Efficient Subgraph Matching by Postponing Cartesian Products

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Never Stand Still | Faculty of Engineering | Computer Science and Engineering

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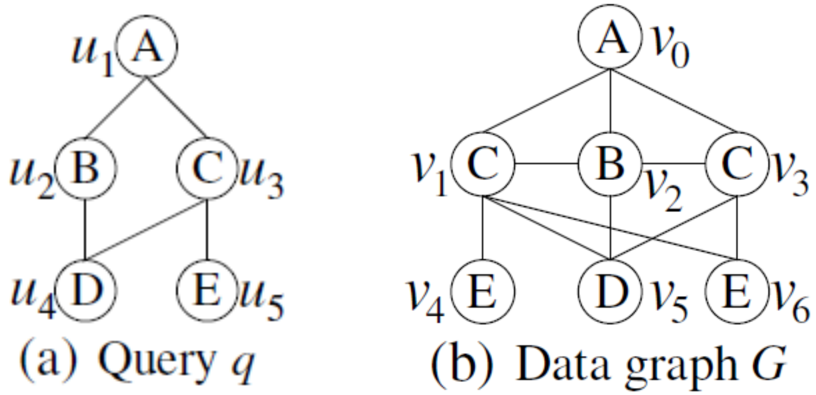
Outline

- Introduction & Existing Works
- Challenges of Subgraph Matching
- Our Approach
  - Core-First Decomposition based Framework
  - Compact Path Index (CPI) based Matching
- Experiments
- Conclusion

Introduction

➢ **Subgraph Matching**

Given a query ***q*** and a large data graph ***G***, the problem is to extract all subgraph isomorphic embeddings of ***q*** in ***G***.



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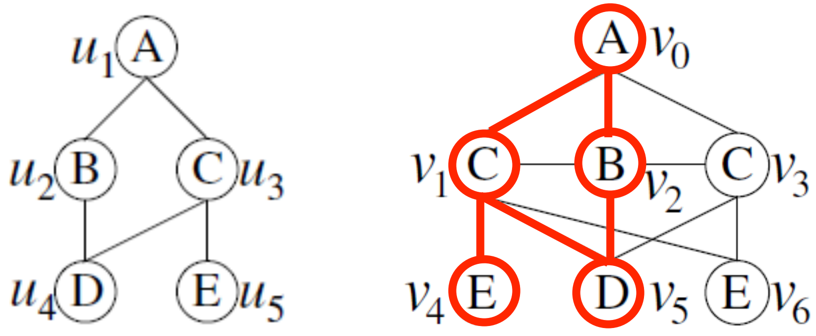

(a) Query q (b) Data graph G

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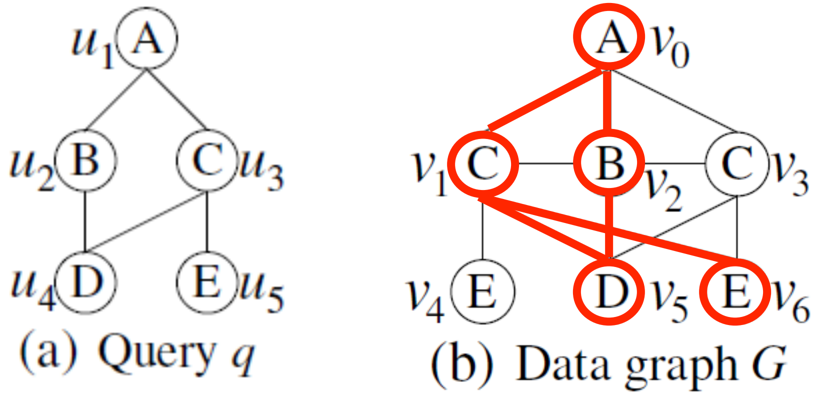

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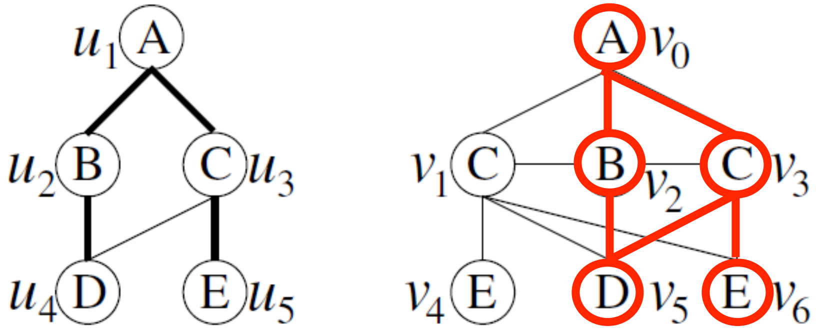
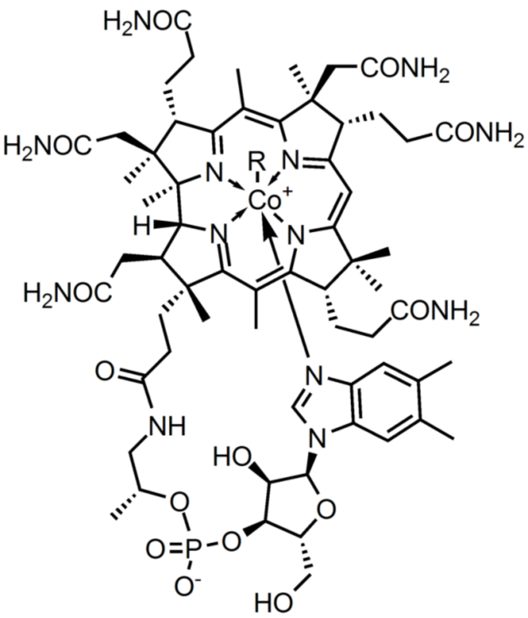


(a) Query q (b) Data graph G

Introduction

- **Applications**
  - Protein interaction network analysis
  - Social network analysis
  - Chemical compound search

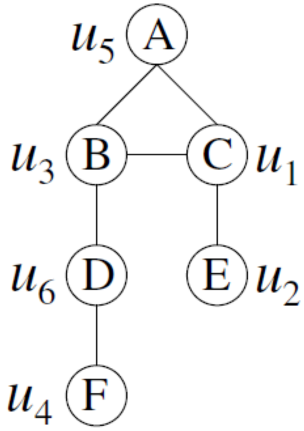


Hardness

- Subgraph Isomorphism Testing is **NP-complete**
  - Decide whether there is a subgraph of ***G*** that is isomophic to ***q***
- Enumerating all subgraph isomorphic embeddings is **NP-hard**
- Many techniques have been developed for efficient enumeration in practice

Existing Work

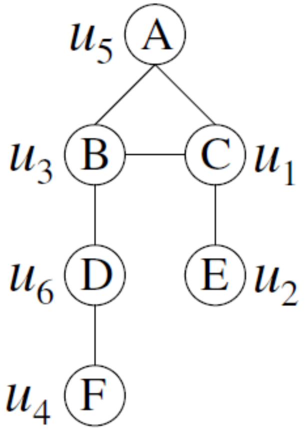
- **Ullmann's algorithm [J.ACM'76]**
  - Iteratively maps query vertices one by one to data vertices, following the **input order** of query vertices.
  - **Cartesian Products** between vertices' candidates.



- **VF2 [IEEE Trans'04] and QuickSI [VLDB'08]**
- **Turbo$_{\text{ISO}}$ [SIGMOD'13]**
- **Boost$_{\text{ISO}}$ [VLDB'15]**

Existing Work

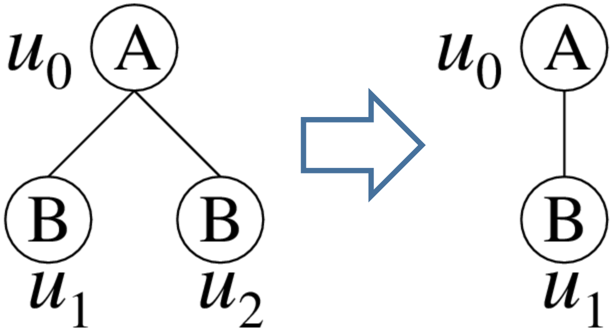
- **Ullmann's algorithm [J.ACM'76]**
- **VF2 [IEEE Trans'04] and QuickSI [VLDB'08]**
  - Independently propose to enforce **connectivity** of the matching order to reduce Cartesian products caused by **disconnected** query vertices.
  - QuickSI further removes false-positive candidates by first processing **infrequent** query vertices and edges.



- **Turbo$_{\text{ISO}}$ [SIGMOD'13]**
- **Boost$_{\text{ISO}}$ [VLDB'15]**

Existing Work

- **Ullmann's algorithm [J.ACM'76]**
- **VF2 [IEEE Trans'04] and QuickSI [VLDB'08]**
- **Turbo$_{\text{ISO}}$ [SIGMOD'13]**
  - **Compress a query graph** by merging together **similar** vertices (i.e., with the same neighborhoods)
    - Reduce Cartesian product caused by **similar** query vertices
  - Build a data structure online to facilitate the search process.
- **Boost$_{\text{ISO}}$ [VLDB'15]**



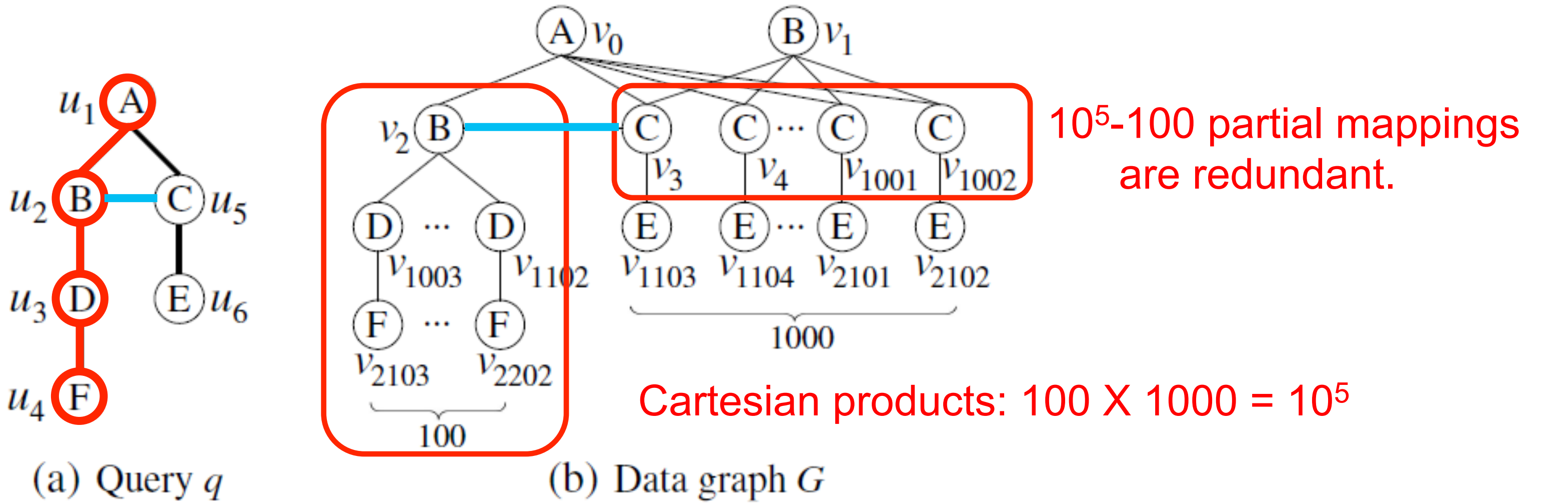
Existing Work

- **Ullmann's algorithm [J.ACM'76]**
- **VF2 [IEEE Trans'04] and QuickSI [VLDB'08]**
- **Turbo$_{ISO}$ [SIGMOD'13]**
- **Boost$_{ISO}$ [VLDB'15, Ren and Wang]**
  - Compress a data graph ***G*** by merging together **similar vertices in *G***.
  - Develop **query-dependent** relationship between vertices in ***G***.
    - **dynamically** reduces duplicate computations.
  - Can be applied to **accelerate all previous techniques** as well as ours

It is still challenging for matching large query graphs.

Challenges of Subgraph Matching

Challenge I: Redundant Cartesian Products by Dissimilar Vertices.



No similar vertices in ***q*** or ***G***.

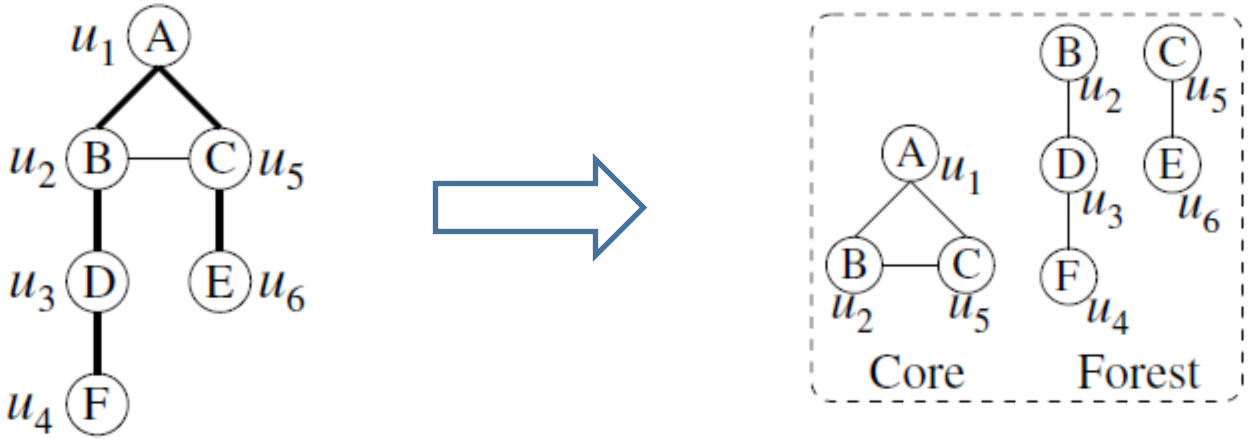
Matching order of **QuickSI** and **Turbo$_{\mathbf{ISO}}$** : (**u_1**, **u_2**, **u_3**, **u_4**, u_5, u_6).

Match dense subgraph first: (u_1, u_2, u_5, u_3, u_4, u_6)

Challenges of Subgraph Matching

Our Solution: Postpone Cartesian products.

- Decompose ***q*** into **a dense subgraph** and **a forest**, and process the dense subgraph first.



- The dense subgraph has **more edge-connectivity information**.

- **We are the first to exploit this feature**.

Challenges of Subgraph Matching

Challenge II: Exponential number of embeddings of query paths in a data graph.

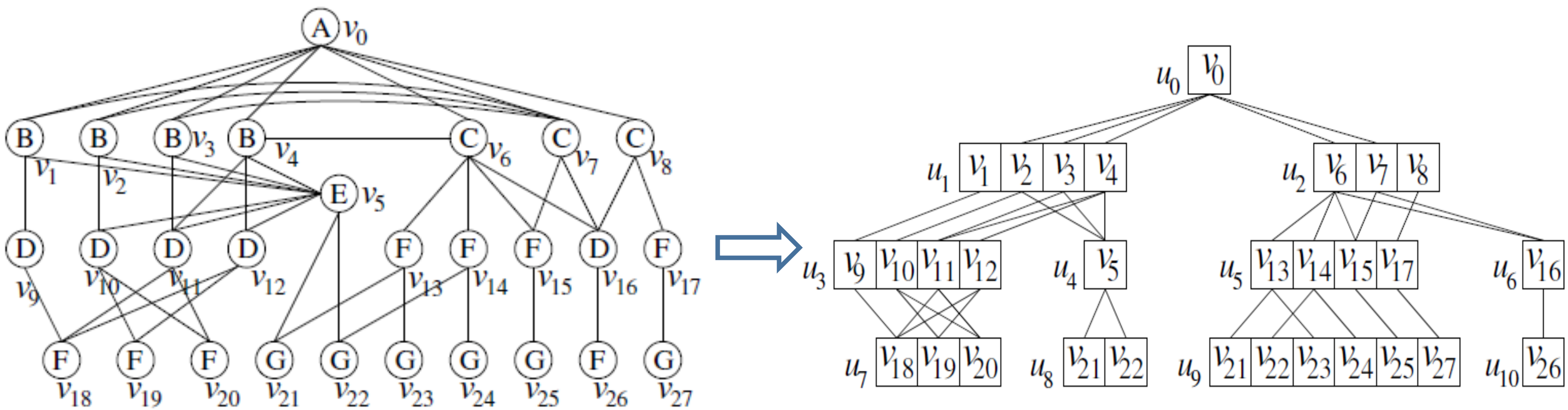
- Turbo$_{ISO}$ builds a data structure that materializes all embeddings of query paths in a data graph
  1. for generating matching order based on estimation of #candidates.
  2. for enumerating subgraph isomorphic embeddings.

- Effective only when the number of embeddings is small

- Worst-case space complexity: **$O(|V(G)|^{|v(q)-1|})$**.

Challenges of Subgraph Matching

Our Solution: We propose a **polynomial-size** data structure to avoid enumerating all embeddings of a query path in the data graph.



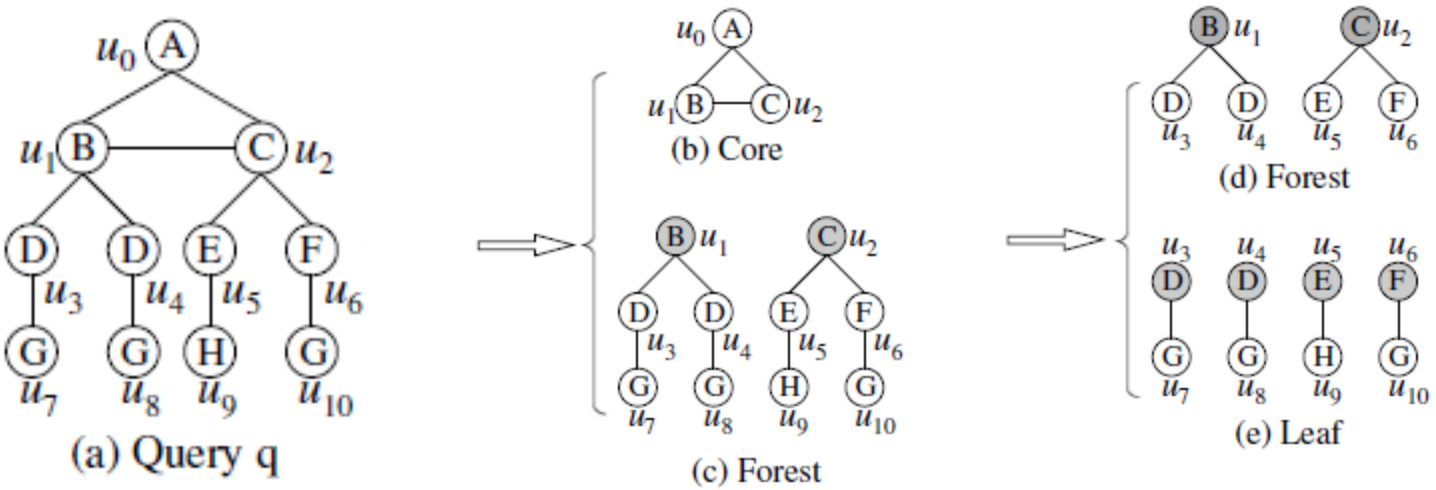
Our Approach

- CFL-Match
  - A Core-First Decomposition based Framework
  - Compact Path-Index (CPI) based Matching

Core-First Decomposition

- Core-Forest Decomposition

  Compute the **minimal connected** subgraph containing **all non-tree edges** of ***q*** regarding any spanning tree.

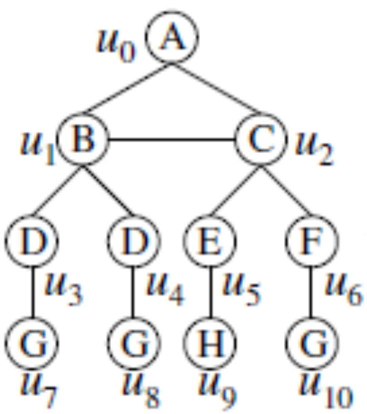


- Forest-Leaf Decomposition

  Compute the set of **leaf vertices** by rooting each tree at its connection vertex.

Framework

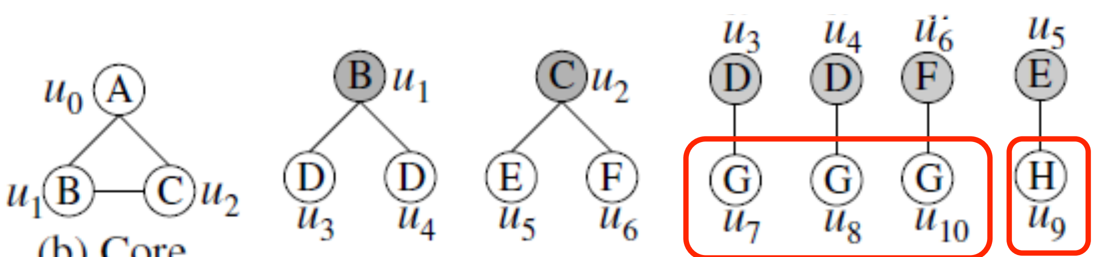
- **A Core-First Decomposition based Framework**
  1) Core-First (Core-Forest-Leaf) Decomposition



(a) Query q

Framework

- **A Core-First Decomposition based Framework**
  1) Core-First (Core-Forest-Leaf) Decomposition
  2) Mapping Extraction
     i. Core-Match
     ii. Forest-Match
     iii. Leaf-Match
        - Categorize leaf nodes according to labels
        - Perform combination instead of enumeration among different labels.

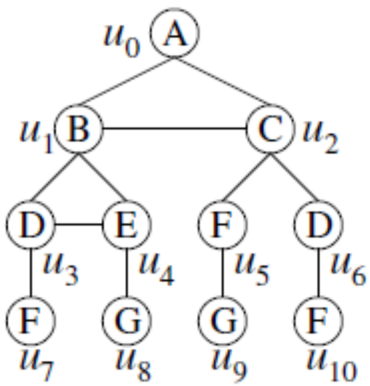


(b) Core (d) Forest (e) Leaf

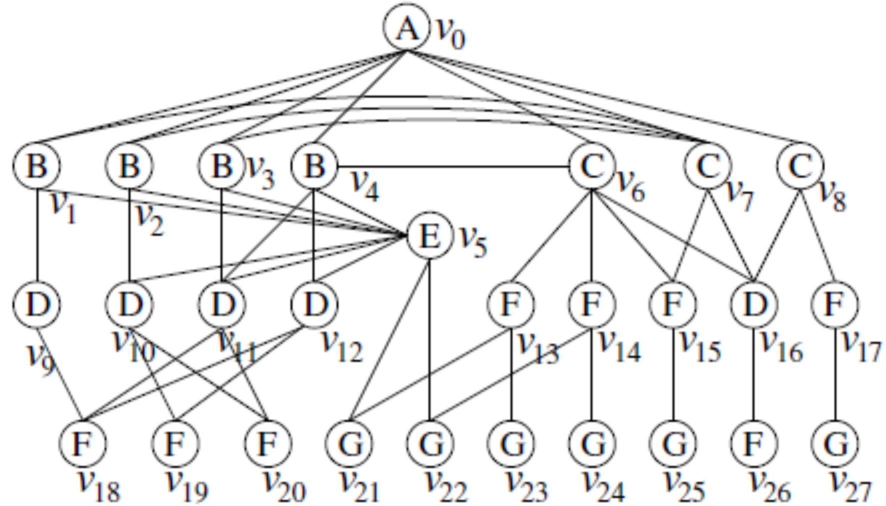
Compact Path-Index based Matching

- **Auxiliary Data Structure: Compact Path-Index (CPI)**
  - Compactly stores candidate embeddings of query spanning trees.
  - Prunes invalid candidates
  - Serves for computing an effective matching order.
    - Estimate #matches for each root-to-leaf query path based on CPI
    - Add query paths to the matching order in increasing order w.r.t. #matches

- **CPI Structure**



(a) Query q



(b) Data graph G

Compact Path-Index based Matching

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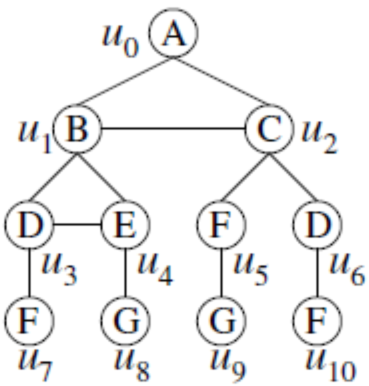
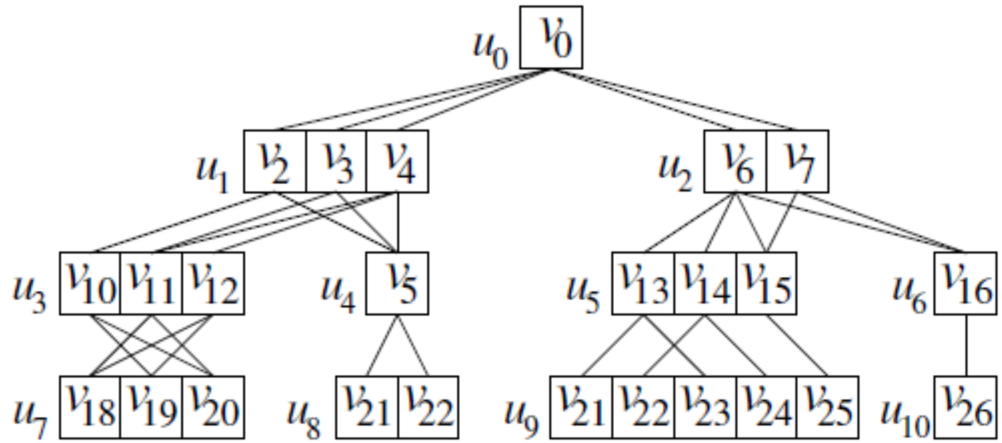
- **CPI Structure**



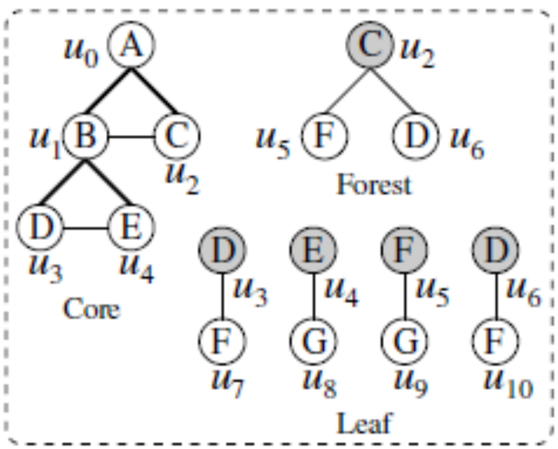
(a) Query q

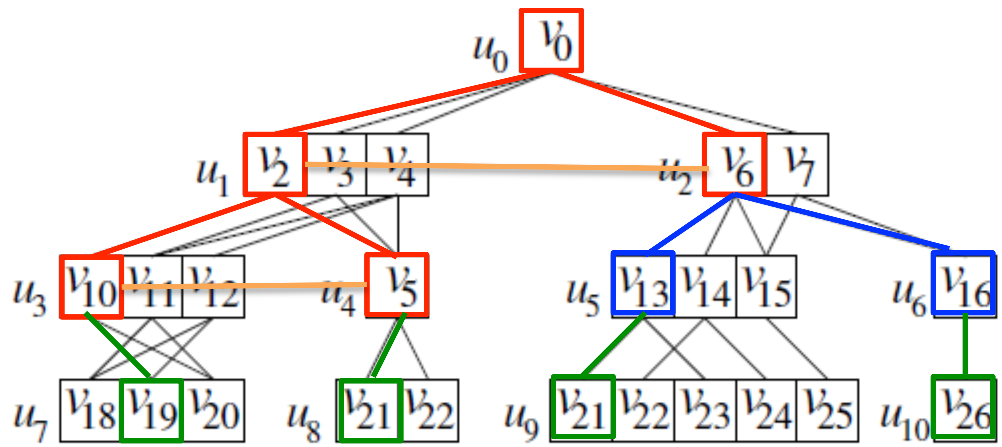


(c) CPI

CPI-based Matching

- **CPI Structure**
  - **Candidate set:** each query node ***u*** has a candidate set ***u.C***.
  - **Edge set:** there is an edge between ***v* ∈ *u.C*** and ***v' ∈ u'.C*** for adjacent query nodes ***u*** and ***u'*** in CPI if and only if ***(v, v')*** exists in ***G***.
- **Traverse CPI to find mappings for query vertices**





(c) CPI

$(u_0, u_1, u_4, u_3, u_2, u_5, u_6, u_7, u_8, u_9, u_{10})$

G is probed only for non-tree edge validation

Minimizing the CPI

- **Benefits of minimizing the CPI**
  - Less memory consumption
  - Fast embedding enumeration

- **Soundness of CPI**

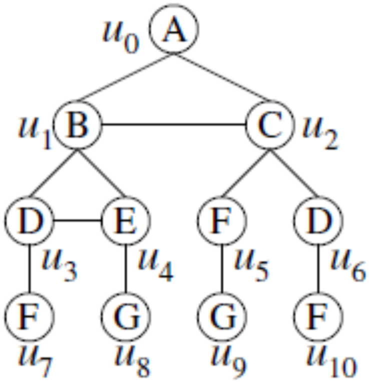
  For every query node ***u*** in CPI, if there is an embedding of ***q*** in ***G*** that maps ***u*** to ***v***, then ***v*** must be in ***u.C***.

Theorem

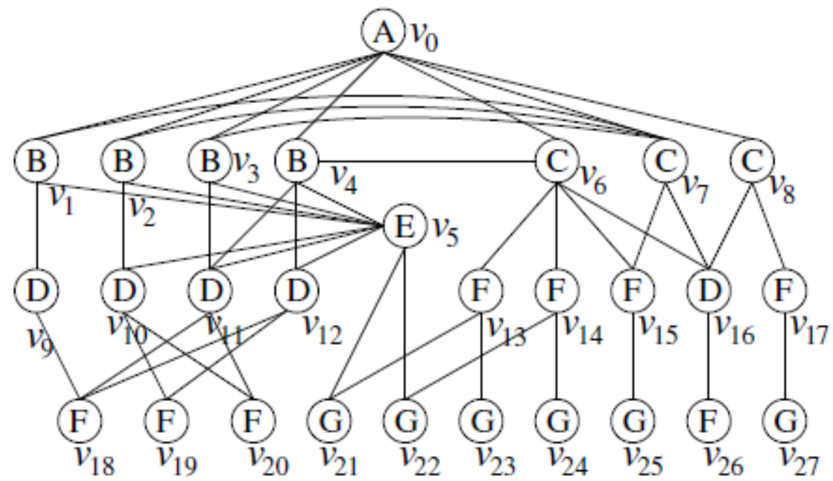
Given a sound CPI, all embeddings of ***q*** in ***G*** can be computed by **traversing only the CPI** while ***G*** is only probed for non-tree edge checkings.

- **It is NP-hard to build a minimum sound CPI.**

CPI Construction

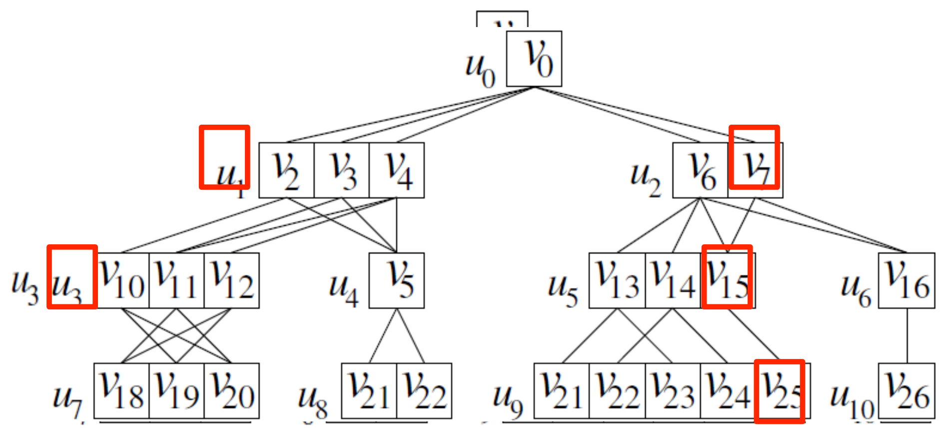


Query *q*



Data graph *G*

$\mathbf{v_9}$ is pruned from $u_3.C \leftarrow$ edge (u_3, u_4);
$\mathbf{v_1}$ is pruned from $u_1.C \leftarrow$ edge (u_1, u_3);
$\mathbf{v_8}$ is pruned from $u_2.C \leftarrow$ edge (u_1, u_2);
$\mathbf{v_{17}}$ is pruned from $u_5.C \leftarrow$ edge (u_2, u_5);
$\mathbf{v_{27}}$ is pruned from $u_9.C \leftarrow$ edge (u_5, u_9).



Auxiliary Data Structure / Compact Path Index

Build a small CPI

- **General Idea**
  - A heuristic approach:

    1) ***u.C*** is initialized to contain all vertices in ***G*** with the same label as ***u***

    2) A data vertex ***v*** is pruned from ***u.C*** ,

       if $\exists\, u' \in N_q(u)$, such that $\nexists v' \in N_G(v)$ & $v' \in u'.C$.

- **A two-phase CPI construction process:**
  - Top-down construction, bottom-up refinement
  - Exploit the pruning power of both directions of every query edge.
  - Construct CPI of **O(|E(G)| X |V(q)|)** size in **O(|E(G)| X |E(q)|)** time

Experiment

- All algorithms are implemented in C++ and run on a machine with 3.2G CPU and 8G RAM.
- **Datasets**
  - Real Graphs

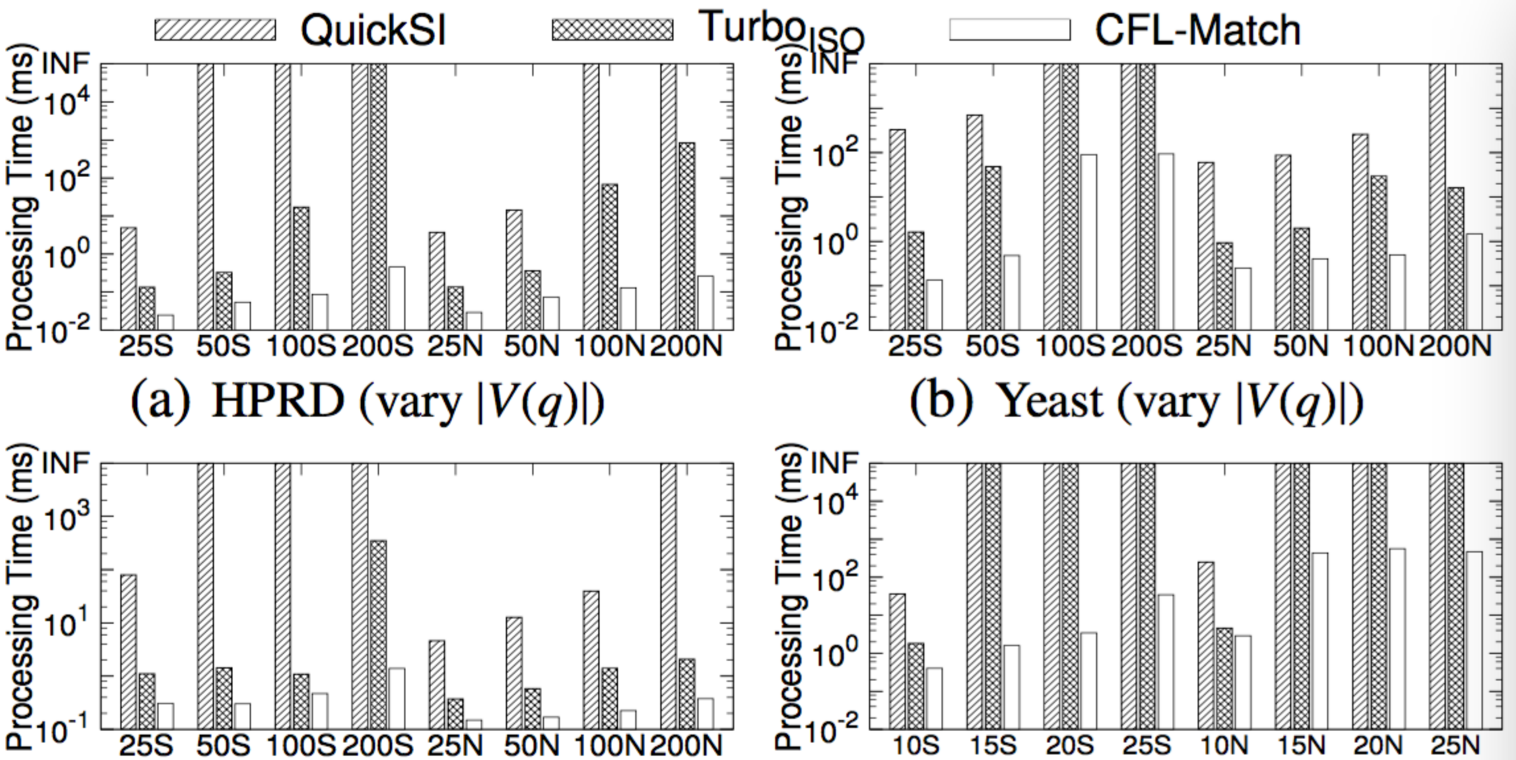
	|V|	|E|	|∑|	Degree
HPRD	9460	37081	307	7.8
Yeast	3112	12519	71	8.1
Human	4674	86282	44	36.9

  - Synthetic Graphs
    - Randomly generate graphs with 100k vertices with average degree 8 and 50 distinct labels.
- **Query Graphs**
  - Randomly generate by random walk
  - Two Categories:

    S: sparse (average degree ≤ 3). N: non-sparse (average degree > 3).

Comparing with Existing Techniques

CFL-Match: our proposed algorithm

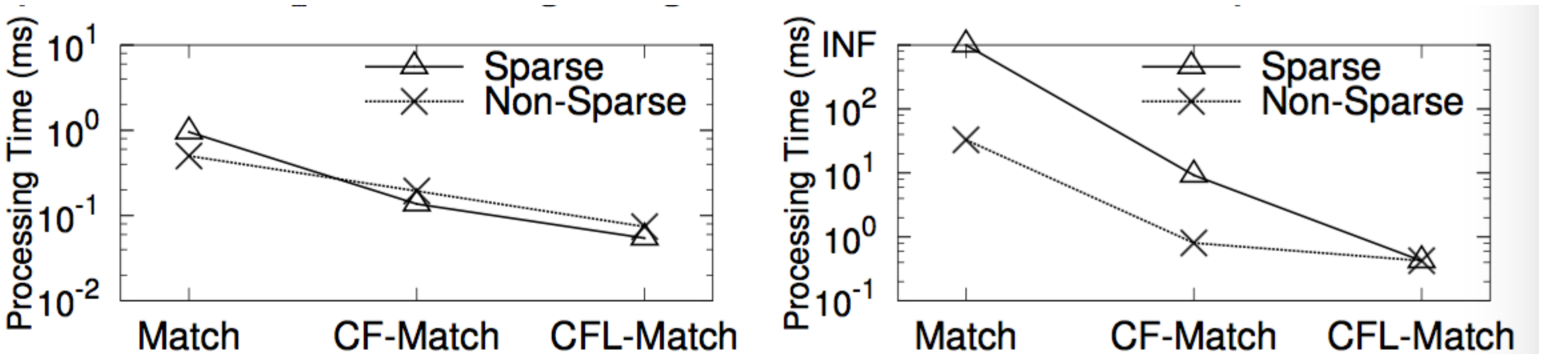


(a) HPRD (vary $|V(q)|$) (b) Yeast (vary $|V(q)|$)
(c) Synthetic (vary $|V(q)|$) (d) Human (vary $|V(q)|$)

Varying the size of query graph |V(q)|

Effectiveness of Our New Framework

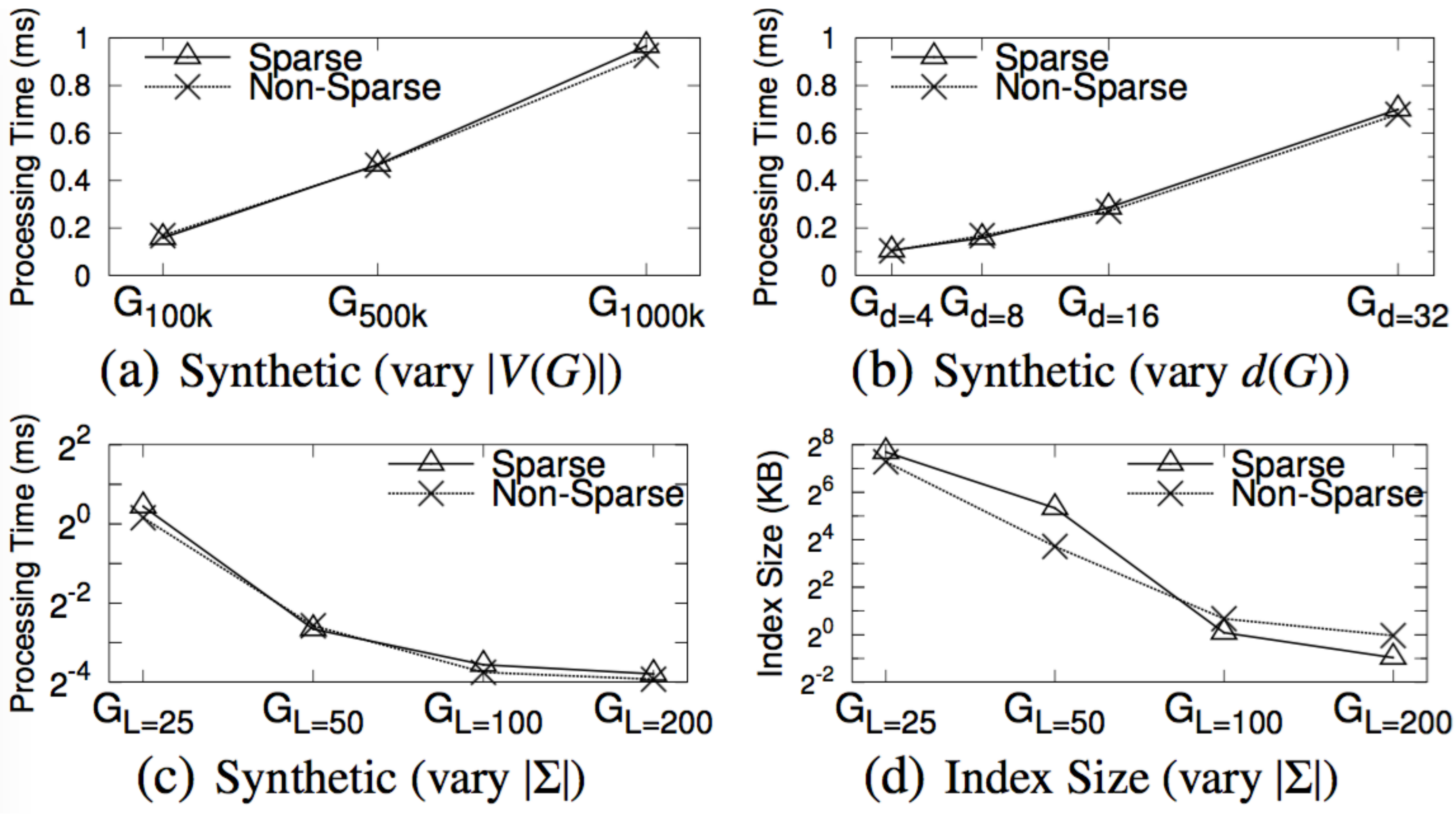
- Match: subgraph matching algorithm with CPI but no query decomposition.
- CF-Match: only core-forest decomposition with CPI.
- CFL-Match: our best algorithm.



(a) HPRD (vary algorithms) (b) Yeast (vary algorithms)

Evaluating our framework

Scalability Testing



(a) Synthetic (vary $|V(G)|$)

(b) Synthetic (vary $d(G)$)

(c) Synthetic (vary $|\Sigma|$)

(d) Index Size (vary $|\Sigma|$)

Conclusion

- A core-first framework for subgraph matching by postponing Cartesian products

- A new polynomial-size path-based auxiliary data structure CPI, and efficient and effective technique for constructing a small CPI

- Efficient algorithms for subgraph matching based on the core-first framework and the CPI

- Extensive empirical studies on real and synthetic graphs

Thank you!

Questions?

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