On Nesting Graphs

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ABSTRACT

Despite the existance of valuable graph operations creating new vertices and edges from existing graphs, such as graph transformations and graph summarization, an operator allowing both to summarize a subgraph content into one single vertex or edge and to keep the information of the contained vertices and edges is missing. This deficiency is not only due to the operators' definitions, but has to be sought on the current graph data model definition not supporting nestings for overlapping subgraphs. In this paper we propose a novel graph data structure for nested property graphs. Based thereon, we also propose a graph nesting operator and a specific algorithm, THoSP, outperforming the solution propoed by graph (Cypher, SPARQL) relational (SQL) and document oriented databases.

ACM Reference Format:

1 INTRODUCTION

Graph data management systems play an increasing role in present data analytics, because they allow flexible analyses of relationships among data objects. In fact, graphs have been already used as a fundamental data structure for representing data within different contexts, such as corporate data [14, 17], social networks [3, 20] and linked data [19]. Despite the increasing production of graph data, a general operator aggregating with a roll-up fashion one single graph is missing. Given one single input graph q, this operator should both preserve the vertices and edges that are not involved in the roll-up operation, and create nested vertices and nested **edges**, which may contain subgraphs of *g*; we would also like that the nested created components may be freely unnested, such that the original graph may be obtained back again. The edges connecting the nested vertices do not necessarily represent a partition of the input graph, but the presence of an edge between two nested vertices may represent the existence (within the input graph) of an edge (or more generally a path) between the subgraphs of gcontained in the aforementioned nested vertices.

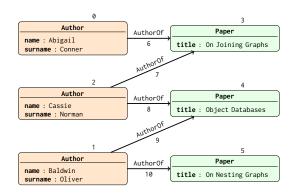
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Conference'17, July 2017, Washington, DC, USA
© 2018 Association for Computing Machinery.
ACM ISBN 978-x-xxxx-xxxx-x/YY/MM...\$15.00
https://doi.org/10.1145/nnnnnnn.nnnnnnn

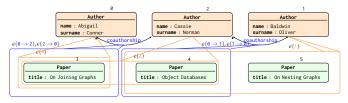
Such desired outcome extends the vertex summarization class of aggregations: those latter strategies mainly group the vertices as in relational Group By strategies, and then aggregate the edges accordingly [11]. These class of operations restrict the ability of aggregating by paths, that are limited to the set of edges connecting the vertices belonging to two (different) class of vertices. It follows that such class of aggregations do not allow to freely aggregate the edges into final nested edges. Since most of such vertex summarization techniques are graph-partition based, most of them fail to aggregate graphs that share some vertices and edges in common [10, 18, 21]. Among all those graph summarization techniques, only HEIDS [5] and Graph Cubes [22] perform graph summarizations of one single graph over a graph collection of non pairwise disjoint subgraphs. On the other hand, these last two techniques require that the set union of such graph collections must be equivalent to the original graph, while data integration and social networks scenarios even consider the possibility of outliers within the data, that are hereby represented in no subgraph belonging to the aforementioned graph collections.

The possibility of performing graph traversals allows *path sum-marizations* as well as vertex summarizations; path summarizations allow the aggregation of multiple paths among source and target vertices that share the same properties. Within pattern matching query languages (described in more detail in Section 2.2), the vertex summarization phase must be necessarily separated from the path summarization one, thus thwarting the advantages of performing vertex and path summarizations contemporarily. In particular, while Cypher queries can perform distinct aggregations only within distinct MATCH clauses, SPARQL 1.1 implementations of the query plan combine these two phases with a UNION operator, thus forcing the algorithm to visit the same graph twice. As a result, the query plan optimizers of such query languages do not allow to avoid to visit one same graph more than once whether possible.

This paper shows that such query language limitations can be reduced by using a graph nesting operator, which embodies both vertex and path summarization queries, which are performed contemporarily within the same operator. We also investigate a data structure to optimize a specific graph nesting use case. To that end, we study the existence of specific graph patterns prone to algorithmic optimizations. Hereby, we show that such algorithmic approaches allow to reduce the time complexity of the visiting and nesting problem, which is going to performed over a data structure that requires less indexing time that its own competitors. In particular, we focus on intersecting graph visiting patterns: one pattern (g_V) is given for vertex summarization, and the other (g_E) is for path summarization into one single edge, thus subsuming which is the shared sub-pattern (α) among the two former ones.



(a) Input bibliographical network.



(b) Nested result: given two Authors a and a', there exist two coauthorship edges, $a \to a'$ and $a' \to a$ if and only if they share some authored paper contained respectively in $\epsilon(a \to a')$ and $\epsilon(a' \to a)$. Moreover, each author a is associated to the set of his authored papers $\epsilon(a)$.

Figure 1: Nesting a bibliographic network: the provenance information is nested within the original node.

Consequently, α is going to be visited only once within the graph, after which either the vertex or the path summarization pattern can be visited in their entirety. We also perform some restrictions over these patterns enhancing such optimizations: for each vertex pattern we're going to elect one vertex as a **vertex grouping reference** (γ_V), in which we're going to nest the matched vertices and edges during the graph traversal. Similarly, each edge path summarization pattern is going to elect a source (γ_E^{src}) and a target (γ_E^{dst}) vertex, which are going to be called **edge grouping references**: such vertces must both coincide with the vertex grouping references, so that the newly generated edge will have as sources and target the previously vertex-nested elements.

Example 1. Given a bibliographic network containing (at least) Authors and Papers as vertices, and where authorOf edges connect each author to the papers he has authored (Figure 1a), we want to "roll up" the network into a coauthorship network, where each Author is connected by a coauthor edge with another Author with which he has published some papers (Figure 1b). In particular, for each resulting Author vertex, nest inside it its papers as vertices, and nest inside each coauthor edge all the papers coauthored by the source and destination Authors. We also want to exclude coauthor hooks over the same vertex.

This problem can be solved by visiting the graph only once; if the current vertex is a Paper, traverse backwards all the authorof edges, thus reaching all of its Authors, that are going to be coauthor



(a) Vertex summarization pattern (g_V) . Author is the vertex grouping reference γ_V .



(b) Path summarization pattern (g_E) . Author_{src} and Author_{dst} are respectively edge grouping references γ_E^{src} and γ_E^{dst} .

Figure 2: Vertex and Path summarization patterns for the query expressed in Example 1. Vertex and edge grouping references are marked by a light blue circled node. As we can see, the vertex grouping reference depicts the same property expressed by edge grouping references.

for at least the current paper. Therefore, I can incrementally define the edge nesting between all such authors in a separated nesting index, since I know that all these authors share the same paper, and partially instantiate the nesting of each author with the papers that has authored via an external index. The remaining types of vertices and edges may be discarded. By doing this, only the edges are visited twice, but the vertices are visited only once. Hereby, with these patterns we reach the optimal solution by visiting the graph only once.

Figure 2 represents the desired vertex and path summarization patterns. The same vertex summarization pattern appears twice within the path summarization: this means that by visiting the path summarization pattern once, we may pre-istantiate two morphisms for the vertex summarization pattern. The two patterns have different key roles: while the vertex summarization retrieves all the papers that one author has published and nest them within one single matched author, the path summarizations return all the papers authored by two different authors and creates an edge between the two previously nested vertices. This construction implies that a join between the two paths must be carried out.

This pattern comparison remarks that, in order to reduce the graph time visit, we must start from visiting the Paper, which is shared among the two distinct patterns, and then keep going with the graph visit by exploring the source and target vertices.

This chapter provides the three following main contributions:

- We implement the aforementioned solution into a nested graph data model, where the logical model differs from the physical one.
- **Graph Nesting Operator** (Section 4); we provide a general definition of the nesting operator which combines the path with the vertex summarization approaches to nesting graphs.
- Two HOP SEPARATED PATTERNS (THoSP) algorithm for a specific graph nesting task (Section 4.1): we compare it to its implementation over both graph (SPARQL, Cypher),

relational (SQL) and document oriented (AQL) query languages. The results of such experiments shows that the sum of both indexing and query evaluation time of our proposed solution outperforms by at least one order of magnitude the aforementioned solutions evaluated on such databases with their respective query languages (Section 5). Consequently, our data model also proved to be curcial in providing an enhanced implementation of the specific graph nesting task.

The source code for THoSP is provided at [Link removed for double-blind review].

2 RELATED WORKS

2.1 Nested Graph Representations

Statecharts [8] were one of the first models representing nested graphs: they were used for representing complex systems at different abstraction levels, where each node represents a state or "configuration" of the system, and each edge represents a transaction between two different states on a given event. Each vertex and edge is labelled, but they do not come with attribute-value associations because this model was not designed for data representations. In order to represent different nesting levels, each node can contain other states and edges connecting such states. As a consequence, there is no distinction between (simple) states and states containing other states. This model allows both external edges and internal edges: we say that edge e is external if its source (or target) is contained by the target (or source) but neither of them contains e; the edge is called *internal* when the containing vertex (either its source or target) also contains the edge. Besides of state representation purposes, this model was been even used for both modelling the evolution of pathophysiological states and to describe the subsequent treatments to which the patient must undergo, where each treatment could be furtherly subdivided in smaller consequential steps to be followed [12].

This model was also adopted as a basis for the hypernode data model [15]: even if hypernodes are subsequent to statecharts, they are less expressive than the former ones, because they do not label the edges and they only allow edges between vertices which are contained within the same vertex: the model neither represents external edges nor internal ones. As previously stated for statecharts, even this model does not allow to fully represent a property graph, since the attribute-value association must be necessarily expressed as a relation between two different vertices [15]. Last, the fact that the vertex containments cannot overlap make such nested model affected from the same data replication representation problem described for semistructured and nested data. A first extension of the hypernode model towards data representation is represented by CoGITaNT [7], where any type of edge (thus including internal and external ones) are included and data is firstly contained inside a node. Nested graphs are also supported by GraphML [2] and GXL

Two different approaches have been used to extend current graph data model for supporting nesting operations: the first ones try to overcome to the basic graph data structure limitations by simply extending the query language, while the other ones try to extend the data structures that are used for both input and intermediate computations.

Among the first type of approaches, the one outlined in [6] propose to define a RDF vocabulary over which the OLAP cube can be defined in RDF. On top of this "structured" RDF graph, an algorithm generates the SPARQL query that will allow to perform either the roll-up or the drill-down operation. This later approach implies that each possible computation has to be always recomputed on top of the row data like for classical ROLAP systems: as a consequence, this MOLAP approach does not benefit from the specific RDF representation, that is not able to represent different aggregation levels and to store intermediate computations.

The last type of approaches have been recently widely investigated, and seem to be more promising with respect to optimization techniques: in [4, 16, 18] graph data structures are associated with external graph indices, thus allowing to connect one graph to its broader one with respect to the roll-up query. As a consequence, these solutions do not allow to freely expand any aggregated component at a time, but they can only backtrack the aggregation to a previous known state.

2.2 Databases and Query Languages

We want now to discuss how current query languages can express graph nesting within their data model of choice. In particular, we must select query languages that either support collections or nested representations allowing to express the same query presented in our running example. The associated proposed listings can be seen in the appendix.

For these reasons, we select PostgreSQL's dialect which, by extending the SQL-3 syntax with JSON data supports, allows to create arrays as a result of a GROUP BY query via array_agg; therefore, instead of using function aggregating a collection into one single summarized value, we can list all the elements that have been aggregated. In particular, in PostgreSQL's dialect, we implement our graph by storing the triples defining an edge as the following relation:

Edge(edgeId, sourceId, edgeLabel, targetId)

Hereby, by grouping the edges by *sourceld* and collecting all the target's ids we obtain a representation of nested vertices. Similarly, if we join the Edge relation with itself and group the join result by two distinct *sourceld* and return the list of all the Papers that they have in common, we can return the list of all the Papers that they have coauthored. As showed in Listing 1, the overall graph nesting cannot be created in one single SQL query, because by the SQL language definition we cannot distinctively group the same dataset in different ways, but we must visit the same data twice and perform two distinct aggregations.

All the other query languages are going to be affected by the same problem, SPARQL included (Listing 2): despite the fact that this query language may represent the graph nesting query as a single statement, even in this case the UNION clause implies a separate visit for the two graph patterns. In particular, the first pattern allows to traverse those graph patterns matching the coauthorship statement in Figure 2b so that they can be nested within the created COAUTHORSHIP edge, while the second part returns all the associations of the Paper that have been authored by one single AUTHOR. In particular, the OPTIONAL. . . FILTER(!bound(. . .)) syntax is adopted instead of FILTER NOT EXISTS, because the latter is only

supported in SPARQL1.1, which is not supported by the current version of *librdf* used to query Virtuoso in our benchmarks. In this case, the edge nesting is performed via the association of different http://cnt.io/nesting properties departing from the ?newedge CoAuthorship between two coauthors. Consequently, even in this case the graph visits two times the same graph patterns.

We also consider the AQL query language supported by ArangoDB, because ArangoDB is a NoSQL database relying on a document-oriented storage, which is hereby prone to both represent and return nested content. An example of how such graph nesting query can be carried out in AQL is presented in Listing 3: in this scenario we assume that we've previously loaded our graph data with the default format, where both vertices and edges are fully stored, and where the former are indexed by id, while the latter are also indexed by source and target vertex id. In particular, we can state that this algorithm provides the exact same result as the one produced by the SQL query, except that JSON documents are returned instead of relational tables containing JSON arrays.

Last, Listing 4 provides an example of Neo4J allowing to nest property graphs: even in this case the property graph model does not directly nest the graphs inside one element. Similar to the previous approaches, we can group by all the graphs returned by the graph pattern by selecting the vertices of interest, and nesting the to-be-grouped remaining objects inside a collection. In particular, we can first match the vertex summarization pattern in Figure 2a and group by AUTHOR, and nest the collection of authored PAPERS within the to-be-created nested vertex; similarly, we can first match the path summarization pattern presented in Figure 2b by source and destination AUTHOR, and then create an edge between the previously created nested vertices by collecting all the coauthored PAPERS appearing in the original graph. Moreover, the Neo4J property graph data model implies that we cannot create an edge if the vertices are not previously known beforehand and, therefore, we always must join the nested vertices with the original matched ones in order to reconstruct the original information and perform the actual matching operation. As it will be observed within the benchmarks, the solution of not separating the elements' ids from their data quickly leads to an intractable solution.

3 NESTED GRAPHS

The term *property graph* usually refers to a directed, labelled and attributed multigraph (each vertex and edge is represented as a relational tuple). In a property graph a single *label* is associated to every vertex and edge (e.g., Author or coAuthorsip). Further on, vertices and edges may have arbitrary named attributes (*properties*) in the form of key-value pairs (e.g., fullname: "Alice McKenzie" or institution: "Bengodi Ltd."). Property-value associations are represented as set as tuples from the relational model. We define the *nested* (*property*) *graphs* as follows:

DEFINITION 1 (NESTED GRAPH DATABASE). Given a set Σ^* of strings, a **nested** (property) graph database G is a tuple $G = \langle \mathcal{V}, \mathcal{E}, \lambda, \ell, \omega, v, \epsilon \rangle$, where \mathcal{V} and \mathcal{E} are disjoint sets, respectively referring to vertex and edge identifiers $(c, i) \in \mathbb{N}^2$. In particular, input data graphs have c = 0 while data views containing new elements may have new vertices or edges with c > 0.

Each vertex and edge is assigned to multiple possible labels through the labelling function $\ell: \mathcal{V} \cup \mathcal{E} \to \wp(\Sigma^*)$. λ is a function $\mathcal{E} \to \mathcal{V}^2$ mapping each edge to its source and target vertex. ω is a function mapping each vertex and edge into a relational tuple.

In addition to the previous components defining a property graph, we also introduce functions representing vertex content $v: (V \cup E) \rightarrow \wp(V)$ and edge content $\epsilon: (V \cup E) \rightarrow \wp(E)$. These functions induce the nesting by associating a set of vertices or edges to each vertex and edge. Each vertex or edge $o \in V \cup E$ induces a **nested (property)** graph as the following pair:

$$G_o = \langle v(o), \{ e \in \epsilon(o) \mid s(e), t(e) \in v(o) \} \rangle$$

Since the content functions ν and ϵ induce the expansion of each single vertex or edge to a graph, we must avoid recursive nesting to support expanding operations. Therefore, we additionally introduce the following constraints to be set at a nested property graph database level:

AXIOM 1 (RECURSION CONSTRAINTS). For each correctly nested property graph, each vertex $v \in V$ must not contain v at any level of containment of ϵ and, any of its descendants c on the underneath level must not contain v itself. That is:

$$\forall v \in \mathcal{V}. \forall c \in v^+(v). \ c \neq v \land v \notin v^+(c)$$

Similarly to vertices, any edge shall not contain itself at any nesting level:

$$\forall e \in \mathcal{E}. \forall c \in \rho^+(e). c \neq e \land e \notin \rho^+(c)$$

A vertex v having a non-empty vertex or edge content is called **nested vertex**, while vertices with empty content are simply referred to **simple vertices**. For edges, we respectively use the terms **nested edges** and **simple edges**.

4 GRAPH NESTING

The graph nesting operator uses a classifier to group all the vertices and edges that shall appear as a member of a cluster C.

Definition 2 (Nested Graph Classifier, g_{κ}). Given a set of cluster labels C, a **nested graph classifier** operator g_{κ} maps a nested property graph G_0 into a nested property graph collection $\{G_C\}_{C \in C, G_C \neq \emptyset}$ of subgraphs of G_0 . Such operator uses a classifier function $\kappa \colon \mathcal{V} \cup \mathcal{E} \to \wp(C)$ mapping each vertex or edge in either no graph or more than one non-empty subgraph. Each nested graph G_C is a pair $G_C = \langle \mathcal{V}_C, \mathcal{E}_C \rangle$ where \mathcal{V}_C (and \mathcal{E}_C) is the set of all the vertices v (and edges e) in G_0 having $C \in \kappa(v)$ (and $C \in \kappa(e)$). Therefore, the nested graph classifier is defined as follows:

$$g_{\kappa}(G_o) = \{ \, \langle \mathcal{V}_C, \mathcal{E}_C \rangle \mid C \in C, \mathcal{V}_C \neq \emptyset, \mathcal{E}_C \neq \emptyset \, \}$$

The former definition is also going to express graph pattern evaluations, where κ may be represented as a graph (cf. Neo4J). In order to represent the subgraphs in $g_{\kappa}(G_o)$ as either vertices and edges, we may use the following USER-DEFINED FUNCTIONS:

Definition 3 (User-Defined Functions). An object user defined function μ_{Ω} maps each subgraph $G_C \in g_{\kappa}(G_o)$ into a pair $\mu_{\Omega}(G_C) = (L,t)$, where $L \in \wp(\Sigma^*)$ is a set of labels and t is a relational tuple.

An edge user defined function μ_E maps each subgraph $G_C \in g_K(G_o)$ into a pair of identifiers $\mu_E(G_C) = (s,t)$ where $s,t \in \mathbb{N}^2$.

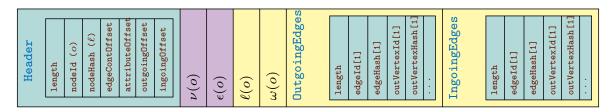


Figure 3: Serialized data structure representing an extended adjacency list for one nested vertex o. The header contains some basic information (such the representation size of o, its id and associated hash) and the offsets to the remaining fields. v and ϵ are empty when the serialized graph represents a basic property graph as the one in Figure 1a.

While μ_{Ω} may be used for transforming subgraphs to both vertices and edges, μ_E is only used to map subgraphs to edges. In order to complete such transformation, we have to map each graph in $g_{\kappa}(G)$ into a new id $(\mathbf{c}, \mathbf{i}) \notin \mathcal{V} \cup \mathcal{E}$, for which an indexing function has to be defined as follows:

$$\iota_G(G_C) = (\max \{ c \mid (c, i) \in V \cup E \} + 1, dt(V_C \cup V_E))$$

where dt is an arbitrary bijection associating a n-tuple in \mathbb{N}^n into one single number \mathbb{N} [13]. The combination of all the previous functions allow the definition of the following nesting operator:

DEFINITION 4 (GRAPH NESTING). Given a nested graph $G_{(c,i)}$ within a nested graph database G, an object user defined function μ_{Ω} , an edge user defined function μ_E and an indexing function ι_G , the graph nesting operator $\eta_{g_V,g_E,\mu_{\Omega},\mu_{E},\iota_G}$ converts each subgraph in $G_C \in g_V(G_{(c,i)})$ (and $G_C \in g_E(G_{(c,i)})$) into a nested vertex (and nested edge) $\iota_G(G_C)$ and adds them in the resulting nested graph:

$$\begin{split} &\eta_{g_{V},g_{E},\mu_{\Omega},\mu_{E},\iota_{G}}^{\pmb{keep}}(G_{(c,i)}) = \\ & \left\langle \{v \in v(c,i) | V(v) = \emptyset \land \pmb{keep} \} \cup \iota_{G}(g_{V}(G_{(c,i)})), \right. \\ & \left. \{e \in \epsilon(c,i) | E(e) = \emptyset \land \pmb{keep} \} \cup \iota_{G}(g_{E}(G_{(c,i)})) \right\rangle \end{split}$$

The vertices and edges in $G_{(c,i)}$ that appear neither in a nested vertex nor in a nested edge may be also returned if **keep** is set to true. As a result, the nested graph database is updated by using the nested graph classifier and user defined functions as follows:

$$\begin{split} & \left\langle \mathcal{V} \cup \iota_G(g_V(G_{(c,i)})), \ \mathcal{E} \cup \iota_G(g_E(G_{(c,i)})), \right. \\ & \lambda \oplus \bigoplus_{G_C \in g_E(G_{(c,i)})} \iota_G(G_C) \mapsto \mu_E(G_C), \\ & \ell \oplus \bigoplus_{G_C \in g_E(G_{(c,i)}) \cup g_V(G_{(c,i)})} \iota_G(G_C) \mapsto \text{fst } \mu_\Omega(G_C), \\ & \omega \oplus \bigoplus_{G_C \in g_E(G_{(c,i)}) \cup g_V(G_{(c,i)})} \iota_G(G_C) \mapsto \text{snd } \mu_\Omega(G_C), \\ & \nu \oplus \bigoplus_{G_C \in g_E(G_{(c,i)}) \cup g_V(G_{(c,i)})} \iota_G(G_C) \mapsto V_C, \\ & \varepsilon \oplus \bigoplus_{G_C \in g_E(G_{(c,i)}) \cup g_V(G_{(c,i)})} \iota_G(G_C) \mapsto E_C \right\rangle \end{split}$$

where $f \oplus g$ denotes the extension of the (finite) function f with another (finite) function g.

4.1 Two HOp Separated Patterns Algorithm

In order to solve our specific graph nesting problem as presented in the introduction, we want to evaluate ν when the non-traversed vertices and edges are not preserved (**keep** = false), where g_V and g_E are the ones represented in Figure 1 and the UDFs associate to each nested vertex the authors' informations and creates nested edges with coAuthorship label and no associated tuple. In particular:

$$\mu_E(G_C) = \left\langle f_C(\gamma_E^{src}), f_C(\gamma_E^{dst}) \right\rangle \quad s.t. \quad g_E \xrightarrow{f_C} G_C$$

$$\mu_{\Omega}(G_C) = \begin{cases} ([\text{``coAuthor''}], \ \emptyset) & G_C \in g_E(G_{(c,i)}) \\ (\ell(f_C(\gamma_V))), \ \omega(f_C(\gamma_V))) & G_C \in g_V(G_{(c,i)}) \end{cases}$$

The input data represnetation for the THoSP algorithm is presented in Figure 3, which represents an extension of the usual graph adjacency lists: in addition to the information pertaining to both the ingoing and outgoing edges, each vertex o has an associated header, where its id (o), its associated hash and the offset pointing to other serialzied fields, such as the information of the nested vertices and edges a set of labels ($\ell(o)$), and eventually its propertyvalue representation ($\omega(o)$). Last, for each edge we store its id and hash value, as well as the hash and the id of the adjacent vertex. Hash values are used within the proposed THoSP algorithm to store the correspondences with the graph patterns in Figure 2; therefore, each $\ell(o)$ is associated to a distinct hash value. We also suppose that the input graph data to be serialized does not represent an exact adjacency list: for this reason, the graph is firstly created in primary memory without the offset information, and then serialized into secondary memory. This first preprocessing step provides the loading and indexing step of our algorithm, where no further ancillary indexing data structures are serialized.

Algorithm 1 provides the desired implementation of the THoSP algorithm using the outcome of the previous preprocessing. We first restrict α to one single vertex and two edges (Line 5): for each vertex (c,v) matched by α (Line 7) we know that we must (possibly) visit all the edges going from (c,v) towards the vertices γ_E^{src} and γ_E^{dst} , that substantially are γ_V . Therefore, having an edge as a constraint in α linking v towards γ_E^{src} or γ_E^{dst} both in g_E and g_V can reduce all the possible computations to the actual edges traversed from (c,v) meeting the grouping references (Line 14). Therefore, we know whether we finished visiting our patterns after exhaustively matching all the elements within the pattern. As a consequence, a "path join" is performed between the two nested

Algorithm 1 Two HOp Separated Patterns Algorithm (THoSP)

```
1: procedure PartitionHashJoin((g_V, \gamma_V), (g_E, \gamma_E^{src}, \gamma_E^{dst}); G_o)
        FILE AdjFile = OPEN(G_o);
        FILE Nesting = OPEN(new);
         Adjacency to Serialize =
             new Map<Vertex,<Edge,Vertex»();</pre>
         \alpha := g_V \cap g_E \setminus (\gamma_V \cup \gamma_E^{src} \cup \gamma_E^{dst});
 5:
         for each vertex (c, v) in AdjFile do
 6:
 7:
            if (c, v) \models \alpha then
               for each ((c', u), e, (c, v)) \models \gamma_V do
 8:
                  u' := dt(1, dt(c', u))
 9:
                   NestingIndex.write(\langle u', u \rangle)
10:
                   NestingIndex.write(\langle u', e \rangle)
11:
12:
                   NestingIndex.write(\langle u', v \rangle)
                  for each ((c'', w), e, (c, v)) \models \gamma_V do
13:
                      if ((c', u), e, (c, v), e', w) \models \gamma_E then
14:
                          w' := dt(1, dt(0, w))
15:
                          \varepsilon := dt(1,\, dt(u,\, w))
16:
17:
                          NestingIndex.write(\langle \varepsilon, u \rangle)
18:
                          NestingIndex. write(\langle \varepsilon, e \rangle)
                          NestingIndex.write(\langle \varepsilon, w \rangle)
19:
20:
                          NestingIndex.write(\langle \varepsilon, e' \rangle)
21:
                          NestingIndex.write(\langle \varepsilon, \upsilon \rangle)
                          to Serialize. \mathtt{put}(u', \langle \varepsilon, \, w' \rangle)
22:
         AdjFile.serialize(toSerialize);
```

patterns (Line 13): this is evident from the two vertex nested for loops appearing in the algorithm.

Our physical data model differentiates the **input data represnetation** from the **query result**. We suppose that the latter is only used by the user to read the outcome of the nesting process as in other query languages (such as SPARQL and SQL) and does not have to produce "materialized views". Therefore, the result of the graph query itself can postpone the creation of a complete "materialized view", which will later use the same representation of the input data by using both the id information and the application of the User Defined Functions. In particular, the dovetailing function is used to associate both the nested vertices, u' and w', and the nested edge ε to their grouping references, thus allowing to easily go back to the original grouping references by using the inverse function of dt, thus allowing the application of the user defined functions.

Last, the association between the nested vertices (and edges) f and its content within the input graph c is stored in a NestingIndex file as a set of pairs $\langle f, c \rangle$. By doing so, we omit the Group By cost which affects the previously seen query languages, thus allowing to an overall better performance.

Please note that if in g_E there is no path connecting α to γ_E^{src} or γ_E^{dst} , the problem may quickly become cubic with respect to the size of the vertices, because we must create all the possible permutations where (c,v) is present alongside another element matching γ_E^{src} or γ_E^{dst} .

5 EXPERIMENTAL EVALUATIONS

Through the following experiments we want to prove that (i) both the time required to serialize our data structure and (ii) the query plan provided for the graph nesting query, outperform the same tasks performed on top on other databases, either graph, relational,

or document oriented. For a first analysis we compare the loading time (the time required to store and index the data structure) and for the second one we time the milliseconds to perform the query over the serialized and indexed data structure. Moreover, we shall jointly compare the time required to query the data with the time spent on the loading phase, because in some cases better query performances may be lead to the creation of several indices.

The query plans are evaluated with respect to the data representation independently to the data attached to it: in this case there is no additional penalty over carrying the values associated to the indices, and only the algorithms used within the data structures are compared. We choose a graph where vertices are only represented by their vertex ids and their label, and edges are represented only by the source and target vertex, alongside with the edge's label. Consequently, within the relational model the whole information can be stored only within one single table regarding the edges. Similar approaches are used in Virtuoso for representing RDF triple stores over a relational engine. We performed our benchmark using a bibliography network using the gMark generator [1], as the previous dataset cannot be used for this other query task. To each author 0f relation a Zipf's Law distribution with parameter 2.5 is associated to the ingoing distribution, while a normal distribution between 0 and 80 is associated to the outgoing distribution. Consequently, each vertex represents either an Author or an authored Paper, and are represented by distinct vertex ids. The resulting graph is represented as a list of triplets: source id, edge label (author of) and target id. The generator was configured to generate 8 experiments by incrementally creating a graph with vertices with a power of 10, that is from 10 to 10^8 .

We performed our tests over a Lenovo ThinkPad P51 with a 3.00 GHz (until 4.00 GHz) Intel Xeon processor and 64 GB of RAM at 2.400 MHz. The tests were performed over a ferromagnetic Hard Disk at 5400 RPM with an NTFS File System. We evaluate THoSP using the two pattern matching queries provided in the running example. We used default configurations for Neo4J, PostgreSQL and **ArangoDB**, while we changed the cache buffer configurations for Virtuoso (as suggested in the configuration file) for 64 GB of RAM; we also kept default multithreaded query execution plan. PostgreSQL queries were evaluated through the psql client and benchmarked using both explain analyze and \timing commands. Virtuoso was benchmarked through the Redland RDF library using directly the librdf_model_query_execute function. AQL queries over ArangoDB were evaluated directly through the arangosh client and benchmarked using the getExtra() method. Cypher queries were evaluated using the Java API through the execute method of an GraphDatabaseService object. All the aforementioned conditions do not degradate the query evaluations. Last, given that all databases (except from Neo4J) were coded in C/C++ and that Neo4J provided the worst overall performances, we implemented our serialization and THoSP only in C++.

At first, we must discuss the operator loading time (Table 1a), directly loaded from the data generated by gMark. We shall compare Virtuoso and PostgreSQL first, since they are both based on a traditional relational database engine using one single table to store a graph. In both cases the graph was only represented in triples: Virtuoso automatically stores an RDF graph, while in PostgreSQL the graph was stored by a table of quadruples, where the first is

| Operands Size | Operand Loading and Indexing Time (C/C++) (ms) | | | | | | | |
|------------------|--|------------|-----------|--------------|---------------------|--|--|--|
| Vertices (V) | PostgreSQL | Virtuoso | ArangoDB | Neo4J (Java) | Nested Graphs (C++) | | | |
| 10 | 8 | 3.67 | 43 | 3,951 | 0.13 | | | |
| 10^{2} | 18 | 6.86 | 267 | 4,124 | 0.33 | | | |
| 10^{3} | 45 | 23.53 | 1,285 | 5,256 | 3.51 | | | |
| 10^{4} | 225 | 371.40 | 11,478 | 11,251 | 31.83 | | | |
| 10^{5} | 1,877 | 3,510.96 | 135,595 | 1,193,492 | 337.00 | | | |
| 10^{6} | 19,076 | 34,636.80 | 1,362,734 | >1H | 3,694.56 | | | |
| 10^{7} | 184,421 | 364,129.00 | >1H | >1H | 44,063.50 | | | |
| 10^{8} | 1,982,393 | >1H | >1H | >1H | 518,361.00 | | | |

(a) Operand Loading and Indexing Time. PostgreSQL and Neo4J have transactions, while Virtuoso and ArangoDB are transactionless. Nested Graphs are our proposed method which is transactionless.

| Operands Size | | Two HOp Separated Pattern Time (C/C++) (ms) | | | | | |
|-----------------------------|--|---|--|--|---|--|--|
| Matched subraphs | SQL Dialect | SPARQL | AQL | Cypher | THoSP (C++) | | |
| $(m_V(G_o) + m_E(G_o))$ | (PostgreSQL) | (Virtuoso) | (ArangoDB) | (Neo4J – Java) | 1 HOSP (C++) | | |
| 3 | 2.10 | 11 | 3.89 | 681.40 | 0.11 | | |
| 58 | 9.68 | 63 | 12.34 | 1,943.98 | 0.14 | | |
| 968 | 17.96 | 63 | 15.00 | >1H | 0.46 | | |
| 8,683 | 69.27 | 364 | 46.74 | >1H | 4.07 | | |
| 88, 885 | 294.23 | 4,153 | 508.87 | >1H | 43.81 | | |
| 902, 020 | 2,611.48 | 50,341 | 7,212.19 | >1H | 563.02 | | |
| 8, 991, 417 | 25,666.14 | 672,273 | 922,590.00 | >1H | 8,202.93 | | |
| 89, 146, 891 | 396,523.88 | >1H | >1H | >1H | 91,834.20 | | |
| | Matched subraphs $(m_V(G_o) + m_E(G_o))$ 3 58 968 8,683 88,885 902,020 8,991,417 | Matched subraphs $(m_V(G_o) + m_E(G_o))$ SQL Dialect (PostgreSQL)32.10589.6896817.968,68369.2788,885294.23902,0202,611.488,991,41725,666.14 | Matched subraphs $(m_V(G_o) + m_E(G_o))$ SQL Dialect (PostgreSQL)SPARQL (Virtuoso)32.1011589.686396817.96638,68369.2736488,885294.234,153902,0202,611.4850,3418,991,41725,666.14672,273 | Matched subraphs $(m_V(G_o) + m_E(G_o))$ SQL Dialect (PostgreSQL)SPARQL (Virtuoso)AQL (ArangoDB)32.10113.89589.686312.3496817.966315.008,68369.2736446.7488,885294.234,153508.87902,0202,611.4850,3417,212.198,991,41725,666.14672,273922,590.00 | Matched subraphs $(m_V(G_o) + m_E(G_o))$ SQL Dialect (PostgreSQL)SPARQL (Virtuoso)AQL (ArangoDB)Cypher (Neo4J – Java)32.10113.89681.40589.686312.341,943.9896817.966315.00>1H8,68369.2736446.74>1H88,885294.234,153508.87>1H902,0202,611.4850,3417,212.19>1H8,991,41725,666.14672,273922,590.00>1H | | |

(b) Graph Nesting Time. Each data management system is grouped by its graph query language implementation. This table clearly shows that the definition of our query plan clearly outperforms the default query plan implemented over those different graph query languages and databases.

an edge primary key and the remaining elements are the gMark representations. Given that Virtuoso is transactionless, it performed better at serializing and index data for very small data sets (from 10 to 10³) while, afterwards, the triple indexing time takes over on the overall performances. On the other hand, ArangoDB has not a relational data representation, and it just serializes the data as JSON objects to which several indices are associated. Given that the only data used to serialize data into ArangoDB are the edges' labels, all the time required to store the data is the indexing time. On the other hand, the Neo4J serialization proves to be inefficient, both because there are no constraints for data duplication and we must always check if the to-be-inserted vertex already exists, and because Lucene invertex indices are more useful to index full text documents than indexing graph data. Finally, our nested graph data structure creates adjacency lists directly when serializing the data, while primary indices are only serialized for granting other possible data accesses, even though they are not directly used by the THoSP algorithm. Please also note that no external primary index will be used during the THoSP query evaluation, given that only the adjacency lists information is required to join the edges in a two hop distance scenario.

Let us now consider the graph nesting time (Table 1b): albeit no specific triplet or key are associated to the stored graph, PostgreSQL appears to be more performant than Virtuoso in performing graph queries. Please also note that the Virtuoso query engine rewrites

the SPARQL query into SQL and, hereby, two SQL queries were performed in both cases. Since both data were represented in a similar way in secondary memory, the completely different performance between the two databases must be attributed to an inefficient rewriting of the SPARQL query into SQL. In particular, the nested representation using ISON array for PostgreSOL proved to be more efficient than returning a full RDF graph represented as triplets, thus arguing in favour of document stores. The PostgreSQL's efficiency is attributable to the run-time indexing time of the relational tables, that is shared with ArangoDB, where the indices are created ad loading time instead: in both cases a single join operation is performed, plus some (either runtime or stored) index access time. Both PostgreSQL and ArangoDB use GROUP BY-s to create collections of nested values, separately for both vertices and edges. As observed in the previous paragraph, no primary index is used while performing the THoSP query, and adjacency graphs are returned using the same data structure used for graph joins: one single vertex is returned alongside the set of outgoing edges. Moreover, the nesting result is not created by using GROUP BY-s, but by sparsely creating an index that associates the container to its content: as a result, our query plan does not generate an additional cost for sorting and collecting all the elements because it is provided during the graph traversal phase. Thus, the choice of representing the nesting information as a separate index proves to be particularly efficient.

6 CONCLUSIONS

This paper introduces an algorithm for graph nesting jointly with graph traversal queries. Moreover, a class of graph traversal queries that can be optimized is identified, among which a graph algorithm (THoSP) is proposed whenever the nesting vertices are generated by two graph vertices appearing at most at two steps within the original graph operand. By comparing the execution of our algorithm with our graph data structures, we also know that our choice of providing the containment as an external index provides better performances, thus avoiding an additional data grouping phase. Moreover, this algorithm shows that the definition of a separate index for providing the algorithmic result of graph nesting is beneficial, because it allows to return the nested graph as a simple graph having additional nesting informations. This solution was possible due to the assumptions of our proposed graph data model, where it is showed that it is possible to refer any time to the elements that are going to be created later on within the computation, by simply deterministically knowing which the id belonging to the element that is going to be created. Therefore, this paper proves that the representation of nested graph may lead to the solution of current graph querying problems in a tractable way. Nevertheless, we believe that further studies will have to be done on the class of GROQ problems, thus extending our work on THoSP.

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A QUERY BENCHMARKS

Listing 1: Graph Nesting in PostgreSQL's SQL dialect. Two distinct tables are created for both vertices and edges.

```
-- Nesting Vertices

SELECT distinct T.sourceId as src,
array_agg(distinct T.dst) as papers

FROM edges-i as T
GROUP BY T.sourceId;

-- Nesting Edges

SELECT distinct T.sourceId as src,
T1.sourceId as dst,
array_agg(distinct T1.targetId) as papers

FROM edges-i as T, edges-i as T1
WHERE T.targetId = T1.targetId

AND T.sourceId <> T1.sourceId
GROUP BY T.sourceId, T1.sourceId;
```

Listing 2: Graph Nesting in SPARQL. We use properties to associate to either vertices and edges the nesting content.

```
CONSTRUCT {
 ?autha ?newedge ?authb.
 ?newedge <http://cnt.io/nesting> ?paper1.
 ?authc <http://my.grph/edge> ?paper2.
} WHERE {
 {
  GRAPH <http://my.grph/g/i/> {
   ?autha <http://my.grph/g/edge> ?paper1.
   ?authb <http://my.grph/g/edge> ?paper1.
  }
  FILTER(?autha != ?authb).
  BIND(URI(CONCAT("http://my.grph/g/newedge/",

    STRAFTER(STR(?autha), "http://my.grph/g/

   id/"),"-",STRAFTER(STR(?authb),"http://

    my.grph/g/id/"))) AS ?newedge).
  } UNION {
   GRAPH <http://my.grph/g/i/> {
    ?authc <http://my.grph/g/edge> ?paper2.
   }
   OPTIONAL {
    ?authd <http://my.grph/g/edge> ?paper2.
```

```
FILTER (?authd != ?authc)
}
FILTER(!bound(?authd))
}
```

Listing 3: Graph Nesting in ArangoDB using AQL. All the fields marked with an underscore represent externally indexed structures.

```
-- Nesting vertices
FOR b IN authorOf
COLLECT au = b._from INTO groups = [b._to]
RETURN {"author" : au, "papers": groups }

-- Nesting edges
FOR x IN authorOf
FOR y IN authorOf
FILTER x._to==y._to && x._from!=y._from
COLLECT src = x._from, dst = y._from
INTO groups = [ x._to ]
RETURN {"src": src, "dst": dst,
"contain": groups}
```

Listing 4: Graph Nesting in Neo4J using Cypher as a Query Language. Please note that, even in this case, is it not possible to return one single nested graph immediately, and hence the nested vertices must be created before creating the nested edges.