be a continuous long standing query that is run periodically on different snapshots of the database. In this more general setting with multiple database and result versions, the challenge is how to efficiently reverse-engineer a query Q' such that $Q'(D_i) = T_i$ for each $i \in [1, \ell]$.

In summary, this paper makes the following contributions. First, we introduce the novel problem of QRE and propose a solution, TALOS, that models the QRE problem as a data classification task with a unique property that we term *at-least-one semantics*. Second, to handle data classification with this new semantics, we develop a new dynamic class labeling technique and propose effective optimization techniques to efficiently compute IEQs. Third, to the best of our knowledge, TALOS is the first comprehensive solution for the query reverse engineering problem that covers three dimensions of the problem space: The original query is known/unknown, the type of IEQ fragement (i.e., SPJ with possibly union/aggregation), and the presence of multiple database versions. Finally, our experimental evaluation of TALOS demonstrates its efficiency and effectiveness in generating interesting IEQs.

Organization In Sect. 2, we provide some basic background and describe an exemplar scenario for QRE that will serve as a running example throughout this article. Section 3 presents the concept of instance-equivalent queries and establishes some complexity results for the QRE problem. Sections 4, 5 and 6 present our solution, TALOS, to derive IEQs. Section 7 discusses criteria for ranking IEQs. Section 8 presents an extension to handle unknown input query, and Sect. 9 presents an extension to support multiple database versions. Section 10 presents an experimental study to evaluate the effectiveness of TALOS. Section 11 presents related work. Finally, we conclude in Sect. 12. Proofs of theoretical results and other details are given in the Appendix of ESM.

2 Preliminaries

The QRE problem takes as inputs a database D, an optional query Q, and the query's output $Q(D)$ (w.r.t. D) to compute one or more IEQs Q', where Q and Q' are IEQs if $Q \equiv_D Q'$. We refer to Q as the *input query*, $Q(D)$ as the *given result table*, and Q' as the *output query*.

In this paper, we consider three fragments of SPJ relational queries for IEQs: (1) SPJ queries, which are the basic Select-Project-Join queries, (2) SPJU queries, which are of the form $Q_1\ union\ Q_2\ \ldots union\ Q_n$, where each Q_i is an SPJ query, and (3) SPJA queries, which correspond to simple SPJ SQL queries with aggregation operators in the select-clause and an optional group-by clause.

Given a query Q, we use *rel(Q)* to denote the collection of relations involved in Q (i.e., relations in SQL's from-clause); *proj(Q)* to denote the set of projected attributes in Q (i.e., attributes in SQL's select-clause); and *sel(Q)* to denote the set of selection predicates in Q (i.e., conditions in SQL's where-clause).

Consider two attributes: attribute A in relation R and attribute B in relation S. If $\pi_B(S) \subseteq \pi_A(R)$, we say that $A covers B$ and refer to A as a *covering attribute* of B. If $\pi_B(S) \cap \pi_A(R) \neq \emptyset$, we say that $A partially covers B$ and refer to A as a *partially covering attribute* of B. Clearly, A partially covers B if and only if B partially covers A.

For ease of presentation and without loss of generality, we express each Q' as a relational algebra expression. To keep our definitions and notations simple and without loss of generality, we shall assume that there are no multiple instances of a relation in Q and Q'.

Given a database, we use $\mathcal{SG}$ to denote its *schema graph* where each node in $\mathcal{SG}$ represents a relation and each edge between two nodes represents a primary-key-foreign-key relationship between the relations corresponding to the nodes.

Running example We use a database housing baseball statistics as our running example as well as in our experiments. Part of the schema is illustrated in Fig. 1, where the key attribute names are shown in bold. The *Master* relation describes information about each player (identified by *pID*): The attributes *name*, *country*, *weight*, *bats*, and *throws* refer to his name, birth country, weight (in pounds), batting hand (left, right, or both), and throwing hand (left or right), respectively. The *Batting* relation provides the number of home runs (*HR*) of a player when he was playing for a team in a specific year and season (*stint*). The *Salaries* relation specifies the salary obtained by a player in a specific year. The *Team* relation specifies the rank obtained by a team for a specified year.

pID	name	country	weight	bats	throws
P1	A	USA	85	L	R
P2	B	USA	72	R	R
P3	C	USA	80	R	L
P4	D	Germany	72	L	R
P5	E	Japan	72	R	R

(a)

pID	**year**	**stint**	team	HR
P1	2001	2	PIT	40
P1	2003	2	ML1	50
P2	2001	1	PIT	73
P2	2002	1	PIT	40
P3	2004	2	CHA	35
P4	2001	3	PIT	30
P5	2004	3	CHA	60

(b)

pID	**year**	salary
P1	2003	80
P3	2002	35
P5	2004	60

(c)

team	**year**	rank
PIT	2001	7
PIT	2002	4
CHA	2004	3

(d)

Fig. 1 Running example—baseball data set D. **a** Master. **b** Batting. **c** Salaries. **d** Team

3 Instance-equivalent queries (IEQs)

3.1 Strong versus weak IEQs

Our basic definition of *instance-equivalent queries (IEQs)* requires that the IEQs Q and Q' produce the same output (w.r.t. some database D), i.e., $Q \equiv_D Q'$. The advantage of this simple definition is that it does not require the knowledge of Q to derive Q', which is particularly useful for QRE applications where Q is either missing or not provided. However, there is a potential "accuracy" trade-off that arises from the simplicity of this weak form of equivalence: An IEQ may be "semantically" quite different from the input query that produced $Q(D)$ as the following example illustrates.

Example 3 Consider the following three queries on the baseball database D in Fig. 1:

$$Q_1 = \pi_{country}(\sigma_{bats=\text{"R"} \wedge throws=\text{"R"}}(Master)),$$
$$Q_2 = \pi_{country}(\sigma_{bats=\text{"R"} \wedge weight \leq 72}(Master)), \text{ and}$$
$$Q_3 = \pi_{country}(\sigma_{bats=\text{"R"}}(Master)).$$

Observe that although all three queries produce the same output after projection ({USA, Japan}), only Q_1 and Q_2 select the same set of tuples $\{P2, P5\}$ from *Master*. Specifically, if we modify the queries by replacing the projection attribute "country" with the key attribute "pID", we have $Q_1(D) =$ { P2, P5}, $Q_2(D) =$ {P2, P5}, and $Q_3(D) =$ {P2, P3, P5}. Thus, while all three queries are IEQs, we see that the equivalence between Q_1 and Q_2 is actually "stronger" (compared to that between Q_1 and Q_3) in that both queries actually select the same set of relation tuples.

If Q is provided as part of the input, then we can define a stronger form of instance equivalence as suggested by the above example. Intuitively, the stricter form of instance equivalence not only ensures that the instance-equivalent queries produce the same output (w.r.t. some database D), but it also requires that their outputs be projected from the same set of "core" tuples. We now formally characterize weak and strong IEQs based on the concepts of *core relations* and *core queries*.

Core relations Given a query Q, we say that $S \subseteq rel(Q)$ is a set of *core relations* of Q if S is a minimal set of relations such that for every attribute $R_i.A \in proj(Q)$, (1) $R_i \in S$, or (2) Q contains a chain of equality join predicates "$R_i.A = \cdots = R_j.B$" such that $R_j \in S$.

Intuitively, a set of core relations of Q is a minimal set of relations in Q that "cover" all the projected attributes in Q. As an example, consider a query $Q = \pi_{R_1.X}\sigma_p(R_1 \times R_2 \times R_3)$ where $p = (R_1.X = R_3.Y) \wedge (R_2.Z = R_3.Z)$. Here, Q has two sets of core relations, $\{R_1\}$ and $\{R_3\}$: $\{R_1\}$ is clearly a set of core relations since the only projected attribute in Q is from R_1, while $\{R_3\}$ is another set of core relations due to the join predicate "$R_1.X = R_3.Y$."

Core queries Given a query Q and a set of relations $S \subseteq rel(Q)$, we use Q_S to denote the query that is derived from Q by replacing $proj(Q)$ with the key attribute(s) of each relation in S. If S is a set of core relations of Q, we refer to Q_S as a *core query* of Q.

Consider two IEQs Q and Q' (w.r.t. a database D), i.e., $Q \equiv_D Q'$. We say that Q and Q' are *strong IEQs* if Q has a set of core relations S such that: (1) ${Q'}_S$ is a core query of Q' and (2) $Q_S(D)$ and ${Q'}_S(D)$ are equal. IEQs that are not strong are classified as *weak IEQs*.

The strong IEQ definition essentially requires that both Q and Q' share a set of core relations such that $Q(D)$ and $Q'(D)$ are projected from the same set of selected tuples from these core relations. Thus, in Example 3, Q_1 and Q_2 are strong IEQs, whereas Q_1 and Q_3 are weak IEQs.

Note that in our definition of strong IEQ, we only impose moderate restrictions on Q and Q' (relative to the weak IEQ definition) so that the space of strong IEQs is not overly constrained and that the strong IEQs generated are hopefully both interesting as well as meaningful.

As in the case with weak IEQs, two strong IEQs can involve different sets of relations. As an example, suppose query Q selects pairs of records from two core relations, *Supplier* and *Part*, that are related via joining with a (non-core) *Supply* relation. Then it is possible for a strong IEQ Q' to relate the same pair of core relations via a different relationship (e.g., by joining with a different non-core *Manufacture* relation).

We believe that each of the notions of query equivalence has useful applications in different contexts depending on the available type of information about the input query and database. At one extreme, if both Q and the database integrity constraints are available, we can compute semantically strong equivalent queries. At the other extreme, if only $Q(D)$ and the database D are available, we can only compute weak IEQs. Finally, if both Q and the database D are available, we can compute both weak and strong IEQs.

3.2 Precise versus approximate IEQs

It is also useful to permit some perturbation so as to include IEQs that are "close enough" to the original query. Perturbations could be in the form of extra records or missing records or a combination thereof. Such generalizations are necessary in situations where there are no precise IEQsand useful for cases where the computational cost for finding precise IEQs is considered unacceptably high. Moreover, a precise IEQ Q' might not always provide insightful characterizations of $Q(D)$, as Q' could be too "detailed" with many join relations and/or selection predicates.

The imprecision of a weak SPJ- or SPJU-IEQ Q' of Q (w.r.t. D) can be quantified by $|Q(D) - Q'(D)| + |Q'(D) - Q(D)|$; the imprecision of a strong IEQ can be quantified similarly. Thus, Q' is considered an approximate (strong/weak) IEQ of Q if its imprecision is positive; otherwise, Q' is a precise (strong/weak) IEQ. For SPJA-IEQs, the imprecision metric is more involved as it needs to take into account matching tuples in $Q(D)$ and $Q'(D)$ that differ only on their aggregated attribute value(s); the details are presented in the Appendix.

3.3 Complexity results

In this section, we establish some complexity results for the QRE problem.

Theorem 1 *Given an input query Q, we define QRE_S to be the problem to find the output query Q', where Q' is a conjunctive query that involves only projection and selection (with predicates of the form "A_i op c", where A_i is an attribute, c is constant, and op $\in \{<, \leq, =, \neq, >, \geq\}$) such that: (1) $Q' \equiv_D Q$ and (2) the number of operators (AND, OR, and NOT) used in the selection condition is minimized. Then QRE_S is unlikely to be in P.*

Theorem 2 *Given an input query Q, we define QRE_U to be the problem to find an SPJU-IEQ Q' of Q w.r.t. a database D of the form $Q' = Q_1\ union \cdots union\ Q_k$ where each Q_i is an SPJ query such that (1) $Q' \equiv_D Q$ and (2) k is minimized. Then QRE_U is NP-hard.*

Theorem 3 *Given an input query Q, we define QRE_A to be the problem to find an SPJA-IEQ Q' of Q w.r.t. a database D where each aggregation operator (SUM or AVG)oes not involve any arithmetic expression in the operator's argument. Then QRE_A is NP-hard.*

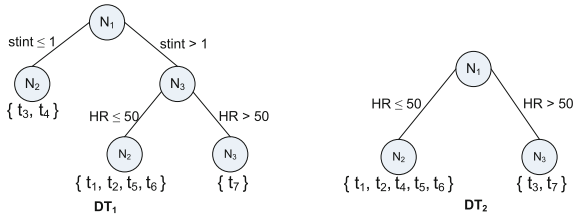
Given the above results, we consider relational queries Q where the select-clause refers to either some relation's attribute, or a value computed by an aggregation operator (COUNT, SUM, AVG, MIN, or MAX) that does not involve any arithmetic expression in the operator's argument to ensure that Q' can be derived from $Q(D)$ efficiently. We also require that $Q(D) \neq \emptyset$ for the problem to be interesting. Other fragments of SQL queries (e.g., SPJA queries with HAVING clause, queries with arithmetic expressions) are beyond the scope of this paper.

	pID	name	country	weight	bats	throws	year	team	stint	HR
t_1	P1	A	USA	85	L	R	2001	PIT	2	40
t_2	P1	A	USA	85	L	R	2003	ML1	2	50
t_3	P2	B	USA	72	R	R	2001	PIT	1	73
t_4	P2	B	USA	72	R	R	2002	PIT	1	40
t_5	P3	C	USA	80	R	L	2004	CHA	2	35
t_6	P4	D	Germany	72	L	R	2001	PIT	3	30
t_7	P5	E	Japan	72	R	R	2004	CHA	3	60

(a)

Name
B
E

(b)



(c)

Fig. 2 Example of deriving IEQs for Q_4 on D. **a** $J = Master \bowtie_{pID} Batting$. **b** $Q_4(D)$. **c** Decision trees DT_1 and DT_2

4 Overview of approach

In this section, we give an overview of our approach, named TALOS (**T**ree-based classifier with **A**t **L**east **O**ne **S**emantics), for the QRE problem.

4.1 Data classification formulation

Given an input result table $Q(D)$, to generate an SPJ Q' that is an IEQ of Q, we basically need to determine the three components of Q': $rel(Q')$, $sel(Q')$, and $proj(Q')$. Clearly, if $rel(Q')$ contains a set of core relations of Q, then $proj(Q')$ can be trivially derived from these core relations.[3] Thus, the possibilities for Q' depend mainly on the options for both $rel(Q')$ and $sel(Q')$. Between these two components, enumerating different $rel(Q')$ is the easier task, as $rel(Q')$ can be obtained by choosing a subgraph G of the schema graph $\mathcal{SG}$ such that G contains a set of core relations of Q: $rel(Q')$ is then given by all the relations represented in G. Note that it is not necessary for $rel(Q) \subseteq rel(Q')$, as Q may contain some relations that are not core relations. The reason for exploring different possibilities for $rel(Q')$ is to find interesting alternative characterizations of $Q(D)$ that involve different join paths or selection conditions from those in Q. TALOS enumerates different schema subgraphs by starting out with minimal subgraphs that contain a set of core relations of Q and then incrementally expanding the minimal subgraphs to generate larger, more complex subgraphs.

We now come to the most critical and challenging part of our solution, which is how to generate "good" $sel(Q')$'s such that each $sel(Q')$ is not only succinct (without too many conditions) and insightful, but also minimizes the imprecision between $Q(D)$ and $Q'(D)$ if Q' is an approximate IEQ. We propose to formulate this problem as a *data classification* task as follows.

Consider the relation J that is computed by joining all the relations in $rel(Q')$ based on the foreign key joins represented in G. Without loss of generality, let us suppose that we are looking for weak IEQs Q'. Let L denote the ordered listing of the attributes in $proj(Q')$ such that the schema of $\pi_L(J)$ and $Q(D)$ are equivalent.[4] J can be partitioned into two disjoint subsets, $J = J_{in} \cup J_{out}$ such that $\pi_L(J_{in}) \subseteq Q(D)$ and $\pi_L(J_{out}) \cap Q(D) = \emptyset$. For the purpose of deriving $sel(Q')$, one simple approach to classify the tuples in J is to label the tuples in J_{out}, which do not contribute to the query's result $Q(D)$, as *negative tuples*, and label the tuples in J_{in} as *positive tuples*.

Example 4 To illustrate how we derive IEQs, consider the following query on the baseball database D:

$Q_4 = \pi_{name}\,(\sigma_{bats=\text{"R"} \wedge throws=\text{"R"}}\ Master)$. Note that $Q_4(D) = \{B, E\}$. Suppose that the schema subgraph G considered contains both *Master* and *Batting*, i.e., $rel(Q'_4) = \{\text{Master, Batting}\}$. The output of $J = \text{Master} \bowtie_{pID} \text{Batting}$ is shown in Fig. 2a. Using t_i to denote the i^{th} tuple in J, we observe that J is partitioned into $J_{out} = \{t_1, t_2, t_5, t_6\}$ and $J_{in} = \{t_3, t_4, t_7\}$, since $\pi_{name}(J_{in}) = Q(D)$ and $\pi_{name}(J_{out}) \cap Q(D) = \emptyset$. We therefore label tuples t_3, t_4 and t_7 as positive tuples, and the other tuples (t_1, t_2, t_5, t_6) as negative tuples.

Given the labeled tuples in J, the problem of finding a $sel(Q')$ can now be viewed as a data classification task to separate the positive and negative tuples in J: $sel(Q')$ is given by the selection conditions that specify the positive tuples. A natural solution is to examine whether an off-the-shelf data classifier can give us what we need. To determine

[3] Note that even though the definition of a weak IEQ Q' of Q does not require the queries to share a set of core relations, we find this restriction to be a reasonable and effective way to obtain "good" IEQs.

[4] If the search is for strong IEQs, then the discussion remains the same except that L is the ordered listing of the key attributes of a set of core relations S of Q, and we replace $Q(D)$ by $Q_S(D)$.

what kind of classifier to use, we must consider what we need to generate our desired IEQ Q'. Clearly, the classifier should be efficient to construct, and the output should be easy to interpret and express using SQL; that is, the output should be expressible in axis parallel cuts of the data space. These criteria rule out a number of classifier systems such as neural networks, k-nearest neighbor classification, Bayesian classifiers, and support vector machines [21]. Rule-based classifiers or decision trees (a form of rule-based classifier) are a natural solution in this context. TALOS uses a decision tree classifier for generating $sel(Q')$.

By computing IEQs in this way, our approach also generates a useful by-product: The set of labeled tuples in J could be used to derive the potential data provenance (i.e., the source tuples) of each output tuple in the query result.

4.1.1 Decision tree construction

We now briefly describe how a simple binary decision tree is constructed to classify a set of data records D. For expository simplicity, assume that all the attributes in D have numerical domains. A decision tree DT is constructed in a top-down manner. Each leaf node N in the tree is associated with a subset of the data records, denoted by D_N, such that D is partitioned among all the leaf nodes. Initially, DT has only a single leaf node (i.e., its root node), which is associated with all the records in D. Leaf nodes are classified into pure and non-pure nodes depending on a given goodness criterion. Common goodness criteria include entropy, classification error, and the Gini index [21]. At each iteration of the algorithm, the algorithm examines each non-pure leaf node N and computes the best split for N that creates two child nodes, N_1 and N_2, for N. Each split is computed as a function of an attribute A and a split value v associated with the attribute. Whenever a node N is split (w.r.t. attribute A and split value v), the records in D_N are partitioned between D_{N_1} and D_{N_2} such that a tuple $t \in D_N$ is distributed into D_{N_1} if $t.A \leq v$; and D_{N_2}, otherwise.

A popular goodness criterion for splitting is the Gini index, which is computed as follows. For a data set S with k distinct classes, its Gini index is given by

$$Gini(S) = 1 - \sum_{j=1}^{k} \left(f_j^2\right) \tag{1}$$

where f_j denotes the fraction of records in S belonging to class j. Thus, if S is split into two subsets S_1 and S_2, then the Gini index of the split is given by

$$Gini(S_1, S_2) = \frac{|S_1|\ Gini(S_1) + |S_2|\ Gini(S_2)}{|S_1| + |S_2|} \tag{2}$$

where $|S_i|$ denotes the number of records in S_i. The general objective is to pick the splitting attribute whose best splitting value reduces the Gini index the most (i.e., the ideal goal is to reduce Gini to 0 resulting in all pure leaf nodes).

Example 5 Continuing with Example 4 when we have labeled tuples t_3, t_4, t_7 as positive and the other tuples as negative. Using the above algorithm, we build the decision tree DT_1 that separates the positive and negative tuples in J, as shown in Fig. 2c. (Ignore for now the decision tree DT_2 in this figure.) The IEQ derived from DT_1 is given by Q'_4: $\pi_{name}\sigma_{stint\leq 1 \vee (stint>1 \wedge HR>50)}\ (Master \bowtie Batting)$.

4.1.2 An overview of TALOS

The overall approach of TALOS is outlined in Algorithm 1. TALOS takes as inputs a query Q, a database instance D, and the query result $Q(D)$ of Q on D. The output of TALOS is a set R of IEQs of Q. First, TALOS derives the set of core relations of Q (line 1). For each schema subgraph G that contains the set of core relations, TALOS computes the join J of relations in G (line 4). TALOS next enumerates a set of decision trees for J and derives an IEQ of Q for each of the decision trees (lines 5-8). Finally, TALOS returns the collection R of IEQs of Q.

Algorithm 1: TALOS(Q, D, Q(D))

```
1 let S be the set of core relations of Q
2 let R be the set of IEQs of Q which is initialized to be empty
3 foreach schema subgraph G that contains S do
4 |   let J be the join of the relations in G
5 |   Enumerate a set of decision trees for J
6 |   foreach decision tree DT for J do
7 |   |   Derive the IEQ Q' corresponding to DT
8 |   |   Add Q' into R
9 return R
```

As the search space for IEQs can be very large, particularly with large complex database schema where each relation has foreign key joins with other relations, the search space could be restricted by providing users with certain control knobs in the form of hint/preference specifications. The following five are some examples of control knobs to limit the search space. The first three knobs enable users to constrainhe complexity of the derived IEQs in terms of the number of relations/conjuncts/disjuncts, while the last two knobs enable users to specify more schema-specific information (relations/attributes) to control the search space.

(K1) Constraining the number of relations in the from-clause of each IEQ to be in the range $[n_{min}, n_{max}]$. This control knob constrains the number of vertices of each schema subgraph G to be in the range $[n_{min}, n_{max}]$.
(K2) Constraining the number of disjunctive clauses in the query's selection condition to be in the range

$[l_{min}, l_{max}]$. Recall that the selection condition of an IEQ is expressed in disjunctive normal form where each disjunctive clause is a conjunction of selection predicates. This is implemented by limiting the number of leaf nodes that are selected in the derived decision trees to be in the range $[l_{min}, l_{max}]$.

(K3) Constraining the number of conjunctions in each disjunctive clause to be in the range $[h_{min}, h_{max}]$. This is implemented by limiting the height of the derived decision trees to be in the range $[h_{min}, h_{max}]$.

(K4) Specifying a specific set of relations to be included in (or excluded from) Q'. This knob controls the space of schema subgraphs considered.

(K5) Specifying a specific set of attributes to be included in (or excluded from) the selection predicates in Q'. This knob controls the space of attributes considered for decision tree construction.

We discuss metrics to rank IEQs for a query in Sect. 7.

4.2 Challenges

There are two key challenges in adapting decision tree classifier for the QRE problem.

4.2.1 Challenge 1: At-least-one semantics

The first challenge concerns the issue of how to assign class labels in a flexible manner without over constraining the classification problem and limiting its effectiveness. Contrary to the impression given by the above simple class labeling scheme, the task of assigning class labels to J is actually a rather intricate problem. The reason is that multiple tuples in J_{in} can be projected to the same tuple in $\pi_L(J_{in})$. Recall that in the simple class labeling scheme described, a tuple t is labeled positive if and only if $t \in J_{in}$. However, note that it is possible to label only a subset of tuples $J^+_{in} \subseteq J_{in}$ as positive (with tuples in $J - J^+_{in}$ labeled as negative) and yet achieve $\pi_L(J^+_{in}) = \pi_L(J_{in})$ (without affecting the imprecision of Q'). In other words, the simple scheme of labeling all tuples in J_{in} as positive is just one (extreme) option out of many other possibilities. For instance, in Example 4, it is possible to label tuples in $J^+_{in} = \{t_3, t_7\} \subset J_{in}$ as positive and tuples in $J - J^+_{in}$ as negative and yet achieve $\pi_{name}(J^+_{in}) = \pi_{name}(J_{in})$.

We now discuss more precisely the various possibilities of labeling positive tuples in J to derive different $sel(Q')$. Let $\pi_L(J_{in}) = \{t_1, \cdots, t_k\}$. Then J_{in} can be partitioned into k subsets, $J_{in} = P_1 \cup \cdots \cup P_k$, where each $P_i = \{t \in J_{in} \mid$ the projection of t on L is $t_i\}$. Thus, each P_i represents the subset of tuples in J_{in} that project to the same tuple in $\pi_L(J_{in})$. Define J^+_{in} to be a subset of tuples of J_{in} such that it consists of at least one tuple from each subset P_i. Clearly, $\pi_L(J^+_{in}) = \pi_L(J_{in})$, and there is a total of $\prod_{i=1}^{k}(2^{|P_i|} - 1)$ possibilities for J^+_{in}. For a given J^+_{in}, we can derive $sel(Q')$ using a data classifier by labeling the tuples in J^+_{in} as positive and the remaining tuples in $J - J^+_{in}$ as negative.

Based on the above discussion on labeling tuples, each tuple in J can be classified as either a *bound tuple* or *free tuple* depending on whether there is any freedom to label the tuple. A tuple $t \in J$ is a *bound tuple* if either (1) $t \in J_{out}$, in which case t must be labeled negative, or (2) t is the only tuple in some subset P_i, in which case t must certainly be included in J^+_{in} and be labeled positive. Otherwise, t is a *free tuple*; that is, t is in some subset P_i that contains more than one tuple. Thus, a free tuple could be labeled positive or negative. In Example 4, J_{in} is partitioned into two subsets: $P_1 = \{t_3, t_4\}$ and $P_2 = \{t_7\}$, where P_1 and P_2 contribute to the outputs "B" and "E," respectively. The tuples in J_{out} (i.e., t_1, t_2, t_5, t_6) and P_2 (i.e., t_7) are bound tuples, while the tuples in P_1 are free tuples.

In contrast to the conventional classification problem where each record in the input data comes with a well defined class label, the classification problem formulated for QRE has the unique characteristic where there is some flexibility in the class label assignment. We refer to this property as *at-least-one semantics* in the sense that at least one tuple from each subset P_i must be labeled positive. For instance, to derive an IEQ of Q_4, at least one of the free tuples in P_1 must be labeled positive. To the best of our knowledge, we are not aware of any work that has addressed the data classification problem involving at-least-one semantics.

An obvious approach to solve the at-least-one semantics variant is to map the problem into the traditional variant by first applying some arbitrary class label assignment that is consistent with the at-least-one semantics. In our experimental study, we compare against two such static labeling schemes, namely (1) `NI`, which labels all free tuples as positive and (2) `RD`, which labels a random non-empty subset of free tuples in each P_i as positive.[5] However, such static labeling schemes do not exploit the flexible class labeling opportunities to compute optimal node splits for decision tree construction.

To avoid the limitations of static labeling schemes, `TALOS` employs a novel *dynamic class labeling scheme* to compute optimal node splits for decision tree construction without having to enumerate an exponential number of combinations of class labeling schemes for the free tuples. Continuing with Example 4, if t_3 is labeled positive and t_4 is labeled negative, then DT_2 in Fig. 2c is a simpler decision tree constructed by partitioning J based on a selection predicate on attribute

[5] We also experimented with a scheme that randomly labels only one free tuple for each subset as positive, but its performance is worse than `NI` and `RD`.

HR. The IEQ derived from DT_2 is Q_4'' : $\pi_{name}\ \sigma_{HR>50}$ $(Master \bowtie Batting)$.

Exactly-k semantics In a more general SQL setting where the query result is a bag instead of a set (i.e., the "distinct" keyword is not used in the select-clause), the at-least-one semantics becomes *exactly-k semantics* in the following sense: If there are m instances of a tuple t_i in the query result $Q(D)$, then the *exactly-k semantics* requires that J_{in}^{+} must contain exactly m tuples from the subset $P_i \subseteq J$ corresponding to t_i. For example, consider the following query:

$Q_{4,k}$: SELECT name
FROM Master, Batting
WHERE Master.pID = Batting.pID
AND bats = "R"AND throws = "R".

We have $Q_{4,k}(D) = \{B, B, D\}$. Suppose that the schema subgraph G considered to derive the IEQs for $Q_{4,k}$ contains *Master* and *Batting*. The output of $J = \text{Master} \bowtie_{pID} \text{Batting}$ is shown in Fig. 2a (similar to the relation J for query Q_4). The partition corresponding to tuple "B" is $P_1 = \{t_3, t_4\}$. The exactly-k semantics requires that J_{in}^{+} contains exactly two tuples from P_1. In this case, both t_3 and t_4 must be labeled positive.

For simplicity and without loss of generality, we will mainly focus on the at-least-one semantics in the following discussion. We defer the discussion about the exactly-k semantics to Sect. 5.2.

4.2.2 Challenge 2: performance issues

The second challenge concerns the performance issue of how to efficiently generate candidates for $rel(Q')$ and optimize the computation of the single input table J required for the classification task. To improve performance, TALOS exploits join indices (discussd in Sect. 6) to avoid a costly explicit computation of J and constructs mapping tables to optimize decision tree construction. TALOS also uses another type of indices, domain indices (discussed in Sect. 8), to efficiently identify covering attributes when the input query is unknown.

5 Data classification with at-least-one semantics

In this section, we address the first challenge of TALOS and present a novel approach for classifying data with the at-least-one semantics and the exactly-k semantics in deriving SPJ-IEQs (Sects. 5.1, 5.2). We then present techniques to derive more expressive IEQs beyond the basic SPJ queries (Sect. 5.3).

5.1 Computing optimal node splits

The main challenge for classification with the at-least-one semantics is how to optimize the node splits given the presence of free tuples that offers flexibility in the class label assignment. We present a novel approach that computes the optimal node split *without* having to explicitly enumerate all possible class label assignments to the free tuples. The idea is based on exploiting the flexibility offered by the at-least-one semantics.

Let us consider an initial set of tuples S that has been split into two subsets, S_1 and S_2, based on a value v of a numeric attribute A (the same principle applies to categorical attributes as well); that is, a tuple $t \in S$ belongs to S_1 iff $t.A \leq v$. The key question is how to compute the optimal Gini index of this split without having to enumerate all possible class label assignments for the free tuples in S such that the at-least-one semantics is satisfied. Without loss of generality, suppose that the set of tuples in S is partitioned into $m+2$ subsets, $P_1, \ldots, P_{m+2}$, where $P_1, \ldots, P_m$ are the partitioned subsets of free tuples (as described in Sect. 4.2) such that each $|P_i| > 1$ and at least one tuple in each of them must be labeled positive; P_{m+1} is the set of bound tuples that are labeled positive; and P_{m+2} is the set of bound tuples that are labeled negative.

Let $n_{i,j}$ denote the number of tuples in $P_i \cap S_j$, $i \in [1, m+2]$, $j \in \{1, 2\}$. Thus, the total number of free tuples in S_j, $j \in \{1, 2\}$, is given by $\sum_{i=1}^{m} n_{i,j}$. Let f_i denote the number of free tuples in S_i, $i \in \{1, 2\}$, that are labeled positive to satisfy the at-least-one semantics. After the free tuples have been labeled, the total number of positive and negative tuples in each S_j, $j \in \{1, 2\}$, are, $n_{m+1,j} + f_j$ and $n_{m+2,j} + \sum_{i=1}^{m} n_{i,j} - f_j$, respectively. By Equation 1, the Gini index of each S_j, $j \in \{1, 2\}$, is given by:

$$Gini(S_j) = 1 - \left(\frac{n_{m+1,j} + f_j}{\sum_{i=1}^{m+2} n_{i,j}}\right)^2 - \left(\frac{n_{m+2,j} + \sum_{i=1}^{m} n_{i,j} - f_j}{\sum_{i=1}^{m+2} n_{i,j}}\right)^2$$

By Equation 2, the Gini index of the split S into S_1 and S_2 is given by:

$$Gini(S_1, S_2) = \alpha_1 \cdot Gini(S_1) + \alpha_2 \cdot Gini(S_2), \quad (3)$$

where $\alpha_j = (\sum_{i=1}^{m+2} n_{i,j})/(\sum_{k=1}^{2}\sum_{i=1}^{m+2} n_{i,k})$, $j \in \{1, 2\}$. After simplification, $Gini(S_1, S_2)$ is of the form

$$Gini(S_1, S_2) = H(f_1, f_2) = c - (a_1 \cdot f_1 + b_1)^2 - (a_2 \cdot f_2 + b_2)^2, \quad (4)$$

where f_1 and f_2 are two variables to be optimized to minimize $Gini(S_1, S_2)$ and c, a_1, a_2, b_1, and b_2 are constants defined as follows:

$$a_j = \frac{\sqrt{2 \cdot \alpha_j}}{\sum_{i=2}^{m+2} n_{i,j}},\ j \in \{1,2\}$$

$$b_j = \sqrt{\frac{\alpha_j}{2}} \cdot \left(\frac{n_{m+1,j} - n_{m+2,j} - \sum_{i=1}^{m} n_{i,j}}{\sum_{i=1}^{m+2} n_{i,j}} \right),\ j \in \{1,2\}$$

$$c = \sum_{j \in \{1,2\}} \alpha_j - \alpha_j \cdot \frac{n_{m+1,j}^2 + (n_{m+2,j} + \sum_{i=1}^{m} n_{i,j})^2 - d}{(\sum_{i=1}^{m+2} n_{i,j})^2}$$

$$d\ \frac{(n_{m+1,j} - n_{m+2,j} - \sum_{i=1}^{m} n_{i,j})^2}{4}.$$

For each partition of free tuples P_i, $i \in [1, m]$, we classify P_i as a SP_1-*set* (resp. SP_2-*set*) if P_i is completely contained in S_1 (resp. S_2); otherwise, P_i is a SP_{12}-*set* (i.e., $n_{i,1} > 0$ and $n_{i,2} > 0$). Let T_j denote the minimum number of free tuples in S_j to be labeled positive, $j \in \{1, 2\}$. Since for each SP_j-set, at least one of its tuples must be labeled positive to satisfy the at-least-one constraint, T_j is equal to the number of SP_j sets.

The following result establishes that the optimal value of $Gini(S_1, S_2)$ is computed by considering only five combinations of f_1 and f_2 values.

Theorem 4 *The optimal value of* $Gini(S_1, S_2)$ *is given by* $\min\{H1, H2, H3, H4, H5\}$, *where*

$$H1 = H\left(\sum_{i=1}^{m} n_{i,1}, \sum_{i=1}^{m} n_{i,2}\right),$$

$$H2 = H\left(\sum_{i=1}^{m} n_{i,1}, T_2\right),$$

$$H3 = H\left(T_1, \sum_{i=1}^{m} n_{i,2}\right),$$

$$H4 = H(T_1, m - T_1),\ \textit{and}\ \ H5 = H(m - T_2, T_2).$$

The five combinations of f_1 and f_2 values considered in Theorem 4 actually correspond to the different ways to maximize the number of positive or negative tuples in S_1 and S_2: $H1$ maximizes the number of positive tuples in both S_1 and S_2; $H2$ maximizes the number of positive tuples in S_1 and maximizes the number of negative tuples in S_2; $H3$ maximizes the number of negative tuples in S_1 and maximizes the number of positive tuples in S_2; and finally, $H4$ and $H5$ correspond to the two possibilities to maximize the number of negative tuples in both S_1 and S_2.

5.2 Updating labels & propagating constraints

Once the optimal $Gini(S_1, S_2)$ is determined for a given node split, we need to update the split of S by converting the free tuples in S_1 and S_2 to bound tuples with either positive/negative class labels. The details of this updating depend on which of the five cases the optimal Gini value was derived from and are summarized by the last four columns in Table 1.

For case H1, which is the simplest case, all the free tuples in S_1 and S_2 will be converted to positive tuples. However, for the remaining cases, which involve maximizing the number of negative tuples in S_1 or S_2, some of the free tuples may not be converted to bound tuples. Instead, the maximization of negative tuples in S_1 or S_2 is achieved by propagating another type of constraints, referred to as "exactly-one" constraints, to some subsets of tuples in S_1 or S_2. Similar to the principle of at-least-one constraints, the idea here is to make use of constraints to optimize the Gini index values for subsequent node splits without having to explicitly enumerate all possible class label assignments. Thus, in Table 1, the fourth and fifth columns specify which free tuples are to be converted to bound tuples with positive and negative labels, respectively; where a'-" entry means that no free tuples are to be converted to bound tuples. The sixth and seventh columns specify what subsets of tuples in S_1 and S_2, respectively, are required to satisfy the exactly-one constraint; where a'-" entry column means that no constraints are propagated to S_1 or S_2.

We now consider the exactly-one constraint, a special case of exactly-k semantics, and explain why it is necessary. An *exactly-one constraint* on a set of free tuples S' requires that exactly one free tuple in S' must become labeled as positive with the remaining free tuples in S' labeled as negative. Consider case H2, which is to maximize the number of positive (resp. negative) tuples in S_1 (resp. S_2). The maximization of the number of positive tuples in S_1 is easy to achieve by converting all the free tuples in S_1 to positive. In this way, the at-least-one constraints on the SP_1-sets and SP_{12}-sets are also satisfied. Consequently, for each SP_{12}-set P_i, all the

Table 1 Optimizing Node Splits

Case	Number of free tuples to be labeled positive		Labeling of free tuples		Exactly-one constraint propagation	
	f_1	f_2	Positive	Negative	S_1	S_2
$H1$	$\sum_{i=1}^{m} n_{i,1}$	$\sum_{i=1}^{m} n_{i,2}$	$S_1 \cup S_2$	–	–	–
$H2$	$\sum_{i=1}^{m} n_{i,1}$	T_2	S_1	SP_{12}-sets in S_2	–	SP_2-sets
$H3$	T_1	$\sum_{i=1}^{m} n_{i,2}$	S_2	SP_{12}-sets in S_1	SP_1-sets	–
$H4$	T_1	$m - T_1$	–	SP_{12}-sets in S_1	SP_1-sets	All subsets
$H5$	$m - T_2$	T_2	–	SP_{12}-sets in S_2	All subsets	SP_2-sets

free tuples in $P_i \cap S_2$ can be converted to negative tuples to maximize the number of negative tuples in S_2. This will not violate the at-least-one constraint on the SP_{12}-set P_i. However, for a SP_2-set P_i, the constraint to maximize the number of negative tuples in P_i while satisfying the at-least-one semantics translates to an exactly-one constraint on P_i. Thus, for case H2, an exactly-one constraint is propagated to each SP_2-set in S_2, and no constraint is propagated to S_1. A similar reasoning applies to the other cases.

Therefore, while the at-least-one constraint is applied to each subset of free tuples P_i in the initial node split, the exactly-one constraint is applied to each P_i for subsequent node splits. This second variant of the node split problem can be optimized by techniques similar to what we have explained so far for the first variant. In particular, the exactly-one semantics means that $f_1 + f_2 = m$ if there are m partitions of free tuples. Consequently, the optimization of the Gini index value becomes simpler and only needs to consider cases H4 and H5.

Example 6 To illustrate how class labels are updated and how constraints are propagated during a node split, consider the following query on the baseball database D: $Q_5 = \pi_{stint}\,(\sigma_{country=\text{"USA"}}\, Master \bowtie_{pID} Batting)$. Suppose that the weak-IEQ Q'_5 being considered has $rel(Q'_5) = \{Master,\ Batting\}$. Let $J = Master \bowtie_{pID} Batting$ (shown in Fig. 2a). Since $Q_5(D) = \{1, 2\}$, we have $J_0 = \{t_6, t_7\}$, $P_1 = \{t_1, t_2, t_5\}$ (corresponding to $stint = 2$), and $P_2 = \{t_3, t_4\}$ (corresponding to $stint = 1$). The tuples in J_0 are labeled negative, while the tuples in P_1 and P_2 are all free tuples.

Suppose that the splitting attribute considered is "weight," and the optimal splitting value for "weight" is 72. The $Gini(S_1,\ S_2)$ values computed (w.r.t. "$weight = 72$") for the five cases, H1 to H5, are 0.29, 0.48, 0.21, 0.4 and 0.4, respectively. Thus, the optimal value of $Gini(S_1, S_2)$ is 0.21 (due to case H3). We then split tuples with $weight \leq 72$ (i.e., $\{t_3, t_4, t_6, t_7\}$) into S_1 and tuples with $weight > 72$ (i.e., $\{t_1, t_2, t_5\}$) into S_2. Thus, P_1 is a SP_2-set, while P_2 is a SP_1-set. Since the optimal Gini index computed is due to case H3 (i.e., maximizing negative tuples in S_1 and maximizing positive tuples in S_2), all the free tuples in S_2 (i.e., t_1, t_2 and t_5) are labeled positive, and an exactly-one constraint is propagated to the set of tuples $P_2 \cap S_1$ (i.e., $\{t_3, t_4\}$).

Handling exactly-k semantics In the following, we discuss how to extend the above technique to handle the *exactly-k* semantics. The exactly-k semantics is required when there is a constraint on the number of instances of a specific tuple in the query result. Recall that the *exactly-k* semantics applied on a set of free tuples S' requires exactly k of its free tuples to be labeled positive and the remaining free tuples in S' to be labeled negative.

Suppose that there are m partitions of free tuples $P_1, \ldots, P_m$ such that exactly k_i tuples from each of P_i needo be labeled positive, where $k_i \in [1, |P_i|]$. Thus, the total number of free tuples to be labeled positive to satisfy the exactly-k_i constraint is given by $f_1 + f_2 = \sum_{i=1}^{m} k_i$. Since each P_i needs exactly k_i free tuples to be labeled positive, minimizing the number of free tuples in $P_i \cap S_1$ to be labeled positive maximizes the number of free tuples in $P_i \cap S_2$ to be labeled positive, and vice versa. Therefore, the minimum number of free tuples to be labeled positive in each $P_i \cap S_j$ is given by $\max\{0, k_i - n_{i,3-j}\}$, and thus, we have $T_j = \sum_{i=1}^{m} \max\{0, k_i - n_{i,3-j}\},\ j \in \{1, 2\}$. Consequently, the optimization of the Gini index value becomes simpler and needs to consider only two cases H'4 and H'5 (analogous to H4 and H5): Case H'4 corresponds to $f_1 = T_1$ and $f_2 = \sum_{i=1}^{m} k_i - T_1$; while case H'5 corresponds to $f_1 = \sum_{i=1}^{m} k_i - T_2$ and $f_2 = T_2$.

In summary, TALOS is able to efficiently compute the optimal Gini index value for each attribute split value considered without enumerating an exponential number of class label assignments for the free tuples.

5.3 Supporting more expressive IEQs

Our discussion so far has focused on IEQs that are simple SPJ queries. In this section, we present techniques to derive more expressive IEQs beyond the basic SPJ queries. The increased expressiveness is important to broaden the range of applications of QRE. Specifically, we discuss the derivation of IEQs that belong to the following two additional query fragments: SPJ with union (SPJU) and SPJ with aggregation (SPJA).

In the default mode of operation, TALOS will attempt to derive IEQs that belong to a simpler fragment before proceeding to the more complex fragments in the following order: SPJ, SPJU, and SPJA. In this way, simpler IEQs (which are preferred) are generated before the more complex IEQs.

5.3.1 Deriving SPJU–IEQs

Since an SPJU-IEQ Q' is a union of some n number of SPJ queries ($n > 1$), Q' is conceptually derived by partitioning $T = Q(D)$ into n non-empty subsets, $T = T_1 \cup \cdots \cup T_n$, where each T_i is produced by some SPJ-IEQ Q'_i. It is desirable to generate a succinct SPJU-IEQ Q' where n is minimized. However, minimizing n is an NP-hard problem as shown by Theorem 2.

TALOS uses a simple greedy heuristic to derive the SPJU-IEQ by generating the Q'_i's iteratively, where the largest candidate T_i is selected at each iteration to derive an IEQ Q'_i. Algorithm 2 shows the heuristic used by TALOS to derive a SPJU-IEQ for an output table T containing k columns $\{C_1, \cdots, C_k\}$ with respect to a database D.

Algorithm 2: TALOS-SPJU (T, D, k)

```
1  foreach column C_i of T do
2      CA_i ← {(A, L) | A is an attribute of some relation R,
       L = {t.rid | t ∈ T, t.C_i ∈ π_A(R)}, L ≠ ∅};
3  SCA ← {((A_1, L_1), ··· , (A_k, L_k)) | (A_i, L_i) ∈ CA_i};
4  Q ← an empty query;
5  while (SCA ≠ ∅) ∧ (T ≠ ∅) do
6      Pick the element ((A_1, L_1), ··· , (A_k, L_k)) from SCA such
       that |L_1 ∩ L_2 ··· ∩ L_k ∩ π_rid(T)| is largest among all possible
       elements from SCA and remove this element from SCA ;
7      T' ← {t ∈ T | t.rid ∈ L_1 ∩ L_2 ··· ∩ L_k};
8      Derive an IEQ Q' using the set of covering attributes
       {A_1, ··· , A_k} w.r.t. the input table T';
9      if Q' exists then
10         Q ← Q ∪ Q'_i;
11         T ← T − Q'(D);
12 return Q;
```

The algorithm first identifies all partially covering attributes for each column C_i of T (line 2). Here, we use $t.A$ to denote the value of attribute A of a tuple t and use rid to refer to an implicit attribute of each tuple that represents the tuple's row identifier (RID). $(A, L) \in CA_i$ if A is a partially covering attribute of C_i, and L represents the set of tuples in T whose C_i column values are "covered" by attribute A.

Next, the algorithm enumerates all combinations of partially covering attributes for all the k output columns and stores them in SCA (line 3). The k attributes in each combination $((A_1, L_1), \cdots, (A_k, L_k))$ can potentially form a join relation that "covers" a partition T_i of T to generate an IEQ Q_i. TALOS uses the metric $|L_1 \cap L_2 \cdots \cap L_k \cap \pi_{rid}(T)|$ as an estimate of the cardinality of the partition T_i corresponding to the combination.

The algorithm generates the SPJ-IEQs iteratively using a greedy heuristic. At each iteration, it picks the combination from SCA that has the largest estimated partition cardinality (line 6). The target partition of tuples in T is given by T' (line 7). The algorithm then tries to generate a SPJ-IEQ Q' (using the previously discussed technique) for the output table T' using $\{A_1, \cdots, A_k\}$ as the set of projected attributes for Q' (line 8). If the IEQ Q' exists, Q' is added as a component to the final SPJU-IEQ Q (line 10), and T is updated by removing the tuples in T that are covered by the output of Q' on D (line 11). Note that $Q'(D)$ may not be equal to T' if Q' is an approximate IEQ for T'. The algorithm terminates when all the combinations in SCA have been considered or if all the tuples in T have been covered.

5.3.2 Deriving SPJA–IEQs

For each output column C_i in the output table T, let $Cover(C_i)$ denote the set of attributes in the database that completely covers C_i. TALOS classifies each C_i as an *aggregated output column* if $Cover(C_i)$ is empty; otherwise, C_i is classified as a *non-aggregated output column*. As the name implies, each aggregated output column in T will be generated by applying some aggregation function on some database attribute. Recall that we do not consider arithmetic expressions in an aggregation operator's argument in this paper.

Specifically, if T consists of $k + m$ output columns where $C_1, \cdots, C_k$ are non-aggregated output columns and $C_{k+1}, \cdots, C_{k+m}$ are aggregated output columns, the SPJA-IEQ Q' derived by TALOS for T is of the form

"SELECT	$B_1, \cdots, B_k, \mathcal{F}_1(A_1), \cdots, \mathcal{F}_m(A_m)$
FROM	$J(G)$
WHERE	p
GROUP BY	$B_1, \cdots, B''_k$.

Here, $J(G)$ refers to the join relation (corresponding to some schema subgraph G) that is formed by joining all the relations contained in G based on their foreign key joins, and p is some selection predicate on $J(G)$. The attributes $B_1, \cdots, B_k, A_1, \cdots, A_m$ are from $J(G)$ such that each $B_i \in Cover(C_i)$, $i \in [1, k]$; and each $\mathcal{F}_i, i \in [1, m]$ is either a COUNT, SUM, AVG, MIN, or MAX aggregation function. We refer to each A_i as an *aggregation attribute*.

To simplify the following presentation, we shall assume that T consists of exactly two columns with one non-aggregated column and one aggregated column. Algorithm 3 shows an overview of the heuristic used by TALOS to derive SPJA-IEQs for an output table T (with respect to database D) consisting of a non-aggregated output column C_g and an aggregated output column C_a. To find candidate aggregation attributes for C_a, TALOS enumerates different schema subgraphs G that contain at least a relation (denoted by R_g) such that R_g has an attribute A_g that completely covers the non-aggregated column C_g. For each such schema subgraph G, TALOS computes the join relation $J(G)$ by joining all the relations in G based on the foreign key joins among the relations in G. Each of the attributes in $J(G)$ (except for A_g)

Algorithm 3: TALOS-SPJA (T, C_g, C_a, D)

```
1  foreach schema subgraph G that contains at least some relation
   R_g, R_g.A_g ∈ Cover(C_g) do
2      Compute the join relation J(G);
3      foreach attribute A_x in J(G), A_x ≠ A_g do
4          foreach aggregation function F ∈ { COUNT, SUM, AVG,
           MIN, MAX } do
5              if F is applicable with A_x as aggregation attribute
               then
6                  Label the tuples in J(G) wrt A_x & F to derive an
                   IEQ Q';
7                  if Q' exists then
8                      return Q';
9  return null;
```

will be considered as a candidate aggregation attribute. In the following, we elaborate on how an SPJA-IEQ is derived for a given candidate aggregation attribute A_x and a candidate aggregate function $\mathcal{F}$ by an appropriate labeling of the tuples in $J(G)$ (line 6).

Suppose that T contains n tuples of the form (g_i, a_i), $i \in [1, n]$, where g_i and a_i are values of columns C_g and C_a, respectively. $J(G)$ can be partitioned into $(n + 1)$ disjoint partitions: $J(G) = P_0 \cup P_1 \cup \cdots \cup P_n$, where each P_i, $i > 0$, is the subset of tuples in $J(G)$ that has the value g_i for attribute A_g, i.e., $P_i = \{t \in J(G) \mid t.A_g = g_i\}$. Thus, P_0 refers to the subset of tuples that do not contribute to any of the output tuples in T, i.e., $\pi_{C_g}(T) \cap \pi_{C_g}(P_0) = \emptyset$.

The tuples in $J(G)$ are labeled as follows. Since none of the tuples in P_0 can contribute to any output tuple in T, the tuples in P_0 are all labeled as negative tuples and the remaining tuples are initially labeled as free tuples. For a candidate aggregation function $\mathcal{F}$ being considered for the IEQ Q', TALOS needs to determine a subset of tuples $P_i' \subseteq P_i$ for each partition P_i, $i > 0$, such that when the tuples in P_i' are labeled as positive and the tuples in $P_i - P_i'$ are labeled as negative, the result of $\mathcal{F}$ on each P_i' is a_i. In the following, we elaborate on how the P_i''s are selected (i.e., how the selection predicate p on $J(G)$ is determined) for each of the three aggregation functions.

For the COUNT aggregation function, it is applicable for an aggregation attribute A_x if the values in the output column C_a are all natural numbers such that $a_i \in \{0, 1, \cdots, |P_i|\}$ for each $(g_i, a_i) \in T$. The semantics of the COUNT aggregation function requires that $|P_i'| = a_i$ for each partition P_i, $i > 0$, which can be solved by imposing the *exactly-k* constraint for labeling tuples as described in Sect. 5.

For the SUM and AVG aggregation functions, the problem of selecting each $P_i' \subseteq P_i$ such that $\mathcal{F}(P_i') = a_i$ can be mapped to the subset-sum/subset-average problem, which is a well-known NP-hard problem [8]. TALOS uses standard pseudo-polynomial algorithms to solve the subset-sum and subset-average problems with time complexities of $O(Kn)$ and $O(Kn^2)$, respectively [8], where $K = a_i$ and $n = |P_i|$; or approximation algorithms [8] to derive approximate IEQs with lower time complexity.

For the MIN aggregation function, for each P_i, there must exist at least one tuple $t_m \in P_i$ such that $t_m.A_x = a_i$. We further partition P_i as follows: $P_i = P_i^- \cup P_i^{alos} \cup P_i^{free}$ where $P_i^- = \{t \in P_i \mid t.A_x < a_i\}$, $P_i^{alos} = \{t \in P_i \mid t.A_x = a_i\}$, and $P_i^{free} = \{t \in P_i \mid t.A_x > a_i\}$. Clearly, at least one tuple in P_i^{alos} must be labeled positive in order for the MIN function applying on P_i to returnhe value a_i. Likewise, all tuples in P_i^- must be labeled negative. Otherwise, the result of the MIN function on P_i will be smaller than a_i. Finally, tuples in P_i^{free} have the flexibility to be assigned positive or negative. The reason is that if any tuples in P_i^{free} are assigned positive class labels, the MIN function applying on P_i still returns the value a_i. A similar scheme will be applied if the aggregated function is MAX.

6 Performance issues

In this section, we address the second challenge of TALOS and discuss several optimization techniques to speed up the derivation of IEQs. We first explain how TALOS adapts a well-known decision tree classifier for performing data classification in the presence of free tuples, whose class labels are not fixed. We then explain the performance challenges of deriving Q' when $rel(Q')$ involves multiple relations and present optimization techniques to address these issues. For ease of presentation and without loss of generality, the discussion here assumes weak IEQs.

6.1 Classifying data in TALOS

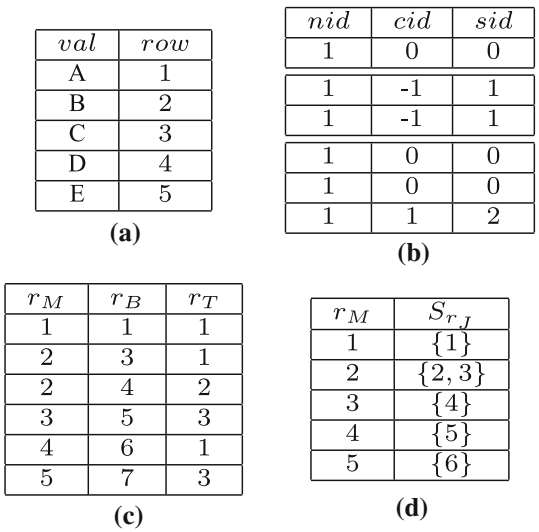
We first give an overview of SLIQ [16], a well-known decision tree classifier, that we have chosen to adapt for TALOS. We then describe the extensions required by TALOS to handle data classification in the presence of free tuples. Finally, we present a non-optimized, naive variant of TALOS. It is important to emphasize that our approach is orthogonal to the choice of the decision tree technique.

Overview of SLIQ SLIQ is an efficient decision tree classifier designed for handling large, disk-resident training data. To construct a binary decision tree on a set of data records D, SLIQ uses two key data structures.

First, a sorted attribute list, denoted by AL_i, is precomputed for each attribute A_i in D. Each AL_i can be thought of as a two-column table (val, row), of the same cardinality as D, that is sorted in non-descending order of val. Each record $r = (v, i)$ in AL_i corresponds to the i^{th} tuple t in D and $v = t.A_i$. The sorted attribute lists are used to speed up the computation of optimal node splits. To determine the optimal node split w.r.t. A_i requires a single sequential scan of AL_i.

Second, a main memory array called *class list*, denoted by CL, is maintained for D. This is a two-column table (nid, cid) with one record per tuple in D. The i^{th} entry in CL, denoted by $CL[i]$, corresponds to the i^{th} tuple t in D, where $CL[i].nid$ is the identifier of leaf node N, $t \in D_N$, and $CL[i].cid$ refers to the class label of t. CL is used to keep track of the tuples location (i.e., in which leaf nodes) as leaf nodes are split.

Class list extension In order to support data classification with free tuples where their class labels are assigned dynamically, we need to extend SLIQ with the following modifications. The class list table $CL(nid, cid, sid)$ is extended with an additional column "sid," which represents a subset



(a)

val	row
A	1
B	2
C	3
D	4
E	5

(b)

nid	cid	sid
1	0	0
1	-1	1
1	-1	1
1	0	0
1	0	0
1	1	2

(c)

r_M	r_B	r_T
1	1	1
2	3	1
2	4	2
3	5	3
4	6	1
5	7	3

(d)

r_M	S_{r_J}
1	{1}
2	{2, 3}
3	{4}
4	{5}
5	{6}

Fig. 3 Example data structures for $Q_4(D)$. **a** AL_{name}. **b** CL. **c** J_{hub}. **d** M_{Master}

identifier, to indicate which subset (i.e., P_i) a tuple belongs to. This additional information is needed to determine the optimal Gini index values as discussed in the previous section. Consider a tuple t that is the i^{th} tuple in D, the cid and sid values in CL are maintained as follows. If t belongs to J_{out}, then $CL[i].cid = 0$ and $CL[i].sid = 0$. If t is a bound tuple in P_j, then $CL[i].cid = 1$ and $CL[i].sid = j$. Otherwise, if t is a free tuple in P_j, then $CL[i].cid = -1$ and $CL[i].sid = j$.

Example 7 Fig. 3 illustrates the two data structures created to compute IEQs for $Q_4(D)$ in Example 4. Figure 3a shows the attribute list created for attribute *Master.name*, and Fig. 3b shows the initial class list created for the relation J = Master $\bowtie_{pID}$ Batting, where all the records are in a single leaf node (with nid value of 1).

Naive TALOS(TALOS$^-$). Before presenting the optimizations for TALOS in the next section, let us first describe a non-optimized, naive variant of TALOS (denoted by TALOS$^-$). Suppose that we are considering an IEQ Q' where $rel(Q') = \{R_1, \cdots, R_n\}$, $n > 1$, that is derived from some schema subgraph G. First, TALOS$^-$ joins all the relations in $rel(Q')$ (based on the foreign key joins represented in G) to obtain a single relation J. Next, TALOS$^-$ computes attribute lists for the attributes in J and a class list for J. TALOS$^-$ is now ready to construct a decision tree DT to derive the IEQ Q' with these structures. The decision tree DT is initialized with a single leaf node consisting of the records in J, which is then refined iteratively by splitting the leaf nodes in DT. TALOS$^-$ terminates the splitting of a leaf node when (1) its tuples are either all labeled positive or all labeled negative; or (2) its tuples have the same attribute values w.r.t. all the splitting attributes. Finally, TALOS$^-$ classifies each leaf node in DT as positive or negative as follows: A leaf node is classified as positive if and only if the ratio of the number of its negative tuples to the number of its positive tuples is no greater than a threshold value given by τ. [6] The selection condition of the IEQ Q' is then derived from the collection of positive leaf nodes in DT as follows. Each internal node in DT corresponds to a selection predicate on some attribute of J, and each root-to-positive-leaf path P_j in DT corresponds to a conjunctive predicate C_j on J. Thus, each decision tree enumerated for G yields a selection predicate for Q' of the form C_1 *or* C_2 $\cdots$ *or* C_ℓ. In the event that all the leaf nodes in DT are classified as negative, the computation of Q' is not successful (i.e., there is no IEQ for $rel(Q')$), and we refer to Q' as a *pruned IEQ*.

6.2 Optimizations

The naive TALOS described in the previous section suffers from two drawbacks. First, the overhead of computing J can be high, especially if there are many large relations in $rel(Q')$. Second, since the cardinality of J can be much larger than the cardinality of each of the relations in $rel(Q')$, building decision trees directly using J entail the computation and scanning of correspondingly large attribute lists, which further increases the computation cost. In the rest of this section, we present the optimization techniques used by TALOS to address the above performance issues.

Join indices & hub table To avoid the overhead of computing J from $rel(Q')$, TALOS exploits pre-computed join indices [30], which is a well-known technique for optimizing joins. For each pair of relations, R and R', in the database schema that are related by a foreign key join, its join index, denoted by $I_{R,R'}$, is a set of pairs of row identifiers referring to a record in each of R and R' that are related by the foreign key join.

Based on the foreign key join relationships represented in the schema subgraph G, TALOS computes the join of all the appropriate join indices for $rel(Q')$ to derive a relation, called the *hub table*, denoted by J_{hub}. Computing J_{hub} is much more efficient than computing J, since there are fewer number of join operations (i.e., number of relevant join indices) and each join attribute is a single integer-valued column.

Example 8 Consider again query Q_4 introduced in Example 4. Suppose that we are computing IEQ Q'_4 with $rel(Q'_4)$ = {*Master*, *Batting*, *Team*}. Figure 3c shows the hub table, J_{hub}, produced by joining two join indices: one for *Master* $\bowtie_{pID}$ *Batting*, and the other for *Batting* $\bowtie_{team,year}$ *Team*. Here, r_M, r_B, and r_T refer to the row identifiers for *Master*, *Batting*, and *Team* relations, respectively.

[6] To generate only precise IEQs, $\tau = 0$. In our experiments, we set $\tau = 1$ to derive a reasonable number of approximate IEQs.

Mapping tables Instead of computing and operating on large attribute lists (each with cardinality equal to $|J|$) as in the naive approach, TALOS operates over the smaller pre-computed attribute lists AL_i for the base relations in $rel(Q')$ together with small *mapping tables* to link the pre-computed attribute lists to the hub table. In this way, TALOS only needs to pre-compute once the attribute lists for all the base relations, thereby avoiding the overhead of computing many large attribute lists for different $rel(Q')$ considered.

Each mapping table, denoted by M_i, is created for each $R_i \in rel(Q')$ that links each record r in R_i to the set of records in J_{hub} that are related to r. Specifically, for each record r in R_i, there is one record in M_i of the form (j, S), where j is the row identifier of r, and S is a set of row identifiers representing the set of records in J_{hub} that are created from r.

Example 9 Figure 3d shows the mapping table M_{Master} that links the *Master* relation in Fig. 1 and J_{hub} in Fig. 3b. The record $(2, \{2, 3\})$ in M_{Master} indicates that the second tuple in *Master* relation (with pID of $P2$), contributed two tuples, located in the second and third rows, in J_{hub}.

Computing class list We now explain how TALOS can efficiently compute the class list CL for J (without having explicitly computed J) by using the attribute lists, hub table, and mapping tables. The key task in computing CL is to partition the records in J into subsets (J_0, P_1, P_2, etc.), as described in the previous section.

For simplicity and without loss of generality, assume that the schema of $Q(D)$ has n attributes $A_1, \cdots, A_n$, where each A_i is an attribute of relation R_i. TALOS first initializes CL with one entry for each record in J_{hub} with the following default values: $nid = 1$, $cid = 0$, and $sid = 0$. For each record, r_k that is accessed by a sequential scan of $Q(D)$, TALOS examines the value v_i of each attribute A_i of r_k. For each v_i, TALOS first retrieves the set of row identifiers RI_{v_i} of records in R_i that have a value of v_i for attribute $R_i.A_i$ by performing a binary search on the attribute list for $R_i.A_i$. With this set of row identifiers RI_{v_i}, TALOS probes the mapping table M_i to retrieve the set of row identifiers JI_{v_i} of the records in J_{hub} that are related to the records referenced by RI_{v_i}. The intersection of the JI_{v_i}'s for all the attribute values of r_k, denoted by P_k, represents the set of records in J that can generate r_k. TALOS updates the entries in CL corresponding to the row identifiers in P_k as follows: (1) The sid value of each entry is set to k (i.e., all the entries belong to the same subset corresponding to record r_k) and (2) the cid value of each entry is set to 1 (i.e., tuple is labeled positive) if $|P_k| = 1$; otherwise, it is set to -1 (i.e., it is a free tuple).

Example 10 We illustrate how TALOS creates CL for query Q_4, which is shown in Fig. 3b. Initially, each row in CL is initialized with $sid = 0$ and $cid = 0$. TALOS then accesses each record of $Q_4(D)$ sequentially. For the first record (with name = "B"), TALOS searches AL_{name} and obtains $RI_B = \{2\}$. It then probes M_{Master} with the row identifier in RI_B and obtains $JI_B = \{2, 3\}$. Since $Q_4(D)$ contains only one attribute, we have $P_1 = \{2, 3\}$. The second and the third rows in CL are then updated with $sid = 1$ and $cid = -1$. Similarly, for the second record in $Q_4(D)$ (with name = "E"), TALOS searches AL_{name} and obtains $RI_E = \{5\}$, and derives $JI_E = \{6\}$ and $P_2 = \{6\}$. The sixth row in CL is then updated with $sid = 2$ and $cid = 1$.

7 Ranking IEQs

As a query generally has many possible IEQs, it is useful to rank and prioritize the presentation of the derived IEQs to the user. Since our preference for simpler and more precise IEQs involves conflicting objectives, we present three reasonable criteria for ranking IEQs: a metric based on the minimum description length (MDL) principle [24] and two metrics based on the F-measure [23].

7.1 Minimum description length

The minimum description length (MDL) principle argues that all else being equal, the best model is the one that minimizes the sum of the cost of describing the data given the model and the cost of describing the model itself. If M is a model that encodes the data D, then the total cost of the encoding, $cost(M, D)$, is defined as: $cost(M, D) = cost(D|M) + cost(M)$. Here, $cost(M)$ is the cost to encode the model (i.e., the decision tree in our case), and $cost(D|M)$ is the cost to encode the data given the model. We can rely on succinct tree-based representations to compute $cost(M)$. The data encoding cost, $cost(D|M)$, is calculated as the sum of classification errors. Thus, an IEQ with a lower MDL encoding cost is considered to be better. The details of the encoding computations are given elsewhere [16].

7.2 F-measure

We now present two useful metrics based on the popular F-measure [23] that represents the precision of the IEQs. The first variant follows the standard definition of F-measure: The F-measure for two IEQs Q and Q' is defined as $F_m = \frac{2\times|p_a|}{2\times|p_a|+|p_b|+|p_c|}$, where $p_a = Q(D) \cap Q'(D)$, $p_b = Q'(D) - Q(D)$, and $p_c = Q(D) - Q'(D)$. We denote this variant as *F-measure* in our experimental study. Here, an IEQ with a higher F-measure value is considered to be a more precise and better query.

Observe that the first variant of F-measure is useful only for approximate IEQsand is not able to distinguish among precise IEQs, as this metric gives identical values for precise

IEQs since p_b and p_c are empty. To rank precise IEQs, we introduce a second variant, denoted by F_m^{est}, which relies on estimating p_a, p_b, and p_c using some data probabilistic models (as opposed to using the actual values from the data set). F_m^{est} captures how the equivalence of queries is affected by database updates, and the IEQ with high F_m^{est} is preferable to another IEQ with low F_m^{est}. For simplicity, we use a simple independent model to estimate F_m^{est}; other techniques such as the Bayesian model by Getoor and others [10] can be applied too. The second variant has the benefit that estimates, which are computed from a global distribution model, may more accurately reflect the true relevance of the IEQs than one computed directly from the data. This of course presupposes that future updates follow the existing data distribution.

The details on computing the F-measure (F_m and F_m^{est}) of a pair of IEQs Q and Q' are discussed in the Appendix.

8 Handling unknown input query

This section considers the problem of how to derive IEQs Q' given only D and the query result $T = Q(D)$ without knowledge of the input query Q. The key challenge is how to efficiently determine candidate core relations for T. We first present the overall framework in Sect. 8.1 followed by a discussion of an optimization technique using domain indices in Sect. 8.2.

8.1 An overview of TALOS

The overall approach of TALOS is outlined in Algorithm 4 which takes as input a database D and an input table T to derive a set of IEQs Q' such that $Q'(D) = T$. Recall from Sect. 5.3 that in the default mode of TALOS, it will attempt to derive IEQs starting from the simplest SPJ-IEQs to the more complex SPJU and SPJA-IEQs.

Algorithm 4: TALOS(D, T)

```
1 let C_1, ..., C_k be the columns in T
2 foreach column C_i in T do
3 |  S_i ← {R.A is an attribute in D | R.A covers C_i}
4 if all S_i's are non-empty then
5 |  foreach R_{i_1}.A_{j_1} ∈ S_1, ..., R_{i_k}.A_{j_k} ∈ S_k do
6 |  |  R ← {R_{i_1}, R_{i_2}, ..., R_{i_k}}
7 |  |  Derive SPJ-IEQs using Algorithm 1 with R as the set of
  |  |  core relations
8 Derive SPJU-IEQs using Algorithm 2
9 Derive SPJA-IEQs using Algorithm 3
```

To generate SPJ-IEQs, TALOS first determines the set of schema attributes S_i that covers each column C_i in T (line 3). If each S_i is non-empty, TALOS then enumerates all possible sets of core relations from $S_1, \ldots, S_k$, and invokes Algorithm 1 to derive SPJ-IEQs for each set of core relations $\mathcal{R}$ (lines 4 to 7). Note that $\mathcal{R}$ is constructed such that each column in T is covered by at least some attribute of some relation in $\mathcal{R}$. SPJU- and SPJA-IEQs for T are generated using Algorithms 2 and 3, respectively (lines 8 & 9).

8.2 Optimization: domain indices

We now describe how TALOS uses a simple but effective indexing technique, called *domain indices*, to optimize the identification of covering attributes.

Recall that the definition of a covering attribute (in Sect. 2) is based on set semantics which ignores the presence of duplicate column values. That is, it is possible for an attribute A in relation R to cover an attribute C in relation T and yet there is some value v that occurs m times in $T.C$ and n times in $R.A$ with $m > n$ and $n \geq 1$. This weaker definition is, however, sufficient for the purpose of identifying candidate core relations because after joining relation R with other relations in the schema subgraph to compute the join relation J, the frequency of a value v in $J.A$ could be higher than that in $R.A$. In this section, for simplicity and without loss of generality, we assume that each column C of T does not contain any duplicate values; otherwise, we simply preprocess C to eliminate duplicates.

To determine whether a column A in relation R covers a column C in T, a straightforward approach is to compute the antijoin $T \triangleright_{T.C=R.A} R$. Then A covers C iff the antijoin result is empty. Thus, all the covering attributes for C could be identified by performing this procedure for every database attribute that has the same domain as C. We refer to this naive solution as TALOS$^-$.

To avoid the cost of computing multiple antijoins, TALOS uses a simple yet effective indexing technique called *domain indices*. Unlike a conventional index which is defined on attribute(s) within a single relation, a domain index is defined on all the attributes in the database that have the same attribute domain.

For each attribute domain d, TALOS maintains a three-column mapping table $M_d(v, attr, count_v)$, where v is a value of type d in the database, $attr$ is the schema attribute that contains v in its column, and $count_v$ is the frequency of v in $attr$'s column. This table has one composite key consisting of v and $attr$, which is indexed by a B$^+$-tree index, that we refer to as the *domain index* for d. The $count_v$ field is used to facilitate index maintenance: $count_v$ is updated accordingly when database records are modified, and when $count_v$ drops to 0, the corresponding value v is removed from its mapping table M_d and domain index.

With the mapping tables and domain indices, TALOS identifies the covering attributes for a column C (with domain d) in the output table T by computing the result $\gamma_{attr,count(v)}\, \pi_{attr,v}(T \bowtie_{T.C=M_d.v} M_d)$. Essentially, TALOS

first joins T and M_d on $T.C = M_d.v$ to find out the set of values in $T.C$ that are covered by each database attribute $attr$ that has the same domain as C and then performs a group-by aggregation to count the number of distinct attribute values in $T.C$ that are covered by each $attr$. Thus, an attribute A covers C iff the aggregated result contains the tuple $(A, acount)$ and the number of distinct values of C is equal to $acount$. Here, $acount$ represents the number of distinct attribute values in C that are covered by A. The implementation details of TALOS$^-$ and TALOS to identify covering attributes are discussed in the Appendix.

9 Handling multiple database versions

In this section, we consider a more general setting of the QRE problem where the input consists of multiple versions of database instead of a single database. Specifically, we consider the following two practical scenarios for this generalization.

9.1 Multiple database versions & single unknown result

In data exploratory/analysis scenarios, it is typically the case that the querying time when a user requests to reverse-engineer a precise query Q' for a result table T occurs much later than the time when T was actually produced. Thus, it may not be meaningful or possible to derive Q' from the current version of the database as this could be very different from the version that T was generated from. Specifically, given a result table T and a sequence of database versions $< D_1, D_2, \cdots, D_\ell >$, where D_i is a more recent version than D_j if $i > j$, a specific goal may be to determine the most recent database version D_i, $i \in [1, \ell]$ and query Q' such that $Q'(D_i) = T$. Depending on the applications, other variations of the problem (e.g., finding the earliest database version or all versions) are also possible. In this section, we focus on the problem of deriving IEQs with respect to the most recent database version. The performance challenge is how to efficiently determine both D_i as well as Q' for a given result T.

The most straightforward solution is to apply the previously described solution developed for a single database version to one database version at a time starting from the most recent version D_ℓ and work progressively "backward" to the next recent version and so on until an IEQ is derived (or none is found). However, if the multiple database versions are not stored independently but are instead organized using a *reference version* (either the earliest or latest version) together with a sequence of forward/backward deltas between successive versions (e.g., [27]), then it is possible to apply well-known join view maintenance techniques [5,19] to optimize the IEQ derivations.

In this section, we assume, without loss of generality, that the database versions are stored using the backward delta storage organization. That is, given a sequence of database versions $D_1, D_2, \cdots, D_\ell$, the database stores the most recent version D_ℓ together with $\delta_{\ell(\ell-1)}, \cdots, \delta_{21}$, where each D_j is derived from D_i and δ_{ij}. For simplicity, we assume that each tuple update operation is modeled by a pair of tuple delete and insert operations. Thus, each delta δ_{ij} consists of a set of tuple insert and delete operations. We use the notation "$X \oplus \delta X$" to denote applying the insert/delete "delta" tuples in δX to update X where X is a database version or a relation. In the backward delta storage organization, we have $D_i = D_{i+1} \oplus \delta_{(i+1)i}$.

Assume that the current database version being considered is D_x; i.e., the database versions $D_\ell, D_{\ell-1}, \cdots, D_{x+1}$ have already been considered but without any IEQs derived from them. The task at hand is to try to derive IEQs from D_x. An obvious approach is to first compute D_x from D_{x+1} and $\delta_{(x+1)x}$ and then try to derive IEQs from the materialized D_x. This simple approach, however, does not leverage any of the computations performed for previously considered database versions.

There are two computations for the current database version D_x that could be optimized by exploiting the computations performed for the previous database version D_{x+1}. The first one is the computation of covering attributes, and the second one is the computation of join relations. As both optimizations are based on the same ideas, we shall focus on the first optimization in the rest of this section and briefly discuss the second optimization at the end of this section.

Recall from Sect. 8.2 that TALOS maintains a mapping table $M_d(v, attr, count_v)$ for each attribute domain d. The mapping table M_d is used to determine the covering attributes for a column C (with domain d) in the output table T by computing $\gamma_{attr,count(v)}\ TM_d$, where $TM_d = \pi_{attr,v}(T \bowtie_{T.C=M_d.v} M_d)$. Here, TM_d determines the set of attribute values of $T.C$ that are covered by each schema attribute $attr$ with the same domain as $T.C$.

Let M_d^i and TM_d^i denote the relations M_d and TM_d with respect to database version D_i. The goal of our optimized approach is to compute TM_d^x from TM_d^{x+1} and $\delta_{(x+1)x}$ without having to explicitly derive D_x and M_d^x. To facilitate this, we need to extend the schema of TM_d^i with an additional attribute $count_v$ to $TM_d^i(attr, v, count_v)$ where $count_v$ indicates the number of times the value v occurs in the database attribute $attr$. Thus, when we start by considering database version D_ℓ, TM_d^ℓ is computed as follows:

$$TM_d^\ell = \pi_{attr,v,count_v}(T \bowtie_{T.C=M_d^\ell.v} M_d^\ell).$$

Subsequently, when we consider database version D_x, $x < \ell$, TM_d^x is derived from TM_d^{x+1} and $\delta_{(x+1)x}$, which we explain in the following.

The derivation of TM_d^x, $x < \ell$, consists of two steps. In the first step, we compute δM_d, which represents the delta tuples required to derive M_d^x from M_d^{x+1}. Specifically, δM_d, which is derived from $\delta_{(x+1)x}$, is a set of tuples of the form $(attr, v, count_v)$ representing the net effect of the insert/delete delta tuples in $\delta_{(x+1)x}$ on the frequency of occurrence (given by $count_v$) of attribute values (indicated by value v of attribute $attr$) that occur in the delta tuples. For example, if $\delta_{(x+1)x}$ consists of m insert tuples that have a value of 10 for attribute A (with domain d) and n delete tuples that have a value of 10 for attribute A, then $(A, 10, m - n) \in \delta M_d$. Tuples in δM_d with a value of zero for $count_v$ are removed. Note that it is possible to derive M_d^x from M_d^{x+1} and δM_d.

Finally, in the second step, we compute TM_d^x from TM_d^{x+1} and δM_d as follows:

$$TM_d^x = \sigma_{count_v>0} \ (\pi_{attr,v,count_v=TM_d^{x+1}.count_v+\delta TM_d.count_v} (TM_d^{x+1} \rtimes_{v,attr} \delta TM_d)), \text{ where}$$
$$\delta TM_d = \pi_{attr,v,count_v}(T \bowtie_{T.C=\delta M_d.v} \delta M_d).$$

δTM_d represents the delta tuples required to derive TM_d^x from TM_d^{x+1}. The full outer-join between TM_d^{x+1} and δTM_d (with equality join predicates on both $attr$ and v attributes) is used to combine[7] the delta tuples in δTM_d with TM_d^{x+1}.

Since $\delta_{(x+1)x}$ is typically much smaller than D_x, the presented approach to compute δM_d and δTM_d to derive TM_d^x is less costly than the straightforward approach to compute D_x and M_d^x to derive TM_d^x.

Another area that could benefit from a similar optimization is the computation of the join relation $J(G)$ corresponding to a selected schema subgraph G. Let $J_i(G)$ denote the join relation for database version D_i. The direct approach to compute $J_x(G)$ is to first derive D_x from $\delta_{(x+1)x}$ and then compute $J_x(G)$ from D_x. However, this can be optimized by instead deriving a set of delta tuples, denoted by $\delta J(G)$, from $\delta_{(x+1)x}$ and computing $J_x(G)$ from $\delta J(G)$ and the previously computed $J_{x+1}(G)$. As the ideas are similar to the first optimization, we omit the elaboration of the second optimization.

9.2 Multiple database and result versions

In the second scenario, the input to the QRE problem is a sequence of database versions and result pairs (D_1, T_1), (D_2, T_2), $\cdots$ (D_ℓ, T_ℓ); where each T_i is the result of the *same* unknown query Q on database version D_i (i.e., $T_i = Q(D_i)$). We assume that all the databases D_i have the same schema.

For example, the T_i's could correspond to weekly reports generated by the same query on weekly versions of the database, or Q could be a continuous long standing query that is run periodically on different snapshots of the database. In this more general setting with multiple database and result versions, the challenge is how to efficiently reverse-engineer a query Q' such that $Q'(D_i) = T_i$ for each $i \in [1, \ell]$.

The most straightforward solution to this problem is to independently derive a set of IEQs S_i for each database and result pair (D_i, T_i) and then intersect all the S_i's to compute the set of IEQs for Q. We refer to this direct approach as `TALOS`$^-$.

In the following, we present a more efficient solution (denoted by `TALOS`) that considers all database and result pairs collectively to derive the IEQs. The trade-off of this more efficient approach is that it could miss even more precise IEQs compared to `TALOS`$^-$.

Similar to `TALOS`$^-$, `TALOS` starts by identifying the set of covering attributes (and hence candidate core relations) for the columns in the output tables. Next, for each schema subgraph G that contains a set of candidate core relations, `TALOS` computes a join relation $J_i(G)$ for each database version D_i by joining all the relations in D_i that are included in G based on their foreign key joins. Note that if the multiple database versions are not stored independently but are instead organized using a reference version as discussed in the previous section, our previously discussed optimization to derive $J_i(G)$ is applicable here as well. At this point, `TALOS` has computed a collection of join relations $J_1(G), \cdots, J_\ell(G)$ wrt G. Instead of deriving IEQs independently for each $J_i(G)$ as in `TALOS`$^-$, `TALOS` derives IEQs from a single unified join relation $J(G)$ that is generated by combining all the join relations, i.e., $J(G) = \bigcup_{i=1}^{\ell} J_i(G)$.

For convenience, let T denote the combined result table; that is, $T = \bigcup_{i=1}^{\ell} T_i$. For each tuple $t_j \in T$, let $X(t_j) = \{i \in [1, \ell] | t_j \in T_i\}$, and let $P_{i,j}$ denote the maximal subset of tuples in $J_i(G)$ that form t_j when they are projected on $proj(Q)$. Note that each $P_{i,j} \subseteq J(G)$ since each $J_i(G) \subseteq J(G)$.

The tuples in $J(G)$ are labeled as follows. The tuples that do not contribute to any result tuples in T (i.e., $J(G) - \bigcup_{t_j \in T, i \in [1,\ell]} P_{i,j}$) are labeled negative and the remaining tuples in $J(G)$ are labeled free. To guarantee that $t_j \in Q'(D_i)$ for each $t_j \in T$ and $i \in X(t_j)$, we need to ensure that at least one free tuple in each $P_{i,j}$ will be eventually labeled positive for the decision tree constructed with respect to $J(G)$. This can be achieved by imposing the at-least-one semantics on the set $\bigcap_{i \in X(t_j)} P_{i,j} - \bigcup_{i \in [1,\ell], i \notin X(t_j)} P_{i,j}$ for the decision tree construction.

In case we need to derive an SPJA-IEQ, the same idea can be applied. For instance, to derive an SPJA-IEQ with SUM/AVG aggregation function, instead of applying the at-least-one semantics on the corresponding subset, i.e., $\bigcap_{i \in X(t_j)} P_{i,j} - \bigcup_{i \in [1,\ell], i \notin X(t_j)} P_{i,j}$, we solve a subset-

[7] Note that in the SQL implementation, null count values are first converted to zero values before being added.

Table 2 Table sizes (number of tuples)

Table	# Tuples
(a) Adult & Baseball	
adult	45,222
Master	16,639
Batting	88,686
Pitching	37,598
Fielding	128,426
Salaries	18,115
Team	2,535
Manager	3,099
(b) TPC-H	
lineitem	6,000,000
order	1,500,000
partsupp	800,000
part	200,000
customer	150,000
supplier	10,000
nation	25

sum/subset-average problem defined on this set of tuples and label the tuples accordingly.

10 Experimental study

This section presents our experimental study to evaluate the performance of our proposed approach, TALOS, for computing IEQs. We first examine its effectiveness in handling at-least-one semantics (Sect. 10.2) and generating IEQs (Sect. 10.3) and then evaluate the efficiency of its optimizations (Sects. 10.4, 10.5).

10.1 Methodology

Algorithms To evaluate the effectiveness of TALOS in dynamically assigning the class labels for free tuples, we compare TALOS against two static class labeling techniques, denoted by NI and RD. Recall that NI labels all the free tuples as positive, while RD labels a random number of at least one tuple from each subset of free tuples as positive.

We also examine the effectiveness of our proposed optimizations by comparing against a non-optimized naive variant of TALOS (denoted by TALOS$^-$).

Data sets and queries We used two real and one synthetic data sets of different sizes for our experiments: Adult, Baseball, and TPC-H with a scale factor of 1.0. The sizes of these data sets are shown in Table 2, and the test queries are given in Table 3 with the cardinality of their results shown in the last column. We also run experiments on three additional data sets: basket ball data set[8], a single-relation data set containing information about laptops that are crawled from ebay[9], and TPC-H with a scale factor of 5.0. The results for these additional data sets are given in the Appendix.

The Adult data set, from the UCI Machine Learning Repository, is a single-relation data set that has been used in many classification works. We use this data set to illustrate the utility of IEQs for the simple case where both the input query Q as well as the output IEQ Q' involve only one relation. There are five queries (A1–A5) on this data set.[10]

The baseball data set is a more complex, multi-relation database that contains Batting, Pitching, and Fielding statistics for Major League Baseball from 1871 through 2006 created by Sean Lahman. The queries used for this data set (B_1–B_6) are common queries that mainly relate to baseball players' performance.

The TPC-H data set is a widely used benchmark. We use the TPC-H data set with a size of 1 GB, and seven test queries T_1–T_7.

Queries A_5, B_5, B_6, T_5, T_6, T_7 are examples of queries in more expressive fragments (SPJU, SPJA), while the remaining queries are examples of SPJ queries.

Control knobs In our experiments, we set the following two control knobs: (K1) the number of relations in the from-clause of the IEQsand (K2) the number of selection predicates in each conjunction of $sel(Q')$. Table 4 shows the range of values set for these knobs for the queries in Adult, Baseball, and TPC-H data sets; these values are chosen to ensure that the generated IEQs are not too complicated.

Testing platforms Our experiments were conducted on a machine running 64-bit Ubuntu OS with four-core Intel(R) Core(TM) i7 CPU Q820 @1.73 GHz CPU and 4 GB RAM. All the algorithms were coded in C++ and compiled and optimized with gcc; and data are managed using MySQL Server 5.0.51. Each experimental timing reported is an average timing over 5 different runs.

10.2 Effectiveness of at-least-one semantics

We compare TALOS against the two static class-labeling schemes, NI and RD, in terms of their efficiency as well as the quality of the generated IEQs. Recall that NI labels all the free tuples as positive, while RD labels a random number of at least one tuple from each subset of free tuples as

[8] http://www.basketballreference.com/.

[9] http://www.ebay.com/.

[10] We use *gain*, *ms*, *edu*, *loss*, *nc*, *hpw*, and *rs*, respectively, as abbreviations for capital gain, marital status, number of years of education, capital loss, native country, hours per week, and relationship.

Table 3 Test queries for Adult (A_1–A_5), Baseball (B_1–B_6) & TPC-H (T_1–T_7)

	Query	$Q(D)$
A_1	$\pi_{nc}\,\sigma_{occ=\text{“Armed-Force”}}\,(adult)$	1
A_2	$\pi_{edu,occ}\,(\sigma_{ms=\text{“Never-married”}\wedge 64\leq age\leq 68\wedge race=\text{“White”}\wedge gain>500\wedge sex=\text{“F”}}\,adult)$	4
A_3	$\pi_{nc,gain}\,(\sigma_{ms=\text{“Never married”}}\,adult)$	137
A_4	$\pi_{id}\,(\sigma_{SKY-LINE(gainMAX,ageMIN)}\,adult)$	4
A_5	$\pi_{age,AVG(hpw)}\sigma_{nc=\text{“US”}}(adult)$	1
B_1	$\pi_{M.name}\,(\sigma_{team=\text{“ARI”}\wedge year=2006\wedge HR>10}\,(Master\bowtie Batting))$	7
B_2	$\pi_{M.name}\,(\sigma_{sum(HR)>600}\,(Master\bowtie Batting))$	4
B_3	$\pi_{M.name}\,(\sigma_{SKY-LINE(HRMAX,SOMIN)}\,(Master\bowtie Batting))$	35
B_4	$\pi_{M.name,T.year,T.rank}\,(\sigma_{team=\text{“CIN”}\wedge 1982<year<1988}\,(Manager\bowtie Team))$	6
B_5	$\pi_{Master.name,Manager.ID}(Master\bowtie Manager)\bigcup\pi_{Master.name,B.teamID}\,\sigma_{year=2006}\,(Master\bowtie Batting)$	583
B_6	$\pi_{name,SUM(salary)}\,(Master\bowtie Salaries)$	3,540
T_1	$\pi_{S.name,N.name}\,\sigma_{S.acctbal>4000\wedge N.regionkey<4}\,(supplier\bowtie nation)$	4,383
T_2	$\pi_{C.name,N.name}\,\sigma_{C.acctbal>3000}\,(customer\bowtie nation)$	95,264
T_3	$\pi_{P.name,S.name}\,\sigma_{PS.avaiqty>3000\wedge S.acctbal>9500}\,(part\bowtie partsupp\bowtie supplier)$	24,672
T_4	$\pi_{O.clerk,L.extendedprice}\,\sigma_{L.quantity<2\wedge orderstatus=\text{“P”}}\,(lineitem\bowtie order)$	3,719
T_5	$\pi_{C.name,N.name}\,\sigma_{mktsegment=\text{“BUILDING”}\wedge C.acctbal>100}\,(customer\bowtie nation)\bigcup\pi_{S.name,N.name}\,\sigma_{S.acctbal>4000}\,(supplier\bowtie nation)$	32,554
T_6	$\pi_{P.name,SUM(PS.supplycost)}\mathcal{G}_{P.name}\,\sigma_{PS.retailprice>2000}\,(part\bowtie partsupp)$	4,950
T_7	$\pi_{C.name,SUM(O.totalprice)}\mathcal{G}_{C.name}\,\sigma_{C.acctbal>3000}\,(order\bowtie customer)$	63,533

Table 4 The control knob values

Control knob	Adult	Baseball	TPC-H
(K1) # relations in the from-clause	[1,1]	[2,4]	[2,3]
(K2) # selection predicates in each conjunction of the where-clause	[0,5]	[0, 5]	[0,5]

positive. The comparison focuses on SPJ test queries for the Adult and Baseball data sets.[11]

For the Adult data set, only weak IEQs are considered as all the labeling schemes would have produced the same strong IEQs due to the absence of free tuples in a single-relation database for computing strong IEQs.

Figure 4a compares the number of the three types of IEQs (precise, approximate, pruned) generated for Adult data set. As the number of decision trees considered is the same for all the schemes, the total number of IEQs generated by the schemes are the same. Observe that the number of precise IEQs from TALOS is consistently larger than that from NI and RD. The better quality IEQs from TALOS is due to its flexible dynamic class label assignment scheme for free tuples which provides more opportunities to derive precise IEQs. We note that it happens that all the tuples are bound for query

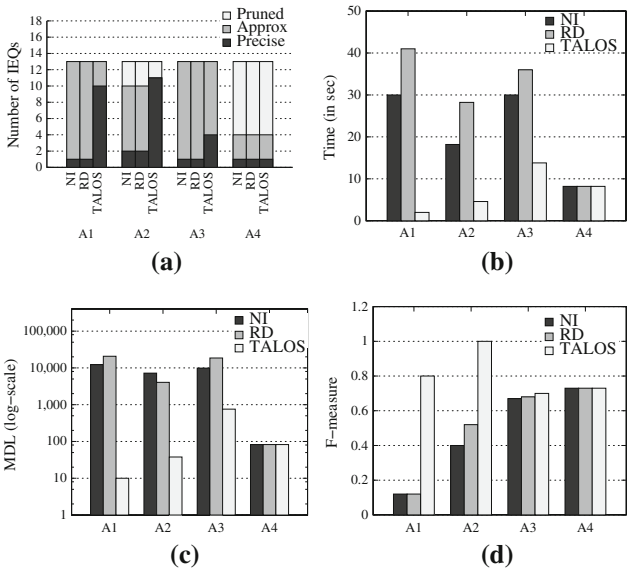


Fig. 4 Comparison of TALOS, NI and RD (Adult data set). **a** Types of IEQs. **b** Running time. **c** MDL metric. **d** F-measure metric

[11] As all the class-labeling schemes are based on the same framework to derive SPJU-IEQs which differ only in how they label free tuples to derive SPJ-IEQs that form the subqueries for SPJU-IEQs, we do not consider SPJU queries here. For SPJA queries, since the free tuples are assigned fixed class labels to satisfy the aggregation conditions before being classified, all the three schemes would have returned the same results for SPJA-IEQs; therefore, SPJA queries are not considered. For the TPC-H queries, it turns out that all the free tuples are bound, and therefore, all the three schemes return the same set of IEQs; therefore, we do not report results for TPC-H data sets.

Table 5 Comparison of decision trees for NI, RD, and TALOS

Query	Average height			Average size		
	NI	RD	TALOS	NI	RD	TALOS
A_1	14.9	19.8	2.1	5,304	9,360	4.7
A_2	16.1	21.8	6.5	3,224	2,970	19.2
A_3	16	20	12	4,386	8,103	334

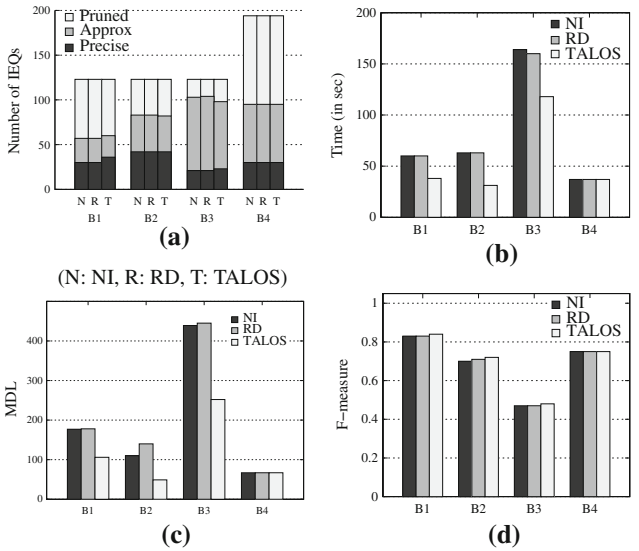


Fig. 5 Comparison of TALOS, NI, and RD (Baseball data set). **a** Types of IEQs(N: NI, R: RD, T: TALOS). **b** Running time. **c** MDL metric. **d** F-measure metric

A_4; hence, the performance results are the same for all three labeling schemes.

Figure 4b compares the running time performance of the three schemes for Adult data set. The results show that TALOS is also more efficient than NI and RD. The reason is due to the flexibility of TALOS's dynamic labeling scheme for free tuples, which results in decision trees that are smaller than those constructed by NI and RD. Table 5 compares the decision trees constructed by TALOS, NI, and RD in terms of their average height and average size (i.e., number of nodes). Observe that the decision trees constructed by TALOS are significantly more compact than those built by NI and RD.

Figure 4c,d compares the quality of the IEQs generated for Adult data set using the MDL and F-measure metrics, respectively. The results show that TALOS produces much better quality IEQs than both NI and RD. For the MDL metric (smaller value means better quality), the average value of the MDL metric for TALOS is low (under 700), while the values of both NI and RD are in the range of [4000, 22000]. For the F-measure metric (larger value means better quality), the average value for TALOS is no smaller than 0.7, whereas the values for NI and RD are only around 0.4.

Figure 5 shows the comparison results for the Baseball data set for strong IEQs. (The strong and weak IEQs for the queries B_1 to B_4 happen to be the same.) The results also demonstrate similar trends with TALOS outperforming NI and RD in both the running time as well as the number and the quality of IEQs generated for queries B_1–B_3. It happens that all the tuples are bound for query B_4; hence, the performance results are the same for all three algorithms.

We observe that the benefit of TALOS over NI and RD is higher for queries A_1–A_3 in Adult data set compared with that for queries B_1–B_3 in Baseball data set. For example, TALOS runs 3–10 times faster than NI and RD for queries A_1–A_3, whereas TALOS runs 2 times faster than NI and RD for queries B_1–B_3. As another example, the MDLs of the IEQs for A_1–A_3 returned by TALOS are 10–1,000 times lower than those of NI (and RD); whereas the MDLs of the IEQs for B_1–B_3 returned by TALOS are 2 times lower than those of NI (and RD). The reason is that the number of free tuples per partition for queries on Baseball data set is smaller (in the order of 10) compared with that for queries on Adult data set (in the order of 100). The flexibility for TALOS, therefore, reduces in queries B_1-B_3; however, TALOS still produces higher quality IEQs than NI and RD.

10.3 Discussion on generated IEQs

In this section, we discuss some of the interesting IEQs generated by TALOS on the running data sets, as shown in Table 6. Discussions for other queries are given in the Appendix We use $X_{i,j}$ to denote an IEQ for the query X_i in Table 3, where $X \in \{A, B, T\}$. For each IEQ, we also show its value for the F-measure metric (i.e., F_m^{est}) given in terms of their $|p_a|$, $|p_b|$ and $|p_c|$ values; recall that an IEQ is precise iff $|p_b| = 0$ and $|p_c| = 0$.

Adult In query A_2, we want to find the occupation and education of white females who are never married and with age in the range [64, 68] and with a capital gain greater than 500. The IEQ $A_{2,1}$ provides additional insight about the query result: Those who are in the age range [64, 66] are highly educated, whereas the rest (i.e., those in the age range [67, 68]) have high capital gains.

Query A_4 is a skyline query looking for people with maximal capital gain and minimal age. Interestingly, the precise IEQ $A_{4,1}$ provides a simplification of A_4: The people selected by this skyline query are either (1) very young ($age \leq 17$) and have capital gain in the range 1055–27,828 or (2) have very high capital gain (>27,828), work in the protective service and whose race is not classified as "others."

Query A_5 is an SPJA query looking for the average number of working hours per week of each age group of people who have native country as "USA" The precise IEQ $A_{5,1}$ reports the number of working hours per week of a particular person in this group. Note that although A_5 and $A_{5,1}$ use different aggregated functions (SUM vs. AVG), these queries are still

Table 6 Examples of IEQsgenerated by TALOS

IEQ		$\|p_a\|$	$\|p_b\|$	$\|p_c\|$
$A_{2,1}$:	$\sigma_{p_1 \vee p_2}\,(adult)$	5	0	0
	$p_1 : 63 < age \leq 66 \wedge edu > 15 \wedge ms =$ "NM"; $p_2 : 66 < age \leq 68 \wedge ms =$ "NM" $\wedge\, gain > 2993$			
$A_{4,1}$:	$\sigma_{p_1 \vee p_2}\,(adult)$	4	0	0
	$p_1 : 1055 < gain \leq 27828 \wedge age \leq 17$; $p_2 : gain > 27828 \wedge occ = \mathrm{P} \wedge race \neq \mathrm{O}$			
$A_{5,1}$:	$\pi_{age,SUM(hpw)}\,\sigma_{age=53 \wedge edu=\text{"Bachelor"} \wedge occ=\text{"Prof-specialty"}}(adult)$	1	0	0
$B_{2,1}$:	$\sigma_{salary>21680700 \wedge throws=\text{"L"}}\,(Master \bowtie Salaries)$	1	0	3
$B_{4,1}$:	$\sigma_{21<L\leq 22 \wedge SB\leq 0 \wedge 67<W\leq 70}\,(Mananger \bowtie Master \bowtie Batting \bowtie Team)$	1	0	5
$T_{1,1}$:	$\sigma_{regionkey\leq 3}(supplier \bowtie nation)$	4,383	3,598	0
$T_{3,1}$:	$\sigma_{3000<availqty\leq 3001 \wedge retailprice\leq 953}\,(part \bowtie partsupp \bowtie supplier)$	1	0	24,671

considered to be equivalent. The reason is that the difference between the aggregated values of the corresponding tuples in $A_5(D)$ and $A_{5,1}(D)$ is less than one and is considered to be the same based on the similarity function that is used.

Baseball In query B_2, we want to find the set of high performance players who have very high total home runs (> 600). The IEQ $B_{2,1}$ indicates that one player in this group is highly paid with a left throwing hand.

Query B_4 is an interesting query that involves multiple core relations. This query asks for the managers of team "CIN" from 1983 to 1988, the year they managed the team as well as the rank gained by the team. In this query, we note that TALOS found alternative join paths to link the two core relations, Manager and Team. The first alternative join path (shown by $B_{4,1}$) involves Manager, Master, Batting, and Team. The second alternative join path (not shown) involves Manager, Master, Fielding, and Team. The IEQ $B_{4,1}$ reveals the interesting observation that there is one manager who was also a player in the same year that he managed the team with some additional information about this manager-player.

Queries B_5 and B_6 are examples of SPJU and SPJA queries. TALOS returns one IEQ for each of these two queries, and the IEQ is exactly the same as the original one. In other words, TALOS is able to reverse-engineer the original queries that are used to derive $B_5(D)$ and $B_6(D)$.

TPC-H Query T_1 retrieves the names of suppliers whose $acctbal$ is greater than 4000 and $regionkey$ is smaller than 4. $T_{1,1}$ is an approximate IEQ of T_1 that does not include the selection condition on $acctbal$ attribute.

Query T_3 retrieves the name of suppliers and parts, where the $acctbal$ of the supplier is greater than 9500 and the $availqty$ of the part is greater than 3000. $T_{3,1}$ is an approximate IEQ that provides details of one tuple in $T_3(D)$, i.e., the tuple has $availqty = 3001$ and $retailprice \leq 953$.

Queries $T_5 - T_7$ are examples of SPJU and SPJA queries. TALOS returns one IEQ for each of these queries, and the IEQ is exactly the same as the original one. In other words, TALOS is able to reverse-engineer the original queries that are used to derive $T_5(D)$, $T_6(D)$ and $T_7(D)$.

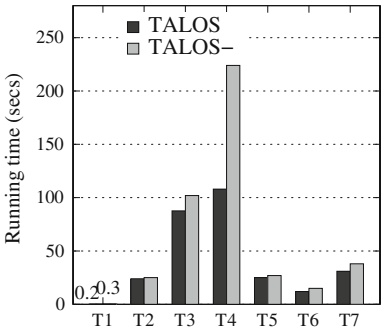


Fig. 6 Effectiveness of join indices

So far, we have studied the effectiveness of TALOS in generating IEQs. In the following, we study the efficiency of the proposed optimizations of TALOS. Our discussion focuses on TPC-H data set and the corresponding queries, as other data sets (Adult and Baseball) have small size, and the optimizations have little effect for those cases.

10.4 Effectiveness of optimizations for one database version

We now consider the case of applying TALOS to generate IEQs given *one* database version.

Effectiveness of join indices First, we evaluate the effectiveness of using join indices to compute the join relation for the decision tree classifier by comparing TALOS (which uses join indices) against TALOS$^-$ (without join indices) for deriving IEQs.

Figure 6 shows the running time comparison of TALOS and TALOS$^-$. Note that the number and quality of IEQs produced by TALOS and TALOS$^-$ are the same, as these qualities are independent of the optimizations. The results show that TALOS is up to two times faster than TALOS$^-$. The reason is that the computation of J_{hub} by TALOS using join indices is more efficient than the computation of join relation

Table 7 Detailed running times of TALOS and TALOS$^-$

Step	T_3		T_4	
	TALOS	TALOS$^-$	TALOS	TALOS$^-$
Join relation	25	36	20	70
Attribute list	1.6	3	36	63
Decision tree	61	63	52	91

J by joining relations directly in TALOS$^-$. In addition, the attribute lists accessed by TALOS, which correspond to the base relations, are smaller than the attribute lists accessed by TALOS$^-$, which are based on J.

To illustrate these observations above, we show the running time comparison of TALOS and TALOS$^-$ to derive IEQs for queries T_3 and T_4 with respect to the three main steps of each algorithm: (1) deriving the join relation, (2) computing attribute lists, and (3) building decision trees. The results in Table 7 clearly demonstrate the effectiveness of TALOS over TALOS$^-$ in these steps. For instance, the step to derive the join relation for T_3 by TALOS is 1.5 times faster than that of TALOS$^-$, since TALOS only needs to join the corresponding join indicesf *part-partsupp* and *partsupp-supplier* consisting of integer-valued columns. In contrast, TALOS$^-$ needs to perform the join between *partsupp*, *part*, and *supplier* relations. In another example, the step to derive join relation for T_4 by TALOS is 3.5 times faster than that of TALOS$^-$, since TALOS only needs to read the corresponding join index (*lineitem-order*); whereas TALOS$^-$ needs to perform the join between *lineitem* and *order* relations.

The attribute lists used by TALOS are also more compact than those used by TALOS$^-$. For instance, the attribute list constructed by TALOS$^-$ for attribute "*part.retailprice*" for query T_3 is 4 times larger than that constructed by TALOS. Thus, the steps to derive attribute lists and building decision trees run more efficiently in TALOS than in TALOS$^-$.

Effectiveness of domain indices We evaluate the effectiveness of using domain indices to identify covering attributes by comparing TALOS (which uses domain indices) against TALOS$^-$ (without domain indices) for deriving IEQs where the input query is unknown.

For each test query T_i, we first compute its answer $T_i(D)$ on the TPC-H data set D and then use $T_i(D)$ and D as inputs to derive IEQs; thus, each input query for this experiment is actually $T_i(D)$ and not T_i. For each query $T_i(D)$, we measured the time to derive the IEQs for $Q_i(D)$. We present each timing in terms of two components: The time taken to computehe covering attributes (denoted by CA) and the remaining time taken to derive the IEQs after the covering attributes have been computed (denoted by DT).

Figure 7 shows the comparison of TALOS and TALOS$^-$ for the TPC-H queries. The results show that TALOS is more efficient than TALOS$^-$ for computing covering attributes

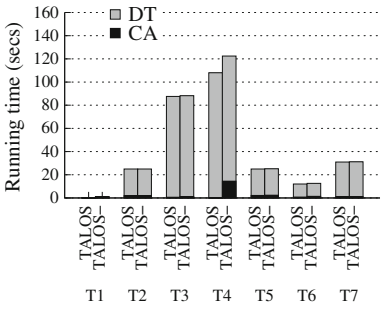


Fig. 7 Effectiveness of domain indices

(i.e., CA component) with TALOS taking a few seconds compared to 10 seconds incurred by TALOS$^-$.

For TPC-H data set with SF = 5.0 (in the Appendix), TALOS took 30 minutes to return three IEQs for query T4 which involved the two largest relations *lineitem* (30M tuples) and *orders* (7.5M tuples). Thus, further research is needed to scale the classification-based approach for very large data.

Storage overhead The storage overhead of TALOS consists of pre-computed join indices built for pairs of relations that have foreign key relationships and the domain indices.

For join indices, basically, for every pair of relations R and S that have foreign key relationship, TALOS builds a join index relation $I_{R,S}(r_R, r_S)$ consisting of k pairs of integers, where k is the number of tuples in the join result of R and S. In addition, TALOS also builds two B$^+$-indices on r_R and r_S column of $I_{R,S}$ to speed up the joins of using join indices. In our experiments, the pre-computed join indices built for TPC-H data set consist of 450 MB versus 1 GB of the whole database.

For the domain indices, the size of domain indices was 272 MB for the 1 GB TPC-H database. [12]

10.5 Effectiveness of optimizations for multiple database versions

In the last set of experiments, we evaluate the effectiveness of the optimizations proposed to derive IEQs for the two contexts with multiple database versions using the TPC-H data set and four queries (T_1 to T_4).

We created two database versions, D_1 and D_2, where D_1 was the original TPC-H database and D_2 was created from D_1 by combining with a set of delta tuples generated from four relations (*supplier*, *customer*, *partsupp*, *orders*)[13] as follows. For each of the four relations R, we randomly selected a subset of k tuples for deletion and also randomly

[12] We remove the *comment* attributes from each relation in TPC-H database.

[13] These four relations are chosen because they appeared in the test queries T_1 to T_4.

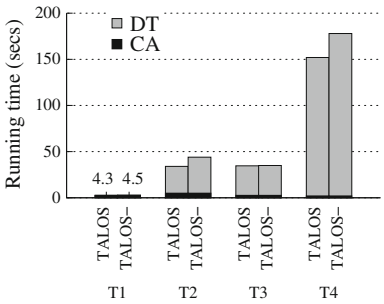


Fig. 8 Optimization for multiple database & result versions

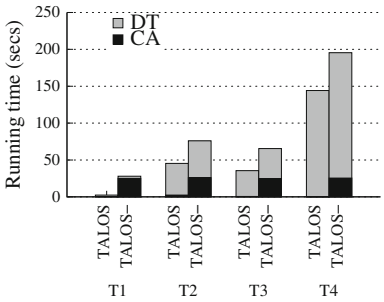


Fig. 9 Optimization for multiple database versions & single result

generated a set of k new tuples for insertion to R, where k is equal to 5 % of the cardinality of R. For each test query T_i, we run T_i on D_1 and D_2 to obtain two output tables $T_i(D_1)$ and $T_i(D_2)$.

The performance timings presented in this section consist of two components: the time to compute the covering attributes (denoted by CA) and the remaining time to derive the IEQs (denoted by DT).

Multiple database & result versions Given the inputs $(D_1, T_i(D_1))$ and $(D_2, T_i(D_2))$, we compare the performance of two algorithms, TALOS$^-$ and TALOS, to derive the IEQs for T_i.

The performance results in Fig. 8 show that TALOS outperforms TALOS$^-$ by a factor of 1.4 times. While both TALOS$^-$ and TALOS incur the same time for computing covering attributes, TALOS$^-$ spends significantly more time for deriving the IEQs because it needs to derive one set of IEQs for each $(D_j, T_i(D_j))$ and combine them to obtain the final result. In contrast, TALOS only needs to derive one set of IEQs using a more efficient approach. For all the test queries, both TALOS$^-$ and TALOS were able to successfully reverse-engineer the original test queries.

Multiple database versions & single unknown result Given the input $T_i(D_1)$, we compare the performance of two algorithms, TALOS$^-$ and TALOS, to derive the most recent database version D_j and IEQs Q'_i such that $Q'_i(D_j) = T_i(D_1)$.

The performance results in Fig. 9 show that TALOS is on average 1.5 times faster than TALOS$^-$. The reason is that TALOS$^-$ incurs a lot of time on computing covering attributes compared to TALOS. CA is in the order of 10 seconds in TALOS versus 60 seconds in TALOS$^-$. To further study the usefulness of the optimization techniques used in TALOS, we present the details of the data structures to derive the covering attributes for T_2 as an example. Recall from Sect. 9.1 that in order to compute the covering attributes which are categorical attributes in this case, TALOS first derives δTM_d as the join between T_2 containing 95k tuples and δM_d containing 600k tuples. The resulting δTM_d contains 15k tuples. Lastly, TALOS performs an outer-join between δTM_d and TM_d^2 containing 100k. This process is much cheaper then TALOS$^-$, which first updates the table M_d^2 containing 4000k by adding 600k tuples from δM_d and then joins the resulting M_d^1 with T_2.

11 Related work

The related work can be broadly classified into three areas: work on deriving instance-equivalent queries, data mining techniques for related problems, and work on reverse query processing.

11.1 Instance-equivalent queries

To the best of our knowledge, our work [29] was the first data-driven approach to generate instance-equivalent queries from an input query and its result on a database. In this paper, we have extended the work to handle an unknown input query, support more expressive IEQs, and handle multiple database versions.

Sarma et al. [25] examined a related problem called *view definitions problem (VDP)* which derives a view definition Q given an input database D and a materialized view V. As the focus there is on analyzing the complexity of variants of the VDP problem, it assumes a very basic setting where D consists of a single relation R and V has the same schema as R. Consequently, the derivation of Q consists of determining the selection predicates on R to generate V, and the paper examines the complexity of the problem for different query fragments in terms of the number of equality/range predicates and whether disjunctions are permitted. In contrast to the theoretical treatment in [25], the setting in our work is more general and focuses on a novel data classification-based approach and optimization techniques to derive IEQs.

An area that is related and complementary to our data-driven approach for QRE is intensional query answering (IQA) or cooperative answering. For a given query Q, the goal of IQA is to augment the query's answer $Q(D)$ with additional intensional information in the form of a semanti-

cally equivalent query[14] that is derived from integrity constraints on the data [9,18]. While semantic equivalence is stronger than instance equivalence and can be computed in a data-independent manner using only integrity constraints (ICs), there are several advantages of adopting instance equivalence for QRE. First, in practice, many data semantics are not explicitly captured using ICs in the database for various reasons [11]. Hence, the effectiveness of IQA could be limited for QRE. Second, even when the ICs in the database are complete, it can be very difficult to derive semantically equivalent queries for complex queries (e.g., skyline queries that select dominant objects). Third, as IQA requires the input query Q to be known, IQA cannot be applied to QRE applications where only $Q(D)$ (but not Q) is available. Thus, we view IQA and our proposed data-driven approach to compute IEQs as complementary techniques for QRE.

11.2 Data mining techniques

A related technique to our approach of classifying tuples in a join relation is the CrossMine approach for multi-relational classification [33]. Given a target relation R with tuples that have fixed class labels (i.e., either positive or negative), CrossMine builds a decision tree classifier for tuples in R using the attributes in R as well as the attributes from other relations that have primary-foreign key relationships with R. Our data classification in TALOS differs from CrossMine in two key ways. First, TALOS has the notion of *free tuples* that are dynamically assigned positive or negative class labels with respect to constraints that are imposed by IEQ derivation problem (i.e., at-least-one semantics, exactly-k semantics, and aggregation constraints). In contrast, CrossMine has the same setting as conventional data classification where all tuples have fixed class labels. Second, whereas CrossMine uses a greedy heuristic to compute node splits in the construction of decision trees, TALOS introduces a novel and efficient technique to compute optimal node splits by exploiting the flexibility enabled by the presence of free tuples.

A somewhat related problem to ours is the problem of *redescription mining* introduced in [22]. The goal in redescription mining is to find different subsets of data that afford multiple descriptions across multiple vocabularies covering the same data set. At an abstract level, our work is different from these methods in several ways. First, we are concerned with a fixed subset of the data (the output of the query). Second, none of the approaches for redescription mining accounts for structural (relational) information in the data (something we explicitly address). Third, redescription mining requires multiple independent vocabulary descriptions to be identified. We do not have this requirement as we are concerned with deriving IEQs within an SQL context.

11.3 Reverse query processing

There are two recent directions that share the same broad principle of "reverse query processing" as QRE but differ completely in the problem objectives and techniques.

The first direction addresses the problem of generating databases to satisfy a set of constraints given an input set of queries and their results. [3] introduced the *reverse query processing* problem, which given an input query Q and a desired result R, generates a database D such that $Q(D) = R$. [4] introduced the QAGen problem, which given an input query Q and a set of target cardinality constraints on the intermediate subexpressions in Q's evaluation plan P, generates a test database such that the execution of P on D satisfies the given cardinality constraints. The QAGen problem was generalized in [14] to consider a workload of queries with the objective of generating a minimal set of database instances such that the results of the workload queries on the database instances satisfy the given cardinality constraints. A more recent work [2] proposed probabilistically approximate algorithms for the QAGen problem. Unlike these works on generating databases, our work on QRE is to generate instance-equivalent queries.

The second direction addresses the problem of *targeted query generation (TQGen)* which aims to generate test queries to meet a given set of cardinality constraints [7,17]. Specifically, given a query Q, a database D, and a set of target cardinality constraints on the intermediate subexpressions in Q's evaluation plan, the objective of TQGen is to generate a modified query Q' (by modifying the constant values in Q's selection predicates) such that the evaluation plan of Q' on D satisfies the given cardinality constraints. Different from the TQGen problem that focuses on cardinality constraints, our work on QRE aims to generate instance-equivalent queries that satisfy the "content" constraints of the query results. In addition, unlike the TQGen problem, the input query may be unknown in our QRE problem and the IEQs generated could be very different from the input query (beyond modifications to selection predicate constants).

More broadly, there has also been work on reverse engineering various aspects of database systems: extracting data models from databases (e.g., [15,20]) and mining database structural information that spans from data dependencies and constraints (e.g., [6,26]) to higher-level semantic structures (e.g., [1,31]) to support browsing of databases with large, complex schemas and data integration applications.

[14] Two queries Q and Q' are *semantically equivalent* if for every valid database D, $Q(D) = Q'(D)$.

12 Conclusion

In this paper, we have introduced the *query reverse engineering* (QRE) problem to derive an instance-equivalent query that produces the same result as a given input result table. The QRE problem has useful applications in database usability, data analysis, and data security. We have proposed a data-driven approach, TALOS, that is based on a novel dynamic data classification formulation and extended the approach to efficiently support the three key dimensions of the QRE problem: whether the input query is known/unknown, supporting different IEQ fragments, and supporting multiple database versions.

There are several directions for further work on the QRE problem. With respect to our proposed method TALOS, one challenging issue that requires further study is the scalability of the approach for very large data sets; in particular, the computation and processing of the hub table could be a bottleneck when the relations involved are very large. It is also interesting to extend TALOS to derive more complex IEQs (e.g., queries with arithmetic expressions, top-*k* queries). An interesting direction to explore beyond TALOS is a hybrid approach that includes an offline phase to mine for soft constraints in the database and an online phase that exploits both the database contents as well as mined constraints. Finally, a more general direction to explore is how to apply the idea of query reverse engineering for querying web data.

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