Capturing Topology in Graph Pattern Matching

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Abstract

Graph pattern matching is often defined in terms of subgraph isomorphism, an NP-complete problem. To lower its complexity, various extensions of graph simulation have been considered instead. These extensions allow pattern matching to be conducted in cubic-time. However, they fall short of capturing the topology of data graphs, *i.e.,* graphs may have a structure drastically different from pattern graphs they match, and the matches found are often too large to understand and analyze. To rectify these problems, this paper proposes a notion of *strong simulation*, a revision of graph simulation, for graph pattern matching. (1) We identify a set of criteria for preserving the topology of graphs matched. We show that strong simulation preserves the topology of data graphs and finds a bounded number of matches. (2) We show that strong simulation retains the same complexity as earlier extensions of simulation, by providing a cubic-time algorithm for computing strong simulation. (3) We present the locality property of strong simulation, which allows us to effectively conduct pattern matching on distributed graphs. (4) We experimentally verify the effectiveness and efficiency of these algorithms, using real-life data and synthetic data.

1. Introduction

Graph pattern matching is being increasingly used in a number of applications, *e.g.,* software plagiarism detection, biology, social networks and intelligence analysis [28, 33, 34, 36]. Given a pattern graph Q and a data graph G, it is to find all subgraphs of G that match Q. Here matching is typically defined in terms of *subgraph isomorphism* (see, *e.g.,* [5, 21] for surveys): a subgraph G_s of G *matches* Q if there exists a *bijective function* f from the nodes of Q to the nodes in G_s such that (1) for each pattern node u in Q, u and $f(u)$ have the same label, and (2) there exists an edge (u, u') in Q if and only if $(f(u), f(u'))$ is an edge in G_s.

However, subgraph isomorphism is a NP-complete problem [35]. Moreover, there are possibly exponential many subgraphs in G that match Q. In addition, as observed in [7, 20], it is often too restrictive to catch sensible matches, as it requires matches to have exactly the same topology as a pattern graph. These hinder its applicability in emerging applications such as social networks and crime detection.

To reduce the complexity, *graph simulation* [30] has been adopted for pattern matching. A graph G matches a pattern Q via *graph simulation* if there exists a binary *relation* $S \subseteq V_Q \times V$, where V_Q and V are the set of nodes in Q and G, respectively, such that (1) for each $(u, v) \in S$, u and v have the same label; and (2) for each node u in Q, there exists v in G such that (a) $(u, v) \in S$, and (b) for each edge (u, u') in Q, there exists an edge (v, v') in G such that $(u', v') \in S$. Graph simulation can be determined in quadratic time [25]. Recently this notion has been extended by mapping edges in Q to (bounded) paths in G [20, 19], with a cubic-time complexity, to identify matches in, *e.g.,* social networks.

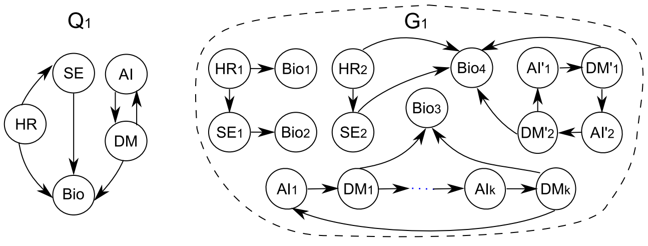


Figure 1: Social matching: query and data graphs

Nevertheless, the low complexity comes with a price: (1) simulation and its extensions [20, 19] do not preserve the topology of data graphs; in other words, they may match a graph G and a pattern Q with drastically different structures. (2) The match relation S is often too large to understand and analyze, as illustrated below.

Example 1: Consider a real-life example taken from [32]. A headhunter wants to find a biologist (Bio) to help a group of software engineers (**SE**s) analyze genetic data. To do this, she uses an expertise recommendation network G_1, as depicted in Fig. 1. In G_1, a node denotes a person labeled with expertise, an edge indicates recommendation, *e.g.,*HR_1 recommends Bio_1, and there is an edge from each DM_i to Bio_3. The biologist Bio needed is specified with a pattern graph Q_1, also shown in Fig. 1. Intuitively, the Bio has to be recommended by: (a) an HR person; (b) an SE, *i.e.,* the Bio has experience working with **SE**s; and (c) a data mining specialist (DM), as data mining techniques are required for the job. Moreover, (d) the SE is also recommended by an HR person, and (e) there is an artificial intelligence expert (AI) who recommends the DM and is recommended by a DM.

When subgraph isomorphism is used, no match can be found, *i.e.,* no subgraph of G_1 is isomorphic to Q_1. In other words, subgraph isomorphism imposes too strict a constraint on the topology of the graphs matched.

When graph simulation or its extensions [20, 19] are adopted, *all* four biologists in G_1 are matches for Bio in Q_1. However, Bio_1 and Bio_2 are recommended by either HR only or by SE only in G_1, and Bio_3 is recommended by neither an HR nor an SE. Hence these are not the ones that the headhunter really wants. Only Bio_4 satisfies all these conditions and makes a good candidate.

This tells us that simulation and its extensions [20, 19] do not preserve the structural properties in graph pattern matching and therefore, may return excessive "matches" that one does not want. Indeed, observe the following.

Topological structure. (a) While Q_1 is a connected graph, G_1 is disconnected, but G_1 matches Q_1 via simulation. (b) Node Bio in Q_1 has three "parents", but it matches nodes Bio_1 and Bio_2 in G_1 that have a single "parent" each. (c) The directed cycle with only two nodes AI and DM in Q_1 matches the long cycle consisting of $\mathsf{AI}_1, \mathsf{DM}_1, \ldots, \mathsf{AI}_k, \mathsf{DM}_k, \mathsf{AI}_1$ in

G_1, and the undirected cycle with nodes HR, SE and Bio in Q_1 matches the tree rooted at HR_1 in G_1.

Match results. The match relation of simulation, when represented as a result graph as suggested in [20], is the entire graph G_1. In general, the result graphs are often large when matching is performed on real-life networks, *e.g.,* LinkedIn [2], which has 19.5M users and yields a graph of 100GB in size. These make it hard to analyze the match results. □

These suggest that we revise the notion of graph simulation to strike a balance between its computational complexity and its ability to capture the topology of graphs. Indeed, graph simulation was proposed for process algebra to mimic steps of a process [30]. To make practical use of it in graph pattern matching, we need to enhance it by incorporating more topological structure of graphs.

Contributions & Roadmap. We introduce a revision of graph simulation that preserves the topology of graphs and has the same complexity as extensions [20, 19] of simulation.

(1) We propose a revision of graph simulation [30] (Section 2), referred to as *strong simulation*, by enforcing two conditions: (a) the duality to preserve the parent relationships and (b) the locality to eliminate excessive matches. For example, matching Q_1 on G_1 of Fig. 1 via strong simulation finds Bio_4 as the only match for Bio in Q_1.

(2) We identify a set of criteria for topology preservation, and show that strong simulation preserves the topology of pattern graphs and data graphs (Section 3). We also prove that the number of matches via strong simulation is linear in the size of the data graph rather than exponential for subgraph isomorphism, and each match has a diameter bounded by the diameter of the pattern graph. Hence strong simulation indeed rectifies the problems of subgraph isomorphism and simulation. Moreover, we show that slight extensions to the notion make graph pattern matching intractable.

(3) We show that strong simulation retains the same complexity as earlier extensions [20, 19] by providing a *cubic*-time computation algorithm (Section 4). We also develop effective optimization techniques, notably a quadratic-time algorithm to minimize strong simulation queries.

In addition, we show that the locality of strong simulation allows us to develop a simple yet effective algorithm to find matches in distributed graphs. To the best of our knowledge, this is among the first distributed algorithms for graph pattern matching, for which the need is evident when processing massive graphs (see *e.g.,* [16, 22, 29]).

(5) Using both real-life data (Amazon and YouTube) and synthetic data, we conduct an extensive experimental study (Section 5). We find that our algorithms for strong simulation scale well with large data graphs (*e.g.,* with 1.5×10^8 nodes). They are able to identify sensible matches that subgraph isomorphism fails to catch, and to eliminate excessive matches of graph simulation that do not make sense. We find 70%-80% matches found by strong simulation are those found by subgraph isomorphism, while only 25%-38% for graph simulation. We also find that our optimization techniques are effective, reducing 1/3 of running time in average.

We contend that strong simulation provides a promising model for graph pattern matching in emerging applications. Indeed, (1) in contrast to subgraph isomorphism, strong simulation is in cubic-time rather than NP-complete, and moreover, due to its locality, it yields a set of matches with cardinality linear in the size of the data graph rather than exponential, where each match is bounded by the diameter of the pattern graph. (2) As opposed to graph simulation, it captures the topology of patterns in its matches, such as parents, connectivity and cycles, by enforcing the duality and locality on matches, while it retains the same complexity as simulation. (3) Unlike simulation, the locality of strong simulation makes it possible to efficiently conduct pattern matching on distributed graphs. (4) As will be seen in Section 3, minor extensions to strong simulation would make graph pattern matching an intractable problem. In other words, strong simulation strikes a balance between the complexity and the capability to capture graph topology.

Due to the space constraint, we defer proofs, distributed matching algorithms and their experimental study to [1].

Related work. There has been a host of work on pattern matching via subgraph isomorphism (*e.g.,* [33, 34, 36]; see [5, 21] for surveys). In light of its intractability, approximate matching has been studied to find inexact solutions, which allows node/edge mismatches [5, 33]. This work differs from approximate matching in that no node/edge mismatches are allowed, and that the number of matches via strong simulation is linear in the size of the data graph rather than exponential for (approximate) subgraph isomorphism.

Closer to this work are bounded simulation [20] and graph pattern queries of [19]. The former extends simulation [30] by allowing bounds on the number of hops in pattern graphs, and the latter further extends [20] by incorporating regular expressions as edge constraints on pattern graphs. Pattern matching via these extensions are in cubic-time [19, 20]. As remarked earlier, these notions of simulation may fail to capture the topology of graphs, and yield false matches or too large a match relation. These are precisely the problems that strong simulation aims to rectify, by imposing additional constraints (duality and locality) on graph simulation.

Schema extraction is to discover the implicit structure of semi-structured data, which has no schema predefined. It has proved effective in query formulation and optimization [3, 23]. Schema of semi-structured data is often extracted via a mild generalization of simulation that deals with labeled edges [3]. Nevertheless, topology preservation is not an issue in schema extraction, and no previous work there has studied how simulation should be refined to capture topology.

Query minimization, as a classical optimization technique, has been well studied for SQL [4], XPath (*e.g.,* [11]), graph simulation [9] and graph pattern queries [19]. This work explores it for pattern matching via strong simulation.

Distributed query processing has been studied for relational data [27] and XML [10, 12]. There has also been recent work on distributed graph processing to manage large-scale graphs [16, 22, 29]. However, to the best of our knowledge, no previous work has studied distributed computation of graph simulation [30] and its extensions[20, 19], not to mention strong simulation proposed in this work.

2. Strong Simulation

In this section, we first present basic notations of graphs. We then introduce the notion of strong simulation.

2.1 Preliminaries

We specify both data graphs and pattern graphs as fol-

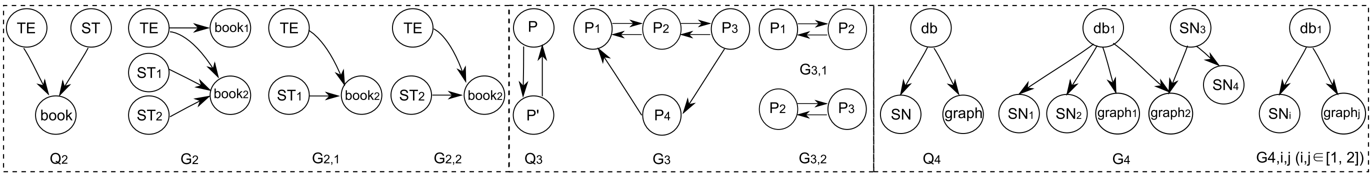


Figure 2: Strong simulation

lows. Let Σ be a (possibly infinite) set of labels.

Graphs. A *node-labeled directed graph* (or simply a *graph*) is defined as $G(V, E, l)$, where (1) V is a finite set of nodes; (2) $E \subseteq V \times V$ is a finite set of edges, in which (u, u') denotes an edge from nodes u to u'; and (3) l is a labeling function that maps each node u in V to a label $l(u)$ in Σ. We denote G as (V, E) when it is clear from the context.

Intuitively, the function $l()$ specifies node attributes, *e.g.,* keywords, blogs, comments, ratings, names, emails, companies [6]; and the label set Σ denotes all such attributes.

We next review some basic notations of graphs.

Subgraphs. Graph $H(V_s, E_s, l_H)$ is a *subgraph* of graph $G(V, E, l_G)$, denoted as $G[V_s, E_s]$, if (1) for each node $u \in V_s$, $u \in V$ and $l_H(u) = l_G(u)$, and (2) for each edge $e \in E_s$, $e \in E$. That is, subgraph $G[V_s, E_s]$ only contains a subset of nodes and a subset of edges of G.

Paths. A *directed* (resp. *undirected*) *path* ρ is a sequence of nodes $v_1, \ldots, v_n$ such that (v_i, v_{i+1}) (resp. either (v_i, v_{i+1}) or (v_{i+1}, v_i)) is an edge in G for $i \in [1, n-1]$. The *length* of ρ is the number of edges in ρ. Abusing notations for trees, we refer to v_{i+1} as a *child* of v_i (or v_i as a *parent* of v_{i+1}).

A *directed* (resp. *undirected*) *cycle* in a graph is a *directed* (resp. *undirected*) path with $v_1 = v_n$, having no repeated nodes other than the start and end nodes v_1 and v_n.

Distance and diameter. Given two nodes u, v in a graph G, the *distance* from u to v, denoted by $\mathsf{dist}(u, v)$, is the length of the shortest *undirected path* from u to v in G.

A graph is *connected* if for each pair of nodes, there exists an undirected path in the graph.

The *diameter* of a connected graph G, denoted by d_G, is the longest shortest distance of all pairs of nodes in G, *i.e.,* $d_G = \mathsf{max}(\mathsf{dis}(\mathsf{u}, \mathsf{v}))$ for all nodes u, v in G.

We assume *w.l.o.g.* that pattern graphs are connected.

2.2 The Definition of Strong Simulation

We define strong simulation by enforcing two conditions on simulation [30]: duality and locality. As will be seen in Sections 3 and 4, these conditions capture the topology of graphs and eliminate excessive matches to a maximum extent, while retaining a low PTIME computational complexity.

Consider a pattern graph $Q(V_q, E_q)$ and a data graph $G(V, E)$. To define strong simulation, we first review the notion of graph simulation [30]. Graph G matches pattern Q via *graph simulation*, denoted by $Q \prec G$, if there exists a binary *match relation* $S \subseteq V_q \times V$ such that (1) for each $(u, v) \in S$, u and v have the same label, *i.e.,* $l_Q(u) = l_G(v)$; and (2) for each node u in V_q, there exists v in V such that (a) $(u, v) \in S$, and (b) for each edge $(u, u') \in E_q$, there exists an edge (v, v') in E such that $(u', v') \in S$.

Intuitively, simulation preserves the labels and the child relationship of a graph pattern in its match. Simulation was proposed for the analyses of programs [30], and studied for schema extraction from semi-structured data [3]. Simulation and its extensions were recently introduced for social networks [7], and for graph pattern matching [20, 19] due to its low PTIME computational complexity [25].

To capture graph topology, we extend simulation by enforcing duality, to preserve the parent relationship as well.

Dual simulation. Pattern graph Q *matches* data graph G via *dual simulation*, denoted by $Q \prec_D G$, if $Q \prec G$ with a binary *match relation* $S \subseteq V_q \times V$, and moreover, for each pair $(u, v) \in S$ and each edge (u_2, u) in E_q, there exists an edge (v_2, v) in E with $(u_2, v_2) \in S$.

Intuitively, dual simulation enhances graph simulation by imposing an additional condition, to preserve both child and parent relationships (downward and upward mappings).

While there may be multiple matches in a graph G for a pattern Q, there exists a unique *maximum* match S_M in G for Q such that for any match S in G for P, $S \subseteq S_M$.

Lemma 1: *For any pattern graph Q and data graph G with $Q \prec_D G$, there is a unique maximum match relation.* □

Locality. To define the locality, we need some notions.

Balls. For a node v in a graph G and a non-negative integer r, the *ball* with *center* v and *radius* r is a subgraph of G, denoted by $\hat{G}[v, r]$, such that (1) for all nodes v' in $\hat{G}[v, r]$, the shortest distance $\mathsf{dist}(v, v') \leq r$, and (2) it has exactly the edges that appear in G over the same node set.

We define the locality by requiring matches to be within a ball of a certain radius. Indeed, as observed in [8], when social distance increases, the closeness of relationships decreases and the relationships may become irrelevant. Hence it often suffices in practice to consider only those matches of a pattern that fall in a small ball. To formalize this, we use the notion of match graphs of a pattern, given as follows.

Match graphs. Consider a relation $S \subseteq V_q \times V$. The *match* graph *w.r.t.* S is a subgraph $G[V_s, E_s]$ of G, in which (1) a node $v \in V_s$ iff it is in S, and (2) an edge $(v, v') \in E_s$ iff there exists an edge (u, u') in Q with $(u, v) \in S$ and $(u', v') \in S$.

We are now ready to define strong simulation.

Strong simulation. Pattern graph Q *matches* data graph G via *strong simulation*, denoted by $Q \prec_D^L G$, if there exist a node v in G and a connected subgraph G_s of G such that (1) $Q \prec_D G_s$, with the maximum match relation S; (2) G_s is exactly the match graph *w.r.t.* S, and (3) G_s is contained in the ball $\hat{G}[v, d_Q]$, where d_Q is the diameter of Q.

We refer to G_s as a *perfect* subgraph of G *w.r.t.* Q.

Intuitively, a match G_s of pattern Q is required to satisfy the following conditions: (1) it preserves both the child and parent relationships of Q (condition 1 above); (2) the nodes and edges needed to match Q are all contained in a ball of a radius decided by the diameter of Q (conditions 2 and 3); this rules out excessively large matches. As will be seen shortly, these conditions are justified for preserving graph topology and retaining low computational complexity.

Example 2: Consider pattern graph Q_1 and data graph G_1 of Fig. 1. Observe the following. (1) No subgraph of G_1 is isomorphic to Q_1. Indeed, there exists no directed cycle in

G_1 that matches the direct cycle $\mathsf{DM}, \mathsf{AI}, \mathsf{DM}$ in Q_1.

(2) When simulation is adopted, the entire data graph G_1 is included in the match relation, which maps HR, SE, Bio, DM and AI in Q_1 to $\{\mathsf{HR}_1, \mathsf{HR}_2\}$, $\{\mathsf{SE}_1, \mathsf{SE}_2\}$, $\{\mathsf{Bio}_1, \mathsf{Bio}_2, \mathsf{Bio}_3, \mathsf{Bio}_4\}$, $\{\mathsf{DM}'_1$, DM'_2, DM_1, $\ldots$, $\mathsf{DM}_\mathsf{k}\}$ and $\{\mathsf{AI}'_1, \mathsf{AI}'_2, \mathsf{AI}_1, \ldots, \mathsf{AI}_\mathsf{k}\}$ in G_1, respectively.

(3) When it comes to strong simulation, the connected component G_c of G_1 that contains Bio_4 is the only match, which maps HR, SE, Bio, DM and AI in Q_1 to $\{\mathsf{HR}_2\}$, $\{\mathsf{SE}_2\}$, $\{\mathsf{Bio}_4\}$, $\{\mathsf{DM}'_1, \mathsf{DM}'_2\}$ and $\{\mathsf{AI}'_1, \mathsf{AI}'_2\}$ in G_1, respectively. Indeed, one can verify the following: (1) $Q_1 \prec_D G_c$, and in its match relation, Bio in Q_1 can only be mapped to Bio_4 in G_1; and (b) the ball with center Bio_4 and radius 3 (the diameter of Q_1) is exactly G_c. As opposed to simulation, the cycle $\mathsf{AI}_1, \mathsf{DM}_1$, $\ldots$, $\mathsf{AI}_k, \mathsf{DM}_k, \mathsf{AI}_1$ in G_1 is not part of the match. Indeed, this cycle is irrelevant and thus should be left out.

As another example, consider pattern graphs Q_2, Q_3, Q_4 and data graphs G_2, G_3, G_4 shown in Fig. 2.

(4) Pattern Q_2 is to find a book recommended by both students (ST) and teachers (TE). When simulation is used, both book_1 and book_2 in G_2 are returned as matches, while book_1 is obviously not a good option. When strong simulation is adopted, book_2 is the only match by the *duality*, in a single match graph (union of $G_{2,1}, G_{2,2}$ in Fig. 2). When it comes to subgraph isomorphism, it returns two match graphs ($G_{2,1}, G_{2,2}$) instead of one, with book_2 as the match.

(5) Pattern Q_3 is to find people (P and P') who recommend each other. When simulation or dual simulation is used, all people (P_1, P_2, P_3 and P_4) in G_3 are found as matches, while P_4 is obviously not a good choice. When strong simulation is adopted, P_1, P_2 and P_3 are the only matches by the *locality*, in a single match graph (union of $G_{3,1}, G_{3,2}$ in Fig. 2). These are also the matches found via subgraph isomorphism, in two match graphs ($G_{3,1}, G_{3,2}$) instead of a single one.

(6) Pattern Q_4 is looking for papers on social networks (SN) cited by papers on databases (db), which in turn cite papers on graph theory (graph). When simulation is used, all papers on SN (SN_1, SN_2, SN_3 and SN_4) in G_4 are matches, while SN_3 and SN_4 are obviously excessive matches. When strong simulation is adopted, SN_1 and SN_2 are the only matches due to the *duality*, returned in a single match graph (union of $G_{4,i,j}$ with $i, j \in [1, 2]$ in Fig. 2). These are also the matches found by subgraph isomorphism, yet returned in four match graphs ($G_{4,i,j}$ for $i, j \in [1, 2]$) instead of one. □

Semantics. Strong simulation is to find, given any pattern graph Q and data graph G, the set of the *maximum* perfect subgraph G_s in each ball such that $Q \prec_D G_s$.

By Lemma 1, one can verify the following, which assures that dual simulation and strong simulation are well defined.

Theorem 2: *For any pattern graph Q and data graph G such that $Q \prec_D^L G$, there exists a unique set of maximum perfect subgraphs for Q and G.* □

Remark. (1) Duality and locality are also imposed by subgraph isomorphism, but not by simulation. (2) One can readily extend strong simulation by supporting bounds on the number of hops and regular expressions as edge constraints on pattern graphs, along the same lines as [20, 19]. We defer this to the full report to simplify the discussion.

We summarize notations in Table 1, in which we use $Q \lhd G$ to denote that Q matches G via subgraph isomorphism.

Notations	Semantics
$G[V_s, E_s]$	A subgraph of G with node set V_s and edge set E_s
$\hat{G}[v, r]$	A ball in a graph G with center v and radius r
$\lhd, \prec$	Subgraph isomorphism and graph simulation
$\prec_D, \prec_D^L$	dual simulation and strong simulation

Table 1: Summary of notations

3. Properties of Strong Simulation

Below we first identify a set of criteria for topology preservation in pattern matching and for bounded match results. Based on the criteria we then evaluate strong simulation, dual simulation, subgraph isomorphism and graph simulation. Finally, we explore possible extensions to strong simulation and show that they lead to intractable problems.

Consider a connected pattern graph $Q = (V_q, E_q)$ with diameter d_Q and a data graph $G = (V, E)$.

3.1 Fundamental Properties

First, one can readily verify that subgraph isomorphism is a stronger notion than the other three, followed by strong simulation, dual simulation and graph simulation in this order. Intuitively, subgraph isomorphism preserves most topological structures between data graphs and pattern graphs.

Proposition 3: *(1) If $Q \lhd G$, then $Q \prec_D^L G$; (2) if $Q \prec_D^L G$, then $Q \prec_D G$; and (3) if $Q \prec_D G$, then $Q \prec G$.* □

We next take a closer look at what structures are preserved by these matching notions, by giving a set of criteria.

(1) Children. If a node u in the pattern graph Q matches node v in the data graph G, then each child of u must match a child of v. All these notions preserve the child relationship.

(2) Parents. If a node u in Q matches node v in G, then each parent of u also matches a parent of v. One can verify that subgraph isomorphism, strong simulation and dual simulation preserve the parent relationship, but simulation does not. A counterexample for simulation is given in Fig. 1.

(3) Connectivity. A connected pattern graph only matches a connected subgraph in the data graph.

As shown in Example 1, connected Q_1 may match a disconnected data graph G_1 via graph simulation. Dual simulation prevents this, as shown below. From this it follows that the stronger notions subgraph isomorphism and strong simulation also preserve the connectivity.

Theorem 4: *If $Q \prec_D G$, then for any connected component G_c of the match graph* w.r.t. *the maximum match relation of Q and G, (1) $Q \prec_D G_c$, and (2) G_c is exactly the match graph* w.r.t. *the maximum match relation of Q and G_c.* □

(4) Cycles. An undirected (resp. directed) cycle in Q must match an undirected (resp. directed) cycle in G.

We show that graph simulation preserves directed cycles, and hence so do the other three matching notions.

Proposition 5: *If $Q \prec G$ and there is a directed cycle in Q, then there must exist a matched directed cycle in the match graph* w.r.t. *any match relation of Q and G.* □

However, as shown in Example 1, graph simulation may match an undirected cycle in a pattern with a tree in a data graph. In contrast, dual simulation (and subgraph isomorphism and strong simulation) preserve undirected cycles.

Matching	children	parents	connectivity	cycles	locality	matches	Bisimilar&b'ed-cycle
$\prec$	✓	×	×	✓ (directed), × (undirected)	×	✓	×
$\prec_D$	✓	✓	✓	✓ (directed & undirected)	×	×	×
$\prec_D^L$	✓	✓	✓	✓ (directed & undirected)	✓	✓	×
$\lhd$	✓	✓	✓	✓ (directed & undirected)	✓	×	✓

Table 2: Topology preservation and bounded matches

Theorem 6: *If $Q \prec_D G$ and there is an undirected cycle in Q, then there must exist a matched undirected cycle in the match graph* w.r.t. *any match relation of Q and G.* □

(5) Locality. The diameter of a matched subgraph in G must be bounded by a function in the size of the pattern graph. This allows us to check a match locally, by inspecting only its neighborhood of a bounded diameter.

Strong simulation has the locality property, and so does subgraph isomorphism. In contrast, neither simulation nor dual simulation has the locality (see Examples 1 and 2).

Proposition 7: *If $Q \prec_D^L G$, then for all perfect subgraphs G_s of G, the diameter of G_s is bounded by $2 * d_Q$, where d_Q is the diameter of Q.* □

(6) Bounded matches. There should be a bounded number of matches, and each match is small enough to inspect. As remarked earlier, subgraph isomorphism may yield exponentially many matched subgraphs. While simulation and dual simulation return a single match relation, the relation is often too large to understand. In contrast, strong simulation strikes a balance: the number of matches is bounded by the number of nodes in the data graph, and each matched subgraph has a bounded diameter (Proposition 7).

Proposition 8: *The number of maximum perfect subgraphs of G is bounded by the number of nodes in G.* □

These results are summarized in Table 2. They tell us that strong simulation preserves much more topological structures between pattern graphs and data graphs than graph simulation, and moreover, possesses the locality property.

3.2 In Search for Tractable Boundary in Matching

One might want to find a notion of graph pattern matching that preserves maximum graph topology, and characterize PTIME along the same lines as how Fagin's theorem characterizes NP [31]. This is, however, very challenging. Indeed, as observed in [24], in graph theory Fagin's theorem implies that "if no logic captures PTIME, then PTIME $\neq$ NP".

Below we present two negative results: extending strong simulation makes its computation from PTIME to NP-hard.

Bounded cycles. Given a pattern graph Q and a data graph G such that $Q \prec G$ with the maximum match relation S, the *bounded cycle problem* is to determine whether the longest cycle in the match graph *w.r.t.* S is bounded by the longest one in Q. Obviously bounded cycle is a desirable locality property that one would have wanted to further impose on strong simulation. Unfortunately, this additional condition would make pattern matching intractable.

Theorem 9: *The bounded cycle problem is* coNP*-hard even when pattern graphs contain a single cycle.* □

Bisimulation. One might be tempted to use graph bisimulation [30] rather than graph simulation in graph pattern matching. A pattern graph Q *matches* a graph G_s via *bisimulation*, denoted by $Q \sim G_s$, if $Q \prec G_s$ with the maximum match relation S and $G_s \prec Q$ with the inverse S^- of S as its maximum match relation. Pattern matching via bisimulation is to find all subgraphs G_s of a graph G such that $Q \sim G_s$. Clearly bisimulation preserves more topological structures than simulation. Indeed, it is a notion stronger than simulation but weaker than isomorphism.

However, pattern matching via bisimulation becomes intractable. Indeed, subgraph bisimulation is NP-hard [18], although graph bisimulation is solvable in PTIME [30]. In contrast, subgraph simulation is equivalent to graph simulation, *i.e.,* checking whether there exists a subgraph G_s of G such that $Q \prec G_s$ is the same as checking whether $Q \prec G$.

4. An Algorithm for Strong Simulation

We next show that graph pattern matching via strong simulation retains the same complexity as earlier extensions [20, 19] of simulation, while it is able to preserve graph topology better. The main results of this section are as follows.

Theorem 10: *For any query graph Q and data graph G, it takes cubic time to check whether $Q \prec_D^L G$, and to find the set of maximum perfect subgraphs of G* w.r.t. *Q.* □

Theorem 11: *For any query graph Q with diameter d_Q, it takes quadratic time to find a minimum query graph Q_m such that Q_m and Q find the same result on any data graph by using d_Q as the radius of balls, via strong simulation.* □

We first prove Theorem 10 by providing a cubic-time algorithm for computing strong simulation. We then show Theorem 11 by proposing optimization techniques. Finally, we briefly discuss how the locality of strong simulation allows us to conduct pattern matching on distributed graphs.

4.1 A Cubic-time Algorithm

Algorithm. The algorithm, refereed to as Match, is shown in Fig. 3. Given a query graph Q and a data graph G, it returns the set of perfect subgraph G_s by inspecting those balls of radius d_Q centered at each node w of G.

To present Match, we first describe its procedures.

Procedure DualSim. It takes as input query graph $Q(V_q, E_q)$ and ball $\hat{G}[w, d_Q]$ with center w and radius d_Q, and finds the maximum match relation S_w of Q and $\hat{G}[w, d_Q]$. For each node v in V_q, it first computes the set $\mathsf{sim}(v)$ of candidate matches u in the ball with the same node label, *i.e.,* $l_{V_q}(u) = l_V(v)$ (lines 1–2). Then the procedure repeatedly removes nodes from $\mathsf{sim}(v)$ for each node v in Q (lines 3–10). A node u is removed from $\mathsf{sim}(v)$ unless (1) if there is a parent node v' of v, then there exists a parent node $u \in \mathsf{sim}(v')$; and (2) if there is a child node v' of v, then there exists a child node $u \in \mathsf{sim}(v')$. Finally, S_w is returned (lines 11–12).

Procedure ExtractMaxPG. It takes as input a query graph Q, ball $\hat{G}[w, d_Q]$, and the maximum match relation S_w. It finds the perfect subgraph G_s in the ball if there exists one. By Theorem 4, the procedure simply finds the connected component containing w in the match graph *w.r.t.* S_w.

Algorithm Match. We are now ready to present Match. For

```
Input: Query graph $Q$ with diameter $d_Q$ and data graph $G(V,E)$.
Output: The set $\Theta$ of maximum perfect subgraphs of $G$ w.r.t. $Q$.

1. $\Theta := \emptyset$;
2. for each ball $\hat{G}[w,d_Q]$ in $G$ do
3.     $S_w :=$ DualSim($Q, \hat{G}[w,d_Q]$);
4.     $G_s :=$ ExtractMaxPG($Q, \hat{G}[w,d_Q], S_w$);
5.     if $G_s \neq nil$ then $\Theta := \Theta \cup \{G_s\}$;
6. return $\Theta$.

Procedure DualSim($Q, \hat{G}[w,d_Q]$)
Input: Query graph $Q(V_q, E_q)$ and ball $\hat{G}[w,d_Q]$.
Output: The maximum match relation $S_w$ of $Q$ and $\hat{G}[w,d_Q]$.

1. for each $v \in V_q$ do
2.     sim($v$) := $\{u \mid u$ is in $\hat{G}[w,d_Q]$ and $l_Q(u) = l_G(v)\}$;
3. while there are changes do
4.     for each edge $(v,v')$ in $E_Q$ and each node $u \in$ sim($v$) do
5.         if there is no edge $(u,u')$ in $\hat{G}[w,d_Q]$ with $u' \in$ sim($v'$)
6.         then sim($v$) := sim($v$) $\setminus \{u\}$;
7.     for each edge $(v',v)$ in $E_Q$ and each node $u \in$ sim($v$) do
8.         if there is no edge $(u',u)$ in $\hat{G}[w,d_Q]$ with $u' \in$ sim($v'$)
9.         then sim($v$) := sim($v$) $\setminus \{u\}$;
10.    if sim($v$) $= \emptyset$ then return $\emptyset$;
11. $S_w := \{(v,u) \mid v \in V_q, u \in$ sim($v$)$\}$;
12. return $S_w$.

Procedure ExtractMaxPG($Q, \hat{G}[w,d_Q], S_w$)
Input: Query $Q$, ball $\hat{G}[w,d_Q]$ with maximum match relation $S_w$.
Output: The maximum perfect subgraph $G_s$ in $\hat{G}[w,d_Q]$ if any.
1. if $w$ does not appear in $S_w$ then return nil;
2. Construct the matching graph $G_m$ w.r.t. $S_w$;
3. return the connected component $G_s$ containing $w$ in $G_m$.
```

Figure 3: Algorithm Match

each node w in the data graph G, (1) it computes the maximum match relation S_w of Q and the ball $\hat{G}[w,d_Q]$ by invoking DualSim (line 2); (2) it finds the perfect subgraph G_s in $\hat{G}[w,d_Q]$ via ExtractMaxPG (line 3); and (3) G_s is added to the set Θ if it exists (line 4). After all balls in G are checked, it returns the set Θ of perfect subgraphs (line 5).

Example 3: Consider pattern graph Q_1 ($d_{Q_1} = 3$) and the ball with center Bio_4 and radius = 3 in data graph G_1 of Fig 1. Note that the ball is exactly the connected component G_c with node Bio_4 in G_1. We show how Algorithm Match works on Q_1 and G_c. Initially, HR, SE, Bio, AI and DM in Q_1 match $\{\text{HR}_2\}$, $\{\text{SE}_2\}$, $\{\text{Bio}_4,\}$, $\{\text{AI}'_1, \text{AI}'_2\}$ and $\{\text{DM}'_1, \text{DM}'_2\}$ in G_c, respectively (lines 1-2, DualSim). The algorithm finds no nodes to be removed from sim(u) for all nodes u in Q_1 in this case (lines 3-10, DualSim). Hence Match returns G_c as the perfect subgraph in the ball (line 6, Match). □

Correctness & Complexity. The correctness of algorithm is assured by the following. (1) There is at most one perfect subgraph in each ball of G (Theorem 2). (2) Procedure ExtractMaxPG returns the perfect graph in ball $\hat{G}[v,d_Q]$, by Theorem 4. (3) The correctness of DualSim can be verified along the same lines as its counterpart for simulation [25].

It takes Procedure BuildBall $O(|V|+|E|)$ time to build a ball $\hat{G}[v,d_Q]$ by using the BFS method [17]. For each ball, Procedure ExtractMaxPG finds its perfect subgraph in $O(|V|)$ time since finding pairwise disconnected components is linear-time equivalent to finding strongly connected components, which is in linear time [14]. By leveraging the algorithm developed in [25], DualSim can be done in $O(|V_q||E|)$ time. Thus algorithm Match is in $O(|V|(|V|+|V_q||E|))$ time.

```
Input: Pattern graph $Q = (V_q, E_q, l_Q)$.
Output: A minimized equivalent pattern graph $Q_m$ of $Q$.

1. Compute the maximum match relation $S$ of $Q \prec_D Q$;
2. Compute equivalent classes of nodes in $Q$ based on $S$;
3. Create a node for each equivalent class in $Q_m$;
4. Connect different equivalent classes with necessary edges in $Q_m$;
5. return $Q_m$.
```

Figure 4: Algorithm minQ

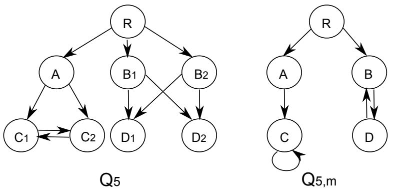


Figure 5: Query minimization

4.2 Optimization Techniques

We next present optimization techniques for algorithm Match, by means of query minimization, dual simulation filtering and connectivity pruning.

Query minimization. We first explore query minimization, which is important for any query language [4].

We say that two pattern graphs Q and Q' are *equivalent*, denoted by $Q \equiv Q'$, iff they return the same result on any data graph. A pattern graph Q is *minimum* if it has the least size $|Q|$ (the number of nodes and the number of edges) among all equivalent pattern graphs.

By the complexity analysis of algorithm Match, smaller pattern graphs lead to better performance.

Theorem 11 follows from Lemmas 12 and 13 given below.

Lemma 12: *For any pattern graph, (1) there exists a unique (up to isomorphism) minimum equivalent pattern graph, via dual simulation, that finds the same maximum match relation on any data graph; and (2) there exists a quadratic time algorithm to find its minimum equivalent query.* □

Lemma 13: *When fixing the radius of balls in strong simulation, two pattern graphs are equivalent via strong simulation iff they are equivalent via dual simulation.* □

Leveraging these, Algorithm Match can be improved as follows. Given query graph Q, we first compute its minimum equivalent query graph Q_m, and then we compute strong simulation *w.r.t.* Q_m and diameter d_Q.

Algorithm. As a proof of Lemma 12, we present Algorithm minQ for minimizing graph patterns, shown in Fig. 11. It takes as input a pattern graph Q, and returns a minimum equivalent pattern Q_m of Q, via dual simulation. For any pattern graph Q, it first computes the maximum match relation S by treating Q as both a pattern graph and a data graph (line 1). It then computes equivalent classes for nodes in Q such that nodes u and v are in the same class iff both $(u,v) \in S$ and $(v,u) \in S$ (line 2). Finally, it constructs the minimum equivalent query Q_m as follows (lines 3-4). (a) For each equivalent class eq, it creates a node eq for Q_m, and (b) there is an edge (eq, eq$'$) in Q_m iff there exist nodes $u \in$ eq and $u' \in$ eq$'$ such that there is an edge (u,u') in Q.

Example 4: Taking as input the pattern graph Q_5 given in Fig. 12, Algorithm minQ works as follows. (1) It first computes the maximum match relation S of Q_5 and Q_5, via dual simulation, yielding $S = \{(R, R), (B_i, B_j), (C_i, C_j),$

```
Input: Pattern graph $Q$, relation $S$ w.r.t. $Q \prec_D G$ and ball $\hat{G}[w, d_Q]$.
Output: The maximum perfect subgraph of $\hat{G}[w, d_Q]$ w.r.t. $Q$.
1.  $S_w$ := project $S$ onto $\hat{G}[w, d_Q]$; filterSet := $\emptyset$;
2.  for each $(u, v) \in S_w$ such that $v$ is a border node do
3.    if $\mathsf{succ}(v) \cap \mathsf{sim}(u_1) = \emptyset$ or $\mathsf{pred}(v) \cap \mathsf{sim}(u_2) = \emptyset$
4.      such that $(u, u_1) \in E_q$, $(u_2, u) \in E_q$
5.    then filterSet.push((u, v));
6.  while (filterSet $\neq \emptyset$) do
7.    (u, v) := filterSet.pop();  $S_w := S_w \setminus \{(u, v)\}$;
8.    for each $(u_2, u) \in E_q$ do
9.      for each $v_2 \in \mathsf{pred}(v) \cap \mathsf{sim}(u_2)$ do
10.       if $\mathsf{succ}(v_2) \cap \mathsf{sim}(u) = \emptyset$ then
11.         filterSet.push($(u_2, v_2)$);
12.   for each $(u, u_1) \in E_q$ do
13.     for each $v_1 \in \mathsf{succ}(v) \cap \mathsf{sim}(u_1)$ do
14.       if $\mathsf{succ}(v) \cap \mathsf{sim}(u_1) = \emptyset$ then
15.         filterSet.push($(u_1, v_1)$);
16. if there exists $u$ in $Q$ such that $\mathsf{sim}(u) = \emptyset$ then $S_w := \emptyset$;
17. return ExtractMaxPG (Q, $\hat{G}[w, d_Q]$, $S_w$)
```

Figure 6: Algorithm dualFilter

$(D_i, D_j)\}$ ($i, j \in [1, 2]$). (2) It then computes five equivalent classes: $\mathsf{eq}_R = \{R\}$, $\mathsf{eq}_A = \{A\}$, $\mathsf{eq}_B = \{B_1, B_2\}$, $\mathsf{eq}_C = \{C_1, C_2\}$, and $\mathsf{eq}_D = \{D_1, D_2\}$. (3) Finally, it constructs the minimum pattern graph $Q_{5,m}$ of Q_5, shown in Fig. 12: (a) For each equivalent class eq_x, where $x \in \{R, A, B, C, D\}$, it creates a node labeled with x; and (b) it creates an edge from node x to y in $Q_{5,m}$ iff there exist node $u \in \mathsf{eq}_x$ and $v \in \mathsf{eq}_y$ such that (u, v) is an edge in Q_5. □

Correctness & Complexity. The correctness of Algorithm minQ is assured by the following. (1) For any data graph G, the match graph *w.r.t.* the maximum match relation S of Q and G is always the same as the the match graph *w.r.t.* the maximum match relation S_m of Q_m and G. Hence, $Q \equiv Q_m$. (2) $|Q_m| \leq |Q'|$ for any Q' such that $Q' \equiv Q$. (3) For any two minimum equivalent pattern graphs Q_m and Q'_m, there is a bijective mapping from Q_m to Q'_m such that (a) for any node u in Q_m, $f(u)$ is a node in Q'_m with the same label, and (b) (u, v) is an edge in Q_m iff $(f(u), f(v))$ is an edge in Q'_m, *e.g.,* Q_m and Q'_m are equivalent up to isomorphism.

Algorithm minQ is in $O(|V_q||E_q| + |V_q|^2)$ time. Indeed, steps (1), (2) and (3) of minQ take $O(|V_q||E_q|)$ time, $O(|V_q|^2)$ time and $O(|E_q|)$ time, respectively.

Dual simulation filtering. Our second optimization technique aims to avoid redundant checking of balls in the data graph. Most algorithms of graph simulation (*e.g.,* [25]) recursively refine the match relation by identifying and removing false matches. As observed in [20], it is much easier to deal with node or edge deletions than their insertions. In light of this, we compute the match relation of dual simulation first, and then project the match relation on each ball to compute strong simulation. This both reduces the initial match set $\mathsf{sim}(v)$ for each node v in Q (line 2, Dualsim), and reduces the number of balls (line 2, Match). Indeed, if a node v in G does not match any node in Q, then there is no need to consider the ball centered at v.

Consider *border* nodes in a ball $\hat{G}[v, r]$, *i.e.,* nodes u with $\mathsf{dist}(v, u) = r$. We refer to those nodes reachable from a border node as *affected* nodes. One can verify the following:

Proposition 14: *The removal process in a ball only needs to deal with its border nodes and their affected nodes.* □

This suggests an order to process nodes in $\hat{G}[v, r]$: starting from its border nodes, we inspect affected nodes only following an increasing order based on their distances from border nodes. This minimizes unnecessary computation. Note that the border nodes can be marked when constructing balls. Hence this incurs little extra complexity.

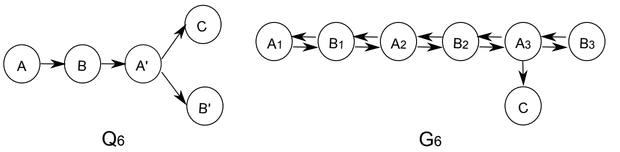


Figure 7: Dual simulation filtering

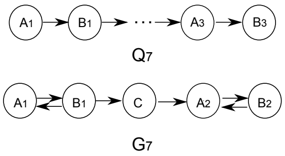


Figure 8: Connectivity pruning

Algorithm. To do this, we first compute the match relation S_G, via dual simulation, over the entire data graph by invoking Procedure DualSim in Fig. 3. We then project S_G onto each ball. When computing the perfect subgraph on a ball, we start with the *border* nodes, and identify invalid matches using Algorithm dualFilter shown in Fig. 14.

We next present Algorithm dualFilter. It takes as input pattern graph Q, the maximum match relation S of Q and G that is found via dual simulation, and ball $\hat{G}[w, d_Q]$. It returns the maximum perfect subgraph of $\hat{G}[w, d_Q]$ *w.r.t.* Q. More specifically, dualFilter first projects match relation S_G onto ball $\hat{G}[w, d_Q]$, yielding relation S_w (line 1). It then iteratively marks and removes those invalid matches stored in a queue *filterSet* (lines 2-15), initially empty. To do this, it first inspects those matches in S_w that contain a border node, to find invalid matches (lines 2-4). The invalid matches found are stored in *filterSet* (line 5). It then processes those marked invalid matches one by one (lines 6-15). Each invalid match $(u,\ v)$ with affected node v is removed from S_w (line 7). The relation S_w is then processed along the same lines as Algorithm Match (lines 8-15), but following the order of invalid matches in *filterSet*. Finally, the algorithm extracts the perfect subgraph by invoking Procedure ExtractMaxPG, and returns the subgraph (line 17).

Example 5: We next illustrate how the filtering technique improves the performance of Algorithm Match by considering pattern graph Q_6 and data graph G_6 given in Fig. 13. The maximum match relation S_{G_6} of Q_6 and G_6 via dual simulation is the set of matches (node pairs) $\{(A, A_2)$, (A, A_3), (B, B_2), (B, B_3), $(C, C)\}$. Hence initially, $\mathsf{sim}(A) = \{A_2, A_3\}$, $\mathsf{sim}(B) = \{B_2, B_3\}$ and $\mathsf{sim}(C) = \{C\}$.

The filtering method then projects the match relation S_{G_6} on each ball, and checks the results. It finds the following.

(i) There exist invalid matches in two balls: $\hat{G}_6(A_1, 3)$ and $\hat{G}_6(B_1, 3)$, by inspecting their border nodes. For $\hat{G}_6(A_1, 3)$, after projecting S_{G_6} on $\hat{G}_6(A_1, 3)$, we get $S_w = \{\mathsf{sim}(A) = \mathsf{sim}(A') = \{A_2\}, \mathsf{sim}(B) = \mathsf{sim}(B') = \{B_2\}\}$. Here B_2 is a border node of $\hat{G}[A_1, 3]$. Starting with B_2, dualFilter finds that there exist invalid matches; similarly for $\hat{G}_6(B_1, 3)$.

(ii) In contrast, there exist no invalid matches in balls $\hat{G}_6(A_2, 3)$, $\hat{G}_6(B_2, 3)$, $\hat{G}_6(A_3, 3)$, $\hat{G}_6(B_3, 3)$ and $\hat{G}_6(C, 3)$. This is found by inspecting border nodes in each ball. Hence the final match relation in any of these balls is exactly the same as the initial projection of S_{G_6} on the ball.

As a result, only two balls ($\hat{G}_6(A_1, 3)$ and $\hat{G}_6(B_1, 3)$) are really processed by dualFiler, while no more processing is needed for the other five balls. That is, the filtering method prunes unnecessary processing and speeds up Match, □

Correctness & Complexity. The correctness of Algorithm dualFiler is asserted by Proposition 14. For its complexity, observe that it takes $O(|V|(|V| + |E|))$ time to construct all balls, and $O(|V_q||E|)$ time to compute the maximum match relation of Q and G via dual simulation, along the same lines as Algorithm Match. For each ball $\hat{G}[w, d_Q]$, it takes at most $O(|V_q||E_{\hat{G}[w,d_Q]}|)$ time. Putting these together, dualFilter takes $O(|V|(|V|+|V_q||E|))$ time in total. Although the worst case complexity is the same as the complexity of Algorithm Match (shown in Fig. 3), as demonstrated by the example and as will be shown by our experimental study, the optimization technique is indeed effective in practice.

Connectivity pruning. Theorem 4 tells us that in a ball $\hat{G}[v, r]$, only the connected component containing the ball center v needs to be considered. Hence, those nodes not reachable from v can be pruned early. Our last main optimization technique does precisely this. It reduces the search space for checking dual-simulation, and can be easily incorporated into Algorithm Match, as illustrated below.

Example 6: Consider pattern graph Q_7 and data graph G_7 shown in Fig. 15, in which diameters $d_{Q_7} = 5$ and $d_{G_7} = 4$. As $d_{Q_7} > d_{G_7}$, a ball with any center node of G is exactly G itself. When conducting dual simulation of Q_7 on ball $\hat{G}_7[A_1, 5]$, for instance, the pruning method first finds an initial sim(v) set for each node v in Q_7, by mapping A_i in Q_7 to A_j in $\hat{G}_7[A_1, 5]$ ($i \in [1, 3]$, $j \in [1, 2]$). This yields two connected component in $\hat{G}_7[A_1, 5]$: SC_1 containing nodes $\{A_1, B_1\}$ and SC_2 containing $\{A_2, B_2\}$, in which only SC_1 contains the center node A_1 (recall the notion of connected graphs from Section 2). By Theorem 4, the pruning method safely removes all those nodes that are not in SC_1 from sim(u), for any node $u \in Q_7$, without affecting the final matches. That is, it prunes invalid matches early and hence, improves the performance of algorithm Match. □

We have implemented a version of Match that supports all optimization strategies, referred to as Match$^+$. As will be seen in Section 5, Match$^+$ significantly outperforms Match.

4.3 Strong Simulation on Distributed Graphs

When evaluating a query on a large dataset, one wants to partition the data and distribute its fragments to multiple machines, such that the query can be evaluated in parallel, as advocated by, *e.g.,* MapReduce [16]. Moreover, it is common to find real-life datasets already partitioned and distributed. For instance, to find the complete information of a person, one may have to query several social networks (*e.g.,* Facebook, Picassa and Youtube) to collect her data. These highlight the need for developing distributed algorithms for evaluating graph queries. However, as observed in [29], graph algorithms often exhibit poor data locality and hence, may incur prohibitive overhead on network traffic.

We next show that strong simulation demonstrates data locality and hence, allows efficient distributed evaluation.

Data locality. Consider a graph G that is partitioned into $(G_1, \ldots, G_k)$ such that each G_i is stored in site M_i for $i \in [1, k]$. We want to evaluate a pattern query Q on G, while minimizing unnecessary data shipment from one site to another. This is, however, rather challenging when pattern matching is defined in terms of graph simulation.

Example 7: Consider again query graph Q_1 and data graph G_1 of Fig. 1. Let G_s be the subgraph of G_1 by removing the connected component with Bio$_4$ from G_1. Suppose that G_s is fragmented and distributed. Then to decide whether $Q_1 \prec G_s$, we have to ship all subgraphs of G_s to a single site to re-assemble G_s. Indeed, (1) the match graph of Q_1 and G_s via graph simulation is the entire G_s; and (2) removing any node or edge from G_s makes $Q_1 \not\prec G_s$. This tells us that it is hard to conduct graph simulation in the distributed setting without incurring high network traffic. □

In contrast, we show that strong simulation has the data locality. Indeed, strong simulation can be computed in the distributed setting, guaranteeing that the total data shipment is bounded by the set of balls $\hat{G}[v, d_Q]$ in G such that v is in some G_i but it has a direct neighbor node not in G_i.

Algorithm. To verify the data locality of strong simulation, we outline a distributed algorithm for pattern matching via strong simulation (see [1] for the details of the algorithm and its related experimental results).

When a site, referred to as *the coordinator*, receives a pattern graph Q, it sends the same Q to each site M_i for $i \in [1, k]$. When a site M_i receives Q, it finds those balls $\hat{G}[v, d_Q]$, where v is in G_i but v has a neighbor node in another fragment G_j. For such nodes v, M_i sends $\hat{G}[v, d_Q]$ to site M_j only if $j < i$. It then invokes algorithm Match to compute the matches of Q in G_i, as a partial result Θ_i of Q in G, at site M_i. It sends Θ_i back to the coordinator.

The coordinator monitors messages sent back from all sites M_i for $i \in [1, k]$. When partial results are returned from all the sites, the coordinator assembles their partial results via union, and returns the final result.

One can readily verify that the algorithm is correct, with the bound on network traffic mentioned above. Furthermore, it is generic: it is applicable to any G *regardless of* how G is partitioned and distributed.

5. Experimental Study

We next present an experimental study of strong simulation. Using both real-life social networks and synthetic data, we conducted two sets of experiments to evaluate: (1) the effectiveness of strong simulation vs. conventional subgraph isomorphism [35] and graph simulation [25], and (2) the efficiency of our centralized algorithm Match.

Experimental setting. We used the following datasets.

Real-life graph data. We used two real-life network datasets.

(1) *Amazon* records a product co-purchasing network with 548,552 product nodes and 1,788,725 product-product directed edges[1]. An edge from products x to y indicates that people buy y with high probability when they buy x.

(2) *YouTube* provides a video network with 155,513 video nodes and 3,110,120 video-video directed edges[2]. An edge from videos x to y indicates that if one watches x, then he is also very likely to watch y.

[1] http://snap.stanford.edu/data/index.html

[2] http://netsg.cs.sfu.ca/youtubedata/

Synthetic graph generator. We adopted the graph-tool library[3] to produce both pattern and data graphs. It is controlled by three parameters: the number n of nodes, the number n^{α} of edges, and the number l of node labels. Given n, α, and l, the generator produces a graph with n nodes, n^{α} edges, and the nodes are labeled from a set of l labels.

Algorithms. We implemented the following algorithms, all in Python: (1) our algorithms Match and Match^{+}, (2) the graph simulation algorithm of [25], denoted by Sim, (3) the approximate matching algorithm TALE of [33], and (4) an approximate matching algorithm, denoted by MCS, that utilizes the approximation algorithm of [26] for computing maximum common subgraphs. We used the VF2 algorithm [13] for subgraph isomorphism in the igraph package [15].

Consider pattern graph $Q(V_q, E_q)$ and data graph $G(V, E)$. For approximate matching algorithms TALE and MCS, there are essentially $2^{|V|}$ number of subgraphs of G to compare with Q, beyond reach in practice. Hence, we chose to compare the subgraphs of G having the same number of nodes as Q. We adopted the same setting as [33] for TALE here. For MCS, a subgraph $G_s(V_s, E_s)$ of G matches pattern graph Q if $\frac{|\mathsf{mcs}(Q,G_s)|}{\max(|V_q|,|V_s|)} \geq 0.7$, where $|\mathsf{mcs}(Q, G_s)|$ is the number of nodes in the maximum common subgraph $\mathsf{mcs}(Q, G_s)$ of Q and G_s computed via the algorithm of [26].

The experiments were run on a cluster of 30 machines, all with Intel Core i7 860 CPU and 16GB of memory. Each test was repeated over 5 times, and the average is reported here.

Experimental results. We next present our findings. In all the experiments, we fixed $l = 200$, and set $\alpha = 1.2$ by default when generating pattern and data graphs.

Exp-1: Quality of matches. In the first set of experiments, we evaluated the quality of matches found by strong simulation vs. matches found by subgraph isomorphism and simulation. We measured the quality of matches as follows.

(1) We first designed pattern graphs, and manually checked the quality of matches returned by Match, VF2 and Sim. We find that Match is able to identify sensible matches. We illustrate this with two example pattern graphs.

Two real-life pattern graphs Q_A and Q_Y are shown in Figures 9(a) and 9(b), respectively. Pattern graph Q_A is to find all "Parenting & Families" books in Amazon network data (a) that are co-purchased with both "Children's Books" and "Home & Garden" books; and (b) that are co-purchased with "Health, Mind & Body" books and vice versa.

Pattern graph Q_Y poses a request on YouTube network data searching for all "Entertainment" videos (a) that are related to "Film & Animation" videos and "Music" videos; and further, (b) for each such "Entertainment" video x, there is another "sports" video that is related to the "Film & Animation" and "Music" videos to which x is related.

In data graphs G_A and G_Y, nodes are books and videos, respectively, labeled with their ids, and they only match the nodes of Q_A and Q_Y with the same geometry shapes, *e.g.,* circles, ellipses, and regular squares and pentagons.

The match results of Q_A and Q_Y are shown in Figures 9(a) and 9(b), respectively. For pattern graph Q_A, subgraph G_A is a sensible match found by Match, but it was not found by VF2. Subgraph G'_A is a match found by Sim in which the "Parenting & Families" books are not co-purchased with both "Children's Books" and "Home & Garden" books, among other things, and was successfully filtered by Match and VF2. These tell us that strong simulation is able to identify sensible matches that subgraph isomorphism fails to catch, and moreover, to eliminate excessive matches by graph simulation that do not make sense.

For pattern graph Q_Y, subgraph G_Y is a match found by Match, while subgraphs $G_{Y,1}$, $G_{Y,2}$ and $G_{Y,3}$ are three matches found by VF2. This example shows how strong simulation reduces the sizes of matches found by subgraph isomorphism, without loss of information.

(2) To further measure the quality of matches found, we use:
closeness = #matches_subIso / #matches_found,
where #matches_subIso and #matches_found are the total numbers of nodes in matches found by VF2 and those by a comparative algorithm (Sim, Match, VF2, TALE, MCS), respectively. Recall that matches found by VF2 are also matches found by Match and Sim, by Proposition 3. Hence closeness is essentially the ratio of matched nodes found by VF2 to the entire matches found by Sim, Match, VF2, TALE or MCS. Note that for VF2, closeness is always 1.

(i) To evaluate the impact of pattern graphs Q, we fixed $|V|$, *e.g.,* Amazon with 31245 nodes, YouTube with 9368 nodes, and synthetic data with 5×10^4 nodes, respectively, while varying $|V_q|$ from 2 to 20.

(ii) To evaluate the impact of data graphs G, we fixed pattern graphs Q with $|V_q| = 10$ and varied the size of data graphs. We varied $|V|$ from 3×10^3 to 3×10^4 nodes for Amazon and from 10^3 to 10^4 for YouTube. For synthetic data, we varied $|V|$ from 10^4 to 10^5. We used relatively smaller data graphs since VF2 does not scale to large graphs.

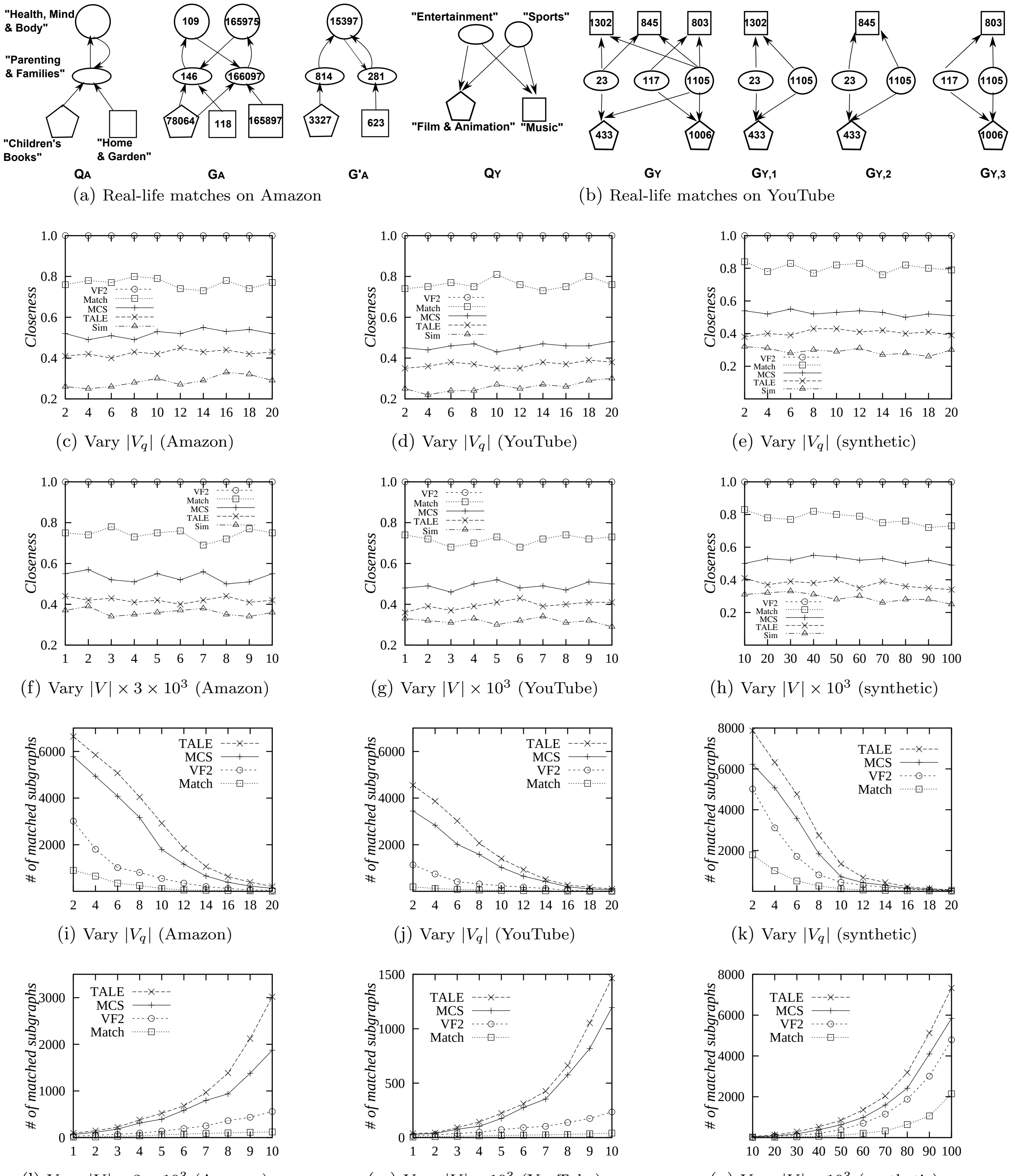
The closeness results are reported in Figures 9(c), 9(d), 9(e), 9(f), 9(g) and 9(h). We can see that the closeness of Match is consistently in the range of [70%, 80%] with various query and data graphs, while Sim is in [25%, 38%], TALE is in [35%, 42%], and MCS is in [46%, 57%], respectively. Hence, Match does much better than Sim (up to 50%), TALE (up to 36%) and MCS (up to 23%) at preserving graph topology. Indeed, 70% to 80% of the matches found by Match are exactly those found by VF2, which enforces strict topological matching. Recall that Match is able to find sensible matches missed by VF2 (Examples 1 and 2 and the above quality test (1)). That is, the [20%, 30%] matches found by Match, but missed by VF2, further contain sensible matches.

In addition, the results tell us that the match quality of Match, Sim, TALE and MCS are *not* sensitive to the size of pattern and data graphs for both real-life and synthetic data, a desirable property when match quality is concerned.

(3) In the same setting as (2) above for testing closeness, we tested the numbers of the matched subgraphs in data graphs returned by Match, VF2, TALE and MCS. We did not report Sim since it always returns at most one matched subgraph.

The results are reported in Figures 9(i), 9(j), 9(k), 9(l), 9(m) and 9(n). They tell us that Match returns much less matched subgraphs than VF2: it returns consistently around 25% to 38% matched subgraphs of VF2, for synthetic graph, Amazon and YouTube alike. For approximate matching algorithm TALE and MCS, it is obvious that they return even much more subgraphs than VF2. Indeed, as shown in Fig. 9(n), for example, Match returns 2144 matched subgraphs compared to 4792 by VF2, 5843 by MCS and 7328

[3] http://projects.skewed.de/graph-tool/



(a) Real-life matches on Amazon

(b) Real-life matches on YouTube

(c) Vary $|V_q|$ (Amazon)

(d) Vary $|V_q|$ (YouTube)

(e) Vary $|V_q|$ (synthetic)

(f) Vary $|V| \times 3 \times 10^3$ (Amazon)

(g) Vary $|V| \times 10^3$ (YouTube)

(h) Vary $|V| \times 10^3$ (synthetic)

(i) Vary $|V_q|$ (Amazon)

(j) Vary $|V_q|$ (YouTube)

(k) Vary $|V_q|$ (synthetic)

(l) Vary $|V| \times 3 \times 10^3$ (Amazon)

(m) Vary $|V| \times 10^3$ (YouTube)

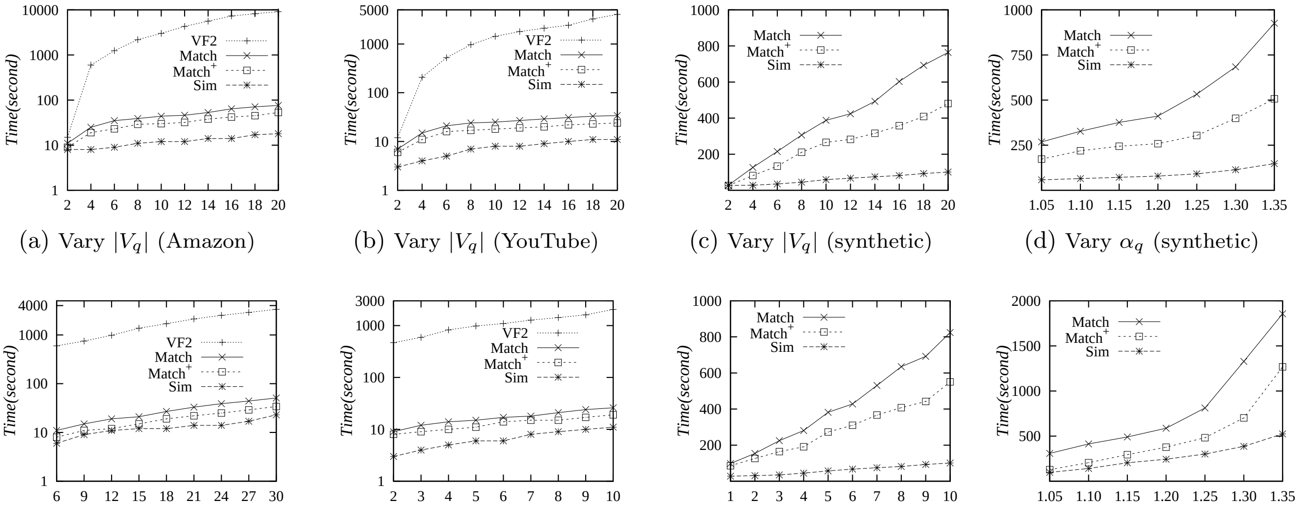
(n) Vary $|V| \times 10^3$ (synthetic)

Figure 9: Match quality evaluation on real-life data

by TALE, on a synthetic data graph with 10^5 nodes. This confirms that Match effectively reduces the sizes of match results, and hence, allows users to effectively analyze the match results on large graphs in practice.

In addition, the number of matched subgraphs decreases when the size of pattern graphs increases, and it increases when the size of data graphs increases, as expected. We also find that although VF2 may find exponentially matches in theory, it does not happen very often in practice.

(4) In the same setting as (2) for testing closeness with



(a) Vary $|V_q|$ (Amazon) (b) Vary $|V_q|$ (YouTube) (c) Vary $|V_q|$ (synthetic) (d) Vary α_q (synthetic)

(e) Vary $|V| \times 10^3$ (Amazon) (f) Vary $|V| \times 10^3$ (YouTube) (g) Vary $|V| \times 10^6$ (synthetic) (h) Vary α (synthetic)

Figure 10: Performance evaluation of centralized algorithms

#nodes	[0, 9]	[10, 19]	[20, 29]	[30, 39]	[40, 49]	≥ 50
Amazon	0	98	23	0	0	0
YouTube	0	21	18	1	1	0
Synthetic	0	187	113	65	6	0

Table 3: Sizes of matched subgraphs

largest possible datasets, *e.g.,* Amazon with 31245 nodes, YouTube with 9368 nodes, and synthetic data with 100000 nodes, we tested the sizes of the matched subgraphs in data graphs returned by Match and Sim.

For Sim, it returns a single matched subgraph with 103, 177 and 311 nodes in Amazon, YouTube and synthetic data, respectively. For Match, the results are reported in Table 3. Their matched subgraphs are typically small, where (a) all matched subgraphs have less than 50 nodes, and (b) over 80% of matches have less than 30 nodes, on real-life and synthetic data. This tells us that strong simulation indeed restricts the sizes of matches, due to the duality and locality.

Exp-2: Performance of centralized algorithms. In the second set of experiments, we evaluated the performance of our algorithms Match, Match$^+$ and algorithms Sim and VF2. Algorithm VF2 does not scale well with large data graphs, *e.g.,* it took VF2 more than *three* hours on data graphs with 5×10^6 nodes (when $\alpha = 1.2$). Hence, we only report the performance of VF2 on the small real-life datasets of Amazon and YouTube that were used to evaluate the quality of matches. For large synthetic data graphs, we only report the other three algorithms Match, Match$^+$ and Sim. In all of our experiments, we also found that TALE and MCS were even much slower than VF2, and hence we did not report the running time of TALE and MCS here.

(1) To evaluate the impact of pattern graphs Q, we used two small real-life datasets (Amazon and YouTube) and one large synthetic dataset. We fixed Amazon, YouTube and the synthetic data to have 3×10^4 nodes, 10^4 nodes and 5×10^6 nodes, respectively, while varying the number $|V_q|$ of query nodes from 2 to 20 or the density α_q of pattern graphs from 1.05 to 1.35 (*i.e.,* increasing pattern edges). The results are reported in Figures 10(a), 10(b), 10(c) and 10(d).

The elapsed time of algorithms over real-life datasets is shown in Figures 10(a) and 10(b). When varying $|V_q|$, VF2 is consistently much slower than the other three algorithms in both cases. It is about 100 times slower than Match$^+$ when $V_q \geq 4$ on the two real-life datasets. For instance, it took VF2 hours on the small Amazon and YouTube datasets. Note that, however, when $|V_q| = 2$, VF2 is almost as efficient as the other algorithms. This is consistent with the complexity analysis of VF2: VF2 is in low PTIME when $|V_q| = 2$.

As shown in Fig. 10(c), all these algorithms scale well with $|V_q|$ on large data graphs, except VF2. When we increased the density α_q of pattern graphs, Figure 10(d) shows that these algorithms scale well with the density α_q on large data graphs, except VF2. Algorithms Match and Match$^+$ are slower than Sim, as expected. Indeed, this is a price that has to be paid in exchange for better match quality. We did not report the performance of VF2 in Figures 10(c) and 10(d) since it could not run to completion when $|V_q| \geq 4$.

Finally, observe that the running time of all algorithms increases when $|V_q|$ or α_q increases. This is consistent with the complexity analyses of these algorithms.

(2) To evaluate the impact of data graphs G, we also used two small real-life datasets (Amazon and YouTube) and one large synthetic dataset. We fixed pattern graphs with $|V_q| = 10$, while varying the number $|V|$ of nodes of Amazon, YouTube and the synthetic data from 6×10^3 to 3×10^4, 2×10^3 to 10^4 and 10^6 to 10^7, respectively, or varying the density α of data graphs from 1.05 to 1.35. The results are shown in Fig. 10(e), Fig. 10(f), Fig. 10(g) and Fig. 10(h).

These results are consistent with the results of varying pattern graph sizes. (a) As shown in Figures 10(e), 10(f), 10(g) and 10(h), all these algorithms except VF2 scale well with the size of data graphs and with the density α of data graphs; (b) algorithms Match and Match$^+$ are slower than Sim; and (c) the running time of VF2 increases far more substantially with the size and density of data graphs than the others. For example, the running time of Match$^+$ increased from about 100s to 600s when the number of nodes of the synthetic data varied from 10^6 to 10^7; in contrast, VF2 spent nearly 4000s on Amazon data with 3×10^4 nodes, but only around 30s on Amazon graphs with 3×10^3 nodes.

(3) The experimental results in (1) and (2) above also verify that our optimization techniques are effective. Indeed, the running time of Match$^+$ is consistently about 2/3 of the time taken by Match, a significant reduction.

Summary. From these experimental results we find the following. (1) Strong simulation is able to identify sensible matches that are not found by subgraph isomorphism, and eliminate those found by graph simulation but are not meaningful. In addition, it finds high quality matches that retain graph topology. Indeed, 70%-80% of matches found by subgraph isomorphism are retrieved by strong simulation, (up to 50%) better than graph simulation, without paying the price of intractable complexity and large number (or size) of matches. (2) Our algorithms for strong simulation are efficient and scale well with the size and density large-scale data graphs, *e.g.,* it took 270 seconds when $|V| = 10^8$, $|V_q| = 10$ and $|M| = 30$. (3) Our optimization techniques are effective, reducing the running time by at least 33%.

6. Conclusion

We have proposed strong simulation to rectify problems of graph pattern matching based on subgraph isomorphism and graph simulation. We have verified, both analytically and experimentally, that strong simulation has several salient features, notably (1) it is capable of capturing the topological structures of pattern and data graphs; (2) it retains the same cubic-time complexity of previous extensions of graph simulation, (3) it demonstrates data locality and allows efficient distributed evaluation algorithms, and (4) it finds bounded matches. Our experimental results have also verified the effectiveness of our optimization techniques.

Several topics are targeted for future work. First, we are to extend strong simulation by incorporating regular expressions on edge types, along the same lines as [19]. Second, our distributed algorithms just aim to demonstrate the data locality of strong simulation. Sophisticated algorithms can be developed in the distributed setting, with better performance guarantees. Third, we are to find metrics to rank matches found by strong simulation, to return top-ranked matches only. Finally, for large graphs, cubic time is still too expensive. We are to explore indexing techniques to speed up the computation, and incremental methods for strong simulation, minimizing unnecessary recomputation in response to (frequent) changes to real-life graphs.

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APPENDIX A: Proofs

Proof of Lemma 1

Let S_1 and S_2 be two distinct matching relations. Based the definition of dual simulation, $S = S_1 \cup S_2$ is also a matching relation. Following from this, it is easy to see that the conclusion is true.

Proof of Theorem 2

One can verify that for any pattern graph Q and data graph G such that $Q \prec_D G$, there exists a unique maximum perfect subgraph in each ball $\hat{G}[v, d_Q]$ if there exists one. This is implied by Theorem 4. Combined with Lemma 1, one can have the conclusion.

Proof of Proposition 3

This can be readily verified by definitions of subgraph isomorphism, strong simulation, dual simulation and graph simulation, which have less restrictions one by one.

Proof of Theorem 4

Assume *w.l.o.g.* that G_c is a connected component of the matching graph *w.r.t.* S.

(1) We first show that $Q \prec_D G_c$. Let v be any node in G_c such that $(u, v) \in S$. For any neighboring node (child or parent) x of u, there must exist a neighboring node y of v such that $(x, y) \in S$. We then recursively consider the neighboring nodes of x, the neighboring nodes of the neighboring nodes of x, …, and until all nodes in Q are considered. This process produces a set of nodes in G_c, and there exists an undirected path from v to any of these nodes. Hence all these nodes belong to G_c. By the definition of dual simulation, it is easy to see that $Q \prec_D G_c$.

(2) We then show that the matching graph *w.r.t.* the maximum matching relation of Q and G_c is exactly G_c. Let $S(G_c)$ be a subset of S such that for each $(u, v) \in S(G_c)$, v is in G_c, and S_c be the maximum matching relation of Q and G_c. To show that G_c is the matching graph *w.r.t.* the maximum matching relation of Q and G_c, it suffices to show $S(G_c) = S_c$ since G_c is a connected component of the matching graph *w.r.t.* S. It is easy to know that $S_c \subseteq S$ since, otherwise, S would not the maximum matching relation of Q and G. Hence, we only need to show that $S(G_c) \subseteq S_c$. This is easy. The previous analysis of (1) implies that $(u, v) \in S_c$ for each $(u, v) \in S(G_c)$.

Putting these together, we can have conclusion.

Proof of Proposition 5

This is verified along the same lines as Theorem 6 by the definition of graph simulation, which considers children only.

Proof of Theorem 6

Assume *w.l.o.g.* that $\rho = u_1/u_2/\ldots/u_k/u_{k+1}$ is a cycle in Q, where $u_1 = u_{k+1}$, and there is an edge (u_i, u_{i+1}) or (u_{i+1}, u_i) in Q for each $i \in [1, k]$. Let G_s be the matching graph of any matching relation S of Q and G. And for each u_i ($i \in [1, k]$) in Q, let $S(u_i)$ be the set of nodes in G_s such that $(u_i, v) \in S$ for each node v in $S(u_i)$. By the definition of dual simulation, for each node $v \in S(u_i)$, there is a node $v' \in S(u_{i+1})$ with an edge (v, v') or (v', v) in G_s. Assume *w.l.o.g.* $S(u_1) = \{v_1, \ldots, v_h\}$, then for each node $v_j \in S(u_1)$, there exists a directed path to a node $v_{j'} \in S(u_{k+1})$. Recall that $u_1 = u_{k+1}$. Hence, for each node $v_j \in S(u_1)$, there exists an undirected path to a node $v_{j'} \in S(u_1)$.

```
Input: Pattern graph $Q = (V_q, E_q, l_Q)$.
Output: A minimized equivalent pattern graph $Q_m$ of $Q$.

Compute the maximum matching relation $S$ of $Q \prec_D Q$;
Compute equivalent classes of nodes in $Q$ based on $S$;
Create a node for each equivalent class in $Q_m$;
Connect different equivalent classes with necessary edges in $Q_m$;
return $Q_m$.
```

Figure 11: Algorithm minQ

We first construct h undirected paths as follows: $\rho_1 = u_1/\ldots/u_{j_1}$, $\rho_2 = u_{j_1}/\ldots/u_{j_2}$, …, and $\rho_h = u_{j_{h-1}}/\ldots/u_{j_h}$. Note that the above analysis implies that there must exist h such directed paths.

We next construct an undirected cycle from the h undirected paths above. By connecting the h paths, we get a longer directed path ρ, in which there are $h + 1$ nodes in $S(u_1)$. Since there are only h distinct nodes in $S(u_1)$, there must exit a node $v_i \in S(u_1)$ that appears at least twice in ρ. Hence, we can easily derive a *simple* cycle from ρ.

Proof of Proposition 7

This can be verified via the definition of strong simulation since balls are connected graphs, and for any two nodes u, u' in perfect subgraph of a ball $\hat{G}(v, r)$, $\mathsf{dist}(u, u') \leq 2r$ since $\mathsf{dist}(u, v) \leq r$ and $\mathsf{dist}(u', v) \leq r$.

Proof of Proposition 8

By the definition of strong simulation, there exists at most one maximum perfect subgraph for each ball $\hat{G}(v, d_Q)$, where v is a node in G, and d_Q is the diameter of Q. The number of balls is bounded by the number of nodes in G, so is the number of maximum perfect subgraphs.

Proof of Theorem 9

We show that the BCP problem is coNP-hard even when pattern graph is a cycle graph by reduction from the longest cycle problem (LCP) to the complement of BCP. The LCP problem is to find whether or not the length of the longest cycle in a graph is greater than or equal to k, and is known to be NP-complete [31].

Given an instance of the LCP problem, we construct an instance of the BCP problem as follows.
(1) We construct a cycle pattern graph Q_1 with $k+1$ nodes, whether all nodes have the same label 'a'.
(2) We construct the data graph G_1 from G, labeling all nodes with the same node label 'a' of pattern graph Q_1

The BCP problem has a negative answer for Q_1 and G_1 iff there is a cycle longer than k in G.

Proof of Theorem 10

This is verified by the correctness and complexity analysis of algorithm Match.

Proof of Theorem 11

This follows from Theorem 12 and Proposition 13.

APPENDIX B: Optimization Techniques

Query minimization. We present details of query minimization optimization for strong simulation evaluation.

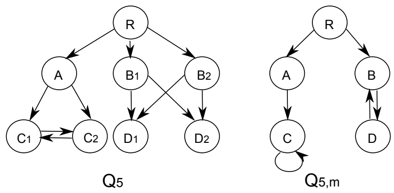

Figure 12: Query minimization

Proof of Lemma 12

We show this by providing algorithm minQ, shown in Fig. 11, that takes as input an pattern graph Q, and returns a minimum equivalent pattern Q_m of Q, via dual simulation. We illustrate algorithm minQ with an example as follows.

Example 8: Consider pattern graph Q_5 in Fig.12, where B_i's, C_i's and D_i's ($i \in [1, 2]$) carry the same labels, respectively. (1) The algorithm first computes the maximum match relation S_5 of Q and Q, via dual simulation, such that $S_5 = \{(R, R), (B_i, B_j), (C_i, C_j), (D_i, D_j)\}$ ($i, j \in [1, 2]$). (2) Given two nodes u, v in Q, we say $u \equiv v$ if $(u, v) \in S$ and $(v, u) \in S$. The algorithm then computes five equivalent classes: $\mathsf{eq}_R = \{R\}$, $\mathsf{eq}_A = \{A\}$, $\mathsf{eq}_B = \{B_1, B_2\}$, $\mathsf{eq}_C = \{C_1, C_2\}$, and $\mathsf{eq}_D = \{D_1, D_2\}$. (3) Finally, it constructs the minimum pattern graph $Q_{5,m}$ of Q_5, via dual simulation. (a) For each equivalent class eq_x ($x \in \{R, A, B, C, D\}$), it creates a node labeled with x. And (b) it creates an edge from nodes x to y iff there is a node $u \in \mathsf{eq}_x$ and a node $v \in \mathsf{eq}_y$ such that there is an edge from u to v in Q_5. The pattern graph $Q_{5,m}$ is shown in Fig. 12. □

Correctness. (I) We first show that for any data graph G, the match graph *w.r.t.* the maximum match relation S of Q and G is always the same as the the match graph *w.r.t.* the maximum match relation S_m of Q_m and G.

By the construction of Q_m in algorithm minQ, we have $Q \prec_D Q_m$ and $Q_m \prec_D Q$. This says that for any data graph G, $Q \prec_D G$ implies $Q_m \prec_D G$, and vice versa. Hence for any node $v \in G$, if v matches a node $u \in Q$, then there exists a node $u_m \in Q_m$ such that v matches u_m, vice versa. (II) We next show that $|Q_m| \leq |Q'|$ for any Q' such that $Q' \equiv Q$ by contradiction. Assume first that $|Q'| < |Q_m|$ and given Q' as input, algorithm minQ outputs Q' (otherwise, we simply use the one generated by minQ). We show that $|Q'| \geq |Q_m|$, which contradicts our assumption.

Let EQ_m and EQ' be the equivalent classes for Q_m and Q', respectively, produced by algorithm minQ. (a) We first show that (1) $|\mathsf{EQ}_m| \leq |\mathsf{EQ}'|$ by constructing a total mapping f from EQ_m to EQ'. (2) We then show that for any $\mathsf{eq}_1, \mathsf{eq}_2 \in \mathsf{EQ}_m$, there is an edge $(\mathsf{eq}_1, \mathsf{eq}_2)$ in Q_m iff $(f(\mathsf{eq}_1), f(\mathsf{eq}_2))$ is an edge in Q'. By (1) and (2), it follows that $|Q_m| = |Q'|$. (1) Let S_1, S_2 be the maximum match relations of $Q' \prec_D Q_m$ and $Q_m \prec_D Q'$, respectively. And let $(\mathsf{eq}, \mathsf{eq}') \in f$ iff there exists $u \in \mathsf{eq}$ and $u' \in \mathsf{eq}'$ with $(u, u') \in S_1$ and $(u', u) \in S_2$. We next show that f is indeed a function by proving (a) f is total; and (b) for any $\mathsf{eq} \in \mathsf{EQ}_m$, there exists only one equivalent class eq' $\in \mathsf{EQ}'$ such that $f(\mathsf{eq}) =$ eq'.

(a) We first how that f is total. Assume that there exists an $\mathsf{eq} \in \mathsf{EQ}_m$ such that for all nodes $u \in \mathsf{eq}$, there exists no $\mathsf{eq}' \in \mathsf{EQ}'$ satisfying that there exists a node $u' \in \mathsf{eq}'$ with $(u, u') \in S_1$ and $(u', u) \in S_2$. For all nodes $u \in \mathsf{eq}$ and all nodes $u' \in \mathsf{eq}'$, there are three possible cases for eq and eq' as follows: (i) $(u, u') \in S_1$ and $(u', u) \notin S_2$; (ii) $(u, u') \notin S_1$ and $(u', u) \in S_2$; and (iii) $(u, u') \notin S_1$ and $(u', u) \notin S_2$.

For all these cases, one can verify that for any $u \in Q_m$, there exists $u' \in Q'$ such that $(u, u') \in S_1$ and $(u', u) \in S_2$. This leads to the total property of f.

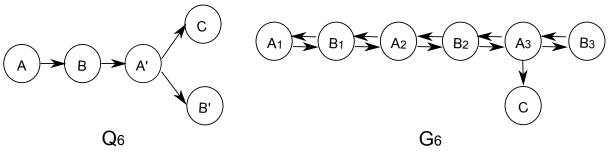

Figure 13: Dual simulation filtering

(b) We next prove that f is a function. Assume to the contrary that there is an equivalent class eq in EQ_m such that there exists two equivalent classes eq'_1 and eq'_2 in EQ', satisfying that $(\mathsf{eq}, \mathsf{eq}'_1) \in f$ and $(\mathsf{eq}, \mathsf{eq}'_2) \in f$. We next show that $\mathsf{eq}_1 = \mathsf{eq}_2$. In fact, we have the following:
(1) From $(\mathsf{eq}, \mathsf{eq}'_1) \in f$, we know that there exits $u_1 \in \mathsf{eq}$ and $u'_1 \in \mathsf{eq}'_1$ such that $(u_1, u'_1) \in S_1$ and $(u'_1, u_1) \in S_2$. (2) From $(\mathsf{eq}, \mathsf{eq}'_2) \in f$, we know that there exits $u_2 \in \mathsf{eq}$ and $u'_2 \in \mathsf{eq}'_2$ such that $(u_2, u'_2) \in S_1$ and $(u'_2, u_2) \in S_2$. (3) $u_1, u_2 \in \mathsf{eq}$ implies that $(u_2, u'_1) \in S_1$ and $(u_1, u'_2) \in S_1$. (4) From $(u'_1, u_1) \in S_2$ and $(u_1, u'_2) \in S_1$, we know that $u'_1 \prec_D u'_2$. (5) From $(u'_2, u_2) \in S_2$ and $(u_2, u'_2) \in S_1$, we know that $u'_2 \prec_D u'_1$. Thus u'_1 and u_2 are dual simulation equivalent, which implies that $\mathsf{eq}'_1 = \mathsf{eq}'_2$, meaning that f is a function. From (a) and (b) we have $|\mathsf{EQ}_m| \leq |\mathsf{EQ}'|$ and for any $\mathsf{eq} \in \mathsf{EQ}_m$, $f(\mathsf{eq}) \in \mathsf{EQ}'$.
(2) From step 3 of algorithm minQ, one can verify that there is an edge $(\mathsf{eq}_1, \mathsf{eq}_2) \in Q_m$ if and only if $(f(\mathsf{eq}_1), f(\mathsf{eq}_2))$ is an edge in Q', which ensures that the number of edges in Q_m is no larger than that in Q'.

With (1) and (2), we have that $|Q_m| \leq |Q'|$.
(III) Observe that the mapping function f proposed above is surjective by proving f^- is total along the same line with above. Hence f is a bijective function from Q^1_m to Q^2_m such that there is an edge $e = (u, v)$ in Q^1_m iff there is an edge $(f(u), f(v))$ in Q^2_m.

Complexity. Steps (1), (2) and (3) of algorithm minQ take $O(|V_Q||E_Q|)$ time, $O(|V_Q|^2)$ time and $O(|E_Q|)$ time, respectively. Hence, in total, it takes $O(|V_Q||E_Q| + |V_Q|^2)$ time, *i.e.,* quadratic time in the size of Q.

Proof of Lemma 13

Consider pattern graph Q and its minimum equivalent Q_m. When the radius of balls is fixed, the balls *w.r.t.* Q and Q_m are exactly the same. As shown by Theorem 12, for any data graph G, the match graph *w.r.t.* the maximum match relation of Q and G is the same as the one *w.r.t.* the maximum match relation of Q_m and G. Hence, it is obvious that Q and Q_m have the same match result on any data graph G, via strong simulation.

Dual simulation filtering. We next provide details about the dual simulation filtering optimization technique. We show that it shares computation among neighbor balls, and hence it improves efficiency of algorithm Match.

This optimization technique firstly computes the match relation S_G, via dual simulation, over the entire data graph via procedure DualSim in Fig. 3. Then it projects S_G onto each ball. When computing the perfect subgraph on a ball, it starts with the *boundary* nodes in the ball, and identifies invalid matches via algorithm dualFilter shown in Fig. 14. Here the *boundary* nodes of a ball $\hat{G}[v, d_Q]$ are the set of nodes u such that $\mathsf{dist}(u, v) = d_Q$. Note that the boundary nodes can be marked early in the ball construction step of

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Input: Pattern graph $Q$, relation $S$ w.r.t. $Q \prec_D G$ and ball $\hat{G}[w, d_Q]$.
Output: The maximum perfect subgraph of $\hat{G}[w, d_Q]$ w.r.t. $Q$.
1.  $S_w$ := project $S$ onto $\hat{G}[w, d_Q]$;  filterSet := $\emptyset$;
2.  for each $(u, v) \in S_w$ such that $v$ is a boundary node do
3.      if $\mathsf{succ}(v) \cap \mathsf{sim}(u_1) = \emptyset$ or $\mathsf{pred}(v) \cap \mathsf{sim}(u_2) = \emptyset$
4.         such that $(u, u_1) \in E_q$, $(u_2, u) \in E_q$
5.      then filterSet.push((u, v));
6.  while (filterSet $\neq \emptyset$) do
7.      (u, v) := filterSet.pop();  $S_w := S_w \setminus \{(u, v)\}$;
8.      for each $(u_2, u) \in E_q$ do
9.         for each $v_2 \in \mathsf{pred}(v) \cap \mathsf{sim}(u_2)$ do
10.           if $\mathsf{succ}(v_2) \cap \mathsf{sim}(u) = \emptyset$ then
11.              filterSet.push($(u_2, v_2)$);
12.     for each $(u, u_1) \in E_q$ do
13.        for each $v_1 \in \mathsf{succ}(v) \cap \mathsf{sim}(u_1)$ do
14.           if $\mathsf{succ}(v) \cap \mathsf{sim}(u_1) = \emptyset$ then
15.              filterSet.push($(u_1, v_1)$);
16. if there exists $u \in Q$ such that $\mathsf{sim}(u) = \emptyset$ then $S_w := \emptyset$;
17. return ExtractMaxPG (Q, $\hat{G}[w, d_Q]$, $S_w$)
```

Figure 14: Algorithm dualFilter

Match. Hence this incurs little extra complexity.

We next explain algorithm dualFilter in more detail. After conducting dual simulation evaluation over the whole data graph G, dualFilter projects S_G onto ball $\hat{G}[w, d_Q]$, resulting in S_w (line 1), and iteratively marks and removes those invalid matches (lines 2-15). Algorithm dualFilter then inspects those matches in S_w that involve with boundary nodes, and checks whether there are invalid matches (lines 2-4). It marks those invalid meaches (line 5). Then it processes those marked invalid matches one by one (lines 6-15). Each invalid match (u, v) with boundary node v is removed from S_w (line 7), and then the affected matches are sought out (lines 8-15). Here the affected matches are ones that violate the constraints of dual simulation (lines 10, 14).

We illustrate how dual simulation filtering technique works with an example by the following.

Example 9: Given the pattern graph Q and data graph G in Fig. 13, S_G is found firstly, *i.e.,* $\mathsf{sim}(u)$ for each node u in Q. Here S_G = {$\mathsf{sim}(A)$, $\mathsf{sim}(B)$, $\mathsf{sim}(A')$, $\mathsf{sim}(B')$, $\mathsf{sim}(C)$}, in which $\mathsf{sim}(A) = \{A_2, A_3\}$, $\mathsf{sim}(B) = \{B_2, B_3\}$ and $\mathsf{sim}(C) = \{C\}$. It then projects the match relation S onto each ball.

First let's consider ball $\hat{G}[A_1, 3]$. After projecting S_G into $\hat{G}[A_1, 3]$, we get $S_w = \{\mathsf{sim}(A) = \mathsf{sim}(A') = \{A_2\}, \mathsf{sim}(B) = \mathsf{sim}(B') = \{B_2\}\}$. Here B_2 is a boundary node of $\hat{G}[A_1, 3]$. Algorithm dualFilter then starts with B_2 and decrementally checks whether there exists invalid matches. In this example it turns out that there are no valid matches *w.r.t.* Q and $\hat{G}[A_1, 3]$. Similar result can be found in ball $\hat{G}[B_1, 3]$.

We now take ball $\hat{G}[A_2, 3]$ as an example. It turns out that there is no invalid matches *w.r.t.* all boundary nodes. Thus the final match relation in the ball is exactly the same as the initial projection of S on all $\hat{G}[A_2, 3]$. Similar conclusions are established for balls $\hat{G}[B_2, 3]$, $\hat{G}[A_3, 3]$, $\hat{G}[B_3, 3]$ and $\hat{G}[C, 3]$. Only $\hat{G}[A_1, 3]$ and $\hat{G}[A_2, 3]$ are really affected by dualFiler. This leads to reductions of redundant computations. □

Proof of Proposition 14

We show this by showing the correctness of dualFilter. Let S_1 and S_2 be the S_w at line 1 and line 17 of algorithm dualFilter, respectively. Let S_3 be the set of match relation returned by algorithm Match over ball $\hat{G}[w, d_Q]$ *w.r.t.* Q. We show that $S_2 = S_3$ by showing $S_2 \subseteq S_3$ and $S_3 \subseteq S_2$. It is obvious that $S_3 \subseteq S_2$. Hence we only need to show that $S_2 \subseteq S_3$.

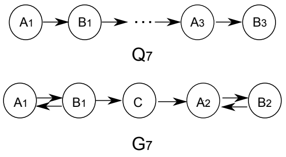


Figure 15: Connectivity pruning

Indeed, it suffices to show that for any (u, v) $\in S_1$, if (u, v) $\notin S_3$, then (u, v) $\notin S_2$. There are two cases to consider: (1) (u, v) is directly removed by the projection (line 1); (2) (u, v) is removed due to the removal of matches at (1). Here a match (u', v') is affected by the removal of (u, v) if (a) u' is a successor (resp. predecessor) of u and (b) v is the only predecessor (resp. successor) of v' that matches u.

Assume there exists (u^1, v^1) $\in S_1$, (u^1, v^1) $\notin S_3$, but (u^1, v^1) $\in S_2$. From (u^1, v^1) $\in S_1$ we know that there exits $u^2 \in \mathsf{succ}(u^1)$ and $v^2 \in \mathsf{succ}(v^1)$ (we consider successors only, it is similar for predecessors) such that (u^2, v^2) $\in S_1$. From (u^1, v^1) $\notin S_3$ we know that for any $v^2 \in \mathsf{succ}(v^1)$, $(u^2, v^2) \notin S_3$. We can verify that (u^2, v^2) remains in S_2, a contradiction. Suppose that (u^2, v^2) is removed by the projection (case (1)). Then (u^1, v^1) is in the affected area of the removal of (u^2, v^2). Similarly, (u^1, v^1) will be an affected match if (u^2, v^2) is removed by case (2). Thus there would exists (u^3, v^3), which is in neither case 1 or case 2, such that $u^3 \in \mathsf{succ}(u^2)$ and $v^3 \in \mathsf{succ}(v^2)$ and (u^3, v^3) $\in S_1$, (u^3, v^3) $\notin S_2$. It is the same for (u^3, v^3). Analogously $u^{(n+1)} \in \mathsf{succ}(u^{(n)})$ and $v^{(n+1)} \in \mathsf{succ}(v^{(n)})$ and ($u^{(n+1)}$, $v^{(n+1)}$) $\in S_1$, ($u^{(n+1)}$, $v^{(n+1)}$) $\notin S_2$ ($\forall n$ = 1, 2, 3, ...). This conflicts with the finiteness of the number of matches in S_1.

As the correctness of dualFilter is guaranteed by proposition 14, we turn to its complexity by the following.

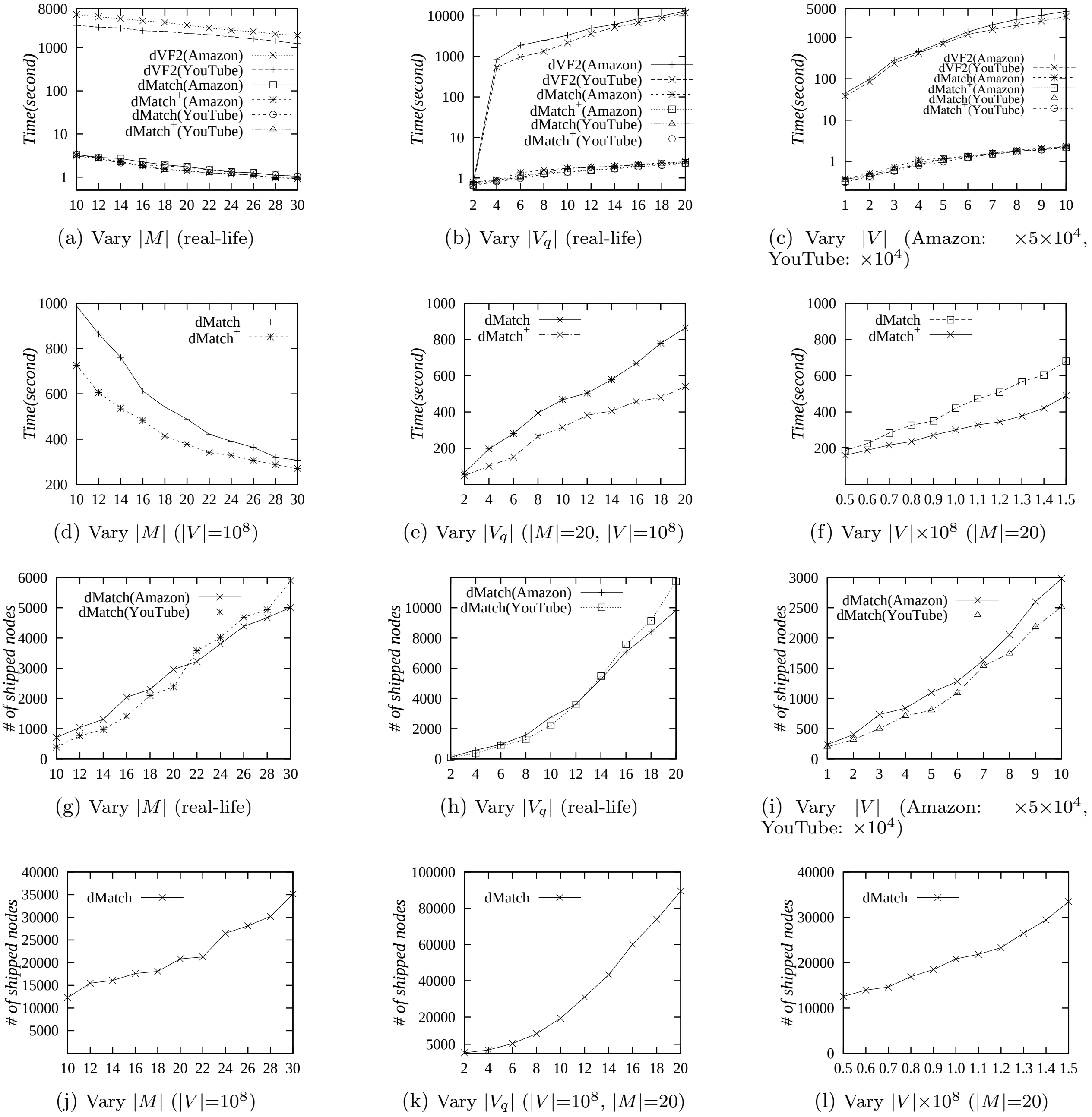
Complexity. It takes $O(|V_q||E|)$ time to get the match relation of the dual simulation of Q on G. For each ball $\hat{G}[v_i, d_q]$, dualFilter takes at most $O(|V_q||E_{\hat{G}[v_i, d_q]}|)$ time. Thus dualFilter takes at most $O(|V_q||V||E|)$ time, the same as the one of algorithm Match shown in Fig. 3.

Connectivity pruning. We firstly illustrate the connectivity pruning optimization with an example as follows. This is inspired by the connectivity property of strong simulation as stated by Theorem 4.

Example 10: Consider pattern graph Q_7 and data graph G_7 shown in Fig. 15. As the diameter of Q_7 is 5 that is larger than the diameter of G_7. Thus each ball of G is exact G itself. When conducting dual simulation of Q_7 on ball $\hat{G_7}[A_1, 5]$, the optimization algorithm first finds an initial sim(v) set for each node v in Q_7, *i.e.,* mapping A_i in Q_7 to A_j in $\hat{G_7}[A_1, 5]$ ($i \in [1, 3]$, $j \in [1, 2]$). This yields two connected component in $\hat{G_7}[A_1, 5]$: SC_1 containing nodes {A_1, B_1} and SC_2 containing nodes {A_2, B_2}. Indeed only SC_1 contains the center node A_1 of the ball. Hence, the rest of nodes u should be removed for any node $v \in Q$ such that $u \in$ sim(v). From this, we can see that this technique prunes accessary matches as early as possible. □

APPENDIX C: Additional Experiments

Exp-3: Performance of distributed algorithms. In the last set of experiments, we evaluated the performance and



(a) Vary $|M|$ (real-life)

(b) Vary $|V_q|$ (real-life)

(c) Vary $|V|$ (Amazon: $\times 5\times10^4$, YouTube: $\times10^4$)

(d) Vary $|M|$ ($|V|$=10^8)

(e) Vary $|V_q|$ ($|M|$=20, $|V|$=10^8)

(f) Vary $|V|\times10^8$ ($|M|$=20)

(g) Vary $|M|$ (real-life)

(h) Vary $|V_q|$ (real-life)

(i) Vary $|V|$ (Amazon: $\times 5\times10^4$, YouTube: $\times10^4$)

(j) Vary $|M|$ ($|V|$=10^8)

(k) Vary $|V_q|$ ($|V|$=10^8, $|M|$=20)

(l) Vary $|V|\times10^8$ ($|M|$=20)

Figure 16: Performance evaluation of distributed algorithms

data shipment of distributed pattern matching algorithms. We used the entire Amazon and YouTube datasets in these experiments. We considered dMatch and dMatch$^+$, our distributed algorithms that support optimization and do not, respectively. We also implemented a distributed algorithm based on subgraph isomorphism, denoted by dSubIso, by replacing Match with SubIso in algorithm dMatch. Note that subgraph isomorphism is a stronger notion than strong simulation and also has data locality property. Unfortunately, there exists no any distributed algorithm based on graph simulation, and graph simulation does not have data locality property, as discussed in Section 4.3. Hence we focused on dMatch, dMatch$^+$ and dSubIso. Here we only report the data shipment of dMatch since algorithms dMatch, dMatch$^+$ and dSubIso incur the same amount of data shipment. We do not report the performance of dSubIso on large synthetic graphs as dSubIso does not run to completion on such data.

(i) To evaluate the impact of the number $|M|$ of machines, we fixed pattern graphs with $|V_q| = 10$ and the number of nodes $|V|$ of data graphs (Amazon: 5×10^5, YouTube: 10^5, and synthetic data: 10^8), while varying $|M|$ from 10 to 30.

(ii) To evaluate the impact of pattern graphs Q, we fixed $|M| = 20$ and the size of data graphs using the same setting as (i), while varying $|V_q|$ from 2 to 20.

(iii) To evaluate the impact of data graphs G, we fixed $|V_q| = 10$ and $|M| = 20$, while varying $|V|$ from 0.5×10^5 to 5.0×10^5, 0.1×10^5 to 1.0×10^5 and 0.5×10^8 to 1.5×10^8 for Amazon, YouTube and synthetic data, respectively.

(iv) In the settings of (i), (ii) and (iii), we also tested the data shipment for our distributed algorithms.

We next report our findings.

(1) The results on the running time of algorithms dSubIso, dMatch and dMatch$^+$ are reported in Figures 16(a), 16(b) and in 16(c) for real-life datasets and Figures 16(d), 16(e) and 16(f) for synthetic datasets, respectively. As shown in these figures, (a) the running time of all algorithms decreases *w.r.t.* the number of machines, and increases *w.r.t.* the pattern graph sizes and data graph sizes, as expected. (b) All algorithms except dSubIso scale well in all cases. When data graphs are large, dSubIso is about 1000 times slower than the other algorithms, as shown in Figures 16(a), 16(b) and 16(c). (c) Our optimization techniques are effective in all cases: dMatch$^+$ takes about 2/3 of the running time of dMatch, which is consistent with the results in the centralized cases. (d) Algorithm dMatch$^+$ is efficient. For instance, it took 270s with $|V| = 10^8$, $|V_q| = 10$ and $|M| = 30$.

(2) The results on the the number of shipped nodes of algorithm dMatch are reported in Figures 16(g), 16(h) and 16(i) for real-life datasets and Figures 16(j), 16(k) and 16(l) for synthetic data, respectively. Observe the following.

(a) The shipped data increases when $|M|$ increases for both real-life and synthetic data, as shown in Fig. 16(g) and Fig. 16(j). Indeed, the data graph is partitioned and distributed across $|M|$ machines. Since the number of border nodes increases with the increase of the number of partitions, the shipped data increases as well. Nevertheless, the amount of data shipped is low: it accounts for 10^{-3} to 10^{-4} of the entire data graph when $|M| = 30$. It is even 4×10^{-4} for synthetic data with 10^8 nodes.

(b) The shipped data increases when the size of pattern graphs increases, as shown in Figures 16(h) and 16(k). When pattern graphs are larger, so are their diameters; hence the increase in the amount of data shipped. Nonetheless, the shipped data accounts for only 10^{-3} of the entire synthetic data even when $|V_q| = 20$.

(c) The data shipped increases when data graphs get larger, for both real-life and synthetic data, as shown in Figures 16(i) and 16(l). The larger the data graphs, the more border nodes and hence, the more data shipped. Again, data shipped only accounts for 10^{-3} of the two real-life datasets, and is 3.5×10^{-4} for synthetic graphs with $|V| = 1.5 \times 10^8$.

As we can see, in all cases strong simulation has a good data locality property. We find that all algorithms except for dSubIso scale well *w.r.t.* large data graphs even on multiple machines, and our optimization techniques are very effective. And, hence, we did not report the running time of algorithm dSubIso on large synthetic datasets. Further, the data shipment of our distributed algorithms is small due to the data locality of strong simulation.