FINDING TOPOLOGICAL FREQUENT PATTERNS FROM GRAPH DATASETS

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Assumptions on graphs

- Undirected
- Connected
- Labeled vertices and edges (not necessarily uniquely)

Graph isomorphism

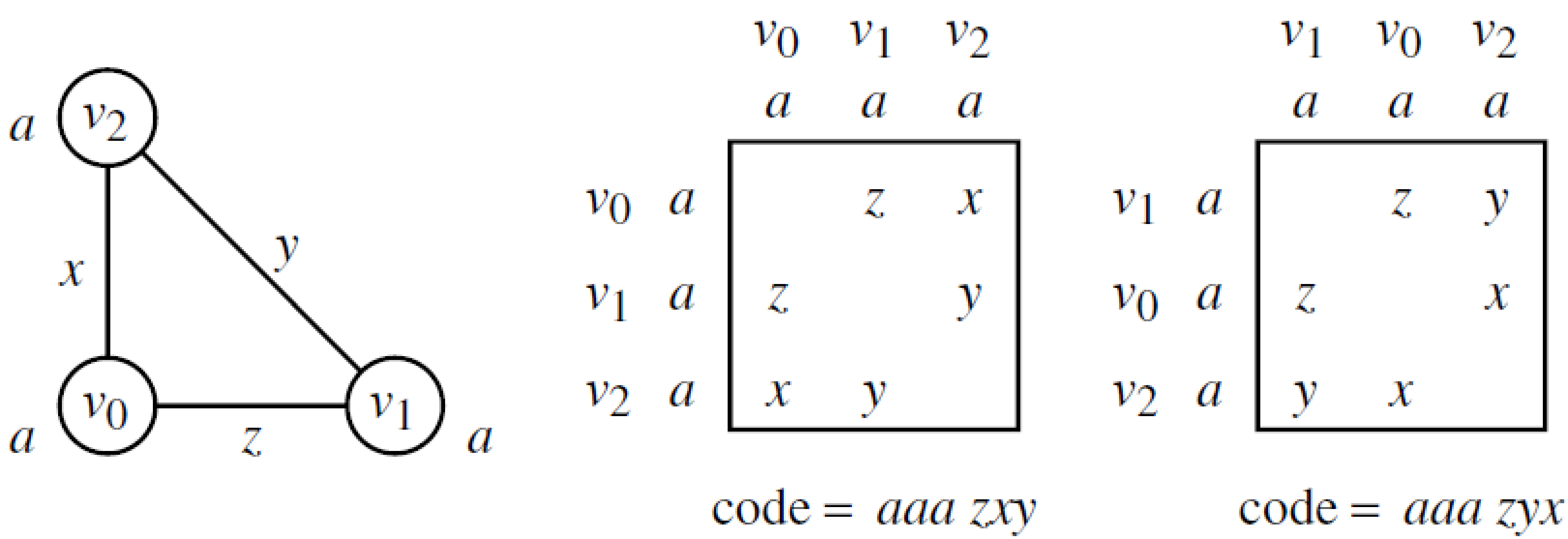
- Subgraph isomorphism
  - Given two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, find an isomorphism between G_2 and a subgraph of G_1 (≈ determine whether or not G_2 is included in G_1)

Graph isomorphism

- Canonical labeling
  - Unique code for the set of graphs with the same topological structure and the same labeling
  - In most cases:
    - Flattened representation of the adjacency matrix
    - Try all permutations in order to find minimum (or maximum) according to lexicographic ordering

Graph isomorphism

- Simple examples of codes and canonical adjacency matrices (from FSG):



(a) G^3 (b) (c)

Graph isomorphism

- Both problems are not known to be either in P or in NP-complete
  - In practice: complexity of canonical labeling is reduced by using various heuristics and properties in set of graphs

Two forms of the input

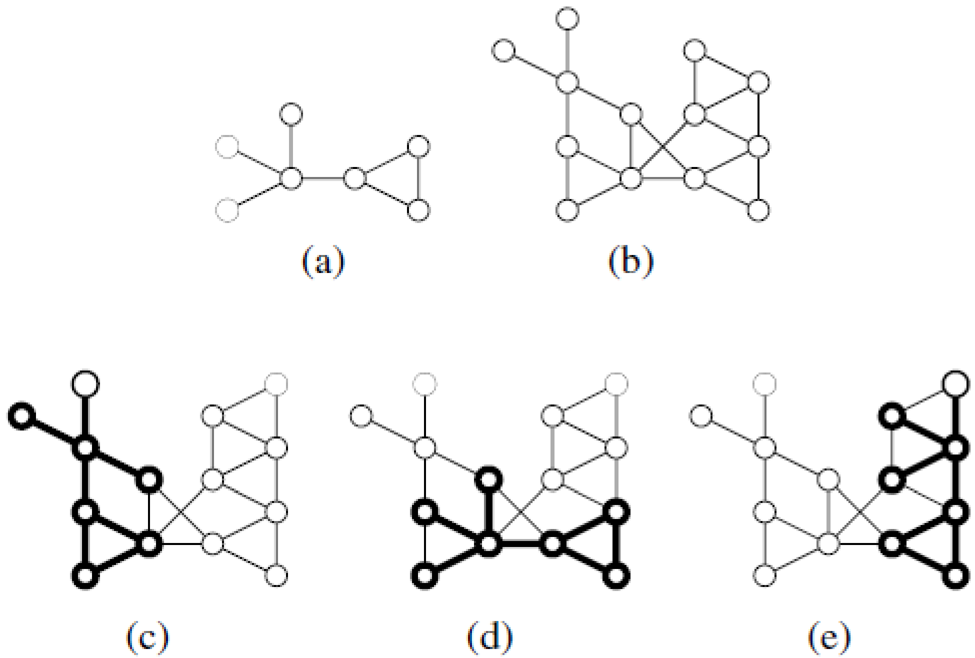
- *Graph-transaction setting*
  - Set of relatively small graphs (*transactions*)
  - Frequency (of a pattern): number of graph transactions that the pattern occurs in

Two forms of the input

- *Single-graph setting*
  - One large graph
  - Frequency: number of pattern occurrences in the single graph.
  - Counting the frequency of edge-disjoint embeddings (using *maximum independent set*)
  - Algorithms can be adapted to solve the first group
  - Examples of algorithms: SUBDUE, SEuS, GREW, SIGRAM, GBI
  - Not discussed further

Two forms of the input

Example:



Overlapped embeddings: (a) subgraph, (b) input graph, (c) embedding 1, (d) embedding 2, (e) embedding 3

Completeness of algorithms

- Complete algorithms
  - All frequent patterns that satisfy a given specification (e.g. minimum support threshold)
  - May become unfeasible
- Heuristic algorithms
  - Return only a subset of all frequent patterns (approximate solution)

Apriori-based algorithms

- FSG [3]
  - Complete
  - Transactional setting, connected graphs
  - Level-by-level expansion as in Apriori
  - Features:
    1. Sparse graph representation
    2. Adding one edge at a time
    3. Using canonical labeling and graph isomorphism
    4. Scales (linearly) with the database size

Apriori-based algorithms

- FFSM (Fast Frequent Subgraph Mining) [4]
  - Canonical form: appended columns from adjacency matrix
  - Competitive with gSpan
  - Algebraic graph framework

Apriori-based algorithms

- AGM (Apriori-based Graph Mining) [5]
  - Code of Adjacency Matrix

$$X_k = \begin{pmatrix} x_{1,1} & x_{1,2} & x_{1,3} & \cdots & x_{1,k} \\ x_{2,1} & x_{2,2} & x_{2,3} & \cdots & x_{2,k} \\ x_{3,1} & x_{3,2} & x_{3,3} & \cdots & x_{3,k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_{k,1} & x_{k,2} & x_{k,3} & \cdots & x_{k,k} \end{pmatrix}$$

$$code(X_k) = x_{1,1}x_{1,2}x_{2,2}x_{1,3}x_{2,3}x_{3,3}x_{1,4}\cdots x_{k-1,k}x_{k,k},$$

- AcGM [6]
    - Complete search of frequent connected (induced) subgraphs in a massive labeled graph dataset within highly practical time

Apriori-based algorithms

- Warmr [7]
  - ILP data mining algorithm
  - Datalog to represent both data and patterns
  - Patterns can reflect one-to-many and many-to-many relationships

Pattern growth algorithms

- gSpan (graph-based Substructure pattern mining) [8]
  - Without candidate generation
  - Adopts depth-first search strategy to mine frequent connected subgraphs
  - Canonical labeling based on DFS traversing of graph
  - Outperforms FSG

Pattern growth algorithms

- GASTON (GrAph/Sequence/Tree extractiON) [9]
  - "Quickstart principle"
    - Various substructures are contained in each other
    - First consider paths, then transform them to trees and finally transform trees to graphs
    - More efficient algorithms for simple substructures, advanced algorithms only when really needed
  - Observation: most frequent substructures in practical graph databases are free trees (trees with no vertex designated as a root)

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