Compact Neighborhood Index for Subgraph Queries in Massive Graphs

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Abstract
Subgraph queries also known as subgraph isomorphism search is a fundamental problem in querying graph-like structured data. It consists to enumerate the subgraphs of a data graph that match a query graph. This problem arises in many real-world applications related to query processing or pattern recognition such as computer vision, social network analysis, bioinformatic and big data analytic. Subgraph isomorphism search knows a lot of investigations and solutions mainly because of its importance and use but also because of its NP-completeness. Existing solutions use filtering mechanisms and optimise the order within witch the query vertices are matched on the data vertices to obtain acceptable processing times. However, existing approaches are iterative and generate several intermediate results. They also require that the data graph is loaded in main memory and consequently are not adapted to large graphs that do not fit into memory or are accessed by streams. To tackle this problem, we propose a new approach based on concepts widely different from existing works. Our approach distills the semantic and topological information that surround a vertex into a simple integer. This simple vertex encoding that can be computed and updated incrementally reduces considerably intermediate results and avoid to load the entire data graph into main memory. We evaluate our approach on several real-word datasets. The experimental results show that our approach is efficient and scalable.

1 Introduction

Graphs are not a new paradigm for data representation and modeling. Their use in these domains dates back to the birth of computer databases with, for example, the work of Bachman on the Network database model [1]. However, the advent of applications related to nowadays connected world with social networks, online crime detection, genome and scientific databases, etc., has brought graphs to greater prominence. This is due mainly to their adaptability to represent the linked aspect of nowadays data but also to their flexibility and scalability when dealing with the main challenge of these kind of applications : Massive data. In this context, subgraph isomorphism search is a fundamental task on which are based search and querying algorithms. Subgraph isomorphism search, also known as exact subgraph matching or subgraph queries, is the problem of enumerating all the occurrences of a query graph within a larger graph called the data graph (cf. Figure 1). Subgraph isomorphism search is an NP-complete problem that knows extensive investigations and solutions mainly because of its importance and use, but also because known solutions are memory and space expensive and consequently do not scale well [14, 5, 18]. Most existing solutions are extensions of the well known Ullmann’s algorithm [19]. These solutions are based on exploring a search space in the form of a recursion tree that maps the query vertices to the data graph’s vertices. However, parsing the recursion tree is exponential in function of the number of vertices in the involved graphs. So, existing solutions never construct entirely the recursion tree and use pruning methods to have smaller search spaces. The most referenced methods such as Ullmann’s algorithm [19], VF2 [4], QuickSI [17], GraphQL [11], GADDI [20], SPath [21], TurboISO [9] and CFL-match [2] have different approaches to tackle this problem. These solutions are surveyed in several papers [12, 14, 5, 18] that analyse and compare them. These comparative studies agree on the fact that there is not a method that outperforms the others for all kind of queries and all graph classes. It seems that the exiting solutions are complementary. This motivated the authors of [12] to propose a framework that allows to run several algorithms on parallel threads on the same query.

In this work, we analyse existing algorithms in regard of the cost of their filtering task and how this task is positioned in respect to the whole matching process. To our knowledge, this issue has not been investigated before. In fact, existing algorithms are generally built around two main tasks: filtering and searching. Filtering is fundamental as it reduces the search space explored by the searching task. Existing algorithms differ by the pruning power of the filtering mechanisms they implement but also by when these filters take place with respect to searching. Our analysis of these two points of difference highlighted four weaknesses in the state of the art algorithms that we address within the proposed framework.
Weakness 1: High filtering cost. The main pruning mechanism used by existing methods during filtering are the features of the $k$-neighborhood of query vertices. This is the amount of information used when matching a query vertex with data vertices. The more information is used, i.e., $k$ is big, the more the pruning of the search space can be important. However, representing compactly the $k$-neighborhood for practical comparisons is a challenging issue. In fact, the representation of this information has a direct impact on its cost which increases with the value of $k$. Besides filtering with the vertex label and the vertex degree, the lightest $k$-neighborhood filter is to consider the features of the one-hop neighborhood, i.e., $k = 1$. For this, recent approaches such as TurboIso [9] and CFL-Mactch [2] use the Neighborhood Label Frequency (NLF) filter [23]. NLF ensures that a data vertex $v$ is a candidate for a query vertex $u$ only if the neighborhood of $v$ includes the neighborhood of $u$ (see lines 5-9 of Algorithm 1).

Algorithm 1: NLF and MND filters.

Data: A potential candidate vertex $v$ for a query vertex $u$

Result: TRUE if $v$ is candidate for $u$ and FALSE otherwise

1 begin
2 if $mnd_G(v) < mnd_Q(u)$ then
3 return (FALSE);
4 end
5 foreach label $l \in \ell(N(u))$ do
6 if $|\{w \in N(v) | \ell(w) = l \}| < |\{w \in N(u) | \ell(w) = l \}|$ then
7 return (FALSE);
8 end
9 end
10 return (TRUE);
11 end

However, NLF is expensive: it is $O(|V(Q)||V(G)|\ell(Q))$ where $|V(Q)|$ is the number of vertices of the query, $|V(G)|$ is the number of vertices in the data graph and $\ell(Q)$ is the set of unique labels of the query graph which is $O(|V(Q)|)$ in the worst case. So, to avoid applying NLF systematically on each vertex, CFL-match [2] proposes the Maximum Neighbor-Degree (MND) filter, which can be verified in constant time for each candidate data vertex. The maximum neighbor-degree of a vertex $u$ in a graph $G$, denoted $mnd_G(u)$, is the maximum degree of all its neighbors [2]. A data vertex $v$ is not a candidate for a query vertex $u$ if $mnd_G(v) < mnd_Q(u)$. As MND is not as powerful as NLF, the idea is to apply it before applying NLF as detailed in Algorithm 1 (see lines 2-3). However, MND is not always effective as we can see in the example depicted in Figure 2 where only 3 vertices are pruned with the MND filter and consequently NLF must be applied for each of the remaining vertices.

It is also worth noting that for some neighborhood configurations filtering is useless and only the searching step is decisive. Let consider the query and data graphs depicted in Figure 3 where all the vertices have the same label and the same degree and let consider that $k = 1000$. Clearly, in this case, the 1000 comparisons required by NLF...
Figure 2: MND Filter on on the Running Example (pruned of the vertices that do not match query labels).

Figure 3: Needless NLF filtering

for each query vertex and each data vertex are needless. This doesn’t mean that filtering is not necessary but that its cost must be reduced. Interestingly, using a less costly filtering with Ullmann’s native subgraph searching subroutine outperforms the state of the art algorithms as showed by our experiments.

Weakness 2: Global filtering Vs local filtering. Depending on its scope, filtering can be characterised as global or local. Local filtering designates the filtering methods that reduce the number of data vertices candidates for a given query vertex, i.e., reduce the size of $C(u_i)$, $i = 1, |V_Q|$, where $C(u_i)$ is the set of vertices of the data graph that are candidates for the query vertex $u_i$. Global filtering designates the filtering methods that can be applied on the entire search space, obtained by joining the above sets, i.e., $C(u_1) \times C(u_2) \times \cdots \times C(u_{|V_Q|})$. Our study of existing algorithms shows that local pruning is predominant. Some mechanisms allow global pruning but they require extra passes of the data graph to be effective. The matching order is such a mechanism. However, it is a very difficult problem to choose a robust matching order mainly because the number of all possible matching orders is exponential in the number of vertices. So, it is expensive to enumerate all of them. For example, TurboIso relies on vertex ordering for pruning. However, to compute this order, it needs to compute for each query vertex a selectivity criteria based on the frequency of its label in the data graph.

To deal with this problem, we introduce the Iterative Local Global Filtering mechanism (ILGF), a simple way to achieve global pruning relying on local pruning filters.

Weakness 3: Late filtering. Our analysis of how filtering and searching are undertaken with respect to each other in the state of the art algorithms revealed that most algorithms apply their filtering mechanisms during subgraph search. In fact, little filtering, reduced mainly to label or degree filtering, is undertaken prior to subgraph search. This means that, the first cartesian products involved by subgraph search are costly. To tackle this, CFL-match [2] applies the MND-NLF filter prior to subgraph search. However, as we can see in Figure 4 the amount of achieved pruning depends on the order within which vertices are parsed. In our example, if $v_2$ is processed before $v_{16}$ the amount of pruning is less than the one obtained with the reverse order. To get caught up, existing solutions rely on additional mechanisms and data structures during subgraph search such as NEC tree in TurboIso [9] and CPI in CFL-mach [2] that both use path-based ordering during subgraph search. However, the underlying data structures are time and space exponential [2]. To avoid constructing and maintaining such data structures, we propose to achieve filtering solely prior to subgraph search. Our experiments show that this approach is as efficient as the state of the art algorithms.
**Weakness 4: lack of scalability.** This drawback results directly from the three above weaknesses. In fact, the lack of global filtering and the necessity to keep the data graph into memory for several passes make these backtracking-based solutions not suitable for graphs that do not fit into main memory. We aim to achieve a single parse of the data graph and reduce as early as possible the search space.

So, our contributions are:

- We propose a novel encoding of vertices, called Compact Neighborhood Index (CNI) that distills all the information around a vertex in a single integer leading to a simple but extremely efficient filtering scheme for processing subgraph isomorphism search. The whole filtering process is based on integer comparisons. CNIs are also easily updatable during filtering.

- We propose an Iterative Local Global filtering algorithm (ILGF) that relies on the characteristics of CNIs to ensure a global pruning of the search space before subgraph search.

- Our encoding mechanism has the advantage to adapt to all graph access models: main memory, external memory and streams. By performing one sequential pass of the disk file (or the stream of edges) of the input graph. This avoids expensive random disk accesses if the graph does not fit into main memory.

- We conduct extensive experiments using synthetic and real datasets in different application domains to attest the effectiveness and efficiency of the proposed scheme.

The rest of this paper is organized as follows. Section 2 first formalizes the problem of subgraph isomorphism search and defines the notations used throughout the paper, then, it discusses related work to motivate our contribution. In Section 3, we introduce our main contribution: the compact neighborhood index and how it is used to solve subgraph isomorphism search. Section 4 presents a comprehensive experimental study on several datasets. Section 5 concludes the paper.

## 2 Background

### 2.1 Problem Definition

We use a data graph to represent objects and their relationships using vertices and edges. More formally, A data graph \( G \) is a 3-tuple \( G = (V(G), E(G), \ell, \Sigma) \), where \( V(G) \) is a set of vertices (also called nodes), \( E(G) \subseteq V(G) \times V(G) \) is a set of edges connecting the vertices, \( \ell : V(G) \cup E(G) \to \Sigma \) is a labeling function on the vertices and the edges where \( \Sigma \) is the set of labels that can appear on the vertices and/or the edges. We use \( |V(G)| \) and \( |E(G)| \) to represent respectively the number of vertices and the number of edges in \( G \).

An undirected edge between vertices \( u \) and \( v \) is denoted indifferently by \((u, v)\) or \((v, u)\). A neighbor of a vertex \( v \) is a vertex adjacent to \( v \). The degree of a vertex \( v \), denoted \( \deg(v) \), is the number of its neighbors. We also use \( \deg_S(v) \) to denote the numbers of neighbors of \( v \) that have a label in the set \( S \). We use \( N(u) \) to represent the neighbors of vertex \( u \). \( \ell_G(u) \) (or simply \( \ell(u) \) when there is no ambiguity) represents the label of vertex \( u \) in \( G \) and \( \ell(u, v) \) is the label of the edge \((u, v)\) in \( G \).

A graph that is contained in another graph is called a subgraph and can be defined as follows:

**Definition 1.** A graph \( G_1 = (V(G_1), E(G_1), \ell_1, \Sigma) \) is a subgraph of a graph \( G_2 = (V(G_2), E(G_2), \ell_2, \Sigma) \) if \( V(G_1) \subseteq V(G_2) \), \( E(G_1) \subseteq E(G_2) \), \( \ell_1(x) = \ell_2(x) \forall x \in V(G_1) \), and \( \ell_1(e) = \ell_2(e) \forall e \in E(G_1) \).
Definition 2. A graph \( Q = (V(Q), E(Q), \ell, \Sigma) \) is subgraph isomorphic to a graph \( G = (V(G), E(G), \ell, \Sigma) \) if and only if there exists an injective mapping \( h \) from \( V(Q) \) to \( V(G) \) such that:

1. \( \forall x \in V(Q) : \ell(x) = \ell(h(x)) \)
2. \( \forall (x, y) \in E(Q) : (h(x), h(y)) \in E(G) \)

For presentation convenience, we focus on non-directed, simple, labeled graphs (graphs with no loops nor multiple edges) but our results can be straightforwardly extended to deal with directed graphs or non simple graphs. For the same reasons, we do not show edge labels on our examples but these labels are considered in our algorithms and datasets. Table 1 summarises our notation.

| Symbol | Description |
|--------|-------------|
| \( G = (V, E, \ell, \Sigma) \) | undirected vertex and edge labeled graph |
| \( \ell \) is a labeling function | |
| \( \Sigma \) is the set of labels | |
| \( V(G) \) | vertex set of the graph \( G \) |
| \( E(G) \) | edge set of the graph \( G \) |
| \( \deg(v) \) | degree of vertex \( v \) in \( G \) |
| \( \deg_S(v) \) | number of neighbors of \( v \) that have a label in \( S \) |
| \( G[X] \) | the subgraph of \( G \) induced by the set of vertices \( X \) |
| \( \mathcal{L}(Q) \) | the set of unique labels in the query \( Q \) |
| \( cni(v) \) | compact neighborhood index of \( v \) |

2.2 Related Work

Many algorithms are proposed to solve the subgraph isomorphism search problem. We can cite without being exhaustive Ullmann’s algorithm [19], VF2 [4], QuickSI [17], GraphQL [11], GADDI [20], SPath [21], TurboISO [9] and CFL-match [2]. One can find in [14] and [12] useful studies that survey and compare most of these methods on several aspects of query processing. These surveys mainly show that none of existing methods is adapted for all kind of queries and graphs and that existing algorithms are somewhat complementary. So, in this section, we review the existing solutions on other facets that outline and justify our contributions. Existing algorithms for subgraph isomorphism search are built onto two basic tasks: Filtering and Searching. Filtering is an important step and determines the efficiency of the algorithm. The searching step is generally based on the Ullmann’s backtracking subroutine [19] that searches in a depth-first manner for matchings between the query graph and the data graph obtained by the filtering step. So, the aim of the filtering step is to reduce the search space on which the searching step operates. Filtering mechanisms can be classified into two categories depending on their scope: local or global.

- Global pruning: as global pruning mechanisms, we can cite vertex ordering and query rewriting. Vertex ordering is the selection of an order within which the vertices of the query are handled. In fact, this order has a direct incidence on the size of the search space as demonstrated by several examples [14]. Query rewriting consists in representing the query in a form that simplifies its matching. Ullmann’s algorithm and SPath do not define any global pruning mechanism and picks the query vertices in a random manner. VF2 and GADDI handle a query vertex only if it is connected to an already matched vertex. However, GADDI uses an additional mechanism: a distance based on the number of frequent substructures between the \( k \)-neighborhoods of two vertices as a mean to prune globally the search space after each established mappings between a query vertex and a data vertex. QuickSI rewrites the query in the form of a tree: a spanning tree of the query. Edges and vertices of the query are weighted by the frequency of their occurrence in the data graph. Based on these weights, a minimum spanning tree is constructed and used to search the data graph. GraphQL selects the vertex that minimises the cost of the ongoing join operation. The cost of a join is estimated by the size of the product of the involved sets of vertices. TurboISO uses the ordering introduced in [22]. This ordering uses the popularity of query vertices in the data graph. Every query vertex \( u \) is ranked by \( \text{rank}(u) = \frac{\text{freq}(G, \ell(u))}{\deg(u)} \) where \( \text{freq}(G, l) \) is the number of data vertices in \( G \) that have label \( l \). This ranking function favors lower frequencies...
and higher degrees which will minimize the number of candidate vertices in the data graph. Furthermore, TurboISO rewrites the query within a tree using this ranking as in QuickSI but TurboISO aggregates the vertices that have the same labels and the same neighbors into a single vertex. This aggregation has been extended to data graphs in [16]. A similar, but more general, compressing-based approach, called SumISO uses modular decomposition of graphs [6] to aggregate vertices that have the same neighborhood into supernodes and undertakes subgraph search on the compressed graphs. More recently, the authors of [2] claim that spanning trees are not the best solutions to represent queries. They show that the edges not included in the spanning tree may have an important pruning power. So, they propose to enhance the tree representation by partitioning the query graph into a core and a forest.

- Local pruning consists mainly in reducing the number of mappings available for each query vertex. In fact, the final search space is the result of joining the sets of available mappings of each query vertex. Thus, given a query graph \( Q = (V(Q), E(Q), \ell, \Sigma) \) and a data graph \( G = (V(G), E(G), \ell, \Sigma) \), the aim is to reduce as much as possible the sets \( C(u_i), i = 1, |V_Q| \), where \( C(u_i) \) is the set of vertices of the data graph that match the query vertex \( u_i \). The final search space is obtained by joining these sets, i.e., \( C(u_1) \times C(u_2) \times \cdots \times C(u_{|V_Q|}) \) [11]. The reduction of \( C(u) \) is generally achieved using the neighborhood information of \( u \). The amount of the obtained pruning depends on the scope of the considered neighborhood. The simplest solution considers the one-hop neighborhood such as the degree of the vertex and/or the labels of the neighbors. Neighborhood at \( k \)-hops is also used in some methods. Ullmann’s Algorithm refines \( C_u \) by removing the vertices that have a smaller degree than \( u \). GraphQL also uses the direct neighborhood by encoding within a sequence the labels of the neighbors of each vertex. Furthermore, GraphQL uses an approximation algorithm proposed in [11] to further reduce the search space by discarding the data vertices that are not compatible with the query vertex using the \( k \)-neighborhood around \( u \). VF2 looks to 2-hops neighborhood. SPath uses the \( k \)-neighborhood by maintaining for each vertex \( u \) a structure that contains the labels of all vertices that are at a distance less or equal than \( k \) from \( u \). SPath uses its encoding of the \( k \)-neighborhood to remove the data vertices that have a \( k \)-neighborhood that does not englobe any \( k \)-neighborhood of query vertices. By rewriting, the query within a tree, QuickSI and TurboISO use also the \( k \)-neighborhood with the particularity that the neighborhood is rooted at a more pruning vertex. The tree representation of TurboISO is also more compact as it aggregates similar vertices.

From the above discussion of existing methods, one can see that the main concern is reducing the search space. The pillar of such quest is the amount of semantic and topological information we maintain for each vertex and how this information is encoded. The more information we use the more pruning we achieve. However, the encoding of this information has a direct impact of its usefulness in pruning. Moreover, existing methods use static encoding of the vertex neighborhood in that it is not updatable after a local pruning. In this paper, we focus on simplifying the encoding of the \( k \)-neighborhood so that : (1) to reduce its cost for filtering and (2) to be able to simply update it after each local pruning to ensure a global pruning of the search space as early as possible without the need of complex data structures.

### 3 A Novel Approach

In this paper, we propose a novel approach to subgraph isomorphism search that aims to reduce the cost of the filtering step. The approach is also adapted for all access methods and especially for big graphs that are accessed within a stream or in external memory. The main task of the proposed framework is a filtering step that relies on integer comparisons. This step is followed by Ullmann’s matching subroutine. The efficiency of the filtering step relies on a novel method to encode a vertex. This encoding distills all the neighboring information that characterise a vertex into a single integer. Unlike existing methods that statically and invariably encode neighboring information, our vertex encoding integer can be dynamically updated leading to an iterative filtering process that allows a global pruning of the search space without additional data structures.

In the following, we first describe this encoding method, called Compact Neighborhood Index, then, we describe the filtering and matching steps of our subgraph matching framework.

#### 3.1 Compact Neighborhood Index (CNI)

In our method the high-level idea is to put into a simple integer the neighborhood information that characterise a vertex. Matching two vertices is then a simple comparison between integers. Given a vertex \( u \), the compact neighborhood index of \( u \), denoted \( cni(u) \), distills the whole structure that surrounds the vertex into a single integer. It is the result of a bijective function that is applied on the vertex’s neighborhood information. This function ensures that two given vertices \( u \) and \( v \) will never have the same compact neighborhood index if they have the same
number of neighbors and the same label unless they are isomorphic at one-hop. Let \( x_1, x_2, x_3, \ldots, x_k \) be the list of \( u \)'s neighbors' labels. The compact neighborhood index of \( u \) in the graph \( G \) is given by:

\[
cni(u) = h(1, x_1) + h(2,x_1 + x_2) + \cdots + h(k,x_1 + x_2 + x_3 + \cdots + x_k).
\]

So, \( cni(u) = \sum_{j=1}^{k} h(j,x_1 + \ldots + x_j) \) where

\[
h(q,p) = \binom{q + p - 1}{q} = \frac{(q + p - 1)!}{q!(p-1)!}.
\]

Theorem 1 states that \( cni(u) \) is a bijection. Its proof is provided in Appendix A.

**Theorem 1.** \( \forall (x_1, x_2, x_3, \ldots, x_k) \in \mathbb{N}^k \) and \( k > 0 \), \( g_k \) is a bijective function from \( \mathbb{N}^k \) in \( \mathbb{N} \), where:

\[
g_k(x_1, x_2, x_3, \ldots, x_k) = \sum_{j=1}^{k} h(j,x_1 + \ldots + x_j)
\]

and

\[
h(q,p) = \binom{q + p - 1}{q} = \frac{(q + p - 1)!}{q!(p-1)!}.
\]

To use this bijection on vertices' labels, we need to assign a unique integer to each vertex label. This assignment can be simply achieved by numbering labels parting from 1 or by using an associative array to store the query labels. We use \( ord(\ell(u)) \) to retrieve the integer associated to the label of vertex \( u \). \( ord(\ell(u)) \) will return 0 if vertex \( u \) has a label that does not belong to \( \mathcal{L}(Q) \). This will systematically prune the neighbors that do not verify the label filter and avoid to consider them in the computation of the CNI of a vertex. Figure 5 illustrates the CNIs for Theorem 1.

**Lemma 1** (Label filter). Given a query \( Q \) and a data graph \( G \), a data vertex \( v \in V(G) \) is not a candidate of \( u \in V(Q) \) if \( \ell(v) \neq \ell(u) \).

**Lemma 2** (Degree filter). Given a query \( Q \) and a data graph \( G \), a data vertex \( v \in V(G) \) is not a candidate of \( u \in V(Q) \) if \( \text{deg}_{\mathcal{L}(Q)}(v) < \text{deg}_{\mathcal{L}(Q)}(u) \).

**Lemma 3** (CNI filter). Given a query \( Q \) and a data graph \( G \), a data vertex \( v \in V(G) \) that verifies the label and degree filters is not a candidate of \( u \in V(Q) \) if \( cni(v) < cni(u) \).

Lemmas 1 and 2 are straightforward. The proof of Lemma 3 is given in Appendix B. We note also that the CNI of a vertex can also be defined to cover the \( k \)-hops neighborhood with \( k > 1 \) as described in Appendix C.

Note that, the CNI filter can be verified in constant time; that is, verifying one candidate vertex \( v \) for a query vertex \( u \) takes \( \mathcal{O}(1) \) time versus \( \mathcal{O}(\mathcal{L}(Q)) \) for NLF.

### 3.2 Iterative Local Global Filtering Algorithm (ILGF)

The aim of the Iterative Local Global Filtering Algorithm (ILGF) is to reduce globally the search space using CNIs. It relies on the fact that \( cni(v) \) can be easily updated after a local filtering giving rise to new filtering opportunities. Algorithm 2 details this iterative filtering process. To verify the CNI filter on a candidate data vertex, the algorithm uses the \( cniMatch() \) subroutine that implements Lemma 3 and consequently allows to verify that a data vertex is a candidate for a given query vertex according to the CNI filter. The ILGF algorithm removes iteratively from \( G \) the vertices that do not match a query vertex using the label, the degree and the CNI filters (see lines 5-7) of the algorithm. Each time a vertex is removed by the filtering process the degree and CNI of its neighbors are updated (lines 8-10) giving rise to new filtering opportunities. Filtering stops when no further vertices are removed. This is implemented by the boolean variable \( \text{stopFilter} \). This iterative filtering leads to an early global filtering of the search space.

Figure 6 illustrates the ILGF algorithm on our example. We can see in these figures that using our three filters we have the following possible mappings between data vertices and query vertices:

- \( u_1 \) has candidates \( v_4 \) and \( v_6 \),
- \( u_2 \) has candidates \( v_8, v_9 \) and \( v_{10} \),
- \( u_3 \) has candidate \( v_{10} \),
- \( u_4 \) has candidates \( v_{11} \), and
Figure 5: CNIs of the Query graph and the Data graph.

Vertices (and the corresponding edges) in dotted lines are not considered in the computation of $\text{deg}_{\mathcal{L}(Q)}(u)$ and $\text{cni}(u)$.

Algorithm 2: ILGF.

Data: A data graph $G$
Result: A filtered version of $G$

begin
    stopFilter ← FALSE;
    cpt ← |$V(G)$|;
    repeat
        foreach vertex $v \in V(G)$ do
            if $\forall u \in V(Q), \text{leniMatch}(v, u)$ then
                remove $v$ from $V(G)$ and the corresponding edges from $E(G)$;
                foreach $x \in N(v)$ do
                    update $\text{cni}(x)$;
                end
            else
                cpt;
            end
        end
        if cpt=0 then
            stopFilter ← TRUE;
        end
    until stopFilter;
    foreach vertex $u \in V(Q)$ do
        $C(u) \leftarrow \{v \in V(G) \text{ such that } \text{cniMatch}(v, u)\}$;
        if $C(u) = \emptyset$ then
            return ($\emptyset$);
        end
    end
    $M \leftarrow \emptyset$;
    SubgraphSearch($M$);
end
Algorithm 3: Function $cniMatch(v, u)$.

**Data:** A data vertex $v$ and a query vertex $u$.

**Result:** returns true if $v$ is a candidate for $u$ according to the label, degree and CNI filters.

\begin{algorithm*}
\begin{algorithmic}[1]
\Function{cniMatch}{v, u}
\State $\text{Data:}$ a data vertex $v$ and a query vertex $u$.
\State $\text{Result:}$ returns true if $v$ is a candidate for $u$ according to the label, degree and CNI filters.
\State \begin{align*}
&\text{return } (\ell(v) = \ell(u) \land \text{deg}_{L(Q)}(v) < \text{deg}_{L(Q)}(u) \land \text{cni}(v) < \text{cni}(u)) \text{ or} \\
&\quad (\ell(v) = \ell(u) \land \text{deg}_{L(Q)}(v) = \text{deg}_{L(Q)}(u) \land \text{cni}(v) = \text{cni}(u))
\end{align*}
\EndFunction
\end{algorithmic}
\end{algorithm*}

Figure 6: Filtering iterations of our running example.

- $u_5$ has candidates $v_2$ and $v_{12}$.

In fact, the first iteration of the ILGF algorithm, finds out that vertices $v_1$, $v_3$, $v_7$, $v_{13}$, $v_{14}$, $v_{15}$, $v_{16}$, $v_{17}$, $v_9$, $v_{20}$ and $v_{21}$ cannot be mapped to any query vertex because:

- $v_7$, $v_{14}$ and $v_{15}$ do not pass the label filter.
- $v_1$, $v_{13}$, $v_{15}$, $v_{16}$, $v_{19}$, $v_{20}$ and $v_{21}$ do not pass the degree filter.
- $v_3$ and $v_5$ do not pass the CNI filter.

After removing these vertices and updating the degree and CNI of their neighbors a new filtering iteration is triggered (see Figure 6 (b)). This second filtering iteration reveals that vertices $v_2$, $v_4$, $v_8$ and $v_{18}$ can also be pruned. In fact, $v_2$ and $v_4$ do not pass the CNI filter and $v_8$ and $v_{18}$ do not pass the degree filter. The final filtered graph is illustrated in Figure 6 (b).

### 3.3 Subgraph Search

After filtering, the data graph contains only the vertices that are candidates for query vertices, i.e., the vertices map at one-hop according to the CNI filter. Subgraph search allows to verify the mapping at k-hops. Algorithm 4 implements this step. It is the depth first search subroutine of Ullmann’s algorithm. It lists the subgraphs of the filtered data graph that are isomorphic to the query by verifying the adjacency relationships. This step allows also to handle edge labels by discarding those that do not match the query labels. The subroutine $\text{neighborCheck()}$ verifies that a mapping $(v, u)$ is added to the current partial embedding $M$ only if $v$ and $u$ have neighbors that also map.

### 3.4 Extension to Larger Graphs

For large data graphs, we aim to keep in memory as few vertices and edges as the three filters can achieve. So, filtering begins while reading the data graph. For this, we compute vertex degrees and CNIs incrementally during graph parsing. Only a single pass of the graph is needed. This is important if we deal with a graph stream or a sequential read of a graph from disk, i.e., a graph that does not fit into main memory and that is loaded part by
Algorithm 4: SubgraphSearch.

Data: a partial embedding \( M \).
Result: All embeddings of \( Q \) in \( G \).

\[
\begin{align*}
1 & \text{begin} \\
2 & \quad \text{if } |M| = |V(Q)| \text{ then} \\
3 & \quad \quad \text{Report } M; \\
4 & \quad \text{end} \\
5 & \quad \text{Choose a non matched vertex } u \text{ from } V(Q); \\
6 & \quad C(u) \leftarrow \{ \text{ non matched } v \in V(G) \text{ such that } \text{cniMatch}(v, u) \}; \\
7 & \quad \text{foreach } v \in C(u) \text{ do} \\
8 & \quad \quad \text{if } \text{neighborCheck}(u, v, M) \text{ then} \\
9 & \quad \quad \quad M \leftarrow M \cup \{(u, v)\}; \\
10 & \quad \quad \quad \text{SubgraphMatch}(M); \\
11 & \quad \quad \quad \text{Remove } (u, v) \text{ from } M ; \\
12 & \quad \quad \text{end} \\
13 & \quad \text{end} \\
14 & \text{end}
\end{align*}
\]

Algorithm 5: Function \text{neighborCheck}(u, v, M).

Data: a partial embedding \( M \), a query vertex \( u \) and a data vertex \( v \).
Result: returns true if \( u \) and \( v \) have neighbors that match.

\[
\begin{align*}
1 & \text{begin} \\
2 & \quad \text{return } \forall (u', v') \in M, ((u, u') \in E(Q) \rightarrow (v, v') \in E(G) \land \ell((u, u')) = \ell((v, v'))) \\
3 & \text{end}
\end{align*}
\]

We keep in memory only the vertices (and the corresponding edges) that verify the label, degree and CNI filters. These are the vertices and edges that will be used during subgraph search. As we parse the data graph, the label filter is straightforward. However, the degree and the CNI can be used when their values, computed incrementally, are sufficient for pruning. However, this depends on how the stream of edges arrives. If edges are sorted, i.e., we access all the edges involving vertex \( i \), then all the edges involving vertex \( i+1 \) and so on, the amount of pruning will be larger during the parse than in the case edges arrive randomly.

Algorithm 6 presents the filtering actions performed during the data graph reading in the case where edges are sorted. In this case, the three filters can be applied as the edges of a vertex are accessed avoiding to store them. When all the edges incident to the current vertex are available (see lines 14-20), we can compute the CNI of the current data vertex and compare it with the CNIs of the query vertices (see lines 21-25), the vertex and all its edges are pruned. The filtered data graph, denoted \( G_Q \) obtained at the end of the reading-filtering process contains only the data vertices that are candidates to query vertices.

4 Experiments

We evaluate the performance of our algorithm, CNI (for Compact Neighborhood Index), over various types of graphs, sizes of queries, number of labels and their distribution on vertices. We also compare it with three state of the art algorithms, CFL-match [2], TurboISO [9] and SumISO [15], a representative algorithm for compressed based subgraph search approaches developed in [13], [16], and [15]. Note that each of CFL-match, TurboISO and SumISO are compared to the other existing solutions, such as QuickSI and SPath, and showed to be more efficient in [9, 16, 2, 15].

All experiments are performed on an Intel i5 2.40 GHz, 64 bits laptop with 8 GB of RAM running windows 7. Algorithms are implemented in C++. For the state of the art algorithms, we used the binaries provided by the authors.

4.1 Datasets

We use seven datasets of real-world graphs to undertake the experiments. We also used synthetic graphs to evaluate the scalability of the algorithms. These datasets can be classified into three categories:
Algorithm 6: Large Data Graph Filtering.

Data: A Data Graph $G$ (stream of edges).

Result: A filtered data graph $G_Q$.

begin
//processing a stream of sorted edges
$V(G_Q) \leftarrow \emptyset$;
$E(G_Q) \leftarrow \emptyset$;
read edge $(x, y)$;
repeat
$current \leftarrow -1$;
if $x \notin V(G_Q)$ and $\ell(x) \in L(Q)$ then
$V(G_Q) \leftarrow V(G_Q) \cup \{x\}$;
end
if $x \in V(G_Q)$ then
$current \leftarrow x$;
end
while $x = current$
do
if $\ell(y) \in L(Q)$ and $y \notin V(G_Q)$ then
$V(G_Q) \leftarrow V(G_Q) \cup \{y\}$;
$E(G_Q) \leftarrow E(G_Q) \cup \{(x, y)\}$;
end
read edge $(x, y)$;
end
compute $\text{cnii}(current)$;
if $\forall u \in V(Q), \text{cniMatch}(current, u)$ then
remove current from $V(G_Q)$;
remove all the edges of $current$ from $E(G_Q)$;
end
until end of stream;
end
1. Small graphs: these graphs are known datasets used by almost all existing methods in their evaluation process. So, we mainly use them as comparative datasets. The underlying graphs represent protein interaction networks coming from three main organisms: human (HUMAN and HPRD datasets), yeast (YEAST dataset) and fish (DANIO-RERIO dataset). The HUMAN and DANIO-RERIO datasets are available in the RI database of biochemical data[3]. The HPRD and YEAST come from the work of [2] and [7].

- **HUMAN**: This dataset consists of one large graph representing a protein interaction network. This graph has 4,675 vertices and 86,282 edges.
- **HPRD**: This is a graph that contains 37,081 edges and 9,460 vertices. The number of unique labels in the dataset is 307.
- **YEAST**: This graph contains 12,519 edges, 3,112 vertices, and 71 distinct labels.
- **DANIO-RERIO**: This graph contains 51,464 edges and 5,720 vertices. We used it with different number of labels (32, 64, 128 and 512) and distributions of them.

To query the HUMAN, HPRD and YEAST datasets, we use the sets of queries generated in [2]. Each query is a connected subgraph of the data graph obtained using a random walk on the data graph. For HPRD an YEAST, the authors of [2] provide 8 query sets, each containing 100 query graphs of the same size. The 8 query sets are denoted 25s, 25n, 50s, 50n, 100s, 100n, 200s, and 200n, where is and in denote query sets with i vertices and, respectively, average degree \( \leq 3 \) (i.e., sparse) and \( > 3 \) (i.e., non-sparse). For HUMAN which is the smallest graph among the considered datasets, the authors constructed smaller queries denoted 10s, 10n, 15s, 15n, 20s, 20n, 25s, and 25n.

We used the DANIO-RERIO dataset to evaluate the algorithms in function of the number of labels and their distribution on the vertices. So, we used this dataset with 4 different number of unique labels 32, 64, 128, and 512 provided by the RI database [3]. We use 2 distributions of the labels on the vertices: a uniform distribution and a Gaussian distribution (normal distribution). The obtained graphs are denoted 32u, 64u, 128u, 512u, 32g, 64g, 128g and 512g where iu and ig denote a DANIO-RERIO data graph with i distinct labels and respectively a uniform distribution and a normal distribution of labels. For all these graphs, we use two sets of queries sparse queries and non sparse queries with the same number of vertices: 128.

2. Large graphs: In this category, we considered a real graph from the Stanford Large Network Dataset Collection called LiveJournal. It is a graph representing an on-line social network with almost 5 million members and over 68 million friendship relations, i.e., edges. We used 200 distinct labels and 4 sets of queries with 100k, 200k, 400k and 500k ( with \( k = 10^3 \) ) vertices. Each set contains 10 query graphs of the same size.

3. Big Graphs (stream of edges): In this category, we considered two graphs from the Stanford Large Network Dataset Collection. They are Twitter and Friendster.

- Twitter is a snapshot of the twitter microblogging social network that corresponds to the period of June-Dec 2009. The vertices represent users and edges correspond to user-follower relationships.
- Friendster is an on-line social network where edges correspond to friendship relations. It contains more than 65 million vertices and more than 180 billion edges.

These graphs do not fit in the main memory of the computer used for the experiments: Twitter is 7.5 GB and Friendster is 30 GB. We used 200 unique labels with a uniform distribution with Twitter and 512 unique labels for Friendster. For these two graphs, we also constructed 4 sets of queries of 100k, 200k, 400k and 500k ( with \( k = 10^3 \) ) vertices. Each set contains 10 query graphs of the same size. Each query graph is a connected subgraph obtained by a random walk in the data graph. We processed these big graphs as a stream of edges by partitioning each disk file into several sequential files that fit into main memory.

We also constructed 3 synthetic graphs with 5 billion, 20 billion and 70 billion vertices respectively. Edges are added following a power law distribution of the degree according to the characteristics of real big graphs. For each of these graphs, we used 512 labels distributed uniformly on the vertices. We queried these graph with a set of 10 queries of 500k vertices each.

Table 2 summarises the characteristics of the datasets. For each graph, we report the number of vertices, the number of edges, the number of unique labels and the compression rate which is the ratio between the number of edges of the compressed graph on the number of edges of the original graph using modular decomposition of graphs as a compression tool of graphs [2] [8] [13]. Modular decomposition compresses graphs by aggregating vertices that

---

1. http://ferrolab.dmi.unict.it/i/ri.html#description
2. http://snap.stanford.edu/
have the same neighbors into one single vertex. The compression ratio is used to show how well the datasets are compressible and consequently how well they are suitable for a subgraph isomorphism search algorithm such as Turbo1iso, its boost version developed in [16] or Sum1iso [15]. For instance, we can see that the HUMAN dataset is highly compressible, i.e., compression rate of 61%.

| Dataset    | |V| | |E| | Number of labels | Compression rate(%) |
|------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| HUMAN      | 4,675       | 86,282      | 44          | 61          |
| HPRD       | 9,460       | 37,081      | 307         | 25          |
| DANIO-RERIO| 5,720       | 51,464      | 32/64/128/512 | 25          |
| YEAST      | 3,112       | 12,519      | 71          | 43          |
| LIVEJOURNAL| 4,847,571   | 68,993,773  | 200         | 30          |
| TWITTER    | 17,069,982  | 476,553,560 | 200         | -           |
| FRIENDSTER | 65,608,366  | 180,606,731,005 | 512     | -           |

### 4.2 Results

In this subsection, we report and comment the results obtained by comparing our algorithm with the state of the art algorithms CFL-match [2], Turbo1iso [9] and Sum1iso [15], the representative algorithm for compression-based subgraph search approaches developed in [10], [13] and [14]. Our main metric is the time performance by varying \(|V(Q)|\), i.e., the number of vertices in the query, \(|E|\), i.e., the number of unique labels, the sparsity of the queries, the distribution of labels, and \(|V(G)|\), i.e., the number of vertices in the data graph. We present the obtained results according to this metrics and by category of graphs (small, large and big). We note also that all the algorithms output the same sets of isomorphic subgraphs for each query graph.

**Against Existing Algorithms by Varying \(|V(Q)|\) within the small datasets:** Figure 7 shows the average total processing time for each query graph on the HUMAN dataset (subfigure (a)), YEAST dataset (subfigure (b)) and the HPRD dataset (subfigure (c)) for the four algorithms. First of all, it is interesting to see that our results are completely different from those obtained in [2] as none of the algorithms exceed 5 hours of execution on the large queries: 100s, 200s, 100n and 200n. In fact, the experiments undertaken in [2] on the same data graphs and the same set of queries report that Turbo1iso exceeds 5 hours running time on these large queries on almost the all three datasets on an Intel i5 3.20 GHz CPU and 8GB memory. We recall that, we used the binaries provided by the authors and consequently no modifications have been done on these algorithms. According to our results plotted on Figure 7, there is practicably no difference between the four algorithms on the HUMAN data graph whatever is the size of the query and its sparsity. We note that this dataset is highly compressible and is suitable for algorithms such as Turbo1iso and Sum1iso. For YEAST and HPRD, we clearly see that CNI outperforms CFL-match and Sum1iso, which behave almost similarly on all queries, and both perform better than Turbo1iso that obtains the worst time performance. This is due to our new neighborhood encoding that allows an easy global pruning step.

**Against Existing Algorithms by Varying \(|E|\) within the small datasets:** Figure 8 shows the average total processing time for each query graph on the DANIO-RERIO for the four algorithms with various numbers of query labels and also two distributions (uniform and Gaussian) of these labels on vertices. These graphs are queried by 2 sets of queries: sparse and non sparse queries. Each set contains 100 query graphs of the same size (128 vertices). We can see on this Figure that the worst results are obtained by Turbo1iso. This can be explained by the complexity of its data structures when we list all the embeddings [2]. CFL-match and sum1iso have very close results on sparse queries on all the considered label numbers and with the two distributions. However, sum1iso behaves better with non sparse queries mainly because the corresponding graphs are more likely compressible. CNI clearly outperforms the three other algorithms which confirms the importance to reduce filtering cost.

**Against Existing Algorithms by Varying \(|E|\) within the large dataset:** Figure 9 shows the average total processing time for each query graph our large dataset LIVEJOURNAL. The obtained results have the same pattern as the results obtained on small graphs. However, the difference between the four algorithms is less pronounced than with small graphs. This can be explained by the fact that the small graphs are more difficult instances for subgraph isomorphism search with denser graphs.

**Against Existing Algorithms by Varying \(|V(Q)|\) within the big datasets:** It was not possible to use CFL-match, Turbo1iso, and Sum1iso with big graphs. So, the results concern only CNI. Figure 10 shows the total processing time of CNI on the two big graphs. We can mainly see that even with a query graph of 500,000 vertices we cannot perceive any exponential shape which confirms the scalability of the approach. This tendency is also
Figure 7: Time performance on small datasets (varying $|V(Q)|$). Results are in logscale.

(a) HUMAN dataset
(b) YEAST dataset
(c) HPRD dataset

Figure 8: Time performance on the small dataset DANIO-RERIO (varying $|\Sigma|$ and the label distribution).

(a) sparse query
(b) non sparse query

Figure 9: Scalability testing on large graphs (varying $|V(Q)|$).
confirmed when we vary the number of vertices of the data graph on Figure 11. These results definitely settle the scalability of the proposed approach.

5 Conclusions

Subgraph isomorphism search is an NP-complete problem. This means a processing time that grows with the size of the involved graphs. Pruning the search space is the pillar of a scalable subgraph isomorphism search algorithm and has been the main focus of proposed approaches since Ullmann’s first solution. In this paper, we proposed CNI, a simple subgraph isomorphism search algorithm that relies on a compact representation of the neighborhood, called Compact Neighborhood Index (CNI), to perform an early global pruning of the search space. CNI distills topological information of each vertex into an integer. This vertex encoding is easily updatable and can be used to prune globally the search space using an iterative algorithm. Furthermore CNI does not require that the entire data graph is loaded into main memory and can be used with a graph stream. Our extensive experiments validate the efficiency of our approach.

As part of future work, it will be interesting to extend CNI to construct a graph index that allows to handle a graph database. For this issue, we plan to compute a vertex CNI that includes the vertex label: \( cni(u) = \sum_{j=1}^{k} h(j, x_1 + ... + x_j) \) where the label of \( u \) is among the \( x_i \) and then compute a compact neighborhood index for the graph using the same formula as follows: \( cni(G) = \sum_{j=1}^{k} h(j, x_1 + ... + x_j) \) where each \( x_i \) is the CNI of a vertex of \( G \). This resulting graph CNI can be used to index a graph in a database of graphs defined on the same set of labels.

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A Proof of Theorem 1

Proof. We need the following lemmas.

Lemma 4. $p < p' \Rightarrow h(k, p) < h(k, p')$

Proof. By deduction from the property of the binomial coefficient: $\binom{n}{k} = \binom{n-1}{k} + \binom{n-1}{k-1}$ (Pascal Formula)

Lemma 5. $\forall k > 0, g(k, x_1, ..., x_k) < h(k, x_1 + ... + x_k + 1)$

Proof. This inequality is trivial for $k = 1$: $g(1, x_1) = x_1$ and $h(1, x_1 + 1) = x_1 + 1$. Assume that, for $k \geq 1$, the inequality holds and let us prove that it also holds for $k + 1$.

By definition of $g_k$, we have:

$$g_{k+1}(x_1, ..., x_{k+1}) = g_k(x_1, ..., x_k) + h(k + 1, x_1 + ... + x_{k+1})$$

we obtain then:

$$h(k, x_1 + ... + x_{k+1} + 1) + h(k + 1, x_1 + ... + x_{k+1}) = h(k + 1, x_1 + ... + x_k + 1 + 1),$$

where $g_{k+1}(x_1, ..., x_{k+1}) < h(k + 1, x_1 + ... + x_{k+1} + 1)

Lemma 6. $\forall k > 0, If g_k(x_1, ..., x_k) = g_k(x'_1, ..., x'_k) then x_1 + ... + x_k = x'_1 + ... + x'_k$

Proof. Assume that $g_k(x_1, ..., x_k) = g_k(x'_1, ..., x'_k)$. According to Lemma 5, we have:

$$h(k, x_1 + ... + x_k) < g_k(x_1, ..., x_k) = g_k(x'_1, ..., x'_k) < h(k, x_1 + ... + x_k + 1)$$

we obtain then: $h(k, x_1 + ... + x_k) < h(k, x_1 + ... + x_k + 1)$. According to Lemma 4, $h(k, p)$ is strictly increasing. So, the inequality $x_1 + ... + x_k \leq x'_1 + ... + x'_k$ holds. Similarly, we prove the inverse inequality. This proves that

$$x_1 + ... + x_k = x'_1 + ... + x'_k.$$ 

To prove Theorem 1, we first prove that $g_k$ is injective from $\mathbb{N}^k$ to $\mathbb{N}$. It is trivial for $k = 1$. In fact, $g_1 = h(1, x_1) = \binom{x_1}{1} = \frac{x_1!}{(x_1-1)!} = x_1$ is the identity in $\mathbb{N}$. For $k \geq 2$, we assume that $g_{k-1}$ is injective and we prove that $g_k$ is also injective. Let $(x_1, ..., x_k)$ and $(x'_1, ..., x'_k)$ such that $g_k(x_1, ..., x_k) = g_k(x'_1, ..., x'_k)$. According to Lemma 6, $x_1 + ... + x_k = x'_1 + ... + x'_k$. We have also by definition of $g_k$:

$$\begin{cases}
g_k(x_1, ..., x_k) = g_{k-1}(x_1, ..., x_{k-1}) + h(k, x_1 + ... + x_k) \\
g_k(x'_1, ..., x'_k) = g_{k-1}(x'_1, ..., x'_{k-1}) + h(k, x'_1 + ... + x'_k)
\end{cases}$$

By subtracting side by side, we obtain $g_{k-1}(x_1, ..., x_{k-1}) = g_{k-1}(x'_1, ..., x'_{k-1})$ which is our induction hypothesis that gives $(x_1, ..., x_{k-1}) = (x'_1, ..., x'_{k-1})$. This implies that $x_k = x'_k$.

Conclusion: $g_k$ is injective.

To show that $g_k$ is also surjective, we recall that $h(k, x_1 + ... + x_k) \leq g_k(x_1, ..., x_k) < h(k, x_1 + ... + x_k + 1)$. As $p \to h(p, p)$ is a strictly increasing sequence, we deduce that each $n$ in $\mathbb{N}$ have an antecedent in $\mathbb{N}^k$.

So, $g_k$ is a bijection from $\mathbb{N}^k$ to $\mathbb{N}$ which proves Theorem 1.

B Proof Sketch of Lemma 3

We prove the lemma by contradiction. Assume $v$ is a candidate of $u$ with $cni(v) < cni(u)$. That is, there is an embedding $M$ that maps $u$ to $v$. This means that $\ell(v) = \ell(u)$ and $deg(v) \geq deg(u)$ and $\ell(N(u)) \subseteq \ell(N(v))$. Let $deg(u) = k$ and $deg(v) = k + t$, $t \geq 1$. Let $(l_1, l_2, \cdots, l_k)$ be the labels of the neighbors of $u$ according to the order given by function $ord()$. Similarly, let $(l_1, l_2, \cdots, l_k, l_{k+1}, \cdots, l_{k+t})$ be the labels of the neighbors of $v$. By construction of, we have $cni(v) = g_{k+1}(l_1, l_2, \cdots, l_{k+t}) = g_k(l_1, l_2, \cdots, l_k) + h(k + 1, l_1 + \cdots + l_{k+1}) + \cdots + h(k + t, l_1 + \cdots + l_{k+t})$. So, $cni(v) = cni(u) + h(k + 1, l_1 + \cdots + l_{k+1}) + \cdots + h(k + t, l_1 + \cdots + l_{k+t})$. As $t > 0$, we reach a contradiction. Thus, the lemma holds.
The compact neighborhood index can also be computed for the $k$-neighborhood with $k > 1$ and can be extended to cover edge labels. The CNI of vertex $v$ featuring its neighborhood at $k$-hops can be computed using the same formula:
\[
cni_k(v) = \sum_{j=1}^{s} h(j, x_1 + \ldots + x_j) \quad \text{where} \quad h(q, p) = \binom{q+p-1}{q} = \frac{(q+p-1)!}{q!(p-1)!},
\]
s is the number of $k$-hops neighbors of $v$, i.e., number of vertices of $G$ that are reachable from $v$ with exactly $k$-hops in a shortest path from $v$, and $x_1, \ldots, x_s$ are the numeric labels of these vertices. For instance, the CNI at $k = 2$ of the query vertex $u_1$ of our running example (see Figure 1) comprises vertices $u_4$ and $u_5$ and can be computed as: $cni_2(u_1) = h(1, 3) + h(2, 4) = 7$. The CNI at $k$-hops can be used to prune the data vertices that are not candidate for a query vertex but that pass through the $(k - 1)$-hop CNI as follows:

**Lemma 7** ($k$-hop Degree filter). Given a query $Q$ and a data graph $G$, a data vertex $v \in V(G)$ is not a candidate of $u \in V(Q)$ if $\deg^k_{E(Q)}(v) < \deg^k_{E(Q)}(u)$ where $\deg^k_{E(Q)}(u)$ is the number of vertices reachable from $u$ with exactly $k$-hops in a shortest path from $u$ and have a label in $L(Q)$.

**Lemma 8** ($CNI_k$ filter). Given a query $Q$ and a data graph $G$, a data vertex $v \in V(G)$ that verifies the $CNI_k$ filter and the $(k + 1)$-hops Degree filter is not a candidate of $u \in V(Q)$ if $cni_{k+1}(v) < cni_{k+1}(u)$.

Lemma 7 is straightforward. The proof of Lemma 8 is similar to the proof of Lemma 3.

To cover edge labels, a CNI can also be computed for the edges at several hops as for vertices. A CNI for edges can be used as a first filter before testing the compatibility of labels edge by edge.