Understanding Data Science Lifecycle Provenance via Graph Segmentation and Summarization

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Abstract—Along with the prosperous data science activities, the importance of provenance during data science project lifecycle is recognized and discussed in recent data science systems research. Increasingly modern data science platforms today have non-intrusive and extensible provenance ingestion mechanisms to collect rich provenance and context information, handle modifications to the same file using distinguishable versions, and use graph data models (e.g., property graphs) and query languages (e.g., Cypher) to represent and manipulate the stored provenance/context information. Due to the schema-later nature of the metadata, multiple versions of the same files, and unfamiliar artifacts introduced by team members, the “provenance graph” is verbose and evolving, and hard to understand; using standard graph query model, it is difficult to compose queries and utilize this valuable information.

In this paper, we propose two high-level graph query operators to address the verbose and evolving nature of such provenance graphs. First, we introduce a graph segmentation operator, which queries the retrospective provenance between a set of source vertices and a set of destination vertices via flexible boundary criteria to help users get insight about the derivation relationships among those vertices. We show the semantics of such a query in terms of a context-free grammar, and develop efficient algorithms that run orders of magnitude faster than state-of-the-art. Second, we propose a graph summarization operator that combines similar segments together to query prospective provenance of the underlying project. The operator allows tuning the summary by ignoring vertex details and characterizing local structures, and ensures the provenance meaning using path constraints. We show the optimal summary problem is PSPACE-complete and develop effective approximation algorithms. The operators are implemented on top of a property graph backend. We evaluate our query methods extensively and show the effectiveness and efficiency of the proposed methods.

I. INTRODUCTION

Provenance capture and analysis is being increasingly seen as a crucial enabler for prosperous data science activities [1]–[5]. Capturing provenance allows the practitioners introspect the data analytics trajectories, monitor the ongoing modeling activities, increase auditability, aid in reproducibility, and communicate the practice with others [2]. Specific systems have been developed to help diagnose dataflow programs [6], [7], ingest provenance in the lifecycle [2], [5], and manage pipelines for high-level modeling paradigms [8], [9].

Compared with well-established data provenance systems for databases [10], and scientific workflow systems for e-science [11], building provenance systems for data science faces an unstable data science lifecycle that is often ad hoc, typically featuring highly unstructured datasets, an amalgamation of different tools and techniques, significant back-and-forth among team members, and trial-and-error to identify the right analysis tools, models, and parameters. Schema-later approaches and graph data model are often used to capture the lifecycle, versioned artifacts and associated rich information [1], [2], [4], which also echoes the modern provenance data model standardization as a result of consolidation for scientific workflows [12] and the Web [13].

Although there is an enormous potential value of data science lifecycle provenance, e.g., reproducing the results or accelerate the modeling process, the evolving and verbose nature of the captured provenance graphs makes them difficult to store and manipulate. Depending on the granularity, storing the graphs could take dozens of GBs within several minutes [14]. More importantly, the verbosity and diversity of the provenance graphs makes it difficult to write general queries to explore and utilize them; there are often no predefined workflows, i.e., the pipelines change as the project evolves, and instead we have arbitrary steps (e.g., trial and error) in the modeling process. In addition, though storing the provenance graph in a graph database seems like a natural choice, most of the provenance query types of interest involve paths [15], and require returning paths instead of answering yes/no queries like reachability [16]. Writing queries to utilize the lifecycle provenance is beyond the capabilities of the pattern matching query (BPM) and regular path query (RPQ) support in popular graph databases [17]–[19]. For example, answering ‘how is today’s result file generated from today’s data file’ requires a segment of the provenance graph that includes not only the mentioned files but also other files that are not on the path that the user may not know at all (e.g., ‘a configuration file’); answering ‘how do the team members typically generate the result file from the data file?’ requires summarizing several query results of the above query while keeping the result meaningful from provenance perspective.

Lack of proper query facilities in modern graph databases not only limits the value of lifecycle provenance systems for data science, but also of other provenance systems. The specialized query types of interest in the provenance domain [15], [16] had often led provenance systems to implement specialized storage systems [20], [21] and query interfaces [22], [23] on their own [11]. Recent works in the provenance community
propose various graph transformations for different tasks, which are essentially different template queries from the graph querying perspective; these include grouping vertices together to handle publishing policies [24], aggregating vertices in a verbose graph to understand commonalities and outliers [25], segmenting a provenance graph for feature extractions in cybersecurity [26]. Our goal with this work is to initiate a more systematic study of abstract graph operators that modern graph databases need to support to be a viable option for storing provenance graphs.

Toward that end, in this paper, we propose two graph operators for common provenance queries to let the user explore the evolving provenance graph without fully understanding the underlying provenance graph structure. The operators not only help our purpose in the context of data science but also other provenance applications which have no clear workflow skeletons and are verbose in nature (e.g., [14], [25], [26]).

First, we introduce a flexible graph segmentation operator for the scenario when users are not familiar with the evolving provenance graph structure but still need to query retrospective provenance between a set of source vertices (e.g., today’s data file) and a set of destination vertices (e.g., today’s result file) via certain boundary criteria (e.g., hops, timestamps, authorship). The operator is able to induce vertices that contribute to the destination vertices in a similar way w.r.t. the given source vertices in the specified boundary. Parts of the segmentation query require a context-free language (CFL) to express its semantics. We study how to support such CFL query in provenance graphs, exploit novel grammar rewriting schemes and propose evaluation techniques that run orders of magnitude faster than state-of-the-art for our graph operator.

Second, we propose a graph summarization operator for aggregating the results of segmentation operations, in order to analyze the prospective provenance of the underlying project (e.g., typical pipeline from the data file to the result file). It allows the user to tune the summary graph by ignoring vertex details and characterizing local structures during aggregation, and ensures the summary is meaningful from the provenance perspective through path constraints. We show the optimal summary problem is PSPACE-complete and develop effective approximation algorithms that obey the path constraints.

We illustrate the operators on provenance data model standards (W3C PROV); the formulations and evaluation techniques are general to many provenance-aware applications. We show how to build such operators on top of modern property graph backends (Neo4j). We present extensive experiments that show the effectiveness and efficiency of our proposed techniques on synthetic provenance graph datasets mimicking real-world data science projects.

Outline: We begin with an overview of our system, introduce the provenance model and unique challenges (Sec. [I]), then describe semantics and evaluation algorithms for segmentation (Sec. [II]) and summarization operators (Sec. [III]). We present extensive experimental evaluation (Sec. [IV]) and summarize the related work from different communities (Sec. [V]).
and entities, ingested via provenance system ingesters (e.g., dataset is copied from some url, Alice changes a pool layer type to AVG in v_2, accuracy in logs v_3 is 0.75).

**Provenance Model:** The ingested provenance of the project lifecycle naturally forms a provenance graph, which is a directed acyclic graph and encodes information with multiple aspects, such as a version graph representing the artifact changes, a workflow graph reflecting the derivations of those artifact versions, and a conceptual model graph showing the involvement of problem solving methods in the project [1, 2].

To represent the provenance graph and keep our discussion general to other provenance systems, we choose the W3C PROV data model [29], which is a standard interchange model for different provenance systems.

We use the core set of PROV data model shown in Fig. 2(b). There are three types of vertices (V) in the provenance graph:

- **a)** Entities (E) are the project artifacts (e.g., files, datasets, scripts) which the users work on and talk about in a project, and the underlying lifecycle management system manages their provenance;
- **b)** Activities (A) are the system or user actions (e.g., train, git commit, cron jobs) which act upon or with entities over a period of time, \([t_i, t_j]\);
- **c)** Agents (U) are the parties who are responsible for some activity (e.g., a team member, a system component).

Among vertices, there are five types of directed edges \(\Delta (E):\)

i) An activity started at time \(t_i\) often uses some entities ("used", \(U \subseteq A \times E\));

ii) then some entities would be generated by the same activity at time \(t_j\) \((t_j \geq t_i)\) ("wasGeneratedBy", \(G \subseteq E \times A\));

iii) An activity is associated with some agent during its period of execution ("wasAssociatedWith", \(S \subseteq A \times U\)). For instance, in Fig. 2(a) the activity `train` was associated with Alice, used a set of artifacts (model, solver, and dataset) and generated other artifacts (logs, weights). In addition:

iv) Some entity’s presence can be attributed to some agent ("wasAttributedTo", \(A \subseteq E \times U\)), e.g., the dataset was added from external sources and attributed to Alice;

v) An entity was derived from another entity ("wasDerivedFrom", \(D \subseteq E \times E\)), such as versions of the same artifact (e.g., different model versions in v_1 and v_2 in Fig. 2(a)).

In the provenance graph, both vertices and edges have a label to encode their vertex type in \([E, A, U]\) or edge type in \([U, G, S, A, D]\). Other provenance records are modeled as properties, ingested by the system during activity executions and represented as key-value pairs.

\(^1\)There are 13 types of relationships among Entity, Activity and Agent. The proposed techniques in the paper can be extended naturally to support more relation types in other provenance systems.
In workflow systems, querying the workflow should be both collaborative in nature, so there is no static workflow skeleton, and no clear boundaries for individual runs in contrast with workflow systems. For instance, the modeling methods may change (e.g., from SVM to neural networks), the data processing steps may vary (e.g., split, transform or merge data files), and the user-committed versions may be mixed with code changes, error fixes, thus may not serve as boundaries of provenance queries for entities. R2: The query facility for snapshots should not assume workflow skeleton and should allow flexible boundary conditions.

Partial Knowledge in Collaboration: Each team member may work on and be familiar with a subset of artifacts and activities, and may use different tools or approaches, e.g., in Example 1 Alice and Bob use different approaches to improve accuracy. When querying retrospective provenance of the snapshots attributed to other members or understanding activity process over team behaviors, the user may only have partial knowledge at query time, thus may find it difficult to compose the right graph query. R3: The query facility should support queries with partial information reflecting users’ understanding and induce correct result.

Verboseness for Usage: In practice, the provenance graph would be very verbose for humans to use and in large volume for the system to manage. R4: The query facility should be scalable to large graph and process queries efficiently.

B. Provenance Query Types of Interest

However, the provenance standards (e.g., PROV, OPM) do not describe query models, as different systems have their own application-level meaning of those nodes. General queries (e.g., SQL, XPATH, SPARQL) provided by a backend DBMS to express provenance retrieval tend to be very complex. To improve usability, a few systems provide novel query facilities, and some of them propose special query languages. Recent provenance systems which adopt W3C PROV data model naturally use graph stores as backends; since the standard graph query languages often cannot satisfy the needs, a set of graph manipulation techniques is often proposed to utilize the provenance. By observing the characteristics of the provenance graph in analytics lifecycle and identifying the requirements for the query facilities, we propose two graph operators (i.e., segmentation and summarization) for general provenance data model, that we illustrate next with examples, and discuss in more depth in the next section.

Segmentation: A very important provenance query type of interest is querying ancestors and descendants of entities. In our context, the users introspect the lifecycle and identify issues by analyzing dependencies among snapshots. Lack of a workflow skeleton and clear boundaries, makes the queries over the provenance graph more difficult. Moreover the user may not be able to specify all interested entities in a query due to partial knowledge. We propose a segmentation operator that takes sets of source and destination entities, and the operator induces other important unknown entities satisfying a set of specified boundary criteria.

Example 3: In Fig. 2(d), we show two examples of provenance graph segmentation query. In Query 1 (Q1), Bob was interested in what Alice did in version v2. He did not know the details of activities and the entities Alice touched, instead he set [dataset], [weight] as querying entities to see how the weight in Alice’s version v2 was connected to the dataset. He filtered out uninterested edge types (e.g., A, D) and excluded actions in earlier commits (e.g., v1) by setting the boundaries as two activities away from those querying entities. The system found connections among the querying entities, and included vertices within the boundaries. After interpreting the result, Bob knew Alice updated the model definitions in model. On the other hand, Alice would ask query to understand how Bob improved the accuracy and learn from him. In Query 2 (Q2), instead of learned weight, accuracy property associated log entity is used as querying entity along with dataset. The result showed Bob only updated solver configuration and did not use her new model committed in v2.

Summarization: In workflow systems, querying the workflow skeleton (aka prospective provenance) is an important use case (e.g., business process modeling) and included in the provenance challenge. In our context, even though a static
workflow skeleton is not present, summarizing the skeleton of similar processing pipelines, showing commonalities and identifying abnormal behaviors are very useful query capabilities. However, general graph summarization techniques are not applicable to provenance graphs due to the subtle provenance meanings and constraints of the data model. We propose a summarization operator to support querying the artifact aspect of the provenance.

Example 4: In Fig. 2(c), an outsider to the team (e.g., some auditor, new team member, or project manager) wanted to understand the activity overview in the project. Segmentation queries (e.g., Q1, Q2 in Fig. 2(d)) only show individual trails of the analytics process at the snapshot level. The outsider issued a summarization query, Query 3 (Q3), by specifying the aggregation over three types of vertices (viewing Alice and Bob as an abstract team member, ignoring details of files and activities), and defining the provenance meanings as a 1-hop neighborhood. The system merged Q1 and Q2 into a summary graph. In the figure, the vertices suffixed name with provenance types to show alternative generation process, while edges are labeled with their frequency of appearance among segments. The query issuer would change the query conditions to derive various summary at different resolutions.

III. SEGMENTATION OPERATION

Among the snapshots, collected provenance graph describes important ancestry relationships which form ‘the heart of provenance data’. Often lineages w.r.t. a query or a run graph trace w.r.t. a workflow are used to formate ancestry queries in relational databases or scientific workflows. However, in our context, there are no clear boundaries of logical runs, or query scopes to cleanly define the input and the output. Though a provenance graph could be collected, the key obstacle is lack of formalisms to analyze the verbose information. In similar situations for querying script provenance, Prolog was used to traverse graph imperatively, which is an overkill and entails an additional skill-set for team members. We design PoSeg to let the users who may only have partial knowledge to query retrospective provenance.

PoSeg semantics induce a connected subgraph to show the ancestry relationships (e.g., lineage) among the entities of interest and include other causal and participating vertices within a boundary that is adjustable by the users.

A. Semantics of Segmentation (PoSeg)

The PoSeg operator is a 3-tuple query \((\mathcal{V}_{\text{src}}, \mathcal{V}_{\text{dst}}, \mathcal{B})\) on a provenance graph \(G\) asking how a set of source entities \(\mathcal{V}_{\text{src}} \subseteq \mathcal{E}\) are involved in generating a set of destination entities \(\mathcal{V}_{\text{dst}} \subseteq \mathcal{E}\). PoSeg induces induced vertices \(\mathcal{V}_{\text{ind}} \subseteq V\) that show the detailed generation process and satisfy certain boundary criteria \(\mathcal{B}\). It returns a connected subgraph \(S(V_S, \overline{E}_S) \subseteq G\), where \(V_S = \mathcal{V}_{\text{src}} \cup \mathcal{V}_{\text{dst}} \cup \mathcal{V}_{\text{ind}}\), and \(\overline{E}_S = \overline{E} \cap \overline{G} \cap \overline{V}_S \times \overline{V}_S\).

When discussing the elements of PoSeg below, we use the following notations for paths in \(G\). A path \(\pi_{v_0, v_n}\) connecting vertices \(v_0\) and \(v_n\) is a vertex-edge alternating sequence \(\langle v_0, e_1, v_1, \ldots, v_{n-1}, e_n, v_n \rangle\), where \(n > 1\), \(\forall i \in [0, n] v_i \in V\), and \(\forall j \in (0, n] e_j = (v_{j-1}, v_j) \in E\). Given a path \(\pi_{v_0, v_n}\), we define its path segment \(\hat{\pi}_{v_0, v_n}\) by simply ignoring \(v_0\) and \(v_n\) from the beginning and end of its path sequence, i.e., \((e_1, v_1, \ldots, v_{n-1}, e_n)\).

A path label function \(\tau\) maps a path \(\pi\) or path segment \(\hat{\pi}\) to a word by concatenating labels of the elements in its sequence order. Unless specifically mentioned, the label of each element (vertex or edge) is derived via \(\lambda_v(i)\) and \(\lambda_e(e)\). For example, from \(a\) to \(c\), there is a path \(\pi_{ac} = (a, e_a, c)\), where \(a, c \in \mathcal{E}\), \(e_a \in \mathcal{E}\) and \(e_b \in U\); its path label \(\tau(\pi_{ac}) = \mathcal{E}G\mathcal{A}\mathcal{U}\), and its path segment label \(\tau(\hat{\pi}_{ac}) = \mathcal{E}G\mathcal{A}\mathcal{U}\). For ease of describing path patterns, for ancestry edges (used, wasGeneratedBy), i.e., \(e_k = (v_i, v_j)\) with label \(\lambda_v(e_k) = U\) or \(\lambda_e(e_k) = G\), we introduce its virtual inverse edge \(\hat{e}_k = (v_j, v_i)\) with the inverse label \(\lambda_v(\hat{e}_k) = U\) or \(\lambda_e(\hat{e}_k) = G\) respectively. A inverse path is defined by reversing the sequence, e.g., \(\pi_{ac} = (c, e_b, a)\), while \(\tau(\pi_{ac}) = \mathcal{E}U\mathcal{A}\mathcal{G}\mathcal{E}\mathcal{A}\mathcal{G}\mathcal{U}\).

1) Source (\(\mathcal{V}_{\text{src}}\)) & Destination Entities (\(\mathcal{V}_{\text{dst}}\)): Provenance is about the entities. In a project, the user know the committed snapshots (e.g., data files, scripts) better than the detailed processes generating them. When writing a PoSeg query, we assume the user believes \(\mathcal{V}_{\text{src}}\) may be ancestry entities of \(\mathcal{V}_{\text{dst}}\). Then PoSeg reasons their connectivity and shows other vertices and the generation process which the user may not know and be able to write query with. Note that users may not know the existence order of entities either, so we allow \(\mathcal{V}_{\text{src}}\) and \(\mathcal{V}_{\text{dst}}\) to overlap, and even be identical. In the latter case, the user could be a program and not familiar with the generation process at all.

2) Induced Vertices \(\mathcal{V}_{\text{ind}}\): Given \(\mathcal{V}_{\text{src}}\) and \(\mathcal{V}_{\text{dst}}\) intuitively \(\mathcal{V}_{\text{ind}}\) are the vertices contributing to the generation process. What vertices should be in \(\mathcal{V}_{\text{ind}}\) is the core question to ask. It should reflect the generation process precisely and concisely to assist the user introspect part of the generation process and make decisions.

Prior work on inducing subgraphs from a set of vertices do not fit our needs. First, lineage query would generate all ancestors of \(\mathcal{V}_{\text{dst}}\), which is not concise or even precise: siblings of \(\mathcal{V}_{\text{dst}}\) and siblings of entities along the paths may be excluded as they do not have path from \(\mathcal{V}_{\text{dst}}\) or to \(\mathcal{V}_{\text{src}}\) in \(G\) (e.g., \(\log\) in \(Q_1\)). Second, at another extreme, a provenance subgraph induced from some paths or all paths among vertices in \(\mathcal{V}_{\text{src}} \cup \mathcal{V}_{\text{dst}}\) will only include vertices on the paths, thus exclude other contributing ancestors for \(\mathcal{V}_{\text{dst}}\) (e.g., model and solver in \(Q_1\)). Moreover, quantitative techniques used in other domains other than provenance cannot be applied directly either, such as keyword search over graph data techniques, which also do not assume that users have full knowledge of the graph, and let users use keywords to match vertices and then induce connected subgraph among keyword vertices. However, the techniques often use tree structures (e.g., least common ancestor, Steiner tree) connecting \(\mathcal{V}_{\text{src}} \cup \mathcal{V}_{\text{dst}}\) and are not aware of provenance usages, thus cannot reflect the ancestry relationships precisely.

Instead of defining \(\mathcal{V}_{\text{ind}}\) quantitatively, we define PoSeg qualitatively by a set of domain rules: \(a\) to be precise, PoSeg includes other participating vertices not in the lineage and not
in the paths among \( \mathcal{V}_{src} \cup \mathcal{V}_{dst} \); b) to be concise, PoSseg utilizes the path shapes between \( \mathcal{V}_{src} \) and \( \mathcal{V}_{dst} \) given by the users as a heuristic to filter the ancestry lineage subgraph. We define the rules for \( \mathcal{V}_{ind} \) as follows and illustrate in Fig. 3.

(a) **Vertices on Direct Path (\( \mathcal{V}_{ind}^{\text{d}} \)):** Activities and entities along any direct path \( \pi_{v_i, v_j} \) between an entity \( v_i \in \mathcal{V}_{src} \) and an entity \( v_j \in \mathcal{V}_{dst} \) are the most important ancestry information. It helps the users answer classic provenance questions, such as reachability, i.e., whether there exists a path; workflow steps, i.e., if there is a path, what activities occurred. We refer entities and activities on such direct path as \( \mathcal{V}_{ind}^{\text{d}} \), which is defined as:

\[
\mathcal{V}_{ind}^{\text{d}} = \bigcup_{v_i \in \mathcal{V}_{src}, v_j \in \mathcal{V}_{dst}} \left\{ v_k | \exists_{v_{ij} \in \pi_{v_i, v_j}} \right\}.
\]

(b) **Vertices on Similar Path (\( \mathcal{V}_{ind}^{\text{s}} \)):** Though \( \mathcal{V}_{ind}^{\text{d}} \) is important, due to the partial knowledge of the user, just considering the direct paths may miss important ancestry information including: a) the entities generated together with \( \mathcal{V}_{dst} \), b) the entities used together with \( \mathcal{V}_{src} \), and c) more importantly, other entities and activities which are not on the direct path, but contribute to the derivations. The contributing vertices are particularly relevant to the query in our context, because data science project consists of many back-and-forth repetitive and similar steps, such as dataset splits in cross-validation, similar experiments with different hyperparameters and model adjustments in a plot (Fig. 3).

To define the induction scope, on one hand, all ancestors w.r.t. \( \mathcal{V}_{dst} \) in the lineage subgraph would be returned, however it is very verbose and not concise to interpret. On the other hand, it is also difficult to let the user specify all the details of what should/should not be returned. Here we use a heuristic: induce ancestors which are not on the direct path but contribute to \( \mathcal{V}_{dst} \) in a similar way, i.e., path labels from \( \mathcal{V}_{ind}^{\text{d}} \) to \( \mathcal{V}_{ind}^{\text{d}} \) are the same with some directed path from \( \mathcal{V}_{src} \). In other words, one can think it is similar to a radius concept \({20}\) to slice the ancestry subgraph w.r.t. \( \mathcal{V}_{dst} \), but the radius is not measured by how many hops away from \( \mathcal{V}_{dst} \) but by path patterns between both \( \mathcal{V}_{ind} \) and \( \mathcal{V}_{src} \) that are specified by the user query. Next we first formulate the path pattern in a context free language \({37}\), \( L(\text{SimProv}) \), then \( \mathcal{V}_{ind}^{\text{s}} \) can be defined as a \( L \)-constrained reachability query from \( \mathcal{V}_{src} \) via \( \mathcal{V}_{dst} \) over \( \mathcal{G} \), only accepting path labels in the language.

A context-free grammar (CFG) over a provenance graph \( \mathcal{G} \) and a PoSseg query \( Q \) is a 6-tuple \((\Sigma, N, P, S, G, Q)\), where \( \Sigma = \{E, A, U\} \cup \{U, G, S, A, D\} \cup \mathcal{V}_{dst} \) is the alphabet consisting of vertex labels, edge labels in \( \mathcal{G} \) and \( \mathcal{V}_{dst} \) vertex identifiers (e.g., \( \text{id} \) in Neo4j) in \( Q \), \( N \) is a set of non-terminals, \( P \) is the set of production rules, and \( S \) is the start symbol. Each production rule in the form of \( l \rightarrow (\Sigma \cup N)^* \) defines an acceptable way of concatenations of the RHS words for the LHS non-terminal \( l \).

Given a CFG and a non-terminal \( l \in N \) as the start symbol, a context-free language (CFL), \( L(l) \), is defined as the set of all finite words over \( \Sigma \) by applying its production rules.

The following CFG defines a language \( L(\text{SimProv}) \) that describes the heuristic path segment pattern for \( \mathcal{V}_{ind}^{\text{s}} \). The production rules expand from some \( v_j \in \mathcal{V}_{src} \) both ways to reach \( v_i \) and \( v_k \), such that the concatenated path \( \pi_{v_i, v_k} \) has the destination \( v_j \) in the middle.

\[
\mathcal{V}_{ind}^{\text{s}} = \bigcup_{v_i \in \mathcal{V}_{src}} \{ v_k | \exists_{v_{ij} \in \pi_{v_i, v_j}} \}
\]

Now we can use \( L(\text{SimProv}) \) to define \( \mathcal{V}_{ind}^{\text{s}} \) as: for any vertex \( v_j \) in \( \mathcal{V}_{ind}^{\text{s}} \), there should be at least a path from a \( v_i \in \mathcal{V}_{src} \) going through \( v_j \in \mathcal{V}_{dst} \) then reaching some vertex \( v_i \), s.t. the path segment label \( \tau(v_{ij}, v_i) \) is a word in \( L(\text{SimProv}) \):

\[
\mathcal{V}_{ind}^{\text{s}} = \bigcup_{v_i \in \mathcal{V}_{dst}} \{ v_k | \exists_{v_{ij} \in \pi_{v_i, v_j}} \}
\]

Using CFG allows us to express the heuristic properly. Note that \( L(\text{SimProv}) \) cannot be described by regular expressions over the path(segment) label, as it can be viewed as a palindromic language \({37}\). Moreover, it allows us to extend the query easily by using other label functions, e.g., instead of \( \lambda_e(v) \) and \( \lambda_e(e) \) whose domains are PROV types, using property value \( \sigma rv(v_i, p_i) \) or \( \omega e(e, p_i) \) in \( \mathcal{G} \) allows us to describe interesting constraints, e.g., the induced path should use the same commands as the path from \( \mathcal{V}_{src} \) to \( \mathcal{V}_{dst} \), or the matched entities on both sides of the path should be attributed to the same agent. For example, the former case can simply modify the second production rule in the CFG as:

\[
U^* \sigma(a_i, p_0) \text{SimProv} \sigma(a_i, p_0) U \quad \text{s.t. } a_i, a_j \in A \land p_0 = \text{command} \land \sigma(a_i, p_0) = \sigma(a_j, p_0)
\]

This is a powerful generalization that can describe repetitiveness and similarly ancestry paths at a very fine granularity.

(c) **Entities Generated By Activities on Path (\( \mathcal{V}_{ind}^{\text{g}} \))**: As mentioned earlier, the sibling entities generated together with \( \mathcal{V}_{dst} \) may not be induced from directed paths. The same applies to the siblings of entities induced in \( \mathcal{V}_{ind}^{\text{d}} \) and \( \mathcal{V}_{ind}^{\text{s}} \). We refer to those entities as \( \mathcal{V}_{ind}^{\text{g}} \) and define it as:

\[
\mathcal{V}_{ind}^{\text{g}} = \bigcup_{v_i \in \mathcal{V}_{src}} \{ v_k | (v_k, v_i) \in \mathcal{G} \land v_k \notin \mathcal{V}_{ind}^{\text{d}} \cup \mathcal{V}_{ind}^{\text{s}} \}
\]

(d) **Involved Agents (\( \mathcal{V}_{ind}^{\text{i}} \))**: Finally, the agents may be important in some situations, e.g., from the derivation, identify who makes a mistake, like git blame in version control settings. On a provenance graph, agents can be derived easily:

\[
\mathcal{V}_{ind}^{\text{i}} = \bigcup_{v_i \in \mathcal{V}} \{ v_k | v_k \in U \land (v_i, v_k) \in S \cup A \}, \text{where } V' \text{ is the union of all query vertices and other induced vertices.}
\]

3) **Boundary Criteria B**: On the induced subgraph, the segmentation operator should be able to express users’ logical boundaries when asking the ancestry queries. It is particularly useful in an interactive setting once the user examines the returned induced subgraph and wants to make adjustments. We categorize the boundary criteria support as a) exclusion constraints and b) expansion specifications.
First, boundaries would be constraints to exclude some parts of the graph, such as limiting ownership (authorship) (who), time intervals (when), project steps (particular version, file path patterns) (where), understanding capabilities (neighborhood size) (what), etc. Most of the boundaries can be defined as boolean functions mapping from a vertex or edge to true or false, i.e., $b_v(v): \mathbb{V} \mapsto \{0, 1\}$, $b_e(e): \mathbb{E} \mapsto \{0, 1\}$, which can be incorporated easily to the CFG framework for subgraph induction. We define the exclusion boundary criteria as two sets of boolean functions ($B_v$ for vertices and $B_e$ for edges), which could be provided by the system or defined by the user. Then the labeling function used for defining $\mathcal{V}_{ind}$ would be adjusted by applying the boundary criteria as follows:

$$\mathcal{F}_v = \begin{cases} 
\lambda_v(v) & \text{otherwise}
\end{cases} \land b_v B_v, \quad \mathcal{F}_e = \begin{cases} 
\lambda_e(e) & \text{otherwise}
\end{cases} \land b_e B_e$$

In other words, a vertex or an edge that satisfies all exclusion boundary conditions, is mapped to its original label. Otherwise the empty word ($\epsilon$) is used as its label, so that paths having that vertex will not satisfy $L$(SmProv).

Second, instead of exclusion constraints, the user may wish to expand the induced subgraph. We allow the users to specify expansion criteria, $B_s = \{b_s(V_i, k)\}$, denoting including paths which are $k$ activities away from entities in $V_i \subseteq \mathcal{V}_{ind}$. In Fig. 2(d), $Q_1$ excludes ($A, D$) edges via $B_s$ and expands by $B_s = \{b_s(weight_v2, 2)\}$, so {update-v2, model-v1} are included.

B. Query Evaluation

1) Overview: Two-Step Approach: Given a PoSeg query, we separate the query evaluation into two steps: 1) induce: induce $\mathcal{V}_{ind}$ and construct the induced graph $S$ using $\mathcal{V}_{src}$ and $\mathcal{V}_{dst}$, 2) adjust: apply $B$ interactively to filter induced vertices or retrieve more vertices from the property graph store backend. The rationale of the two-step approach is that the operator is designed for the users with partial knowledge who are willing to understand a local neighborhood in the provenance graph. Any induction heuristic applied would be unlikely to match the user’s implicit interests and would require back-and-forth explorations.

In the rest of the discussion, we assume a) the provenance graph is stored in a backend property graph store, with constant time complexity to access arbitrary vertex and arbitrary edge by corresponding primary identifier; b) given a vertex, both its incoming and outgoing edges can be accessed equally, with linear time complexity w.r.t. the in- or out-degree. In our implementation, Neo4j satisfies the conditions – both nodes and edges are accessed via their id.

2) Induce Step: Given $\mathcal{V}_{src}$ and $\mathcal{V}_{dst}$, PoSeg induces $\mathcal{V}_{ind}$ with four categories. We mainly focus our discussion on inducing vertices on direct and similar paths, as the other two types can be derived in a straightforward manner by scanning 1-hop neighborhoods of the first two sets of results.

Cypher: The definition of vertices on similar path requires a context-free language, and cannot be expressed by a regular language. When developing the system, we realize it can be decomposed into two regular language path segments, and express the query using path variables [38], [39]. We handcraft a Cypher query shown in Query 1. The query uses $\mathcal{V}_{src}$ (b) and $\mathcal{V}_{dst}$ (e1) to return all directed paths $\mathcal{V}_{ind}$ via path variables (p1), and uses Cypher with clause to hold the results. The second match finds the other half side of the SmProv via path variable p2 which then joins with p1 to compare the node-by-node and edge-by-edge conditions to induce $\mathcal{V}_{ind}$. If we do not need to check properties, then we can use $\text{length}(p1) = \text{length}(p2)$ instead of the two extract clauses. However, as shown later in the evaluation (Sec. V), Neo4j takes more than 12 hours to return results for even very small graphs with about a hundred vertices. Note that RPO with path variables are not supported well in modern graph query languages and graph database [19], [38], we develop our own PoSeg algorithm for provenance graphs.

CFL-reachability: Given a vertex $v$ and a CFL $L$, the problem of finding all vertices $u$ such that there is a path $\pi_{u,v}$ with label $\tau(\pi_{u,v}) \in L$ is often referred as single source CFL-reachability (CFLR) problem or single source L-Transitive Closure problem [40], [41]. The all-pairs version, which aims to find all such pairs of vertices connected by a $L$ path of the problem, has the same complexity. As $\mathcal{V}_{src}$ would be all vertices, we do not distinguish between the two in the rest of the discussion. Though the problem has been first studied in our community [40], there is little follow up and support in the context of modern graph databases (Sec. VII). CFLR finds its main application in programming languages and is recognized as a general formulation for many program analysis tasks [41].

State of the art CFLR algorithm [42] solves the problem in $O(n^3/\log(n))$ time and $O(n^2)$ space w.r.t. the number of vertices in the graphs. It is based on a classic cubic time dynamic programming scheme [41], [43] which derives production facts non-repetitively via graph traversal, and uses the method of four Russians [44] during the traversal. In the rest of the paper, we refer it as CronB. We analyze it on provenance graphs for $L$(SmProv), then present improvement techniques. The details of CronB and proofs are included in Appendix.

Given a CFG, CronB works on its normal form [37], where each production has at most two RHS symbols, i.e., $N \rightarrow AB$ or $N \rightarrow A$. The normal form of SmProv is listed in Fig. 6. At a high level, the algorithm traverses the graph and uses grammar as a guide to find new production facts $N(i, j)$, where $N$ is a LHS nonterminal, $i, j$ are graph vertices, and the found fact $N(i, j)$ denotes that there is a path from $i$ to $j$ whose path label satisfies $N$. To elaborate, similar to BFS, it uses a worklist $W$
how to utilize them are described below, which can be used to avoid repetition and future queries. In SmProv (Fig. 4), the start symbol is $R$, and $P = (V_1, V_2)$ facts include all $v_j$, s.t. between them there is $\tau(\pi_{ij}) \in L(SmProv)$.  

$L(SmProv)$-reachability on PROV: In our context, the prove graph is often sparse, and both the numbers of entities that an activity uses and generates can be viewed as a small constant, however the domain size of activities and entities are potentially large. The following lemma shows show the fast set method is not suitable for PROV graph.

**Lemma 1**: CFLR reduces $L(SmProv)$-reachability on a PROV graph in $O(|V||E|/\log{|A|} + |E|/|A|^{2}\log{|E|})$ time if using fast set. Otherwise, it solves in $O(|G||E| + |U||A|)$ time.

The lemma also reveals a quadratic time scheme for $L(SmProv)$-reachability if we can view the average in-/out-degree as a constant. Note that the quadratic time complexity is not surprising, as SmProv is a linear CFL, i.e., there is at most one nonterminal on RHS of each production rule. The CFLR time complexity for any linear grammar on general graphs $G(V,E)$ have been shown in theory as $O(|V||E|)$ by a transformation to general transitive closures [40].

**Rewriting SmProv**: Most CFLR algorithms require the normal form mentioned earlier. However, under the normal form, it a) introduces more worklist entries, and b) misses important grammar properties. Instead, we rewrite SmProv as shown in Fig. 4 and propose SmProvAlg and SmProvTst by adjusting CFLR. Comparing with standard normal forms, $r_1'$ and $r_2'$ have more than two RHS symbols. SmProvAlg utilizes the rewritten grammar and PROV graph properties to improve CFLR. Moreover, SmProvTst solves $L(SmProv)$-reachability on a PROV graph in linear time and sublinear space if viewing $|V_{del}|$ as constant. The properties of the rewritten grammar and how to utilize them are described below, which can be used in other CFLR problems:

a) **Reduction for Worklist tuples**: Note that $r_2'$ in Fig. 4, $A(a_1, a_2) \rightarrow G'(a_1, e_1) E(e_1, e_2) G(e_2, a_2)$, combines rules $r_1, r_3$ in the normal form, i.e., $R(a_1, a_2) \rightarrow L(a_1, e_2) G(e_2, a_2)$ and $L(a_1, e_2) \rightarrow G'(a_1, e_1) R(e_1, e_2)$. Instead of enqueuing $L(a_1, e_2)$ and then $R(a_1, a_2)$, SmProvAlg adds $A(a_1, a_2)$ to $W$ directly. In the normal form, there may be other cases that can also derive $A(a_1, a_2)$, i.e., in presence of $L(a_1, e_1)$ and $G(e_1, a_2)$. In the worst case, CFLB enqueued $E$ number of $L(a_1, e_2)$ in $W$ which later find the same fact $R(a_1, a_2)$. It’s worth mentioning that in SmProvAlg because $A(a_1, a_2)$ now would be derived by many $E(e_1, e_2)$ in $r_2'$, before adding it to $W$, we need to check if it is already in $W$. We use two pairs of bijection for $E$ and $A$ for $W$ and $H$, the space cost is $O(|E|^2/\log{|E|} + |A|^2/\log{|A|})$. Compressed bijection would be used to improve space usage at the cost of non-constant time random read/write.

b) **Symmetric property**: In the rewritten grammar, both nonterminals $E$ and $A$ are symmetric, i.e., $E(e_1, e_2)$ implies $E(e_2, e_1)$, $A(a_1, a_2)$ implies $A(a_2, a_1)$, which is not held in normal forms. Intuitively $E(e_1, e_2)$ reduces some path label from $e_1$ to $e_i \in V_{src}$ is the same with some path label from $e_2$ to $e_i$. Using symmetric property, in SmProvAlg, we can use a straightforward pruning strategy: only process $(e_1, e_2)$ in both $H$ and $W$ if $id(e_1) \leq id(e_2)$ and $(a_1, a_2)$ if $id(a_1) \leq id(a_2)$; and an early stopping rule: for any $A(a_1, a_2)$ that both $a_1$’s and $a_2$’s order of being is before all $ProSen$ query $V_{src}$ entities, we do not need to proceed further. Note the early stopping rule is SmProv and PROV graph specific, while solving general CFLR, even in the single-source version, cannot take source information and we need to evaluate until the end. Though both strategies do not improve the worst-case time complexity, they are very useful in realistic PROV graphs (Sec.[]).

c) **Transitive property**: By definition SmProv does not have transitivity, i.e., given $E(e_1, e_2)$ and $E(e_2, e_3)$, it does not imply $E(e_1, e_3)$. This is because a $ProSen$ query allows multiple $V_{src}$, $E(e_1, e_2)$ and $E(e_2, e_3)$ may be found due to different $v_j \in V_{src}$. However, if we evaluate $v_j \in V_{src}$ separately, then $E$ and $A$ have transitivity, which leads to a linear algorithm SmProvTst for each $v_j$; instead of maintaining $E(e_1, e_2)$ or $A(a_1, a_2)$ tuples in $H$ and $W$, we can use a set $\{e_m\}$ or $\{a_m\}$ to represent an equivalence class at iteration $m$ or $n$ where any pair in the set is a fact of $E$ or $A$ respectively. If at iteration $m$, the current $W$ holds a set $\{e_m\}$, then $r_2': A(a, a) \rightarrow G'(a, e) E(e, e) G(e, a)$ is used to infer the next $W$ (a set $\{a_{m+1}\}$); otherwise, $W$ must hold a set $\{a_{m}\}$, then similarly $r_1'$ is used to infer next equivalence class $\{a_{m+1}\}$ as the next $W$. In the first case, as there are at most $|G|$ possible $(a, e)$ tuples, the step takes $O(|G|)$ time; in the later case, similarly the step takes $O(|U|)$ time. The algorithm returns vertices in any equivalence classes $\{V_{i}\}$, s.t. $v_j \in V_{src}$. Overall, because there are multiple $V_{src}$ vertices, the algorithm runs in $O(|V_{src}| |G| + |V_{src}| |U|)$ time and $O(|E|/\log{|E|} + |A|/\log{|A|})$ space. The early stop rule can be applied, instead of a pair of activities, in SmProvTst all activities in an equivalent class $\{a_m\}$ are compared with entities in $V_{src}$ in terms of the order of being; while the pruning strategy is not necessary, as all pairs are represented compactly in an equivalent class.

**Theorem 2**: SmProvTst solves $L(SmProv)$-reachability in $O(|G| + |U|)$ time, if viewing $|V_{del}|$ as a constant.

3) **Adjust Step**: Once the induced graph $S(V_S, E_S)$ is derived, the adjustment step applies boundary criteria to filter existing vertices and retrieve more vertices. Comparing with induction step, applying boundary criteria is rather straightforward. For exclusion constraints $B_i$ and $B_e$, we apply them on vertices and edges in $S(V_S, E_S)$ linearly if present. For $B_i$, we traverse the backend store with specified entities for $2k$ hops through $G^2$ and $U^r$ to edges to their ancestry activities and
entities. To support back and forth interaction, we cache the induced graph instead of inducing multiple times. We expect $k$ is small constant in our context as the generated graph is for humans to interpret, otherwise, a reachability index is needed.

IV. Summarization Operation

In a collaborative analytics project, collected provenance graph of the repetitive modeling trails reflects different roles and work routines of the team members and records steps of various pipelines, some of which having subtle differences. Using PoSeq, the users can navigate to their segments of interest, which may be about similar pipeline steps. Given a set of segments, our design goal of PoSum is to produce a precise and concise provenance summary graph, Psg, which will not only allow the users to see commonality among those segments of interests (e.g., yesterday’s and today’s pipelines are almost the same), but also let them understand alternative routines (e.g., an old step excluded in today’s pipeline).

Though no workflow skeleton is defined, with that ability, Psg would enable the users to reason about prospective provenance in evolving workflows of analytics projects.

A. Semantics of Summarization (PoSum)

Although there are many graph summarization schemes proposed over the years [33] (Sec. VI), they are neither aware of provenance domain desiderata [25] nor the meaning of PoSeq segments. Given a set of segments $\mathbb{S}$, each $S_i$ of which is a PoSeq result, a PoSum query is designed to take a 3-tuple $(S, \mathcal{K}, \mathcal{R}_k)$ as input which describes the level of details of vertices and constrains the rigidity of the provenance; then it outputs a provenance summary graph (Psg).

1) Property Aggregations & Provenance Types of Vertices: To combine vertices and edges across the segments in $\mathbb{S}$, we first introduce two concepts: a) property aggregation ($\mathcal{K}$) and b) provenance type ($\mathcal{R}_k$), which PoSum takes as input and allow the user to obfuscate vertex details and retain structural constraints.

Property Aggregation ($\mathcal{K}$): Similar to an attribute aggregation summarization query on a general graph [45], depending on the granularity level of interest, not all the details of a vertex are interesting to the user and some properties should be omitted, so that they can be combined together; e.g., in Example 7, the user may neither care who performs an activity, nor an activity’s detailed configuration; in the former case, all agent type vertices regardless of their property values (e.g., name) should be indistinguishable and in the latter case, the agent type vertices regardless of their property values (e.g., training parameters) in various P

2) Provenance Summary Graph (Psg): Next, we define the output of PoSum, the provenance summary graph, Psg.

Properties such as version of the entity, details of an activity, names of the agents are ignored.

Provenance Type ($\mathcal{R}_k$): In contrast with general-purpose graphs, in a provenance graph, the vertices with identical labels and property values may be very different [25]. For example, two identical activities that use different numbers of inputs or generate different entities should be considered different (e.g., update-v2 and update-v3 in Fig. 2(d)). In [25], Moreau proposes to concatenate edge labels recursively over a vertex’s $k$-hop neighborhood to assign a vertex type for preserving provenance meaning. However, the definition ignores in-/out-degrees and is exponential w.r.t. to $k$.

We extend the idea of preserving provenance meaning of a vertex and use the $k$-hop local neighborhood of a vertex to capture its provenance type; given a PoSeq segment $S(S, E_S)$, and a constant $k$, $k \geq 0$, provenance type $\mathcal{R}_k(v)$ is a function that maps a vertex $v \in S$ to its $k$-hop subgraph in its segment $S, \mathcal{R}_k \subseteq S$. For example, in Fig. 2(e), $k = 1$, thus provenance type of vertices is the 1-hop neighborhood, vertices with label ‘update’, ‘model’ and ‘solver’ all have two different provenance types (marked as ‘11’, ‘12’).

Note one can generalize the definition of $\mathcal{R}_k(v)$ as a subgraph within $k$-hop neighborhood of $v$ satisfying a pattern matching query, which has been proposed in [46] with application to entity matching where similar to provenance graphs, just using the vertex properties are not enough to represent the conceptual identity of a vertex.

Vertex Equivalence Relation ($\equiv_k$): Given $\mathbb{S} = \{S(V_S, E_S)\}$, denoting the union of vertices as $V_S = \bigcup V_{S_i}$, with the user specified property aggregation $\mathcal{K}$ and provenance type $\mathcal{R}_k$, we define a binary relation $\equiv_k$ over $V_S \times V_S$, s.t. for each vertex pair $(v_i, v_j) \in \equiv_k$:

- $v_i$ labels are the same, i.e., $\lambda_k(v_i) = \lambda_k(v_j)$;
- all property values in $\mathcal{K}$ are equal, i.e., $\forall p \in \mathcal{K} \sigma(v_i, p) = \sigma(v_j, p)$;
- $\mathcal{R}_k(v_i)$ and $\mathcal{R}_k(v_j)$ are graph isomorphic w.r.t. the vertex label and properties in $\mathcal{K}$, i.e., there is a bijection $f$ between $V_i \in \mathcal{R}_k(v_i)$ and $V_j \in \mathcal{R}_k(v_j)$, s.t., $f(v_m) = v_n$ if $1)$ $\lambda_k(v_m) = \lambda_k(v_n)$, $2)$ $\forall p \in \mathcal{K} \sigma(v_m, p) = \sigma(v_n, p)$,
- $\mathcal{R}_k(v)$ is a subgraph in its segment $S$, $\mathcal{R}_k \subseteq S$.

It is easy to see that $\equiv_k$ is an equivalence relation on $V_S$ by inspection. Using $\equiv_k$, we can derive a partition $P^{\equiv_k}$ of $V_S$, s.t., each set in the partition is an equivalence class by $\equiv_k$, denoted by $[v]$, s.t., $\{[v_i] \cap [v_j] = \emptyset \}$ and $\bigcup [v_i] = V_S$. For each $[v]$, we can define its canonical label, e.g., the smallest vertex $i$, for comparing vertices.

In other words, vertices in each equivalence class $[v]$ by $\equiv_k$ describe the homogeneous candidates which can be merged by PoSum. Its definition not only allows the users to specify property aggregations $\mathcal{K}$ to obfuscate unnecessary details in different resolutions, but also allows the users to set provenance types $\mathcal{R}_k$ to preserve local structures and ensure the meaning of provenance of a merged vertex.
Desiderata: Due to the nature of provenance, the produced Psg should be precise, i.e., we should preserve paths that exist in one or more segments, at the same time, we should not introduce any path that does not exist in any segment. On the other hand, Psg should be concise; the more vertices we can merge, the better summarization result it is considered to be. In addition, as a summary, to show the commonality and the rareness of a path among the segments, we annotate each edge with its appearance frequency in the segments.

Minimum Psg: PoSum combines vertices in their equivalence classes and ensures the paths in the summary satisfy above conditions. Next we define a valid summary graph.

Given a PoSum($\mathcal{S}, \mathcal{K}, \mathcal{R}_k$) query, a provenance summary graph $\text{Psg}(\mathcal{M}, E, \rho, \gamma)$, is a directed acyclic graph, where

- $a$) each $\mu \in \mathcal{M}$ represents a subset of an equivalence class $\mu \subseteq [\mathcal{V}], w.r.t. \equiv^\mu_\mathcal{S}$ over $\mathcal{V}_\mathcal{S}$, and one segment vertex $v$ can only be in one Psg vertex $\mu$, i.e., $\forall \mu, \mu_n \in \mathcal{M}, \mu_n \cap \mu = \emptyset$; the vertex label function $\rho : \mathcal{M} \mapsto P^\mathcal{S}$ maps a Psg vertex to its equivalence class;
- $b$) an edge $e_{mn} = (\mu_m, \mu_n) \in E$ exists if there is a corresponding segment edge, i.e., $\exists S_m, \mu_n \times \mu_m \cap \mathcal{E}_{\mathcal{S}} \neq \emptyset$; the edge label function $\gamma : E \mapsto [0, 1]$ annotates the edge’s frequencies over segments, i.e., $\gamma(e_{mn}) = ||S_m \times \mu_n \cap \mathcal{E}_{\mathcal{S}}|/||S||$;
- $c$) there is a path $\pi_{mn}$ from $\mu_m$ to $\mu_n$ iff $\forall S_m, \forall_\mathcal{V}_n, \exists \mu_m \times \mu_n \cap \mathcal{E}_{\mathcal{S}} \land \exists v \subseteq \mu_m \times \mathcal{V}_n$, there is a path $\pi_{\mathcal{V}n}$ from $v$ to $v$ in $\mathcal{S}_n$; their path labels are the same $\tau(\pi_{mn}) = \tau(\pi_{\mathcal{V}n})$. Note that in Psg, we use equivalence classes’ canonical label (e.g., smallest vertex id) as the vertex label in $\tau$.

It is easy to see $\bigcup \mathcal{S}_n$, union of all segments in $\mathcal{S}$, is a valid Psg. We are interested in a concise summary with fewer vertices. The best Psg one can get is the optimal solution of the following problem.

Problem 1 (Minimum Psg): Given a set of segments $\mathcal{S}$ and a PoSum($\mathcal{S}, \mathcal{K}, \mathcal{R}_k$) query, find the provenance summary graph $\text{Psg}(\mathcal{M}, E, \rho, \gamma)$ with minimum $|\mathcal{M}|$.

B. Query Evaluation

Given $\mathcal{S} = (\mathcal{S}(\mathcal{V}_\mathcal{S}, \mathcal{E}_\mathcal{S}))$, after applying $\mathcal{K}$ and $\mathcal{R}_k$, Psg $g_0 = \bigcup \mathcal{S}_n$ is a labeled graph and contains all paths in segments; to find a smaller Psg, we have to merge vertices in $\mathcal{V}_\mathcal{S} = \bigcup \mathcal{V}_\mathcal{S}_n$ in $g_0$ while keeping the Psg invariant, i.e., not introducing new paths. To describe merging conditions, we introduce trace equivalence relations in a Psg. $a$) in-trace equivalence ($\equiv^\text{in}_{\mathcal{S}}$): If for every path $\pi_{mn}$ ending at $u \in \mathcal{V}_\mathcal{S}$, there is a path $\pi_{nv}$ ending at $v \in \mathcal{V}_\mathcal{S}$ with the same label, i.e., $\tau(\pi_{mn}) = \tau(\pi_{nv})$, we say $u$ is in-trace dominated by $v$, denoted as $u \leq^\text{in}_{\mathcal{S}} v$. The $u$ and $v$ are in-trace equivalent, written $u \equiv^\text{in}_{\mathcal{S}} v$, iff $u \leq^\text{in}_{\mathcal{S}} v \land v \leq^\text{in}_{\mathcal{S}} u$. $b$) out-trace equivalence ($\equiv^\text{out}_{\mathcal{S}}$): Similarly, if for every path starting at $u$, there is a path starting at $v$ with the same label, then we say $u$ is out-trace dominated by $v$, written $u \leq^\text{out}_{\mathcal{S}} v$, and $v$ are out-trace equivalent, i.e., $u \equiv^\text{out}_{\mathcal{S}} v$, iff $u \leq^\text{out}_{\mathcal{S}} v \land v \leq^\text{out}_{\mathcal{S}} u$.

Lemma 3: Merging $u$ to $v$ does not introduce new paths, if and only if 1) $u \equiv^\text{in}_{\mathcal{S}} v$, or 2) $u \equiv^\text{out}_{\mathcal{S}} v$, or 3) $u \leq^\text{in}_{\mathcal{S}} v \land u \leq^\text{out}_{\mathcal{S}} v$.

The lemma defines a partial order over the vertices in $\mathcal{V}_\mathcal{S}$. By applying the above lemma, we can merge vertices in a Psg greedily until no such pair exist, then we derive a minimal Psg. However, the problem of checking in-/out-trace equivalence is PSPACE-complete [47], which implies that the decision and optimization versions of the minimum Psg problem are PSPACE-complete.

Theorem 4: Minimum Psg is PSPACE-complete.

Instead of checking trace equivalence, we use simulation relations as its approximation [48], [49], which is less strict than bisimulation and can be computed efficiently in $O(|V_\mathcal{S}||E_\mathcal{S}|)$ in Psg $g_0$ [48]. A vertex $u$ is in-simulate dominated by a vertex $v$, written $u \leq^\text{in}_{\mathcal{S}} v$, if $a$) their label is the same, i.e., $\rho(u) = \rho(v)$ and $b$) for each parent $p_n$ of $u$, there is a parent $p_i$ of $v$, s.t., $p_n \leq^\text{in}_{\mathcal{S}} p_i$. We say $u, v$ in-simulate each other, $u \equiv^\text{in}_{\mathcal{S}} v$, iff $u \leq^\text{in}_{\mathcal{S}} v \land v \leq^\text{in}_{\mathcal{S}} u$. Similarly, $u$ is out-simulate dominated ($\leq^\text{out}_{\mathcal{S}}$) by $v$, if $\rho(u) = \rho(v)$ and for each child $c_n$ of $u$, there is a child of $c_i$ of $v$, s.t., $c_n \leq^\text{out}_{\mathcal{S}} c_i$; and $u, v$ out-simulate each other $u \equiv^\text{out}_{\mathcal{S}} v$ iff they out-simulate dominate each other. Note that a binary relation $r_a$ approximates $r_p$, if $(e_i, e_j) \in r_a$ implies $(e_i, e_j) \in r_p$ [49]. In other words, if $(u, v)$ in-/out-simulates each other, then $(u, v)$ is in-/out-trace equivalence. By using simulation instead of trace equivalence in Lemma 3 to merge, we can ensure the invariant.

Lemma 5: If 1) $u \equiv^\text{in}_{\mathcal{S}} v$, or 2) $u \equiv^\text{out}_{\mathcal{S}} v$, or 3) $u \leq^\text{in}_{\mathcal{S}} v \land u \leq^\text{out}_{\mathcal{S}} v$, merging $u$ to $v$ does not introduce new paths.

We develop the PoSum algorithm by using the partial order derived from Lemma 3 to merge a Psg (initialized as $g_0$) to merge vertices. To compute $\leq^\text{in}_{\mathcal{S}}$, and $\leq^\text{out}_{\mathcal{S}}$, we apply the similarity checking algorithm in [48] twice in $O(|V_\mathcal{S}||E_\mathcal{S}|)$ time. From Lemma 3 we can ensure there is no new path introduced, and the merging operation does not remove paths, so PoSum algorithm finds a valid Psg. Note unlike Lemma 3 as the reverse of Lemma 3 does not hold, so we may not be able to find the minimum Psg, as there may be $(u, v)$ is in trace equivalence but not in simulation.

V. Experimental Evaluation

In this section, we study the proposed operators and techniques comprehensively. All experiments are conducted on a Ubuntu Linux 16.04 machine with an 8-core 3.0GHz AMD FX-380 processor and 16GB memory. For the backend property graph store, we use Neo4j 3.2.5 community edition in embedded mode and access it via its Java APIs. Proposed query operators are implemented in Java in order to work with Neo4j APIs. To limit the performance impact from the Neo4j, we always use id to seek the nodes, which can be done in constant time in Neo4j’s physical storage. Unless specifically mentioned, the page cache for Neo4j is set to 2GB and the JVM version is 1.8.0-25 and -Xmx is set to 4GB.

Dataset Description: Unless lifecycle management systems are used by the practitioners for a long period of time, it is difficult to get real-world provenance graph from data science teams. Publicly available real-world PROV provenance graph datasets in various application domains [25] are very small (KBs). We instead develop several synthetic PROV graph generators to examine different aspects of the proposed operators. The datasets and the generators are available online.2

2Datasets: http://www.cs.umd.edu/~hui/code/provdbquery
(a) Provenance Graphs & PoSeg Queries: To study the efficiency of PoSeg, we generate a provenance graphs dataset (Pd) for collaborative analytics projects by mimicking a group of project members performing a sequence of activities. Each project artifact has many versions and each version is an entity in the graph. An activity uses one or more input entities and produces one or more output entities.

To elaborate, given N, the number of vertices in the output graph, we introduce |U| = ⌊log(N)⌋ agents. To determine who performs the next activity, we use a Zipf distribution with skew s_v to model their work rate. Each activity is associated with an agent and uses 1 + m input entities and generates 1 + n output entities. m and n are generated from two Poisson distributions with mean λ_v and λ_o to model different input and output size. In total, the generator produces |A| = ⌊N/(2 + λ_o)| activities, so that at the end of generation, the sum of entities |E|, activities |A| and agents |U| is close to N. The m input entities are picked from existing entities; the probability of an entity being selected is modeled as the pmf of a Zipf distribution with skew s_v at its rank in the reverse order of being. If s_v is large, then the activity tends to pick the latest generated entity, while s_v is small, an earlier entity has better chance to be selected.

We use the following values as default for the parameters: s_v = 1.2, λ_v = 2, λ_o = 2, and s_e = 1.5. We refer Pd as the graph with about n vertices. In Po graphs, we pick pairs (ν_vv, ν_va) as PoSeg queries to evaluate. Unless specifically mentioned, given a Po dataset, ν_vv are the first two entities, and ν_va are the last two entities, as they are always connected by some path and the query is the most challenging PoSeg instance. In one evaluation, we vary ν_vv to show the effectiveness of the proposed pruning strategy.

(b) Similar Segments & PoSum Queries: To study the effectiveness of PoSum, we design a synthetic generator (Sn) with the ability to vary shapes of conceptually similar provenance graph segments. In brief, the intuition is that as at different stages of the project, the stability of the underlying pipelines tends to differ, the effectiveness of summary operator could be affected; e.g., at the beginning of a project, many activities (e.g., clean, plot, train) would happen after another one in no particular order, while at later stages, there are more likely to be stable pipelines, i.e., an activity type (e.g., preprocessing) is always followed by another activity type (e.g., train). For PoSum, the former case is more challenging.

In detail, we model a segment as a Markov chain with k states and a transition matrix $M \in [0, 1]^{k \times k}$ among states. Each row of the transition matrix is generated from a Dirichlet prior with the concentration $\alpha$, i.e., the $i$th row is a categorical distribution for state $i$; each $M_{ij}$ represents the probability of moving to state $j$, i.e., pick an activity of type $j$. We set a single $\alpha$ for the vector $\alpha$; for higher $\alpha$, the transition tends to be a uniform distribution, while for lower $\alpha$, the probability is more concentrated, i.e., fewer types of activities would be picked from. Given a transition matrix, we can generate a set of segments $S$, each of which consists of $n$ activities labeled with $k$ types, derived step by step using the transition matrix. For the input/output entities of each activity, we use $\lambda_v$, $\lambda_o$, and $s_e$ the same way in Po, and all introduced entities have the same equivalent class label.

Segmentation Operator: We compare our algorithms SmProvAlg and SmProvTst with the state-of-the-art general CFLR algorithm, Cflrb [42], and the Cypher query in Sec. [III] in Neo4j. We implement the fast set using a) Java BitSet to have constant random access time, b) RoaringBitMap which is the state-of-the-art compressed bitmap (Cbm) with slower random access but better memory usages [50], [51].

(a) Varying Graph Size N: In Fig. 5(a) we study the scalability of all algorithms. x axis denotes $N$ of the Po graph, while y axis shows the runtime in seconds to finish the PoSeg query. Note the figure is log-scale for both axes. As we see, SmProvAlg and SmProvTst run at least one order of magnitude faster than Cflrb on all Po datasets, due to the utilization of the properties of the grammar and efficient pruning strategies. Note Cflrb runs out of memory on Pd10k due to much faster growth of the worklist, as the normal forms introduce an extra level; SmProvAlg without Cbm runs out of memory on Pd10k due to $O(n^2/\log(n))$ space complexity and 32bit integer interface in BitSet. With Cbm, Cflrb still runs out of memory on Pd50k due to the worklist growth. Both SmProv algorithms reduce memory usages however become several times slower; In particular, SmProvAlg uses 64bit RoaringBitMap and is scalable to larger graphs. For very large graphs, disk-based batch processing is needed and Datalog evaluation can be used (Sec. [VI]).

SmProvAlg runs slightly faster than SmProvTst for small instances while becomes much slower for large instances, e.g., Pd50k, it is 3x slower than SmProvTst for the query. The reason is the because SmProvTst run $|V_{ds}|$ times on the graph and each run’s performance gain is not large enough. When the size of the graph instance increases, the superiority of the SmProvTst by using the transitivity property becomes significant.

On the other hand, the Cypher query can only return correct result for the very small graph Pd50 and takes orders of magnitude longer. Surprisingly, even for small graph Pd100, it runs over 12 hours and we have to terminate it. By using its query profile tool, we know that Neo4j uses a path variable to hold all paths and joins them later which is exponential w.r.t. the path length and average out-degree. Due to the expressiveness of the path query language, the grammar properties cannot be used by the query planer.

(b) Varying Input Selection Skew $s_e$: Next, in Fig. 5(b) we study the effect of different selection behaviors on Pd10k. The x axis is $s_e$ and the y axis is the runtime in seconds in log-scale. In practice, some types of projects tend to always take an early entity as input (e.g., dataset, label), while some others tend to take new entities (i.e., the output of the previous step) as inputs. Tuning $s_e$ in opposite directions can mimic those project behaviors. In Fig. 5(b) we vary $s_e$ from 1.1 to 2.1, and the result is quite stable for SmProvAlg, SmProvTst and Cflrb, which implies the algorithms can be applied to different project types with similar performance.
(c) Varying Number of Activities \( n \): Given a large graph, e.g., SNAP [45]. To make graphs and preserves path among keyword pairs and was used in the context of searching graphs. We discuss the effectiveness of Early Stopping

(d) Effectiveness of Early Stopping: The above evaluations all use the most challenging PoSeg query on start and end entities. In practice, we expect the users will ask queries whose result they can understand by simple visualization. CFLRB and general CFL don’t have early stopping properties. Our algorithms use the temporal constraints of the provenance graph to support early stopping growing the result. In Fig. 5(d), we vary the \( V_{src} \) and study the performance on P10k. The \( x \) axis is the starting position among all the entities, e.g., \( x = 20 \) means \( V_{src} \) is selected at the end of 20\% percentile w.r.t. the ranking of the order of being. As we can see, the shorter of the temporal gap between \( V_{src} \) and \( V_{dst} \), the shorter our algorithms’ runtime. Using the property of PROG graphs, we get better performance empirically even though the worst case complexity does not change.

Summarization Operator: Given a \( S = (S(V_{src}, E_{src})) \), PSum generates a precise summary graph Pseg(\( M, E \)) by definition. Here we study its effectiveness in terms of conciseness. We use the compaction ratio defined as \( c_r = |M|/|U \cup V_S| \). As there are few graph query result summarization techniques available, the closest applicable algorithm we can find is pSum [52] which is designed for summarizing a set of graphs from keyword search graph queries. pSum works on undirected graphs and preserves path among keyword pairs and was shown to be more effective than summarization techniques on one large graph, e.g., SNAP [45]. To make pSum work on PoSeg segments, we introduce a conceptual \( (start, end) \) vertex pair as the keyword vertices, and let the \( start \) vertex connect to all vertices in \( S \) having 0 in-degree, and similarly let the \( end \) vertex connect to all vertices having 0 out-degree. In the rest of the experiments, by default, \( \alpha = 0.1, k = 5, n = 20 \) and \( |S| = 10 \), and \( y \) axis denotes \( c_r \).

(a) Varying Transition Concentration \( \alpha \): In Fig. 5(e), we change the concentration parameter to mimic segment sets at various stage of a project with different stableness. \( x \) axis denotes the value of \( \alpha \) in log-scale. Increasing \( \alpha \), the transition probability tends to be uniform, in other words, the pipeline is less stable, and paths are more likely be different, so the vertex pairs which would be merged become infrequent. As we can see, PoSeg algorithm always performs better than pSum, and the generated Pseg is about half the result produced by pSum, as pSum cannot combine some \( \approx_{in}^t \) and \( \approx_{out}^t \) pairs, which are important for workflow graphs.

(b) Varying Activity Types \( k \): Next, in Fig. 5(f), we vary the possible transition states, which reflects the complexity of the underlying pipeline. It can also be viewed as the effect of using property aggregations on activities (e.g., distinguish the commands with the same name but different options). Increasing \( k \) leads to more different path labels, as shown in the Fig. 5(f), and it makes the summarization less effective. Note that when varying \( k \), the number of activities \( n \) in a segment is set to be 20, so the effect of \( k \) on compaction ratio tends to disappear when \( k \) increases.

(c) Varying Segment Size \( n \): We vary the size of each segment \( n \) when fixing \( \alpha \) and \( k \) to study the performance of Pseg. Intuitively, the larger the segment is, the more intermediate vertices there are. The intermediate vertices are less likely to satisfy the merging conditions due to path constraints. In Fig. 5(g), \( c_r \) increases as the input instances are more difficult.

(d) Varying Number of Segments \( |S| \): With all the shape parameters set \( (\alpha = 0.25) \), we increase the number of similar segments. As the segments are derived by the same transition matrix, they tend to have similar paths. In Fig. 5(h), \( c_r \) becomes better when more segments are given as input.
Provenance Systems: Provenance studies can be roughly categorized in two types: data provenance and workflow provenance. Data provenance is discussed in dataflow systems, such as RDBMS, Pig Latin, and Spark, while workflow provenance studies address complex interactions among high-level conceptual components in various computational tasks, such as scientific workflows, business processes, and cybersecurity. Unlike query facilities in scientific workflow provenance systems, their processes are predefined in workflow skeletons, and multiple executions generate different instance-level provenance run graphs and have clear boundaries. Taking advantages of the skeleton, there are lines of research for advanced ancestry query processing, such as defining user views over such skeleton to aid queries on verbose run graphs, querying reachability on the run graphs efficiently, storing run graphs generated by the skeletons compactly, and using visualization as examples to ease query construction.

Most relevant work is querying evolving script provenance. Because script executions form clear boundary, query facilities to visualize and difference execution run graphs are proposed. In our context, as there are no clear boundaries of run graphs, it is crucial to design query facilities allowing the user to express the logical run graph segments and specify the boundary conditions first. Our method can also be applied on script provenance by segmenting within and summarizing across evolving run graphs.

Data Science Lifecycle Management: Recently, there is emerging interest in developing systems for managing different aspects in the modeling lifecycle, such as building modeling lifecycle platforms, accelerating iterative modeling process, managing developed models, organizing lifecycle provenance and metadata, auto-selecting models, hosting pipelines and discovering reference models, and assisting collaboration. Issues of querying evolving and verbose provenance effectively are not considered in that work.

Context Free Language & Graph Query: Parsing CFL on graphs and using it as query primitives has been studied in early theory work, later used widely in programming analysis and other domains such as bioinformatics, which requires high expressiveness language to constrain paths. Recently it is discussed as a graph query language and SPARQL extension in graph databases. In particular, CFLR is a general formulation of many program analysis tasks on graph representations of programs. Most of the CFL used in program analysis is a Dyck language for matching parentheses. On provenance graphs, our work is the first to use CFL to constrain the path patterns to the best of our knowledge. CFL allows us to capture path similarities and constrain lineages in evolving provenance graphs. We envision many interesting provenance queries would be expressed in CFLR and support human-in-the-loop introspection of the underlying workflow.

Query Results & Graph Summarization: Most work on graph summarization focuses on finding smaller representations for a very large graph by methods such as compression, attribute-aggregation and bisimulation, while there are a few works aiming at combining a set of query-returned trees or graphs to form a compact representation. Our work falls into the latter category. Unlike other summarization techniques, our operator is designed for provenance graphs which include multiple types of vertices rather than a single vertex type; it works on query results rather than entire graph structure; the summarization requirements are specific to provenance graphs rather than returned trees or keyword search results. We also consider property aggregations and provenance types to allow tuning provenance meanings, which is not studied before to the best of our knowledge.

We described the key challenges in querying provenance graphs generated in evolving workflows without predefined skeletons and clear boundaries, such as the ones collected by lifecycle management systems in collaborative analytics projects. At query time, as the users only have partial knowledge about the ingested provenance, due to the schema-later nature of the properties, multiple versions of the same files, unfamiliar artifacts introduced by team members, and enormous provenance records collected continuously. Just using standard graph query model is highly ineffective in utilizing the valuable information. We presented two graph query operators to address the verbooseness and evolving nature of such provenance graphs. First, the segmentation operator allows the users to only provide the vertices they are familiar with and then induces a subgraph representing the retrospective provenance of the vertices of interest. We formulated the semantics of such a query in a context free language, and developed efficient algorithms on top of a property graph backend. Second, the summarization operator combines the results of multiple segmentation queries and preserves provenance meanings to help users understand similar and abnormal behavior. Extensive experiments on synthetic provenance graphs with different project characteristics show the operators and evaluation techniques are effective and efficient. The operators are also applicable for querying provenance graphs generated in other scenarios where there are no workflow skeletons, e.g., cybersecurity and system diagnosis.
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APPENDIX

A. Notation Table

We summarize the notations used for defining operators’ semantics in the paper in Table 1.

| **Provenance Graph:** $G(V, E, A, U, \lambda, \sigma, \omega)$ |
| $G$ | PROV graph |
| $V$ | Vertices ($E, A, U, H$) |
| $A$ | Agent |
| $U$ | Used |
| $E$ | Edges ($U, A, H, A, D$) |
| $\lambda$ | Vertex label |
| $\alpha$ | Edge label |
| $\beta$ | Property type |
| $\sigma$ | Vertex property |
| $\omega$ | Edge property |
| $\lambda$ | wasAttributedTo |
| $\mu$ | inCol |
| $\nu$ | inCol |
| $\pi$ | inRow |
| $\rho$ | wasGeneratedBy |
| $\tau$ | wasAssociatedWith |
| $\theta$ | wasDerivedFrom |

| **Segmentation Operator:** $PeSeg(V_{src}, V_{dst}, B)$ |
| $V_{src}$ | Source entities |
| $V_{dst}$ | Destination entities |
| $B$ | Boundary criteria |
| $\tau$ | Path label function |
| $\alpha$ | Empty word |

| **Summarization Operator:** $PeSum(S, K, R_k)$ |
| $K$ | Property Aggregation |
| $R_k$ | Provenance Type |
| $\pi$ | Vertex Eqv. class |
| $\gamma$ | Summary graph |

Table 1

**Summary of Notations**

B. Segmentation Operation

**CFLRB Algorithm for $L(SimProv) \rightarrow \text{reachability}$:** CFLRB [42] (shown in Alg. 1) is a subcubic algorithm to solve general CFLR problem. Given a CFG, CFLRB works on its normal form [37], where each production has at most two RHS symbols, i.e., $N \rightarrow AB$ or $N \rightarrow A$. We show the normal form of SimProv in Fig. 6 (domain of LHS of each production rule is shown in the caption). At a high level, the algorithm traverses the graph and uses grammar as a guide to find new production facts $N(i, j)$, where $N$ is a LHS nonterminal, $i, j$ are graph vertices, and the found fact $N(i, j)$ denotes that there is a path from $i$ to $j$ whose path label satisfies $N$. To elaborate, similar to BFS, it uses a worklist $W$ (queue) to track newly found fact $N(i, j)$ and a fast set data structure $H$ with time complexity $O(n^4/\log(n))$ for set diff/union and $O(1)$ for insert to memorize found facts.

In the beginning, all facts $F(i, j)$ from all single RHS symbol rules $F \rightarrow A$ are enqueued. In SimProv case ($r_0; Q_0$ in Fig. 6), each $v_j \in V_{src}$ is added to $W$ as $Q_0(v_j)$. From $W$, it processes one fact $F(i, j)$ at a time until $W$ is empty. When processing a

\[
\begin{align*}
q_0 & : Q_0 \rightarrow v_j & q_{v_j} & \in V_{src} \\
q_1 & : L_B \rightarrow G^4 Q_0 & q_2 & : L_B \rightarrow A R g & q_3 & : L_B \rightarrow U^r & q_4 & : L_B \rightarrow U^s & \end{align*}
\]

**Algorithm 1 CFLRB:** Subcubic time CFLR [42] for SimProv
1. $W \leftarrow \{(v, Q_b, v) | v \in V_{src}\}$
2. while $W \neq \emptyset$ do
3. 
4. for each production rule $A \rightarrow CB$ do
5. 
6. end for
7. for each production rule $A \rightarrow BC$ do
8. $W \leftarrow \{(u, A, v') | v' \in \text{Row}(v, C) \setminus \text{Row}(u, A)\}$
9. end for
10. end while

dequeued fact $F(i, j)$, if $F$ appears in any rule in the following cases:

\[
\begin{align*}
N(i, j) & \rightarrow F(i, j); \\
N(i, v) & \rightarrow F(i, j) A(j, v); \\
N(u, j) & \rightarrow A(u, i) F(i, j)
\end{align*}
\]

the new LHS fact $N(i, j)$ is derived by set diff $\{v \in A(j, v) \mid v \in N(i, v)\}$ or $N(u, j)$ by $\{u \in A(u, i) \mid u \in N(u, j)\}$ in $H$. As in SimProv, only the later two cases are present, in Alg. 1 line 4 6 and line 7 9 show the details of the algorithm. Row and Col accesses outgoing and incoming neighbors w.r.t. to a LHS symbol and is implemented using the fast set data structure. Then the new facts of $N$ are added to $H$ to avoid repetition and $W$ to explore it later. Once $W$ is empty, the start symbol $L$ facts $L(i, j)$ in $H$ include all vertices pairs $(i, j)$ which have a path with label that satisfies $L$. If a grammar has $k$ rules, then the worst case time complexity is $O(kn^3/\log(n))$ and $W \rightarrow D$ takes $O(n^2)$ space. If path is needed, a parent table would be used similar to BFS using standard techniques. In SimProv (Fig. 6), the start symbol is $R$, $V_i \in V_{sim}$, $R(v_i, v_j)$ facts include all $v_i$, s.t. between them there is $\tau(\tilde{R}_i, j) \in L(SimProv)$.

**Proof of Lemma 1:** The proof of Lemma 1 is the following: On SimProv normal form (Fig. 6), for $i \in [1, 8]$, CFLRB derives $r_i$ LHS facts by a $r_{i-1}$ LHS fact dequeued from $W$ (Note it also derives $r_1$ from $r_0$). For $i \in \{1, 2\}, r_1(u, v)$ uses $G$ edges in the graph during the derivation, e.g., from $r_0$ LHS $Re$ to $r_1 \rightarrow L_B(u, v) \rightarrow G(u, k)$ Re$(k, v)$. As Re$(k, v)$ can only be in the worklist $W$ once, we can see that each 3-tuple $(u, k, v)$ is formed only once on the RHS and there are at most $|G| |E|$ of such 3-tuples. To make sure Lg$(u, v)$ is not found before, $H$ is checked. If not using fast set but a $O(1)$ time procedure for each instance $(u, k, v)$, then it takes $O(|G| |E|)$ to produce the LHS; on the other hand, if using a fast set on $u'$’s domain $A$ for each $u$, for each Re$(k, v)$, $O(|A| |E|)$ time is required, thus it takes $O(|A| |E|)^2/\log |A|)$ in total. Applying similar analysis on $r_0$ and $r_0$ using $U$ to derive new facts, we can see it takes $O(|A| |E|)^2/\log |A|)$ with fast set and $O(|U| |A|)$ without fast set. Finally $r_3, r_4, r_7, r_8, r_9$ can be viewed as following a vertex self-loop edge and do not affect the complexity result.

C. Query Evaluation Discussion

**Validity of Segments** Validity of provenance graph is an important constraint [26], [34]. In our system, the PeSeg operator does not introduce new vertices or edge. As long as the original provenance graph is valid, the induced subgraph
is valid. However, at query time, the boundaries criteria could possibly let the operator result exclude important vertices. As an interactive system, we leave it to the user to adjust the vertex set of interest and boundary criteria in their queries.

**Two-step approach Revisit:** For other purposes where the two-step approaches are not ideal, the exclusion constraints $B_v$ and $B_e$, and expansion criteria $B_x$ can be evaluated together using CflrB, SimProvAlg and SimProvTst with small modifications on the grammar. In CflrB the label function $F_v$ of $B_v$ can be applied at $r_0, r_3, r_7, r_8$ on $\mathcal{A}$ or $\mathcal{E}$, while $F_e$ of $B_e$ can be applied at rest of the rules involving $U$ and $G$. For SimProvAlg and SimProvTst, $F_v$ and $F_e$ can be applied together at $r'_1, r'_2$.

**Ad-hoc query:** We mainly focus on developing ad-hoc query evaluation schemes. As of now, the granularity of provenance in our context is at the level of commands executions, the number of activities are constrained by project members’ work rate. In case when the PROV graph becomes extremely large, indexing techniques and incremental algorithms are more practical. We leave them as future steps.

**D. Summarization Operation**

**Alternative Formation** We consider alternative of formulation of the summary graph. One way to combine PSEG segment graphs is to use context-free graph grammars (CFGG) [32] which are able to capture recursive substructures. However without a predefined workflow skeleton CFGG, and due to the workflow noise resulting from the nature of analytics workload, inferring a minimum CFGG from a set of subgraphs is not only an intractable problem, but also possibly leads to complex graph grammars that are more difficult to be understood by the users [71]. Instead, we view it as a graph summarization task by grouping vertices and edges in the set of segments to a PSEG.

Though requiring all paths in PSEG must exist in some segment may look strict and affect the compactness of the result, PoSum operator allows using the property aggregation ($\mathcal{K}$) and provenance types ($\mathcal{R}_g$) to tune the compactness of PSEG. Due to the rigidity and the utility of provenance, allowing paths that do not exist in any segment in the summary would cause misinterpretation of the provenance, thus would not be suitable for our context. In situations where extra paths in the summary graph is not an issue, problems with objectives such as minimizing the number of introduced extra paths, and minimizing the description length are interesting ones to be explored further. We leave them as future steps.

**E. System Design Decision**

Note the design decision of using a general purpose native graph backend (Neo4j) for high-performance provenance ingestion may not be ideal, as the volume of ingested provenance records would be very large in some applications, e.g., whole-system provenance recording at kernel level [14], [20] would generate GBs of data in minutes. The support of flexible and high performance graph ingestion on modern graph databases and efficient query evaluation remain an open question [72].

We leave the issue to support similar operators for general PROV graph for our future steps. The proposed techniques in the paper focus on enabling better utilization of the ingested provenance information via novel query facilities and are orthogonal to the storage layer.