

#### **Graph Indexing: Tree + Delta >= Graph**

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#### **An Overview**

- Graph containment query
- The framework and query cost model
- Some existing path/graph based solutions
- A new tree-based approach
- Experimental studies
- Conclusion

## **Graph Containment Query**

• Given a graph database  $G = \{g_1, g_2, ..., g_N\}$  and a query graph q, find the set  $sup(q) = \{g_i | q \subseteq g_i, g_i \in G\}$ 



• Infeasible to check subgraph isomorphism for every  $g_i$  in *G*, because subgraph-isomorphism is NP-Complete.

#### **The Framework**

- Index construction generates a set of features, *F*, from the graph database *G*. Each feature, *f*, maintains a set of graph ids in *G* containing, *f*, *sup(f)*.
- Query processing is a *filtering-verification* process.
  - Filtering phase uses the features in query graph, q, to compute the *candidate set*.

$$C_q = \bigcap_{f \subseteq q \land f \in \mathcal{F}} sup(f)$$

• Verification phase checks subgraph isomorphism for every graph in  $C_q$ . False positives are pruned.

# **Query Cost Model**

- The cost of processing a graph containment query q upon G is modeled as  $C = C_f + |C_q| \times C_v$ 
  - $C_f$ : the filtering cost, and
  - $C_v$ : the verification cost (NP-Complete)
- Several Facts:
  - To improve query performance is to minimize  $|C_q|$ .
  - The feature set F selected has great impacts on  $C_f$  and  $|C_q|$ .
  - There is also an **index construction cost**, which is the cost of discovering the feature set F.

## **Existing Solutions: Paths vs Graphs**

- Path-based Indexing Approach: GraphGrep (*PODS'02*)
  - All paths up to a certain length  $l_p$  are enumerated as indexing features
    - An efficient index construction process
    - Index size is determined by  $I_p$
    - Limited pruning power, because the structural information is lost.
- Graph-based Indexing Approach: gIndex (*SIGMOD'04*)
  - Discriminative frequent subgraphs are mined from *G* as indexing features
    - A costly index construction process
    - Compact index structure
    - Great pruning power, because structural information is wellpreserved

- Regarding paths and graphs as index features:
  - The cost of generating **path** features is small but the candidate set can be large.
  - The cost of generating frequent **graph** features is high but the candidate set can be small.
- The key observation: the majority of frequent graph-features (more than 95%) are trees.
- How good can tree features do?

## A New Approach: Tree+ $\Delta$

- To explore indexability of path, tree and graph.
- A new approach Tree+ $\Delta$  :
  - To select frequent tree features.
  - To select a small number of discriminative graphfeatures that can prune graphs effectively, on demand, *without costly graph mining*.

## **Indexability of Path, Tree and Graph**

- We consider three main factors to answer indexability.
  - The frequent feature set size: |F|
  - The feature selection cost (mining):  $C_{FS}$
  - The candidate set size:  $|C_q|$

#### The Frequent Feature Set Size: |F|

- 95% of frequent graph features are trees. Why?
- Consider non-tree frequent graph features g and g'.
  - Based on Apriori principle, all g's subtrees, t<sub>1</sub>, t<sub>2</sub>, ..., t<sub>n</sub> are frequent.
  - Because of the structural diversity and vertex/edge label variety, there is a little chance that subrees of g coincide with those of g'.

#### **Frequent Feature Distributions**



The Real Dataset (AIDS antivirus screen dataset)  $N = 1,000, \sigma = 0.1$ 

## The Feature Selection Cost: C<sub>FS</sub>

- Given a graph database, G, and a minimum support threshold, σ, to discover the frequent feature set F from G.
  - *Graph*: two prohibitive operations are unavoidable
    - Subgraph isomorphism
    - Graph isomorphism
  - *Tree*: one prohibitive operation is unavoidable

- Tree-in-Graph testing

• *Path*: polynomial time

## The Candidate Set Size: $|C_q|$

• Let pruning power of a frequent feature, *f*, be

$$\mathsf{power}(f) = \frac{|\mathcal{G}| - |sup(f)|}{|\mathcal{G}|}$$

• Let pruning power of a frequent feature set  $S = \{f_1, f_2, ..., f_n\}$ 

$$\mathsf{power}(\mathcal{S}) = \frac{|\mathcal{G}| - |\bigcap_{i=1}^n sup(f_i)|}{|\mathcal{G}|}$$

• Let a frequent subtree feature set of graph, g, be

 $T(g) = \{t_1, t_2, ..., t_n\}.$  power(g)  $\ge$  power(T(g))

• Let a frequent subpath feature set of tree, t, be  $P(t) = \{p_1, p_2, ..., p_n\}$ . **power(t) \ge power(P(t))** 

**The Pruning Power** 



The Real Dataset (AIDS antivirus screen dataset) N = 1,000,  $\sigma = 0.1$ 

## **Indexability of Tree**

- The frequent tree-feature set dominates (95%).
- Discovering frequent tree-features can be done much more efficiently than mining frequent general graph-features.
- Frequent tree features can contribute similar pruning power as frequent graph features *do*.

## **Add Graph Features On Demand**

- Consider a query graph q which contains a subgraph g
  - If power(T(g)) ≈ power(g), there is no need to index the graph-feature g.
  - If power(g) >> power(T(g)), it needs to select g as an index feature, because g is more *discriminative* than T(g), in terms of pruning.
- Select discriminative graph-features on-demand, without mining the whole set of frequent graph-features from *G*.
  - The selected graph features are additional indexing features, denoted ∆, for later reuse.

## **Discriminative Ratio**

A discriminative ratio, ε(g), is defined to measure the similarity of pruning power between a graph-feature g and its subtrees T(g).

$$\varepsilon(g) = \begin{cases} \frac{\mathsf{power}(g) - \mathsf{power}(T(g))}{\mathsf{power}(g)} & \text{if } \mathsf{power}(g) \neq 0 \\ 0 & \text{if } \mathsf{power}(g) = 0 \end{cases}$$

A non-tree graph feature, g, is discriminative if
 ε(g) ≥ ε<sub>0</sub>.

## **Discriminative Graph Selection (1)**

- Consider two graphs g and g', where  $g \blacksquare g'$ .
  - If the gap between power(g') and power(g) is large, reclaim g' from G. Otherwise, do not reclaim g' in the presence of g.
- Approximate the *discriminative* between g' and g, in the presence of frequent tree-features discovered.

$$\begin{array}{ccc} sup(g)(?) & \overbrace{\phantom{aaaaa}}^? & sup(g')(?) \\ \\ \epsilon(g) \ge \epsilon_0 & & \uparrow \epsilon(g') \ge \epsilon_0 \\ \\ sup(\mathcal{T}_g) & \frac{|sup(\mathcal{T}(g))| \ge \sigma |\mathcal{G}|}{|sup(\mathcal{T}(g'))| \ge \sigma |\mathcal{G}|} & sup(\mathcal{T}_{g'}) \end{array}$$

#### **Discriminative Graph Selection (2)**

• Let *occurrence probability* of g in the graph DB be

$$Pr(g) = \frac{|sup(g)|}{|\mathcal{G}|} = \sigma_g$$

• The *conditional occurrence probability* of g', w.r.t.

g:  

$$Pr(g'|g) = \frac{Pr(g \land g')}{Pr(g)} = \frac{Pr(g')}{Pr(g)} = \frac{|sup(g')|}{|sup(g)|}$$

 When Pr(g'|g) is small, g' has higher probability to be discriminative w.r.t. g.

#### **Discriminative Graph Selection (3)**

• The upper and lower bound of Pr(g'|g) become

$$Pr(g'|g) = \frac{|sup(g')|}{|sup(g)|} \le \frac{|\mathcal{G}| - \frac{|\mathcal{G}| - |sup(\mathcal{T}(g')|)}{1 - \epsilon_0}}{\sigma |\mathcal{G}|} = \frac{\sigma_{\mathcal{T}(g')} - \epsilon_0}{(1 - \epsilon_0)\sigma}$$
$$Pr(g'|g) = \frac{|sup(g')|}{|sup(g)|} \ge \frac{\sigma |\mathcal{G}|}{|\mathcal{G}| - \frac{|\mathcal{G}| - |sup(\mathcal{T}(g)|)}{1 - \epsilon_0}} = \frac{\sigma(1 - \epsilon_0)}{\sigma_{\mathcal{T}(g)} - \epsilon_0}$$

because  $\varepsilon(g) \ge \varepsilon_0$  and  $\varepsilon(g') \ge \varepsilon_0$ . recall:  $\sigma_x = |\sup(x)| / |G|$ 

#### **Discriminative Graph Selection (4)**

Because 0 ≤ Pr(g'|g) ≤ 1, the conditional occurrence probability of Pr(g'|g), is solely upper-bounded by T(g').

$$\sigma_{\mathcal{T}(g)} \ge \max\{\epsilon_0, \sigma + (1 - \sigma)\epsilon_0\}$$
$$\max\{\epsilon_0, \sigma\} \le \sigma_{\mathcal{T}(g')} \le \sigma + (1 - \sigma)\epsilon_0$$
$$(\sigma_{\mathcal{T}(g)} - \epsilon_0)(\sigma_{\mathcal{T}(g')} - \epsilon_0) \ge [\sigma(1 - \epsilon_0)]^2$$

## An Experimental Study

- We compared our Tree+∆ with **gIndex** (X. Yan, P.S. Yu, and J. Han, SIGMOD'04) and **C-Tree** (H. He and A.K. Singh, ICDE'06).
- We used AIDS Antiviral Screen Dataset from the Developmental Theroapeutics Program in NCI/NH (http://dtp.nci.nih.gov/docs/aids/aids\_data.html)
  - $\frac{1}{1000} + \frac{1}{100} + \frac{1$
  - 42,390 compunds from DTD's Drug Information System.
  - 63 kinds of atoms (vertex labels).
  - On average, a compond has 43 vertices and 45 edges.
  - At max, 221 vertices and 234 edges.
- We also used the graph generator (M. Kuramochi and G. Karypis, ICDM'01).
- We tested on a 3.4GHz Intel PC with 2GB memory.

#### **Index Construction (Real Dataset)**



**Feature Size** 





#### **Real Dataset: False Positive Ratio** (|Cq|/|sup(q)|)



N=1,000

## Conclusion

- Tree is an effective and efficient graph indexing feature to answer graph containment queries.
- We analyze the indexibility for tree features.
- We propose a Tree+∆ approach that holds a compact index structure, achieves better performance in index construction, and provides satisfactory query performance for answering graph containment queries.