Reachability Queries with Label and Substructure Constraints on Knowledge Graphs

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Abstract—Since knowledge graphs (KGs) describe and model the relationships between entities and concepts in the real world, reasoning on KGs often correspond to the reachability queries with label and substructure constraints (LSCR). Specially, for a search path $p$, LSCR queries not only require that the labels of the edges passed by $p$ are in a certain label set, but also claim that a vertex in $p$ could satisfy a certain substructure constraint. LSCR queries is much more complex than the label-constraint reachability (LCR) queries, and there is no efficient solution for LSCR queries on KGs, to the best of our knowledge. Motivated by this, we introduce two solutions for such queries on KGs, UIS and INS. The former can also be utilized for general edge-labeled graphs, and is relatively handy for practical implementation. The latter is an efficient local-index-based informed search strategy. An extensive experimental evaluation, on both synthetic and real KGs, illustrates that our solutions can efficiently process LSCR queries on KGs.

Index Terms—Knowledge graph, Reachability query, Label constraint, Substructure constraint.

1 INTRODUCTION

NOWADAYS, numerous highly formatted databases are utilized to construct domain specific KGs [21], reasoning on which is widely used in various applications, e.g. criminal link analysis [15], [16], suspicious transaction detection [12], e-commerce recommendation [10], etc. In such applications, reasoning between two entities often relates to the reachability queries with both label and substructure constraints [18], [22], as KGs can be considered as edge-labeled graphs.

For example, we model a financial KG as $G$, where (i) each vertex represents a person; (ii) each edge $e=(u, l, v)$ correlates to an account transfer or a relationship from vertex $u$ to vertex $v$; (iii) the label $l$ of $e$ is either a timestamp that corresponds to the transfer occurred time, or a social relationship (e.g. friend-of, parent-of, married-to, etc.). In some detection tasks, to verify the economic criminal relationship between Suspect $C$ and Suspect $P$, with the known information: “An indirect transaction from $C$ to $P$ occurred in April 2019, in which one of the middlemen of the transaction and Amy are married …”, as depicted in Figure 1(a).

If the economic criminal relationship exists, a transaction path $p=<C, e_0, v_0, ..., v_{k-1}, e_k, P>$ from $C$ to $P$ exists in $G$ as shown in Figure 1(b), where (i) $l_0, ..., l_k$ represent the labels of edges $e_0, ..., e_k$, respectively, and the timestamps of $l_0, ..., l_k$ are in April 2019; (ii) $\exists X \in v_0, ..., v_{k-1}$, which is one of the passing vertex of $p$, represents a person in $G$ who married Amy. Note that $G$ could contain multiple married couples, maybe only some of those couples could satisfy the above conditions.

Moreover, such queries can also be used in a variety of situations, e.g. traffic navigation [9], domain specific anomaly detection [3], etc., asking the following question: Can a vertex $s$ reach to a vertex $t$ by a path $p$, where the edge labels in $p$ are in a certain label set (label constraint), and $p$ passes a certain substructure (substructure constraint)?

Even though the label- and substructure-constraint reachability (LSCR) queries on KGs are quite useful for the above reasoning tasks, as far as we know, there is no particular solution. The reason is that the LSCR problem is much more complicated than the label-constraint reachability (LCR) problem, originated in [6]. According to [6], there are two kinds of techniques for LCR queries, online search (DFS/BFS) and full transitive closure (TC) precomputing.

The former can be applied directly, for the LCR queries. Assuming the input KG contains $|V|$ vertices and $|E|$ edges, the time complexity of DFS/BFS applied in LCR queries is $O(|V|+|E|)$, as the label constraint prunes the search space of DFS/BFS. Unfortunately, the problem of LSCR queries on KGs is too complex. As analyzed in Section 3, the time complexity of implementing traditional BFS/DFS for LSCR queries is about $O(|V| \times (|V|+|E|))$ for the worst case. Thus, the former techniques can hardly be adopted to solve our problem.

The latter aims to precompute a full TC of the input graph to answer LCR queries efficiently, but the space complexity of storing a full TC for a graph $G$ is $O(|V|^2 \times 2^{|L|})$, where $L$ is the label set of $G$. Hence, many works [6], [23], [19] are proposed to reduce the space complexity of indexing...
an input graph. However, the indexing time complexity of the above methods are too high to index a large KG, as discussed in Section 5.2. Note that, in this paper, we do not consider the approximate techniques of LCR queries, e.g. [17], because KG reasoning applications require exact results, like the above criminal detection scenario.

Contributions. In this paper, we provide a comprehensive study of LSCR queries on KGs with efficient solutions. Our work conquers the practical unbearable indexing time of the traditional landmark indexing method [19], with a local index. Plus, we overcome the inefficiency of the algorithm (Section 4) that implements the subgraph matching techniques for LSCR queries on KGs, by developing an informed search strategy based on local index. With the detailed experimental evaluation, our work could address the LSCR queries on KGs efficiently.

Our main contributions are as follows:

- We first define the problem of reachability queries with label and substructure constraints, which is the basis of reasoning on KGs.
- We develop an uninformed search algorithm, named UIS, for LSCR queries. It has a great potential for practical implementation on general labeled graphs, as UIS is not overly complex, and does not require any of the characteristics of KGs.
- Then, we develop an intuition idea of implementing SPARQL engines [11], called UIS*, to address LSCR queries and overcome the disadvantage of UIS. That is because: (i) current KGs are based on the standard of OWL [2] in the form of RDF [11], usually can be accessed by SPARQL; (ii) a substructure constraint can be expressed in SPARQL (Section 2).
- After that, we propose an efficient informed search algorithm, i.e. INS, with a novel index, local index. INS could break the fixed search direction of the uninformed search algorithms, and could process the vertices in the input KG with priorities, by developing two data structures as an evaluation function based on the entries of local index.
- Finally, we conduct extensive experiments on both real and synthetic datasets to evaluate the introduced search algorithms. The experimental results show that the informed search algorithm could address LSCR queries on KGs efficiently.

The rest of this paper is organized as follows. The problem of LSCR queries on KGs is formally defined in Section 2. We introduce UIS, UIS* and INS in Section 3, Section 4 and Section 5 respectively. The experimental results are presented in Section 6. Finally, we draw a conclusion in Section 7.

2 Problem Definition

We formally define the LSCR queries on KGs, with a table of frequently used notations (Table 1) and two KG schematic views (Figure 2 and Figure 3).

Knowledge Graph (KG). In essence, KGs [2] are graphs that consist of vertices and labeled edges. However, different from normal edge-labeled graphs, KGs often correspond to rich information of the real world, and the sizes of KGs are relatively large. For example, at the end of 2014, Freebase [2] included 68 million entities, 1 billion pieces of relationship information and more than 2.4 billion factual triples. In practice, KGs are stored by RDF triples [11], and formatted by RDFS [5] (RDF schema). RDFS defines a set of RDF vocabularies (e.g. “rdfs:Class”, “rdfs:subClassOf”, “rdfs:range”) with special meanings, which could structure RDF resources and format the knowledge representations. From the perspective of graph classification, RDFS represents KGs as scale-free networks [20], in which the relative commonness of vertices with a degree greatly exceeds the average.

Figure 2 draws a simple KG with some RDF vocabularies, in which (i) “eg:Researcher” represents a class of the researchers in the real world; (ii) “eg:workWith” is an edge label entity, and the edges labeled by “eg:workWith” are incident to (“rdfs:domain”) and also points to (“rdfs:range”) an instance of “eg:Researcher”; (iii) Taylor and Walker are real persons and all researchers (instances of “eg:Researcher”), who also work together (with the edges labeled by “eg:workWith”). Certainly, in KGs, a vertex u corresponding to real world instances has high degree, like “eg:Researcher”. Besides, a class vertices, like “eg:Person” is more important for the KG structure than an instance vertex, e.g. “eg:Researcher”.

In a word, KGs are basically edge-labeled graphs, in the form of RDF, and structured by RDFS. The formal definition of a KG is demonstrated in Definition 2.1.

Definition 2.1. A knowledge graph G is a quadruple (V, E, L, Lₘ), where: (1) V is the vertex set of G and L is the edge label set; (2) E ⊆ V ∩ L ∩ V is the labeled edge set of G, and for ∀e ∈ E, e = (s, l, t) is an edge from s to t with a label l; (3) Let λ: E → L be a label mapping function, i.e. λ(e) = l, then L = ∪λ∈E(λ(e)); (4) Lₘ confines the RDF triples of G.

Note that, we illustrate the following definitions based on an input KG G = (V, E, L, Lₘ).

Label constraint. A label constraint in this paper relates to a subset of L in the KG G, for example, in Figure 3(a), a label constraint can be {friendOf, follows}.

Substructure Constraint. In order to define the substructure constraints in the KG G, we first formalize a variable-substructure γ in G as a triple (Vₛ, Eₛ, Eₗ), where (i) Vₛ ⊆ V, Eₛ ⊆ E and ∀(u, l, v) ∈ Eₛ, u, v ∈ Vₛ; (ii) Eₗ = {(u, l, v)|u ∈ Vₛ, l ∈ L} ∪ {(u, l, v)|v ∈ Vₛ, l ∈ L}, and an element e ∈ Eₗ matches zero or multiple edges in E. Then, the substructure constraint is defined as follows:

Definition 2.2. A substructure constraint S is referred to a tuple (?x, Vₛ, Eₛ, Eₗ), where (Vₛ, Eₛ, Eₗ) corresponds...
to a variable-substructure in \( G \), and, \( \exists e \in E_r, e \) is incident to \( ?x \) or points \( ?x \).

For instance, Figure 3(b) demonstrates a substructure constraint \( S_0 \) of \( G_0 \) in Figure 3(a), where \( S_0 = \{ ?x, \{ v_3 \}, \{ ?x, \text{friendOf}, v_3 \}, \{ v_3, \text{likes}, ?y \} \} \).

Note that, although the substructure constraints can be defined in multiple ways, we only study the most widely used one, in this paper, and the other forms can be derived from this definition.

**Reachability.** For clarity, we let \( L(p) \) and \( V(p) \) denote the label set and the vertex set of a path \( p \), respectively, and let \( P(s,t) \) represent the set of all the paths from a vertex \( s \) to a vertex \( t \). Obviously, if \( s \) reaches \( t \), there is a path from \( s \) to \( t \) (\( P(s,t) \neq \emptyset \)). We utilize symbol \( s \rightsquigarrow t \) and symbol \( s \rightarrow t \) to describe the reachability and non-reachability from a vertex \( s \) to a vertex \( t \), respectively.

**Label-constraint reachability (LCR).** Similarly, if a vertex \( s \) reaches a vertex \( t \) under a label constraint \( L \) (denoted by \( s \rightsquigarrow L, t \)), one path \( p \) forms \( s \) to \( t \) exists, where each edge label in \( p \) is an element of \( L \), i.e. \( L(p) \subseteq L \).

In contrast, given a label constraint \( L \), if \( s \rightsquigarrow L \), we say \( L \) is a sufficient path label set. Furthermore, if \( \forall L' \subseteq L \text{ and } s \rightsquigarrow L', t \), \( L \) is a minimal sufficient path label set. For the collection of all the minimal sufficient path label sets (CMS) from \( s \) to \( t \) is denoted by \( M(s,t) \), and defined in Definition 2.3.

**Definition 2.3.** A collection of label sets \( M(s,t) \) is a CMS from \( s \) to \( t \), if \( M(s,t) = \{ L(p) | p \in P(s,t) \text{ and } L(p) \subseteq P(s,t), i \neq j, \text{ such that } L(p_j) \subseteq L(p_i) \} \).

For example, \( M(v_0,v_3) = \{ \{ \text{friendOf} \}, \{ \text{advisorOf}, \text{follows} \}, \{ \text{likes}, \text{follows} \} \} \) as shown in Figure 3(a).

**Substructure-constraint reachability.** Firstly, we say a vertex \( u \) satisfies a substructure constraint \( S = \{ ?x, V_S, E_S, E_T \} \), if we replace \( ?x \) with \( u \) whose result is still a substructure or a variable-substructure of \( G \). For instance, for the substructure constraint \( S_0 \) (Figure 3(b)) and two vertices \( v_1 \) and \( v_2 \), the replaced results are depicted in Figure 3(c) and Figure 3(d), respectively. As the replaced results of \( v_1 \) and \( v_2 \) are a variable-substructure of \( G_0 \), \( v_1 \) and \( v_2 \) satisfy \( S_0 \).

Then, if a vertex \( s \) reaches a vertex \( t \) under a substructure constraint \( S \) (denoted by \( S \rightsquigarrow t \)), there is a path \( p \) from \( s \) to \( t \), where \( \exists u \in V(p) \) and \( u \) satisfies \( S \). For example, in Figure 3(a), \( v_0 \rightsquigarrow v_4, v_0 \rightsquigarrow v_3 \) and \( v_3 \rightsquigarrow v_4 \).

**Overall.** Theorem 2.1 presents the condition for the existence of \( S \rightsquigarrow t \), which states that a vertex \( s \) reaches a vertex \( t \) under a label constraint \( L \) and a substructure constraint \( S \). For example, in Figure 3(a), given a label constraint \( L = \{ \text{likes}, \text{follows} \} \), \( v_0 \rightsquigarrow L_{S_0} v_4 \), while, \( v_0 \rightsquigarrow L_{S_0} v_3 \).

**Theorem 2.1.** \( S \rightsquigarrow L_{S_0} t \) in a KG \( G \), iff \( \exists p \in P(s,t), L(p) \subseteq L \) and \( \exists u \in V(p) \wedge u \text{ satisfies } S \).

**Proof 2.1.** That can be easily proved by the above definitions.

**Problem Definition.** According to the above definitions, we define the problem in Definition 2.4.

**Definition 2.4.** A LSCR query \( Q \), on KG \( G=(V,E,L,L_s) \), is a quadruple \( (s,t,L,S) \), where \( s,t \in V, L \subseteq S \) and \( S \) is a substructure constraint of \( G \). If \( s \rightsquigarrow L_{S_0} t \) in \( G \), then the answer of \( Q \) is true. Otherwise, the answer of \( Q \) is false.

**Additional.** For the KG \( G \) and a substructure constraint \( S \), we let \( V(S,G) \) denote a vertex set, which contains all the vertices in \( G \) that satisfy the substructure constraint \( S \).

Besides, a substructure constraint \( S \) can be expressed by a SPARQL \( ^{24} \) query. For instance, \( S_0 \) (Figure 3(b)) can be modeled as ‘Select ?x where {?x (friendOf) v_3, v_3 (likes) ?y}’.

### 3 Uninformed Search

The most straightforward way of answering reachability queries on KGs is the uninformed (blind) search strategies \( ^{13} \): DFS and BFS, which process an input query with no additional information beyond that in problem definition. Simply using label constraint to reduce the search space, we can adopt DFS or BFS to solve LCR queries \( ^{6} \).

Unfortunately, LSCR queries are too complex, and neither DFS nor BFS can be utilized to such queries directly, as they never revisit the passed vertices in the query processing. For example, supposing a label constraint \( L = \{ \text{likes}, \text{hates}, \text{friendOf} \} \), in order to verify the existence of \( v_3 \rightsquigarrow L_{S_0} v_4 \) in Figure 3(a), a search algorithm needs to walk on the path \( p =< v_3, \text{likes}, v_4, \text{hates}, v_1, \text{friendOf}, v_3, \text{likes}, v_4 > \), because only \( v_1 \) and \( v_2 \) could satisfy \( S_0 \).

To process a LSCR query \( Q=(s,t,L,S) \) on a KG \( G=(V,E,L,L_s) \), at least two procedures are required in DFS or BFS. One searches in the space whose vertices can be reached by \( s \) under the label constraint \( L \); the another one is executed only when the former discovers a vertex \( v \) that satisfies the substructure constraint \( S \), and runs from \( v \) to \( t \) by walking on the vertices that can be reached by \( v \) under the label constraint \( L \). This process stops, when the former stops, or the latter returns true.

Then, we analyze the time complexity of the above process, assuming a substructure constraint \( S=\{ ?x, V_S, E_S, E_T \} \). The former procedure requires \( O(|V|(|V_S|+|E_S|+|E_T|)+|E|) \), as it runs in the space with
Algorithm 1 UIS Algorithm($G, Q$)

Input: $G = (V, E, L, L_S)$ represents a KG,
       $Q = (s, t, L, S)$ is a LSCR query.

Output: The answer of $Q$.
1. Let $S$ be a stack with one element $s$
   // The initial values in close are set to $N$
2. close[$s$] ← SCck($s, S$)
3. while $S$ is not empty do
4.   Take an element $u$ from $S$
5.   for each edge $e = (u, l, v), l \in L$, incident to $u$ do
6.     // We explore $v$ in the following cases
7.     if close[$u$] = $T$ \&\& close[$v$] $\neq T$ (case 1) then
8.       Add $v$ into $S$, close[$v$] $\leftarrow T$
9.     else if close[$v$] = $N$ (case 2) then
10.    Add $v$ into $S$, close[$v$] $\leftarrow$ SCck($v, S$)
11.   if $v = t$ \&\& close[$v$] = $T$ then
12.    return $Q = T$
13. return $Q = F$

evaluating whether each passed vertex can satisfy $S$ or not.
Each invocation of the latter procedure needs $O(|V|+|E|)$.
We execute the latter up to $|V(S, G)|$ times, which is less than $|V|$.
Hence, we summarize the time complexity in Theorem 3.1.

Theorem 3.1. The time complexity of applying DFS/BFS is
$O(|V|(|V_S|+|E_S|)+|E_S|+|V|+|E|)) = O(|V|(|V|+|E|)).$

Proof 3.1. It can be easily proved by the above discussion.

Due to the high time complexity of utilizing the above techniques, we introduce a novel uninformed online search strategy (UIS, Algorithm 1) for LSCR queries (Section 3.1), which could be scaled on general labeled graphs, and provides a baseline for LSCR queries. After that, we discuss the usability of adopting current LCR methods on our problem (Section 3.2).

3.1 Baseline of LSCR Queries
The algorithm UIS($G, Q$) starts with putting an element $s$
into a stack $S$ (Line 1), and runs until $S$ is empty ($s \xrightarrow{L_S} t$,
Line 12) or $s \xrightarrow{L} t$ is proved (Line 11). In UIS, we devise a
function SCck($v, S$) to verify whether $v$ can satisfy $S$.
Furthermore, in order to manage the recalling process of UIS,
we develop a surjection close:$V \rightarrow \{N, T, F\}$ as illustrated in Definition 3.1.

Definition 3.1. A surjection close:$V \rightarrow \{N, T, F\}$ in a search
algorithm for LSCR queries is as follows: (i) initially, \forall $u \in V$, close[$u$] = $N$, which represents that $u$ have not
been explored; (ii) if $s \xrightarrow{L_S} u$ and $s \xrightarrow{L} u$ have been proved by the search strategy, we set close[$u$] to $T$ and $F$, respectively.

Note that, this surjection is used throughout this paper.

After setting close[$s$] to SCck($s, S$) (Line 2), the loop
(Lines 3-11) takes an element $u$ from $S$ (Line 4), and processes each edge $e = (u, l, v)$ with the edge label $l$ belonging to $L$.
Thus, the algorithm only traverses in the space that $s$
reaches to under $L$, i.e. $s \xrightarrow{L} u$ exists. We explore $v$ in the following cases (Lines 5-11).
1. close[$u$] = $T$ \&\& close[$v$] $\neq T$, which means that $s \xrightarrow{L} u$ exists. As $u \xrightarrow{L} v$ and $e = (u, l, v) \wedge l \in L$,
$s \xrightarrow{L} v$ exists so that close[$v$] = $T$. (2) close[$u$] $\neq T$ \&\& close[$v$] = $N$, where, if SCck($v, S$) returns true, i.e. $v$ satisfies $S$, we set close[$v$] = $T$ ($s \xrightarrow{L} v$), otherwise, we set close[$v$] = $F$.

Analysis. In order to analyze the proposed algorithm, we first introduce the search tree in LSCR queries.
For general consideration, in the following discussion, we assume SCck($s, S$) returns false, and loop (Line 3-11) starts with close[$s$] = $F$. Figure 4 draws a tree search example, in which, $\forall v \in V$, we make a distinction between close[$v$] = $T$ and close[$v$] = $F$, and mark them with colors.

In order to illustrate the vertex exploring process, in Lines 5-8 we mark three edges with numbers 1, 2, and 3, which denote $e_1 = (u, l_1, v_1)$, $e_2 = (u, l_2, v_2)$, and $e_3 = (u, l_3, v_3)$, respectively. $e_1$ and $e_2$ appear, iff, in case 2, SCck($v_1, S$)$ =$true and SCck($v_2, S$)$ =$false, respectively; $e_3$ appears, iff, in case 1, we explore vertex $v_3$. In contrast, the edges in the search tree can only be generated in the above three ways, because we only explore a vertex in case 1 and case 2. We formally define the search tree in Definition 3.2.

Definition 3.2. A search tree of a LSCR query $Q = (s, t, L, S)$
is formalized as $T$, where (i) the root of $T$ is $s$; (ii) supposing $N^T$ denotes the node set of $T$, there is an injection $f : V \rightarrow N^T$ and, $\forall u \in V$, $u$ points at most two nodes $v^f$ and $v^T$ in $N^T$; (iii) $v^f$ ($close[v] = F$) and $v^T$ ($close[v] = T$) represent the states of $v$ in close when vertex $v$ is passed by a searched algorithm.

Finally, we prove the algorithm correctness and the time complexity in Theorem 3.2 and Theorem 3.3 respectively.

Theorem 3.2. (Correctness of Algorithm 1) $Q$ is a true query, iff, UIS($G, Q$) returns true.

Proof 3.2. ($\Rightarrow$) $Q$ is a true query, iff, $\exists p \in P(s, t) \wedge \exists v \in p$ and $v$ satisfies the substructure constraint $S$. Supposing $p = \langle s, e_0, \ldots, e \rangle \wedge v$ is the first vertex in $p$, where $s \xrightarrow{L} v$, $v \xrightarrow{L} t$ and close[$v$] = $T$ exist. As UIS has the ability of recalling a vertex $w$, where the state of $w$ in close is $F$, the statement is obvious valid.

($\Leftarrow$) If UIS returns true, a node $v^T$ exists in $T$. Thus, $s \xrightarrow{L} t$, and $Q$ is a true query.

Theorem 3.3. The time complexity of UIS($G, Q$) is $O(|V| \times (|V_S|+|E_S|+|E_T|))$, assuming $S = (?x, V_S, E_S, E_T)$.

Proof 3.3. The time complexity of function SCck($v, S$) is $O(|V_S|+|E_S|+|E_T|)$. We invoke such function up to $|V|$ times. Plus, UIS traverses $G$ at most twice, according to

Fig. 4. An UIS search tree, where we make a distinction between close[$v$] = $T$ (red) and close[$v$] = $F$ (blue) by colors.
Definition 3.2 Hence, the time complexity of UIS traverses $G$ is $O(|V| + |E|)$. Thus, the statement is proved.

3.2 Analysis of LCR Methods

In this section, we first give a brief review of current LCR methods, then discuss why such methods cannot be applied on our problem.

Review. The problem of LCR queries is originated in [6]. They aim to address the high space complexity problem in the graph full transitive closure (TC) precomputation, with a tree-based index framework. This framework contains a spanning tree (or forest) and a partial transitive closure of a tree-based index framework. This framework contains all the information of the full TC to respond the LCR queries.

[25] decomposes an input graph into several strongly connected components. For each component a local transitive closure is computed, that is, they precompute all the CMSs of every vertex pair in a local transitive closure. Then, they transfer each component into a bipartite graph. For the vertex pairs $(u, v)$ that $u$ and $v$ are not in the same component, both the CMSs from $u$ to $v$ and from $v$ to $u$ can be found in the topological order of bipartite graph union. That is, the CMSs of the vertices in different components are also precomputed. Thus, the precomputed index contains all the information of the full TC.

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To our knowledge, the current state-of-the-art solution of LCR queries is [19]. Given a label set $L$ of an input edge-labeled graph, they first choose $k$ landmarks. For each landmark vertex $v$, they precompute all CMSs from $v$ to every vertex that $v$ reaches. Besides, for accelerating LCR query processing, they also index each non-landmark vertex with $b$ CMSs. Plus, let $R_L(v)=\{w \in V|v \xrightarrow{L} w\}$, $v$ is a landmark, and $\forall L \subseteq L$, $|L| \leq |L|/A + 1$, they precompute $R_L(v)$ for each landmark vertex $v$, to accelerate false-queries.

Discussion. Even though such techniques are fast on answering LCR queries, they cannot be scaled for indexing the relatively large KGs, due to the prohibitively high indexing time complexity.

Based on the report in [3] (Table 1 of [3] and Table 2 of [4]), the indexing time of spanning tree increases linearly with the increasing of the graph density $D = |E|/|V|$, as depicted in Figure 5(a). Plus, the indexing time of spanning tree exponentially grows as $|V|$ grows, which is demonstrated in Figure 5(b). When $|V| = 100,000$ and $D = 1.5$, the indexing time is about $10^5 \times 11.57d$.

[25] represents a baseline of [19], and, in [19], they illustrate that [25] do not scale well on large graphs ($|V| > 5.4k$). Besides, the indexing time complexity of [19] is $O((|V| \log |V| + |E| + |V|b(|V| - k))|V|^{2k/4})$, where $k$ is the number of selected landmarks, $b$ is the value of the indexed entries for each non-landmark vertex. In the experimental settings of [19], $k=1250+\sqrt{|V|}$ and $b=20$, so the time complexity of [19] is equal to $O(|E||V|^{2|L|} + |V|^{2k/4})$.

Therefore, for a relatively large graph, the above methods can hardly be adopted.

4 Improved Uninformed Search

For an LSCR query $Q=(s, t, L, S)$ on a KG $G$, UIS has to evaluate each vertex of each search path $p$ with the function $SCck$, until $\exists v \in V(p) \wedge v \in V(S, G)$ exists $(v$ satisfies the substructure constraint $S)$. The time complexity of the above operation highly depends on the given substructure constraint $S$. Thus, UIS could not be accelerated by implementing the techniques for LCR queries, as mentioned in Section 3.2.

As substructure constraints can be formatted as SPARQL queries (Section 3), we could obtain $V(S, G)$ by implementing SPARQL engines [11] rather than checking the vertices in $G$ one by one. Then, a LSCR query $Q$ can be solved by recursively verifying the existence of $\exists v \in V(S, G)$, $s \xrightarrow{L} v \wedge v \xrightarrow{L} t$. For example, in Figure 3, $V(S_0, G_0) = \{v_1, v_2\}$. Then, for a LSCR query $Q_0= (v_3, v_4, L_0=\{likes, hates, friendOf\}, S_0)$, the query process can be done throughout the sequence of verifying $v_3 \xrightarrow{L} v_1$ and $v_1 \xrightarrow{L} v_4$.

Thus, in this section, we present the intuition idea of utilizing SPARQL engines on our problem, named UIS∗ (Algorithm 2). The algorithm description and analysis of UIS∗ are demonstrated in Section 4.1 and in Section 4.2, respectively.

Note that, in this paper, we treat the elements in $V(S, G)$ as disordered, because existing (top-k) SPARQL engines [9], [23] only can order the matched subgraphs with their own properties.

4.1 Algorithm Description

In Algorithm 2, a global stack $S$ is initialized with an element $s$ (Line 1), and used throughout the algorithm. The surjection close is introduced in Definition 3.1. To be notice, the definition of the UIS∗ search tree is same to Definition 3.2 the correctness of which is proved in Lemma 4.3.

Loop (Lines 12) processes each vertex $v \in V(S, G)$, with a function $LCS(s^*, t^*, L, B)$ (Lines 14–24) to evaluate the reachability from a vertex $s^*$ to a vertex $t^*$ under a label constraint $L$. The value of parameter $B$ is in the range of $\{T, F\}$, where, if $s^* \in V(S, G)$, $B=T$, otherwise, $B=F$. For clarity, we draw two sequences of the search trees with an assumption $(g, h \in V(S, G) \wedge g \xrightarrow{L} t)$, which are shown in Figure 6 and Figure 7 respectively.

For general consideration, supposing $s \notin V(S, G)$ in the demonstration of the UIS* running process. Thus, in the first iteration of the loop, $\forall v \in V(S, G)$, $close[v] = N$. We process $v$ in Lines 14–20 to verify the existence of $s \xrightarrow{L} v$ (Line 16 and Line 17). Such that, the function LCS is invoked with the parameters $s^* = s, t^* = v, L = L$ and $B = F$ ($s^* = s \notin V(S, G)$). Since $B = F$, function LCS only explores the vertices $w$ with $close[w] = N$ (case 2, Line 20) and change the state...
Algorithm 2 UIS* Algorithm\((G, Q)\)

Input: \(G = (V, E, L, L_S)\) represents a KG,  
\(Q = (s, t, L, S)\) is a LSCR query,  
\(V(S, G)\) is obtained by a SPARQL engine.

Output: The answer of \(Q\).

1. Let \(S\) be a global stack with an element \(s\)
2. \(\text{close}[s] \leftarrow F\)  // The initial values in \(\text{close}\) are set to \(N\)
3. for each vertex \(v\) in \(V(S, G)\) do
4.   if \(\text{close}[v] = N\) then
5.      if \(v = s\) or \(v = t\) then
6.         return \(Q = \text{LCS}(s, t, L, F)\)
7.      else if \(\text{LCS}(s, v, L, F)\) then
8.         if \(\text{LCS}(v, t, L, T)\) then
9.            return \(Q = T\)
10.   else if \(\text{close}[v] = F\) then
11.     if \(\text{LCS}(v, t, L, T)\) then
12.        return \(Q = T\)
13. return \(Q = F\)
14. Function: \(\text{LCS}(s^*, t^*, L, B)\)  // \(B\) is a boolean
15.   if \(B = T\) then
16.      \(\text{close}[s^*] \leftarrow T\), add \(s^*\) into \(S\)
17.    while \(B = F \land S \neq \emptyset\) or \(B = \text{close}[S, \text{first}] = T\) do
18.      Take an element \(u\) from \(S\)
19.      for each edge \(e = (u, l, w), l \in L_s\) incident to \(u\) do
20.         // We explore \(w\) in the following cases
21.            if \(B = T \land \text{close}[w] \neq T\) (case 1) or \(B = F \land \text{close}[w] = N\) (case 2) then
22.               Add \(w\) into \(S\), \(\text{close}[w] \leftarrow B\)
23.               if \(w = t^*\) then
24.                  return \(\text{true}\)
25.    Remove \(x\) from \(S\), if \(\text{close}[x] = T\), then return \(\text{false}\)

of the explored vertices in \(\text{close}\) to \(F\) (Line 21). In the following illustration, we discuss UIS* by the results of the first invocation of LCS, where \("true" and \("false\) relate to \(s \xrightarrow{L_S} v\) and \(s \xrightarrow{L} v\), respectively.

\(s \xrightarrow{L} v\). Assuming \(v = g\), Figure 5(a) depicts the search tree after the first invocation of LCS. As \(s \xrightarrow{L} g\) is proved, we start the function LCS, and set the parameters \(s^*\), \(t^*\), \(L\), and \(B\) to \(g\), \(t\), \(L\), and \(T\) (\(s^* = g \in V(S, G)\)), respectively, in Line 3. Then, with \(B = T\) (\(s \xrightarrow{L} s^*\)), we add an element \(s^*\) into \(S\) and set \(\text{close}[s^*] \rightarrow T\) (Line 15). Then, for each edge \(e = (u, l, w)\) that is incident to a taken out element \(u\) (Line 18), with \(l \in L_s\), we additionally explore \(w\) in case 1 (Line 20) with changing \(\text{close}[w]\) to \(B\) (Line 21).

Since the implemented data structure \(S\) is a stack, in which the elements obey the LIFO (last-in-first-out) principle, the new added elements in this invocation of LCS are processed first. Certainly, in the second invocation of LCS, if an element \(x\) in \(S\) and \(\text{close}[x] = T\), then \(s \xrightarrow{L_S} x\), while, if \(\text{close}[x] = F\), the existence of \(s \xrightarrow{L_S} x\) is unknown.

Thus, the loop in LCS runs until \(s \xrightarrow{L_S} t^*\) is proved, or the state of first element in \(S\) is \(F\) (\(\text{close}[S, \text{first}] \neq T\)), where:

(i) In the former condition, as \(s \xrightarrow{L_S} s^*, s^* \in V(S, G)\), \(s \xrightarrow{L_S} t^*\) and \(t^* = t\) all exist, we have \(s \xrightarrow{L} t\) in the main function. Thus, UIS* stops and returns \(Q = T\) (Line 9 and Line 12).
(ii) In the latter condition, Line 24 removes the elements in \(S\) that have been passed in this invocation (whose states in \(\text{close}\) are equal to \(T\)). For instance, in Figure 6(b), the elements \(x\) and \(y\) are removed from \(S\), as the node \(x^T\) and the node \(y^T\) are already in the search tree. Furthermore, Figure 6(c) describes a possible later sequence of Figure 6(b), as \(h \in V(S, G)\).

\(s \xrightarrow{L} v\). Since \(B = F\), after the first invocation of LCS, \(\forall w \in V, s \xrightarrow{L} w, close[w] = F,\) and, if \(s \xrightarrow{L} w, close[w] = N\), and the stack \(S\) is empty. In other words, UIS* has traversed all the vertices that \(s\) reaches to. Figure 7(a) demonstrates the search tree of UIS* at this time. In a later iteration of loop (Lines 3-12), only when \(\text{close}[w] = F\) (Line 10), we evaluate the existence of \(v \xrightarrow{L} t\) (Line 11). A schematic view of this sequence is depicted in Figure 7(b). Based on the above analysis, we present a theorem to show that the order of processing the elements in \(V(S, G)\) dominates the efficiency of UIS*.

Theorem 6.1. If, in the \(j^{th}\) invocation of LCS with \(B = F\), LCS returns false, then, after the \(j^{th}\) invocation, \(\forall w \in V \land s \xrightarrow{L} w, close[w] \neq N\).

Proof 6.1. That can be proved by the above discussion.

4.2 Analysis
In this section, we analyze the correctness and time complexity of UIS*(\(G, Q\)), where \(G = (V, E, L, L_S)\) is a KG and \(Q = (s, t, L, S)\) is a LSCR query. Plus, we prove that the search tree of UIS* can be formalized as that of UIS in Lemma 6.3.

Lemma 6.2. Assuming \(s \xrightarrow{L} s, \forall w \in V, s \xrightarrow{L} v, if f, close[v] \neq N\).

Proof 6.2. \(\forall w \in V\), the value of \(\text{close}[v]\) is initialized to \(N\), which can only be changed in Line 7 and function LCS (Lines 14-24). Thus, with the assumption, we prove the statement by induction on the LCS invocation times:
Theorem 4.4. This lemma is valid based on Lemma 4.2 and Lemma 4.3. is as defined in Definition 3.2.

In order to address LSCR queries on KGs, two uninformed search strategies are introduced, UIS (Algorithm 1) and UIS* (Algorithm 2). The former is a baseline method for LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR queries; the latter obtains UIS LSCR strategies are depicted in Section 5.1.2, followed by the correctness and complexity analysis.

5.1 Indexing Strategy

The intuition idea of our local index on a KG $G=(V,E,L,L_S)$ is similar to landmark indexing [19] (Section 5.2). The difference is that we could bound the indexing time complexity, by only precomputing each chosen landmark in a specific subgraph of $G$, instead of in the whole input KG.

In the following part, we overview our indexing technique in Section 5.1.1 in which the local index is formally defined. Then, the algorithm description of the indexing strategy are depicted in Section 5.1.2, followed by the correctness and complexity analysis.

5.1.1 Overview

This overview starts from the illustration of the difference between [19] and local index, with an example (Figure 9), then presents a formal definition of the local index.

According to the description of [19] in Section 5.2 we formalize the traditional landmark indexing as a surjection $f : I \rightarrow \{G\}$, where $I$ denotes the set of the chosen landmarks.
landmarks (highest degrees), and \( \{G\} \) represents the index ranges of the landmarks in \( \mathcal{I} \). For example, in Figure 9(a), \( \mathcal{I} = \{\text{the highlighted vertices of Figure 9(a)}\} \), and, for each vertex \( v \) in \( \mathcal{I} \), [19] precomputes the CMs from \( v \) to any other vertices in Figure 9(a). Obviously, when the size of \( G \) grows, the indexing time of such method grows exponentially, as we discussed in Section 3.2.

To conquer the unbounded indexing time complexity, we aim to narrow the range of the precomputation for each chosen landmark from the whole \( G \) to a subgraph, as shown in Figure 9(b). For formal description, a bijection \( F: \mathcal{I} \to \mathcal{G} \) exists in our indexing strategy (Algorithm 1), where \( \mathcal{I} \) is the set of the chosen landmarks, and, for a landmark \( u \in \mathcal{I} \), \( F(u) \in \mathcal{G} \) is the subgraph that the landmark \( u \) belongs to. Importantly, for each non-landmark vertex \( v \in \mathcal{F}(u) \), we stipulate that the vertex \( u \) reaches the vertex \( v \), and, for a subgraph \( \mathcal{F}(u) \in \mathcal{G}, u \) is the only one chosen landmark. Plus, the result of combining all the subgraphs in \( G \) does not necessarily contain all elements of \( G \).

**Definitions.** An entry in the local index is related to one landmark \( u \in \mathcal{I} \), and is formalized by \( II[u] \cup EI^T[u] \cup D[u] \). Before introducing the details about such entry, we present some local-index-related definitions. Assuming \( G_u = F(u) \) is a subgraph of \( G \), the vertex set and edge set are denoted by \( V_u \) and \( E_u \), respectively. Firstly, a path set \( P(s,t,G_u) \) is a subset of \( P(s,t,G) \), where, \( \forall p \in P(s,t,G_u) \), each edge \( e \) such that \( L \in M(s,t,G_u) \) as follows.

**Definition 5.1.** A collection of label sets \( M(s,t,G_u) \) is a CMS from \( s \) to \( t \) in a subgraph \( G_u \) of \( G \), if \( M(s,t,G_u) = \{L(p_j) \mid p_j \in P(s,t,G_u) \} \), such that \( \mathcal{L}(p_j) \in \mathcal{L}(t) \} \).

Then, supposing \( E_o = \{(v,l,w) \mid v \in V_u \land w / \in V_u \} \) is an edge set of \( G \), where each edge in \( E_o \) is incident to a vertex in \( \mathcal{F}(u) \), and points to a vertex that is not in \( \mathcal{F}(u) \), we define two sets of (vertex, collection of label sets) key-value pairs, \( II[u] \) and \( EI[u] \). The former \( II[u] = \{(v,M(s,t,G_u),E_o) \mid v \in V_u \} \) and the latter \( EI[u] = \{(v,L) \mid \exists (v,l,w) \in E_o, L = \{L \land L \in M(s,t,G_u) \} \} \).

The meaning of the pairs in \( II[u] \) is obvious. For a pair \( (w, L) \) in \( EI[u] \), the following statement exists: Given a label constraint \( L \), if \( \exists w \in L \land w \subseteq L \), then \( u \prec_w w \). It can be easily proved by the definition of \( EI[u] \). For the requirement of query efficiency, in practice, we reverse the pairs in \( EI[u] \) and restore them as (label set, vertex set) key-value pairs in \( EI^T[u] \), where \( EI^T[u] = \{(v,L) \mid \exists (w,L) \in EI[u] \land L \subseteq L \land w \in E_o \} \). Here, we further discuss \( EI^T[u] \) in Theorem 5.1.

**Theorem 5.1.** If \( L_u \subseteq L \), then \( \forall v \in V_u \land u \prec_v v \), where \( (L_u , V_u) \) is a pair in \( EI^T[u] \), and \( L_u \) is a label constraint.

**Proof.** \( \forall (L_u , V_u) \) in \( EI^T[u] \), for each vertex \( w \) in \( V_u \), there must be an entry \( (w, L) \) in \( EI[u] \) that \( L_u \subseteq L \), based on the above definitions. If \( L_u \subseteq L \land L \subseteq L_u \), then \( u \prec_w w \).

Finally, to present a preliminary estimate of the correlation degree between two subgraphs \( F(u) \) and \( F(v) \) in \( G \), we develop \( D[u]=\{|v,D(u,v)|v|E|\} \), where \( D(u,v) \) is the number of the pairs \( (w, L) \) in \( EI[u] \) whose first element \( w \) is a vertex in \( F(v) \).

**Algorithm 3** Indexing Algorithm\( (G) \)

**Input:** \( G = (V,E,L,D,G) \) represents a KG.

**Output:** Local index: \( II[u] \cup EI^T[u] \cup D[u] \) entries \((u \in \mathcal{I}) \).

1. \( \mathcal{I} \leftarrow \operatorname{LandmarkSelect}(L_S,k) \) // Select k landmarks
2. \( \mathcal{BFS}(G_u) / \forall a.A_{\mathcal{F}} = u \leftrightarrow F(u) \) contains \( w \)
3. For vertex \( u \in \mathcal{I} \) do
   4. LocalFullIndex\( (u) \)

5. **Function:** LocalFullIndex\( (u) \)
   6. \( II[u], EI[u], EI^T[u] \leftarrow \emptyset \) (key, value) pair sets
   7. Let \( Q \) be a queue with an element \( \{(u, \{} \} \)
   8. While \( Q \) is not empty do
      9. Take a pair \((v,L)\) from \( Q \)
      10. If \( \exists (v,L) = (u,L) \) true then
          11. For each edge \((v,l,w)\) incident to \( v \) do
              12. If \( w.A_F = u \) then
                  13. Add pair \((w,L \cup \{l\})\) into \( Q \)
              14. Else \( \{u,L \cup \{l\}, EI[u]\} \)
              15. \( EI^T[u], D[u] \leftarrow \text{Compute}(EI[u]) \)

16. **Function:** Insert\( (v, L, index[u]) \)
   17. If \( v = u \land L = \emptyset \) then return true
   18. If \( \exists (v,L) \in index[u] \) then
      19. Add pair \((v,L)\) into \( index[u] \), then return true
   20. Let \((v,L)\) represent a pair in \( index[u] \)
   21. Remove each label set \( L_i \) \( \in \mathcal{L}_i \), if \( L \subseteq L_i \)
   22. Add \( L_i \) into \( \mathcal{L}_i \), then return true
   23. return false

24. **Function:** BFSTraverse\( (G) \)
   25. \( Q \leftarrow \text{Initialize}(I) \) // Each element in \( Q \) is a queue
   26. While \( Q \) is not empty do
      27. Take an element \( Q_u \) from \( Q \)
      28. Take an element \( v \) from \( Q_u \)
      30. For each edge \( e = (v,l,w) \) incident to \( v \) do
          31. If \( \text{explored}[w] = \text{false} \) then
              32. \( w.A_F = u \), add \( w \) into \( Q_u \), explored\( [w] \leftarrow \text{true} \)
      33. If \( Q_u \) is not empty then
          34. Add \( Q_u \) to \( Q \)

5.1.2 Algorithm Description

In this part, we introduce Algorithm 3 for the construction process of both bijection \( F \) and the local index entry \( II[u] \cup EI^T[u] \cup D[u] \).

The landmark selection process in INS is more complicated than that in 19, where 19 directly chooses the vertices with the highest degrees. According to the description of KGs in Section 2, the entities with many real-world instances often relate to the vertices with relatively high degrees in a KG, as shown in Figure 2. Plus, the edges that are incident to or point to such vertices often labeled by a set of RDF vocabularies, e.g. “rdf:type”, “rdfs:subclassOf”. Selecting the vertices with the highest degrees will cause the labels of the associated edges between the landmarks and non-landmarks to be simple. In other words, when an input label constraint do not contain any of the RDF vocabularies, the local index based on such landmarks is useless.

In order to select a sound set of landmarks (\( \mathcal{I} \)), the
landmark selection process (Line 1) of INS is based on the RDF schema \( L_S \) of the input KG \( G \). INS first randomly select a set of classes in \( L_S \), then it even marks \( k \) instances of the selected classes as landmarks \((I)\). Since, the smaller \(|I|\) is, the smaller the chances of encountering the landmarks in a query processing are, in INS, we set \(|I| = k = \log |V| \times \sqrt{|V|}\).

After that, to construct \( F \) (Line 2), we start a BFS (Function BFSTraverse, Lines 24-34) from all vertices in \( I \) simultaneously, and traverse their surrounding vertices, with following rule: For an edge \( e = (v, l, w) \in E \), if both \( v \) and \( w \) belong to the subgraph \( F(u) \), \( e \) is an edge of \( F(u) \). With the consideration of the practical requirement for efficiently searching the subgraph that a vertex \( v \) belongs to, we introduce an additional attribute \( A_F \) for each \( v \) in \( G \), where \( w.A_F = u \) represents the vertex \( w \) belongs to a subgraph \( F(u) \) (Line 32 and Line 12).

Besides, function \( \text{insert}(v, L, \text{index}[u]) \) (Lines 16-24) is proposed to add a pair \((v, L)\) into \text{index}[u] that represents \( II[u] \) or \( EI[u] \), from Line 16 to Line 24. If \( \exists (v, L) \in \text{index}[u] \), we add a new pair \((v, L)\) into \( \text{index}[u] \) (Lines 18-19), otherwise, we use \((v, L)\) to update the value of pair \((v, L)\), which is demonstrated in Lines 20-24.

Then, for each vertex \( u \) in \( I \), we index \( u \) in function \( \text{LocalFullIndex}(u, F) \) (Lines 3-15), in which \( II[u] \), \( EI[u] \) and \( ET[u] \) are empty (key, value) sets (Line 6). This function utilizes a queue in which each element is a (vertex, label) set pair. Loop (Lines 8-14) starts, after adding the first pair \((u, \{\})\) into \( Q \), and runs until \( Q \) is empty. Each iteration of this loop takes a pair \((v, L)\) from \( Q \) (Line 6). We explore the edges that are incident to \( v \) (Lines 11-14), except in the following case: \((v, L)\) cannot be added into \( II[u] \) (Lines 10) by function insert. Then, in Lines 11-14, for each edge \((v, l, w)\), we add a pair \((w, L \cup \{l\})\) into either \( EI[u] \) or \( EI[u] \), which is dependent on whether vertex \( w \) is in \( F(u) \).

Finally, we re-compute the elements in \( EI[u] \) to obtain \( ET[u] \) and \( D[u] \) in Line 15 according to their definitions.

Analysis. We study the correctness (Theorem 5.2) and complexity (Theorem 5.3 and Theorem 5.4) of Algorithm 5 on a KG \( G = (V, E, L, L_S) \).

**Theorem 5.2.** The consistency exists between the definition of an entry \( II[u] \cup ET[u] \cup D[u] \) and the indexing result of \( \text{LocalFullIndex}(u, F) \).

**Proof 5.2.** \( II[u] \): For an element \((v, L=M(u, v)F(u))\) in \( II[u] \), given substructure constraint \( L \), the statement is correct, if, \( \forall \ell' \in L \land L' \subseteq L \Rightarrow u.\ell', v \in F(u), (\Rightarrow) \) Based on function insert, this is correct certainly. \((\Rightarrow) \) If, in \( F(u) \), \( u.\ell \rightarrow v \), then a path \( p \) exists in \( F(u) \) that \( \ell(p) \subseteq L \). If \( \exists \ell' \in L \land L' \subseteq L \), then at least one passed edge is not processed by function \( \text{LocalFullIndex} \). However, in this function, we only skip the vertices in the case that all the possible path label sets from \( u \) to that vertices have been searched. Thus, the assumption does not hold.

\( ET[u] \cup D[u] \): Based on function insert, the consistency also exists for \( ET[u] \). Thus, the statements about \( ET[u] \) and \( D[u] \) are correct (Line 15).

**Theorem 5.3.** The indexing time complexity is \( O(|F| \times (|E| + |V| \log 2|L|)) \).

**Proof 5.3.** Assuming, for a landmark \( u, F(u) \) contains \( n \) vertices and \( m \) edges. In function \( \text{LocalFullIndex}(u) \), we push at most \( n2|L| \) entries into the queue in this function. Each push costs \( O(1) \) time and each call of function insert takes \( O(\log 2|L|) \) time. Thus, the indexing time complexity is \( \sum_{u \in L} O((n + m)2|L| + n2|L| \log 2|L|) \leq O(|F| \times (|E| + |V| \log 2|L|)) \).

**Theorem 5.4.** The indexing space complexity is \( O(|F| \times (|F| + |L|)) \).

**Proof 5.4.** Each entry \( II[u] \cup EI[T][u] \cup D[u] \) of the local index contains \( O(n2|L|) \) elements, assuming \( F(u) \) contains \( n \) vertices. The size of each element is \( O(|V| + |L|) \). Hence, the total indexing space complexity is \( \sum_{u \in L} O(n2|L|(|V| + |L|)) = O(|F| \times (|F| + |L|)) \).

Comparing to the reported indexing time and space complexities of the traditional landmark indexing strategy \([19]\) in Section 3.2, our local index could bound the indexing consumption, which is independent of the number of the chosen landmarks \(|I| \).

5.2 Search Algorithm

In order to provide INS (Algorithm 4), the ability of perceiving a better search direction, and breaking the fixed search directions of traditional uniform search methods, we implement two data structures: a priority heap \( H \) (Line 1) and a priority queue \( Q \) (Line 2) to be an “evaluation function” in our informed search strategy. Before introducing the priorities of \( H \) and \( Q \), we let \( \rho(s, t) \) denote an estimate distance from a vertex \( s \) to a vertex \( t \), where \( \rho(s, t) = D(s, A_F, t, A_F) \) (Section 5.1).

Firstly, the main function of INS is similar to that of UIS* from Line 1 to Line 14 while, in each iteration of loop (Line 14), INS takes the top element \( v \) out of \( H \). Note that, for two vertices \( u, v \in V(S, G) \), \( u \) is on the top of \( v \) in \( H \), when: (i) \( \text{close}[u] = F \) and \( \text{close}[v] = N \); (ii) if \( \text{close}[u] = \text{close}[v] = F, \rho(u, t) \leq \rho(v, t) \) or \( u \in I \land v \notin I \); (iii) if \( \text{close}[u] = \text{close}[v] = N, \rho(s, u) \leq \rho(s, v) \) or \( u \in I \land v \notin I \).

Similar to UIS*, INS also initialize a global variable throughout the algorithm. Instead of implementing a stack, we use a queue \( Q \) to increase the probability of encountering the vertices in \( I \) of the bijection \( F \), as the local index covers a portion of the full TC (Section 3.2) of the input KG \( G \). Even though \( Q \) is initialized in the main function with an element \( s \) (Line 2), the other operations of adding an element into \( Q \) or taking an element out of \( Q \) are in function \( \text{LCS}(s^*, t^*, L, B) \). Besides, for two vertices \( u \) and \( v \) in \( Q \), it stores \( u \) in front of \( v \), when: (i) \( \text{close}[u] = T \land \text{close}[v] = F \); (ii) \( u.A_F \neq t.A_F \land v \notin I \); (iii) \( u \in I \land v \notin I \); (iv) \( \rho(u, t^*) \leq \rho(v, t) \); (v) \( u, v \notin I \), \( \text{close}[u] = N \land \text{close}[v] = N \); (vi) otherwise, \( u \) is added into \( Q \) before \( v \).

Note that, for two elements \( x \) and \( y \) in \( Q \), if \( x \) and \( y \) represent a same vertex in \( G \), \( Q \) deletes the first added element. Plus, according to the above \( Q \) priority rules, if \( \text{close}[x] = T \land \text{close}[y] = F, x \) is in the front of \( y \) in \( Q \). Then, in INS, the elements, which are added into \( Q \) in the \( k^\text{th} \) function LCS invocation with parameter \( B = T \), are processed first in this invocation.
In function LCS($s^*, t^*, L, B$), for each element $u$ taken out from $Q$ (Line 20), we traverse the edges $(e=(u, l, w) \land l \in L)$ that are incident to $u$ by a loop (Lines 21-29). Initially, if $t^* A_x = w$ (subgraph $F(w)$ contains vertex $t^*$), in Line 22 we implement a function Check($II[w], t^*$) to evaluate the existence of $u \overset{L}{\leadsto} t^*$, where if $\exists (t^*, \xi) \in II[w] \land L_x \subseteq L$ and $L_I \subseteq L_I$, function Check returns true, otherwise, false.

Then, in Line 24 if $w \notin I$, two functions in LCS, $\text{Cut}(II[w])$ and $\text{Push}(\varepsilon I^T[w])$, are introduced with the pre-computed local index $II[w]$ and $\varepsilon I^T[w]$, to prune the space and improve the query efficiency. For a pair $(x, \xi)$ in $\varepsilon I^T[w]$, the former set close[x] to $B$, if close[x] $\neq T$ and $\exists l x \in L_x \land L_x \subseteq L$; for a pair $(L_x, V) \in \varepsilon I^T[w]$, the latter adds each vertex $u \in V$ into $Q$, and changes close[u] to $B$, if $L_x \subseteq L \land B = T \land close[u] \neq T$ or $L_x \subseteq L \land B = F \land close[u] = N$. After that, in Line 26 if $w \notin I$, we add $w$ into $Q$ and set close to $B$ in the cases that close[w] = $N$ or close[w] = $F \land B = T$, which is same to UIS$^*$. Theorem 5.5. The time complexity of the search strategy is $O(|E| + |V| \times (\log |V| + 2|E|))$.

Proof 5.5. Each entry $II[u] \cup ET[u] \cup D[u]$ in the local index contains $O(n2^{|L|})$ elements, supposing $F(w)$ contains $n$ vertices. In the worst case, we visit all the landmarks of $I$ in one query processing so that the total local index visiting time complexity is $O(|V|2^{|E|})$. We at most traverse the input KG $G$ twice. Thus, the graph traversing time complexity is $O(|V| + |E|)$. Besides, we perform a complete ordering of the $|V|$ elements in $Q$, but the above operation can occur once only, so its time complexity is $O(|V| \log |V|)$. Overall, the total complexity is $O(|E| + |V| \times (\log |V| + 2|E|))$.

Theorem 5.6. $Q$ is a true query, iff, INS returns true.

Proof 5.6. INS is different to UIS$^*$ in the following aspects: (i) INS utilize a local index constructed by Algorithm 5; (ii) INS processes the elements in $V(S, G)$ with orders; (iii) INS applies the global variable with a priority queue instead of a stack, and INS does not contain the operation that is in Line 24 of UIS$^*$. According to Theorem 5.2, both (i) and (ii) do not affect the correctness of INS. Then, the global variable could automatically remove duplicate elements, and keep the elements with the values in the surjection $close$ are $T$ in the front of the queue. Hence, INS still holds the correctness.

6 EXPERIMENTAL RESULTS

In this section, we evaluate the performance of the proposed algorithms: UIS, UIS$^*$ and INS, on both synthetic and real KGs. Specially, since the effect of the label constraints on the query performance has been widely studied [8, 19], in this section, we are interested in: the indexing time and space consumption of our local index; the influence of the KG scales on the query performance; the impact of the substructure constraints on the query efficiency, including the selectivity of the substructure constraint and the number of the vertices that could satisfy the substructure constraint.

After introducing the settings and measures in experimental evaluation as follows, we detailedly illustrate the experiments on synthetic and real datasets in Section 6.1 and Section 6.2 respectively. In addition, based on all the experimental results, we present a discussion in Section 6.3.

Settings. Our experiments run on a machine with the intel i7-9700 CPU, 64 GB RAM, and 1TB disk space. We implement all the proposed algorithms in this paper with Java. Plus, to avoid the effect of the implementation language, the traditional landmark indexing method [19] is also implemented with Java, and the indexing parameters $k$ and $b$ of [19] are set to $1250+\sqrt{|V|}$ and 20, respectively, as that in the experiments of [19]. Note that, the indexes that build by local index and [19] are stored by the same data structure and on disk.

Then, we utilize the SPARQL engine that is present in [20] for both UIS$^*$ and INS, which is also rewritten with Java. The adoption of the SPARQL engine is due to its high efficiency in the experimental setting of this paper. As that provides the query results with the controlling of parameter...
We randomly generate datasets D0–D5 (Table 2), by applying LUBM. Even though D0 contains 40k vertices and 230k edges, and is only utilized to compare the indexing consumption of our local index and the traditional landmark indexing [19], its scale still greatly exceeds that of the most datasets used in [6, 19]. Based on D0–D5, we evaluate the indexing time and space consumption of both local index and the traditional landmark indexing method [19]. The results are demonstrated in Table 2, which confirm our theoretical analysis that, compared to [19], the indexing consumption of our local index is affordable, and increases linearly with the input KG scale. Note that, the indexing processes are limited within eight hours.

After that, we conduct groups of experiments, and each group is related to a certain substructure constraint in S1–S5 (expressed in SPARQL, Table 3), and runs on D1–D5. The reason, why we do not consider the queries provided in LUBM [4], is that they are designed for evaluating the performance of the RDF engine query optimizers and the not-ontology-reasoning [14], and are useless for our evaluation.

We demonstrate the query generation method and the experimental result analysis for the above groups in Section 6.1.1 and Section 6.1.2 respectively, after introducing the characteristics of S1–S5. Assuming D is a dataset generated by LUBM, whose vertex set is \( V \). S1 is a simple and matches only the vertices whose research interest is ‘Research12’. We treat S1 as our substructure constraint baseline among S1–S5, where \( |V(S1,D)| \approx 1\% \). Comparing to S1, S2 contains a normal selectivity, which matches the vertices which also should be associate professors, and \( |V(S2,D)| \approx 50\% \). Then, we devise S3, where \( |V(S3,D)| \approx 120\% \), which means there is a large set of vertices in \( D \) that could satisfy S3. Then, S4 is related to high selectivity and \( |V(S4,D)| \approx 1\% \), where the vertices in \( |V(S4,D)| \approx 120\% \) are named ‘GraduateStudent4’, take a course \( ?y1 \), etc. Specially, \( |V(S5,D)| \approx 1\% \).

6.1.1 Evaluation query generation

Generating an evaluation query \( Q=(s,t,L,S) \) in our experiments is intricate, because, if \( s \) reaches \( t \) only with a few steps, \( Q \) cannot test the limits of the search algorithms. Plus, due to the existence of the irrelevant factors that affect query performance, we must ensure our experiments are immune to such irrelevant factors.

Method of controlling irrelevant variable. Apparently, label constraint is one of the main factors that affect the query efficiency, but we do not focus on that in the experiments, because the impact of the label constraints on the query efficiency is widely studied in the LCR works. Supposing \( t \) is the size of an input KG label set, for each group of queries, we guarantee the sizes of the label constraints are in the range of \([0.2t, 0.8t]\), and ensure a uniform distribution of the such sizes among the ranges of \([0.2t, 0.4t]\), \([0.4t, 0.6t]\) and \([0.6t, 0.8t]\). Besides, for a group of false-LSCR queries, the performances of the search methods may be affected by the types of false queries. For example, a false-LSCR query \( Q=(s,L) \) has three possibilities: \( s \sim^{L,t} s \), \( s \sim^{L,t} s \), and \( s \sim^{L,t} s \). Thus, for a group of the generated false queries, we also guarantee a uniform proportion of the above possibilities.

Query generation method. For a substructure constraint Si of Table 3 and a dataset Dj of Table 2 we generate two groups of LSCR queries: 1,000 true-queries (Qi) and 1,000 false-queries (Qf). Assuming \( Q=(s,t,L,S) \), the process starts with randomly selecting \( s \) and \( L \) on Dj. Due to the restriction for controlling the irrelevant variables, if \( Q \) cannot be added into \( Q_i \) or \( Q_f \), we re-generate \( L \). Then, to select a sound target vertex \( t \) of \( Q \), we start a BFS from \( s \), and stop it after \( \log |V| \) iterations, after which \( t \) is a BFS-unexplored vertex. This is for filtering out the vertices that \( s \) reaches only with a few steps. In addition, we apply UIS to find out whether \( Q \) is a true query (\( Q=T \)) or not (\( Q=F \), and

### Table 2

| Dataset | Vertex | Edge | Local index | Traditional |
|---------|--------|------|-------------|-------------|
|         |        |      | IT(s) | IS(MB) | IT(s) | IS(MB) |
| D0      | 0.06M  | 0.23M| 25    | 4     | 27,171 | 11,700 |
| D1      | 3.7M   | 13.3M| 1,540 | 136   | -      | -      |
| D2      | 7.5M   | 26.6M| 3,119 | 273   | -      | -      |
| D3      | 11.3M  | 40.0M| 4,538 | 411   | -      | -      |
| D4      | 15.1M  | 53.4M| 6,203 | 546   | -      | -      |
| D5      | 18.9M  | 66.7M| 7,699 | 684   | -      | -      |

### Table 3

Five typical subgraph constraints on the synthetic datasets.

| Name | Description in SPARQL |
|------|-----------------------|
| S1   | SELECT ?x WHERE { ?x (ub:researchInterest) 'Research12'.} |
| S2   | SELECT ?x WHERE { ?x (ub:researchInterest) 'Research12', ?x (rdf:type) (ub:AssociateProfessor).} |
| S3   | SELECT ?x WHERE { ?x (rdf:type) (ub:UndergraduateStudent), ?x (ub:takesCourse) ?y, ?y (rdf:type) (ub:Course).} |
| S4   | SELECT ?x WHERE { ?x (ub:courseName) 'GraduateStudent4', ?x (ub:takesCourse) ?y1, ?x (ub:advisor) ?y2, ?x (ub:memberOf) ?y3, ?y1 (ub:takesCourse) ?y5, ?y2 (ub:teachesCourse) ?y6, ?y3 (ub:workFor) ?y7, ?y4 (ub:subOrganizationOf) ?y8.} |
| S5   | SELECT ?x WHERE { ?x (ub:emailAddress) 'FullProfessor@Department0.University0.edu.', ?x (ub:undergraduateDegreeFrom) ?y1, ?x (ub:masterDegreeFrom) ?y2, ?x (ub:doctoralDegreeFrom) ?y3.} |
record the number of the nodes in the search tree, denoted by $|T|$. With a random number $\min \in [10 \log |V|, 100/1000 |V|]$, if $|T| < \min$, we discard $Q$. If $Q=T$ and $|Q_j| < 1,000$, we add $Q$ into $Q_j$; if $Q=F \land |Q_j| < 1,000$ and $Q_j \cup Q$ satisfies the above restriction, $Q$ belongs to $Q_j$.

6.1.2 Experimental result analysis

For the results about UIS on LSCR queries related to S1, the average running times, of both true (Figure 10(a)) and false (Figure 10(b)) queries, all show a linear upward trend with the increase of the input KG scale. The average passed-vertex number of UIS on such queries is about $10^2$. For the results about UIS on LSCR queries related to S2, (Figure 11(c) and Figure 11(d)), Comparing to S1, the query performances of UIS, corresponding to S2 (normal selectivity) and S4 (high selectivity), are basically unchanged, according to Figure 11 and Figure 13. However, for the true-LSCR queries under the substructure constraint S3 (Figure 12), UIS consumes five times running time, compared to S1. Plus, the ranges of the average running times, of both true and false queries corresponding to S5 (Figure 14), are $[3s, 35s]$ and $[1s, 9s]$, respectively, while the average passed-vertex number is still around $10^6$ of either true or false queries. That is because, the bigger $|V(S,D_j)|$ is, the earlier UIS meets a vertex $v \ (v \in V(S,G))$ in a search path. Such results reflect that $|V(S,D_j)|$ effects the performance of UIS to some extent.

We observe that the average running times of both UIS and INS also grow linearly with the increase of the KG scale. The substructure constraints with normal (S2, Figure 11) and high (S4, Figure 13) selectivity do not show a significant effect on the query efficiency of either UIS or INS, comparing to S1. Furthermore, based on the results shown in Figure 12 and Figure 14, the number of the vertices in an input KG that satisfy the given substructure constraint also effects the query performance of both UIS and INS. Then, even though UIS is an improved algorithm of UIS, the performance of UIS on actual queries is not satisfactory, and the linear increase slope of UIS is greater than that of UIS, except in the case of S5 (Figure 14). That is because the order of the vertices in a $V(S,G)$ is random, causing that UIS always falls into a bad direction. The results shown

Fig. 10. Results related to the substructure constraint S1.

Fig. 11. Results related to the substructure constraint S2.

Fig. 12. Results related to the substructure constraint S3.

Fig. 13. Results related to the substructure constraint S4.
in Figure 12 and Figure 14 demonstrate that the impact of the bad direction (Theorem 4.1) is much greater than that of the high selectivity. However, with a local index pruning the search space and selecting a better search direction, INS overcomes the above disadvantage of UIS, and achieves a much higher efficiency than UIS and UIS*, based on experimental results reported in Figures 10-14.

6.2 Experiments on YAGO

The utilized dataset YAGO includes about 4M vertices and 13M edges. The indexing time and space consumption of local index on YAGO are 4,993s and 86MB, respectively.

Evaluation query generation. We develop sets of evaluation queries, where: (i) if \( r \) is in the same order of magnitude as mentioned above, the average running time of UIS shows a downward trend from the experiments on \( Q(T, 10^4) \) (about 7s) to that on \( Q(T, 10^5) \) (about 3s), as drawn in Figure 15(a). For the false queries (Figure 15(b)), the average running time of UIS does not change significantly from \( Q(F, 10^4) \) to \( Q(F, 10^5) \), which is approximately stable at 5.5s. Additionally, its change trend of the average passed-vertex number is similar to that of the average running time, according to Figures 15(c)-15(d).

The query performance of UIS* is still worse than that of UIS, especially in the experiments related to the false queries (Figure 15(c)), while the passed-number of UIS* is almost equal to that of UIS. Such results further prove that UIS* has a higher percentage of traversing the vertices in the input KG repeatedly. With the local index pruning the search space and accelerating query processing, the performance of INS is the best throughout the experiments. The average online search time consumption of INS is about one thousandth of either UIS or UIS* on both true-LSCR and false-LSCR queries.

However, the above results seems different from that in Section 6.1, where we observe \( |V(S, G)| \) highly dominates the query efficiency of a LSCR query \( Q=(s, t, L, S) \). That is because the potential search spaces of the randomly generated evaluation queries are affected by \( m \): (i) for a group of true queries \( Q(T, m) \), a larger \( m \) means more vertices in the input KG that satisfy the randomly generated substructure constraint, which makes searching from a vertex to another relatively easier, so the efficiency shows a slight increase; (ii) for a group of false queries \( Q(F, m) \), as the search algorithms are runs in the space that a vertex \( s \) reaches to under the given substructure constraint, in which each vertex can be traversed at most twice, the efficiency can be hardly affected by \( m \).

6.3 Discussion

For the experimental results demonstrated in Section 6.1 and Section 6.2, we observe that: (i) comparing to [19], the
indexing time and space consumption are affordable; (ii) comparing to UIS and UIS*, INS achieves a great performance on the different scales of the input KGs, even though, on a large KG, different degrees of the query performance degradation exist in the three algorithms; (iii) the selectivity of a substructure constraint \( S \) hardly affects the query performances of the proposed three algorithms, on a LSCR query \( Q = \langle s, t, L, S \rangle \), while, \( |V(S,G)| \) is a main factor that dominates the query efficiency.

7 Conclusion

This paper introduces a new variant of the reachability problem on KGs, i.e. LSCR queries, which contains both label and substructure constraints. The LSCR queries on KGs is much more complicated than the existing reachability queries, which only consider the label constraints. On the one hand, the query processing time complexity of applying traditional online search strategies (DFS/BFS) cannot be afforded. On the other hand, indexing a relatively large KG with the techniques of LCR queries is unrealistic, as the indexing time grows exponentially with the input KG scale. This work first presents a baseline method (UIS) for LSCR indexing time and space consumption are affordable; (ii) comparing to UIS and UIS*, INS achieves a great performance on the different scales of the input KGs, even though, on a large KG, different degrees of the query performance degradation exist in the three algorithms; (iii) the selectivity of a substructure constraint \( S \) hardly affects the query performances of the proposed three algorithms, on a LSCR query \( Q = \langle s, t, L, S \rangle \), while, \( |V(S,G)| \) is a main factor that dominates the query efficiency.

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