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Inter-University Research Institute Corporation /
Research Organization of Information and Systems
National Institute of Informatics

Graph Mining

Data Mining 03 (データマイニング)

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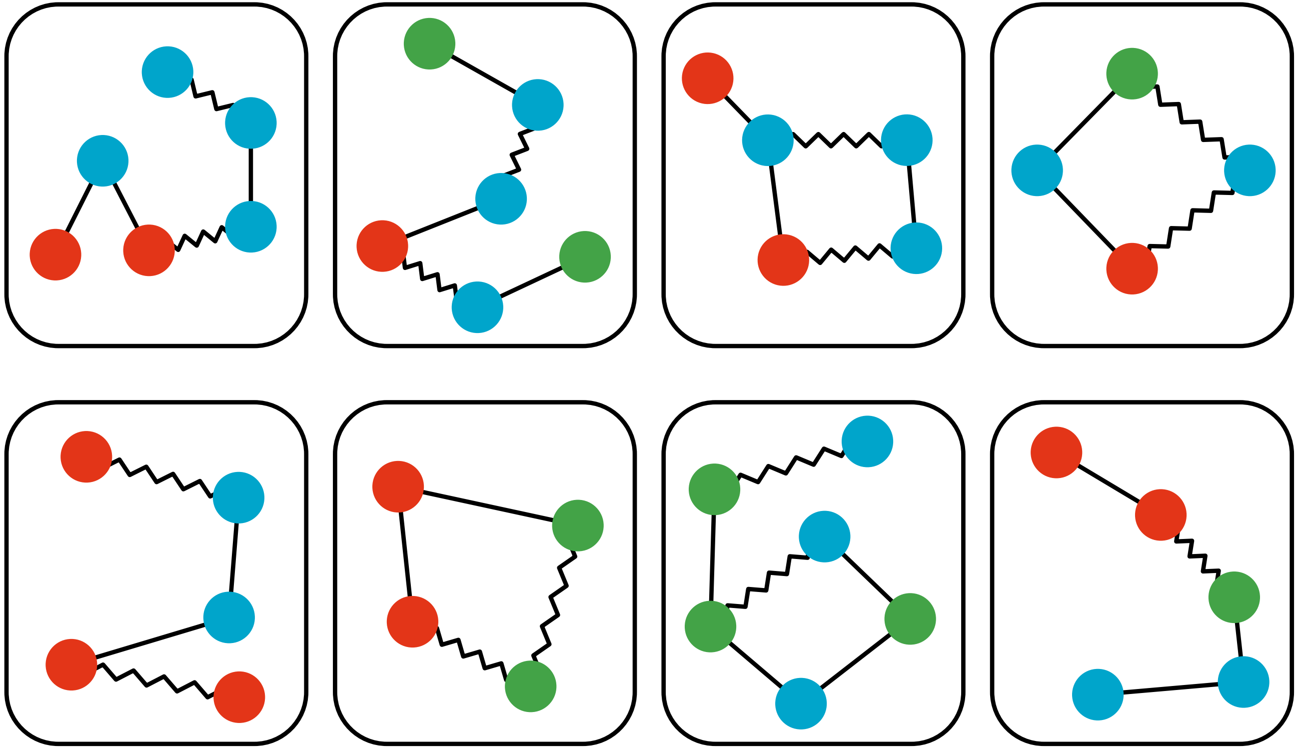
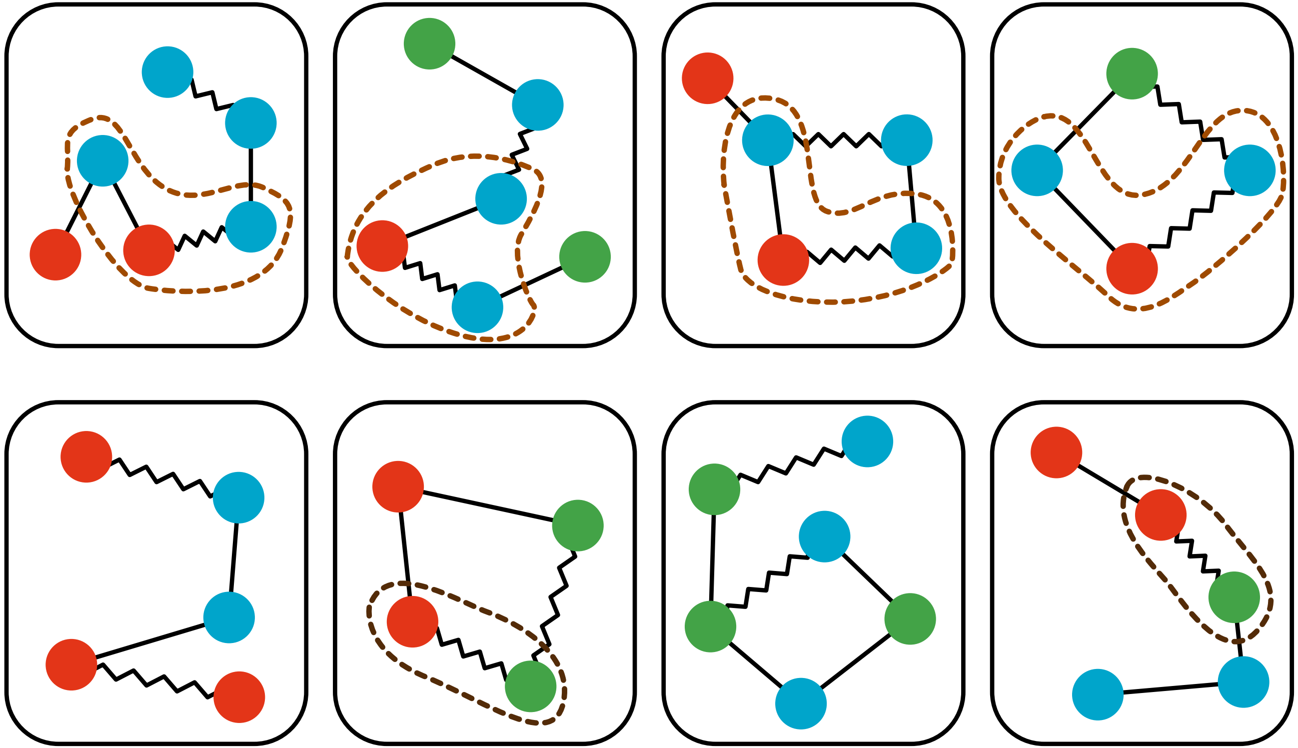
Today's Outline

- A primer of graphs
  - Subgraph isomorphism
- Graph mining
  - How to find (sub)graphs from graph databases?
  - Revisiting the Apriori principle to avoid combinatorial explosion
  - The canonical DSF code for graph representation

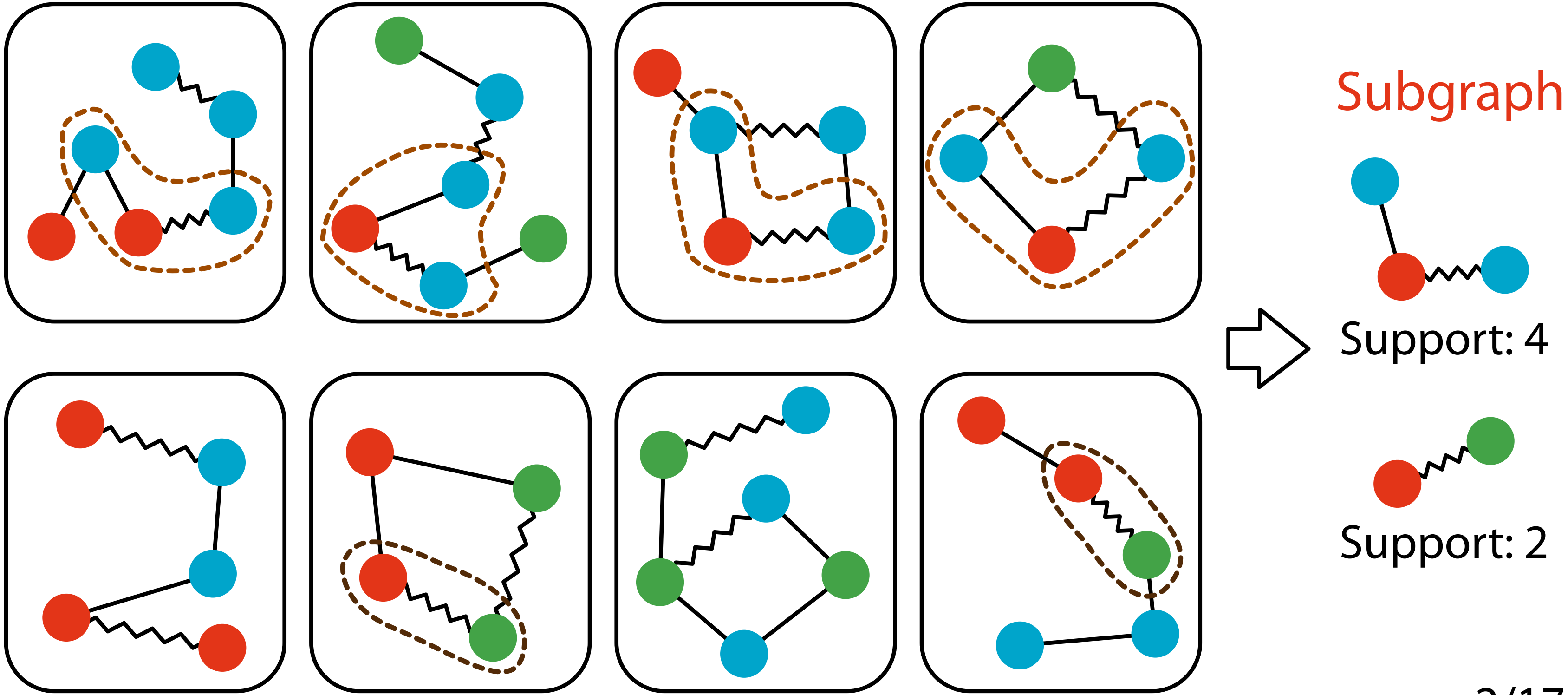
Graph Mining: Overview



Graph Mining: Overview



Graph Mining: Overview



Graphs

- An (unlabeled) graph $G = (V, E)$
  - V: a vertex set, $E \subseteq V \times V$: an edge set
  - For $(u, v) \in E$, u, v are adjacent, v is a neighbor of u
    - (u, v) and (v, u) are identified if the graph is undirected
  - $N(v) = \{u \in V \mid (v, u) \in E\}$, the set of all neighbors

- A labeled graph $G = (V, E, \varphi)$
  - $\varphi : V \cup E \to \Sigma$, where Σ is the set of vertex and edge labels

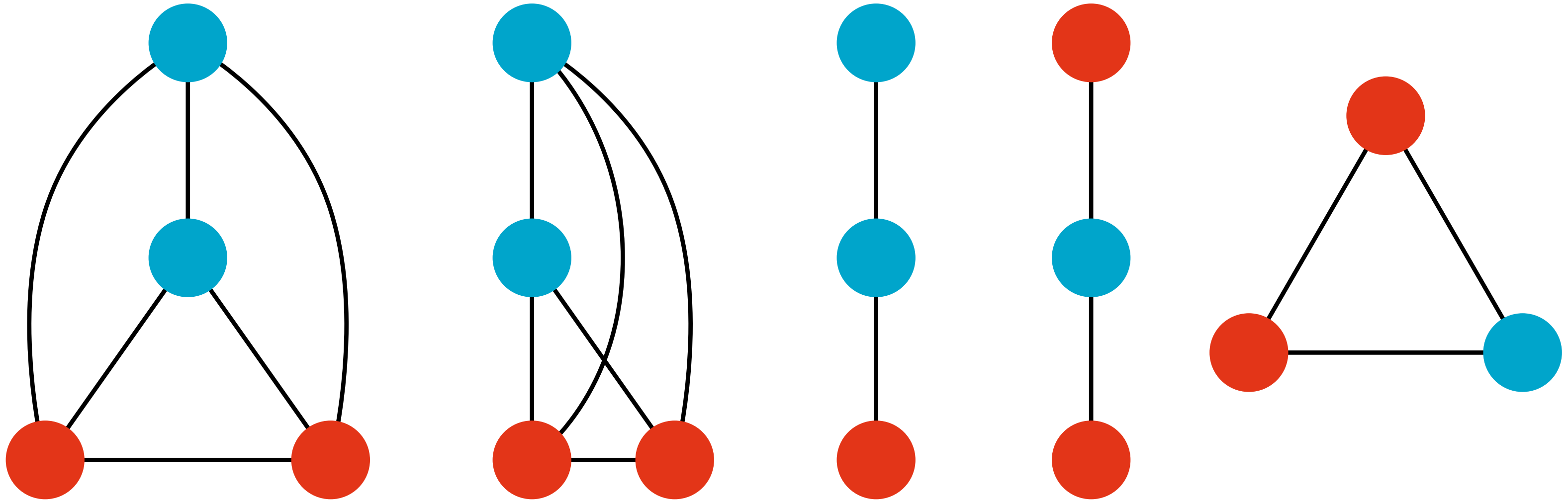
Subgraph Isomorphism

- A graph $G' = (V', E')$ is a subgraph of $G = (V, E)$, denoted by $G' \sqsubseteq G$, if $V' \subseteq V$ and $E' \subseteq (V' \times V') \cap E$

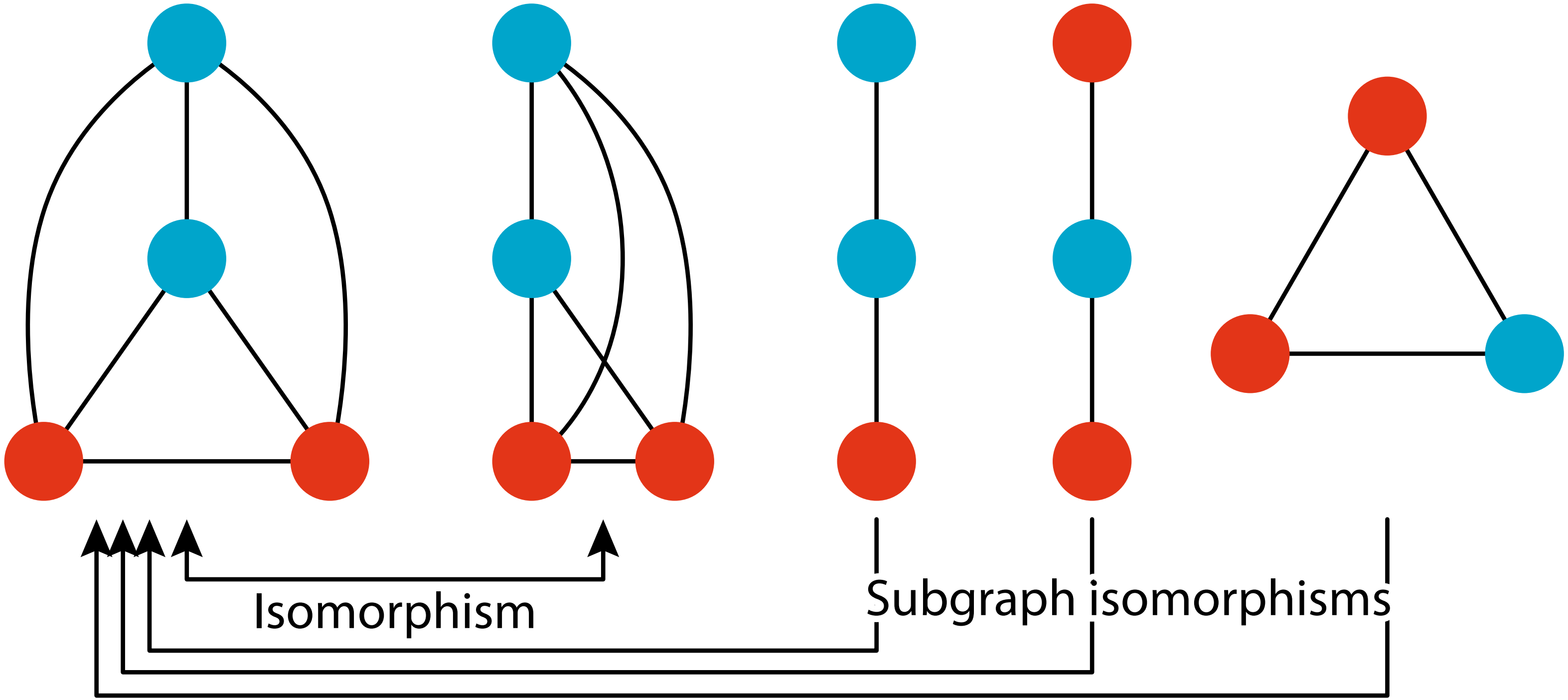
- A graph G' is isomorphic to G if there exists a bijective function $\pi : V' \to V$ such that
  (i) $(u, v) \in E' \iff (\pi(u), \pi(v)) \in E$
  (ii) $\forall v \in V', \varphi(v) = \varphi(\pi(v))$
  (iii) $\forall (u, v) \in E', \varphi(u, v) = \varphi(\pi(u), \pi(v))$

- If π is injective but not surjective: $G \setminus \mathrm{range}(\pi) \neq \emptyset$, G' is subgraph isomorphic to G, denoted by $G' \sqsubseteq G$
  - Testing whether $G' \sqsubseteq G$ is NP-complete (computationally heavy!)

Subgraph Isomorphism



Subgraph Isomorphism



Subgraph Mining

- In graph mining, pattern $\iff$ (sub)graph
- S: the set of graphs (can be infinite), a dataset D is a multiset of S
  - D is a collection of graphs: $D = \{G_1, G_2, \ldots, G_n\}$
- The frequency $\eta(G)$ of a graph G is obtained as

$$\eta(G) = \frac{|\{G_i \in D \mid G \sqsubseteq G_i\}|}{|D|} = \frac{1}{|D|} \sum_{H \sqsupseteq G} \mathbf{1}_D(H)$$

- **Frequent subgraph mining problem:**
  Given a threshold σ, enumerate the set $F = \{G \in S \mid \eta(G) \geq \sigma\}$

Two Problems in Graph Mining

1. Combinatorial explosion of the search space
   - More massive than itemset mining
   - The number of subgraphs with m vertices: $O(2^{m^2})$
     - $O(m^2)$ possible edges
   - The number of subgraphs with m vertices and s labels: $O(s^{m^2})$
2. Subgraph isomorphism checking
   - When we obtain a subgraph G', computing $\eta(G')$ is heavy as we need to repeat subgraph isomorphism checking for every $G_i \in D$

- **Solution:** Use the Apriori principle and the (canonical) DFS code

Graph Mining Algorithms

- The first algorithm that achieves graph mining is AGM
  - Inokuchi, A. and Washio, T. and Motoda, H., **An Apriori-Based Algorithm for Mining Frequent Substructures from Graph Data**, PKDD 2000
- The standard method is gSpan
  - Yan, X. and Han, J., **gSpan: Graph-based substructure pattern mining**, ICDM 2002
- The state-of-the-art is GASTON
  - Nijssen, S. and Kok, J. N., **A Quickstart in Frequent Structure Mining Can Make a Difference**, SIGKDD 2004

DFS Code (1/3)

- The DFS code represents a graph G as a sequence of tuples based on depth first search (DFS)
  - There can be multiple DFS codes for a single graph
- Perform DFS traversal on a graph G and index each vertex according to the order of discovery in the DFS
  - Edges included in the DFS are forward edges, other edges are backward edges
- Each edge (i, j) is represented as a tuple $(i, j, \varphi(i), \varphi(j), \varphi(i, j))$
  - $i < j$ is it is a forward edge and $i > j$ if backward

DFS Code (2/3)

- Introduce the (total) order "$<_t$" between two tuples $t_1 = (i_1, j_1, \varphi(i_1), \varphi(j_1), \varphi(i_1, j_1))$ and $t_2 = (i_2, j_2, \varphi(i_2), \varphi(j_2), \varphi(i_2, j_2))$
- First, introduce the order $<_e$ between $e_1 = (i_1, j_1)$ and $e_2 = (i_2, j_2)$:
  $e_1 <_e e_2 \iff$
  - If both e_1 and e_2 are forward edges, (a) $j_1 < j_2$ or (b) $j_1 = j_2$ and $i_1 > i_2$
  - If both e_1 and e_2 are backward edges, (a) $i_1 < i_2$ or (b) $i_1 = i_2$ and $j_1 < j_2$
  - If e_1 and e_2 are forward and backward edges, $i_1 < j_2$
  - If e_1 and e_2 are backward and forward edges, $j_1 < i_2$
- $(\varphi(i_1), \varphi(j_1), \varphi(i_1, j_1)) <_l (\varphi(i_2), \varphi(j_2), \varphi(i_2, j_2)) \iff$ $\varphi(i_1) < \varphi(i_2)$, $\varphi(j_1) < \varphi(i_1)$, and $\varphi(i_1, j_1) < \varphi(i_2, j_2)$

DFS Code (3/3)

- $t_1 = (i_1, j_1, \varphi(i_1), \varphi(j_1), \varphi(i_1, j_1)) <_t t_2 = (i_2, j_2, \varphi(i_2), \varphi(j_2), \varphi(i_2, j_2)) \iff$

  (i) $(i_1, j_1) <_e (i_2, j_2)$, or
  (ii) $(i_1, j_1) = (i_2, j_2)$ and $(\varphi(i_1), \varphi(j_1), \varphi(i_1, j_1)) <_l (\varphi(i_2), \varphi(j_2), \varphi(i_2, j_2))$

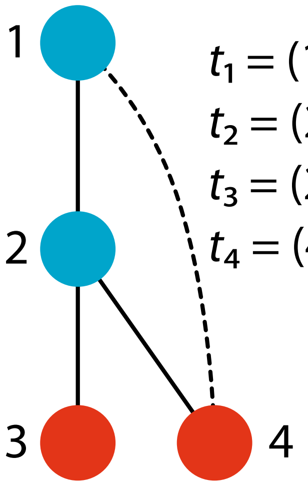
- The DFS code of a graph is a sequence of tuples sorted according to the order "<"

Canonical DFS Code

- Finally, introduce the order $<$ between two DFS codes $\boldsymbol{t} = (t_1, t_2, \dots, t_m)$ and $\boldsymbol{t}' = (t'_1, t'_2, \dots, t'_n)$
- $\boldsymbol{t} < \boldsymbol{s} \iff$ (i) or (ii)
  - (i) $\exists k$ s.t. $0 \le k \le \min(m, n)$, $t_1 = t'_1,\ t_2 = t'_2,\ \dots,\ t_{k-1} = t'_{k-1},\ t_k < t'_k$
  - (ii) $m \le n$ and $t_1 = t'_1,\ t_2 = t'_2,\ \dots,\ t_m = t'_m$
- The canonical DFS code of a graph G is the smallest DFS code of G according to the order "$<$"

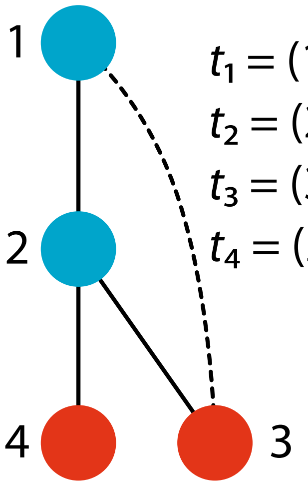
Canonical DFS Code

Canonical



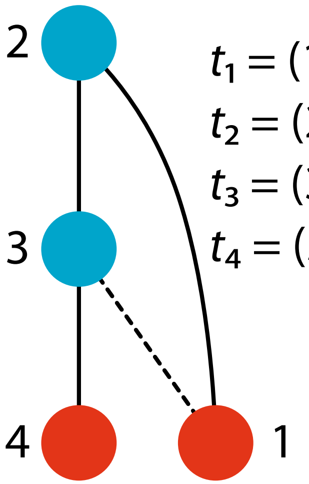
$t_1 = (1, 2, {\color{cyan}\bullet}, {\color{cyan}\bullet})$
$t_2 = (2, 3, {\color{cyan}\bullet}, {\color{red}\bullet})$
$t_3 = (2, 4, {\color{cyan}\bullet}, {\color{red}\bullet})$
$t_4 = (4, 1, {\color{red}\bullet}, {\color{cyan}\bullet})$

Noncanonical



$t_1 = (1, 2, {\color{cyan}\bullet}, {\color{cyan}\bullet})$
$t_2 = (2, 3, {\color{cyan}\bullet}, {\color{red}\bullet})$
$t_3 = (3, 1, {\color{red}\bullet}, {\color{cyan}\bullet})$
$t_4 = (2, 4, {\color{cyan}\bullet}, {\color{red}\bullet})$

Noncanonical



$t_1 = (1, 2, {\color{red}\bullet}, {\color{cyan}\bullet})$
$t_2 = (2, 3, {\color{cyan}\bullet}, {\color{cyan}\bullet})$
$t_3 = (3, 4, {\color{cyan}\bullet}, {\color{red}\bullet})$
$t_4 = (3, 1, {\color{cyan}\bullet}, {\color{red}\bullet})$

Rightmost Path Extension

- During the DFS traversal on a graph G, the rightmost path is the path from the root to the rightmost leaf (leaf with the largest index)

- Rightmost path extension achieves systematic candidate graph generation from an existing graph G by either
  (i) adding a backward edge from the rightmost vertex to other vertex on the rightmost path, or
  (ii) adding a forward edge from a vertex on the rightmost path

The gSpan Algorithm

Algorithm 1: Algorithm gSpan

// $C \leftarrow \varnothing$ for the initial call

gSpan(C, D, σ)

    $\mathcal{E} \leftarrow$ RightmostPathExtension(G, D)

    foreach $(t, \eta_t) \in \mathcal{E}$ **do**

        $C \leftarrow C \cup \{t\}$

        $\eta(C) \leftarrow \eta_t$

        if $\eta(C) > \sigma$ *and* isCanonical(C) **then**

            gSpan(C, D, σ)

Subprocesses in gSpan

- RightmostPathExtension(G, D)
  - Receive a graph G and a dataset D
  - Return all possible rightmost path extensions of G
    - A set of pairs of tuples and frequencies $\mathcal{E} = \{(t_1, \eta_{t_1}), (t_2, \eta_{t_2}), \ldots, (t_m, \eta_{t_m})\}$
- isCanonical(C)
  - Receive a DFS code C
  - Return TRUE if C is canonical and FALSE otherwise

Conclusion

- gSpan achieves graph mining
- The keys are:
  - Canonical DFS codes
  - Rightmost path extension
  - Combine them with the Apriori principle