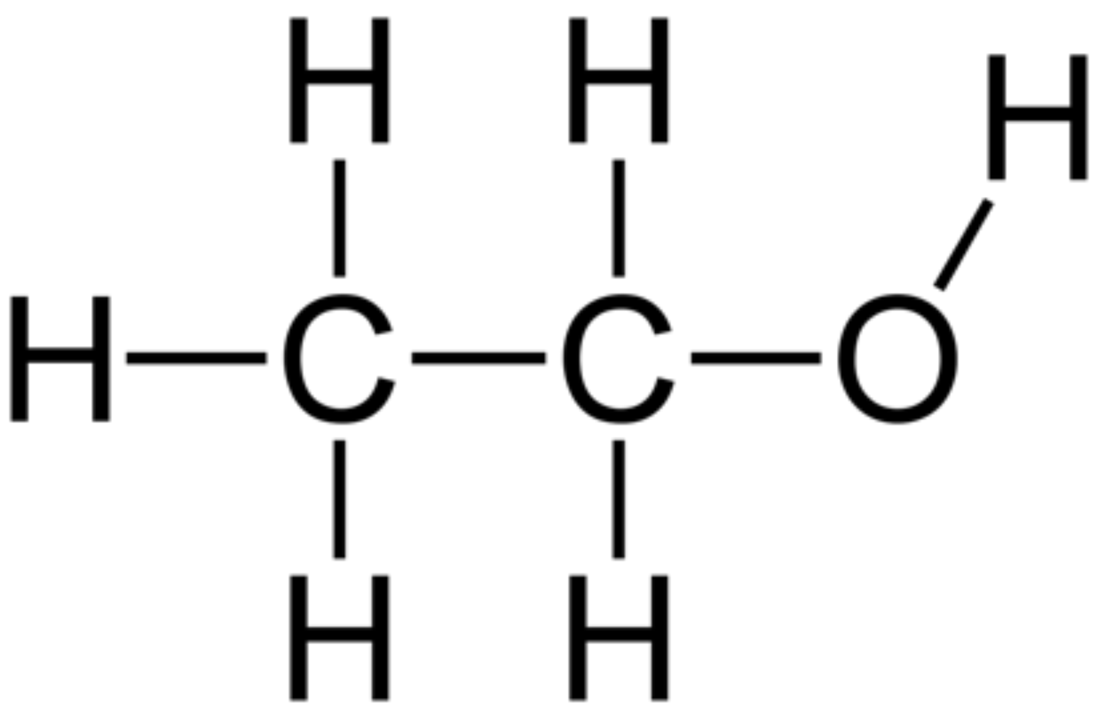
Topic II.1: Frequent Subgraph Mining

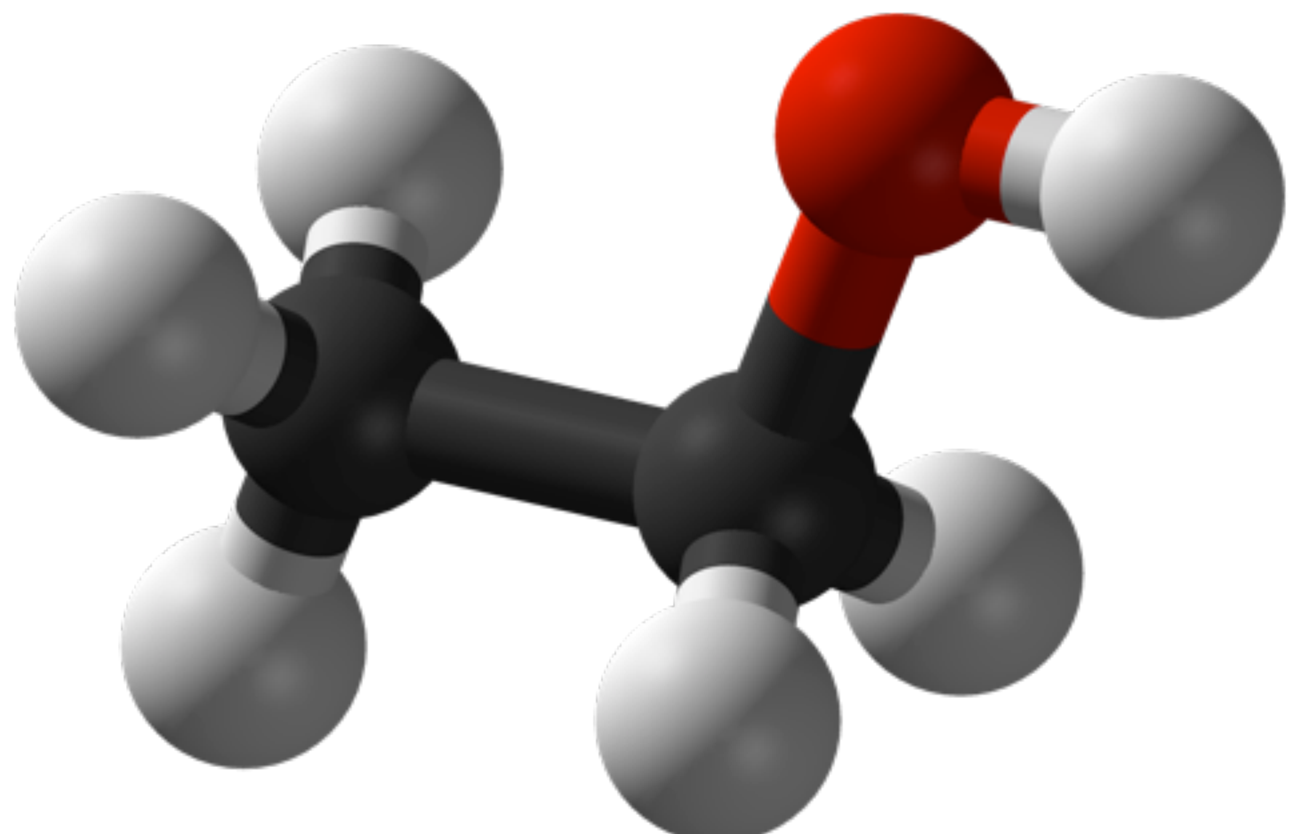
Discrete Topics in Data Mining
Universität des Saarlandes, Saarbrücken
Winter Semester 2012/13

TII.1: Frequent Subgraph Mining

Definitions and Problems

- The data is a set of graphs $D = \{G_1, G_2, \ldots, G_n\}$
  - Directed or undirected
- The graphs G_i are *labelled*
  - Each vertex v has a label $L(v)$
  - Each edge $e = (u, v)$ has a label $L(u, v)$
- Data can be e.g. molecule structures





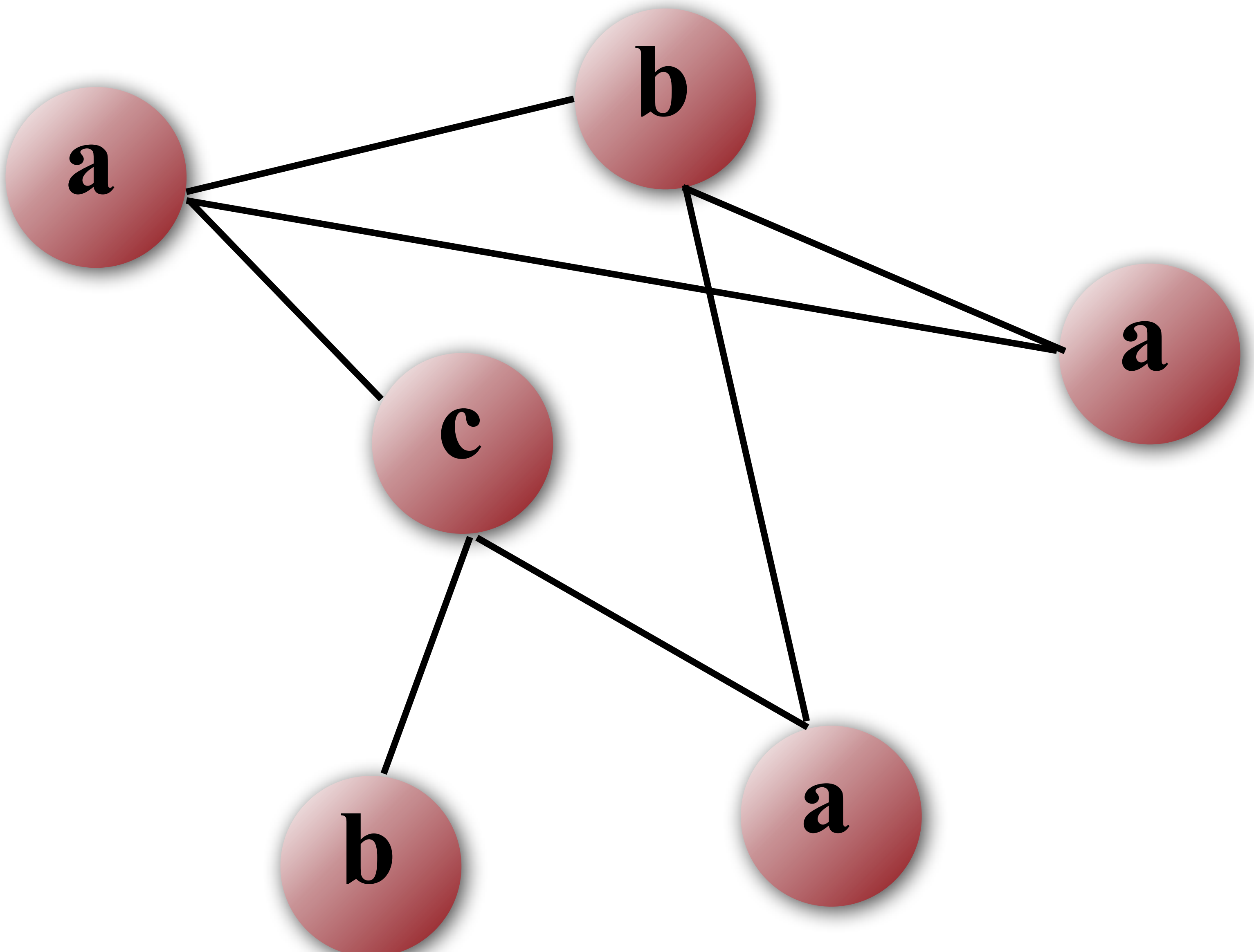
Graph Isomorphism

- Graphs $G = (V, E)$ and $G' = (V', E')$ are **isomorphic** if there exists a bijective function $\varphi: V \to V'$ such that
  - $(u, v) \in E$ if and only if $(\varphi(u), \varphi(v)) \in E'$
  - $L(v) = L(\varphi(v))$ for all $v \in V$
  - $L(u, v) = L(\varphi(u), \varphi(v))$ for all $(u, v) \in E$
- Graph G' is *subgraph isomorphic* to G if there exists a subgraph of G which is isomorphic to G'
- No polynomial-time algorithm is known for determining if G and G' are isomorphic
- Determining if G' is subgraph isomorphic to G is NP-hard

Equivalence and Canonical Graphs

- Isomorphism defines an equivalence class
  - id: $V \to V$, $\mathrm{id}(v) = v$ shows G is isomorphic to itself
  - If G is isomorphic to G' via φ, then G' is isomorphic to G via φ^{-1}
  - If G is isomorphic to H via φ and H to I via χ, then G is isomorphic to I via $\varphi \circ \chi$
- A **canonization** of a graph G, $canon(G)$ produces another graph C such that if H is a graph that is isomorphic to G, $canon(G) = canon(H)$
  - Two graphs are isomorphic if and only if their canonical versions are the same

An Example of Isomorphic Graphs



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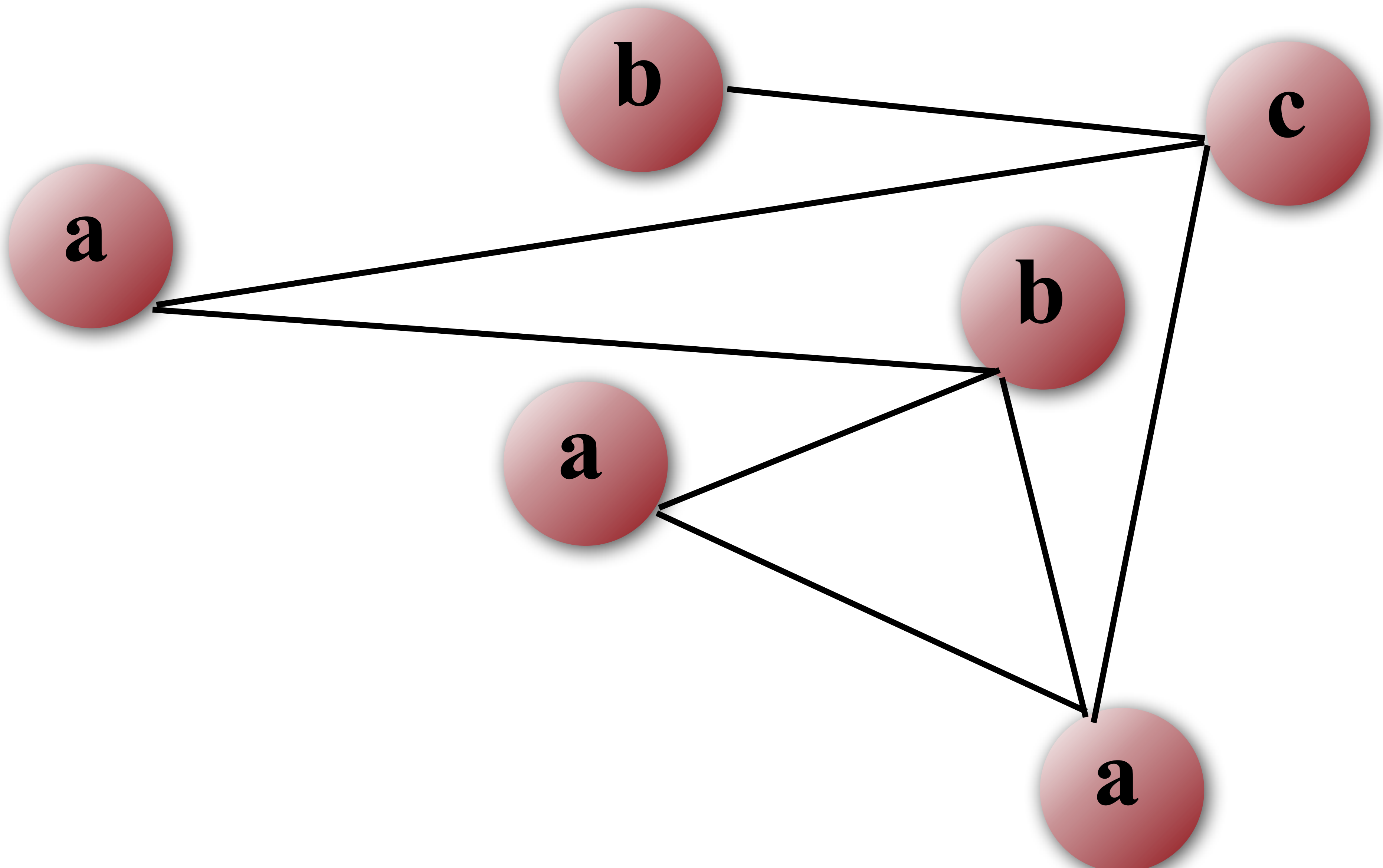

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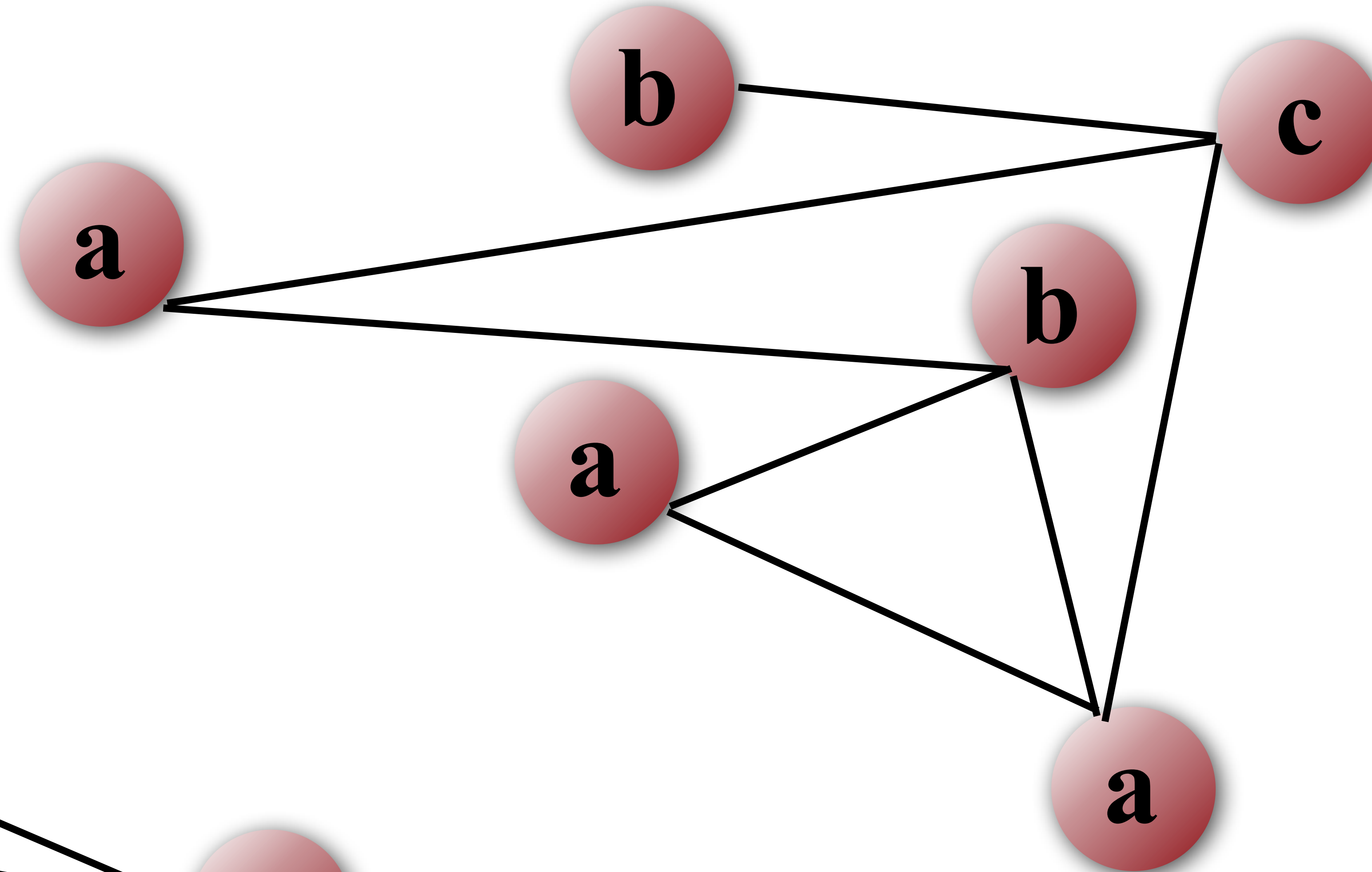

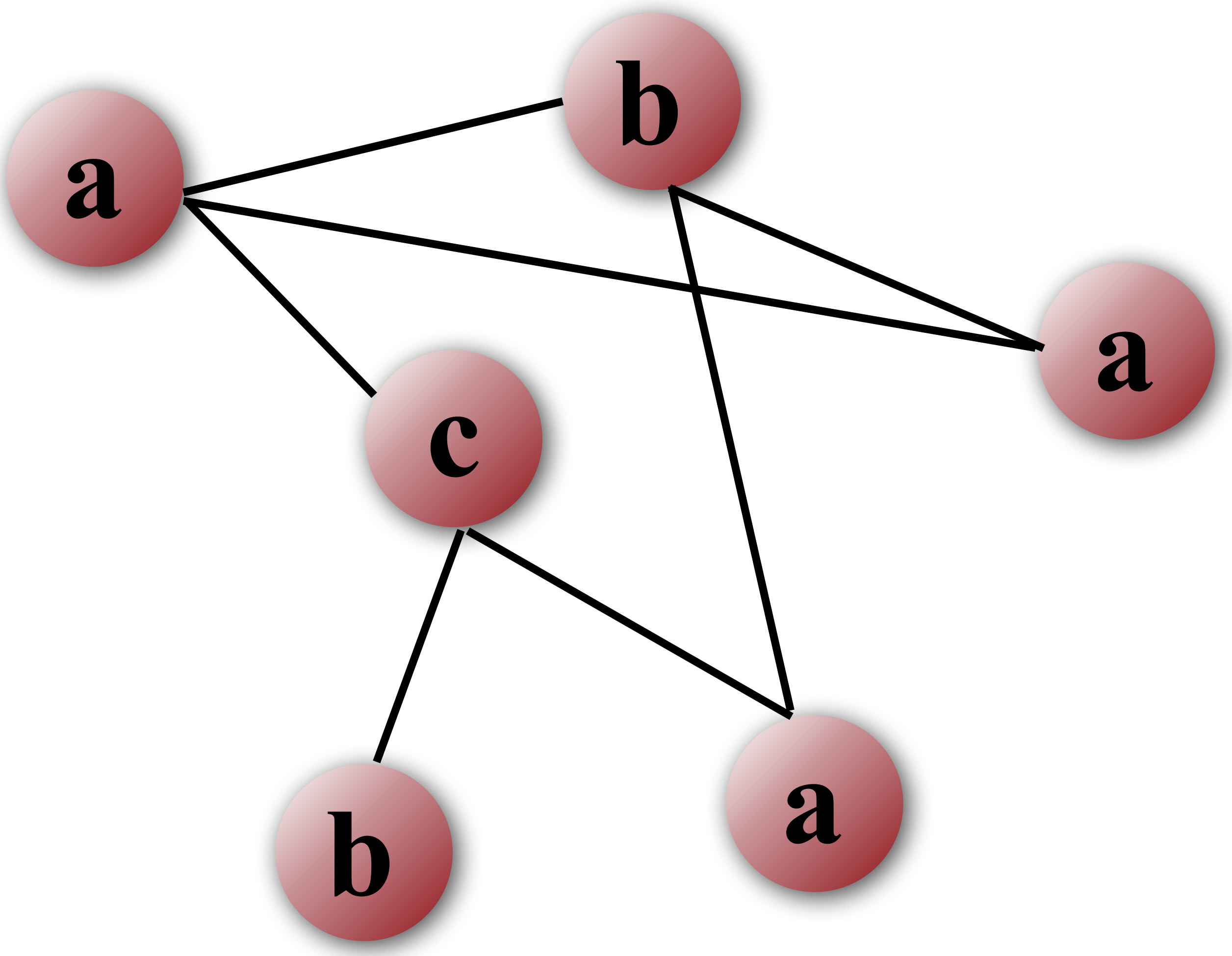

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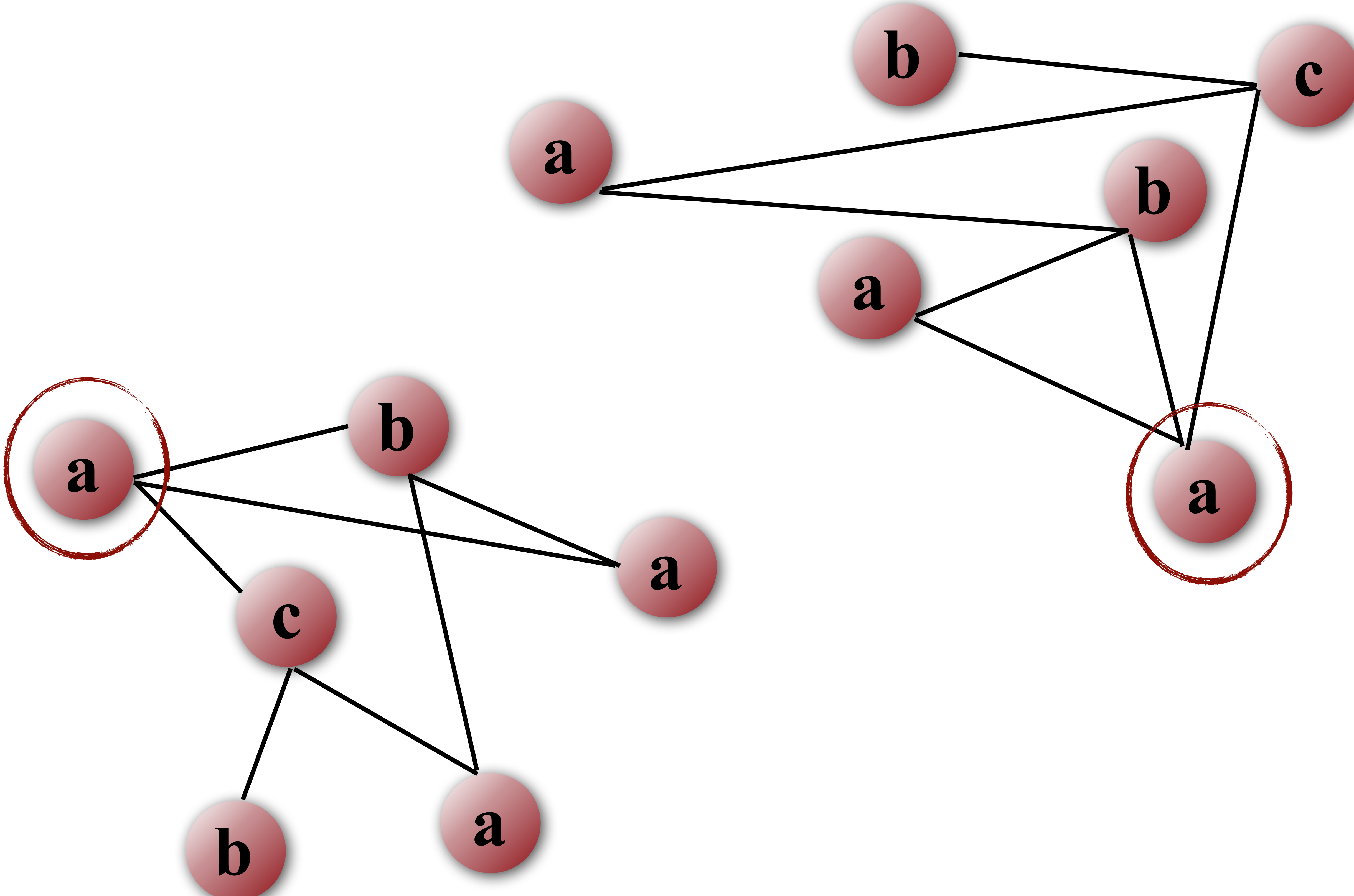

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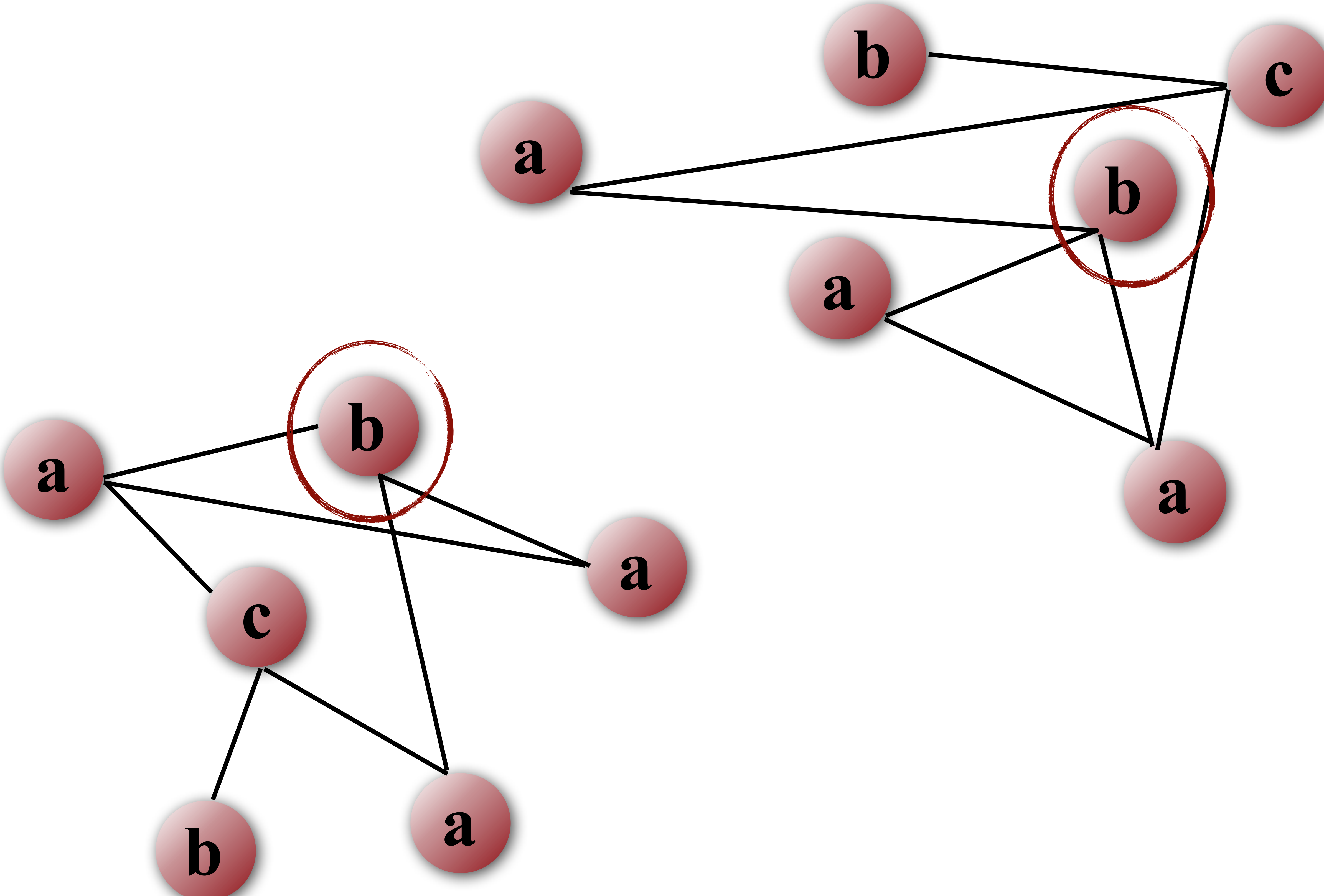

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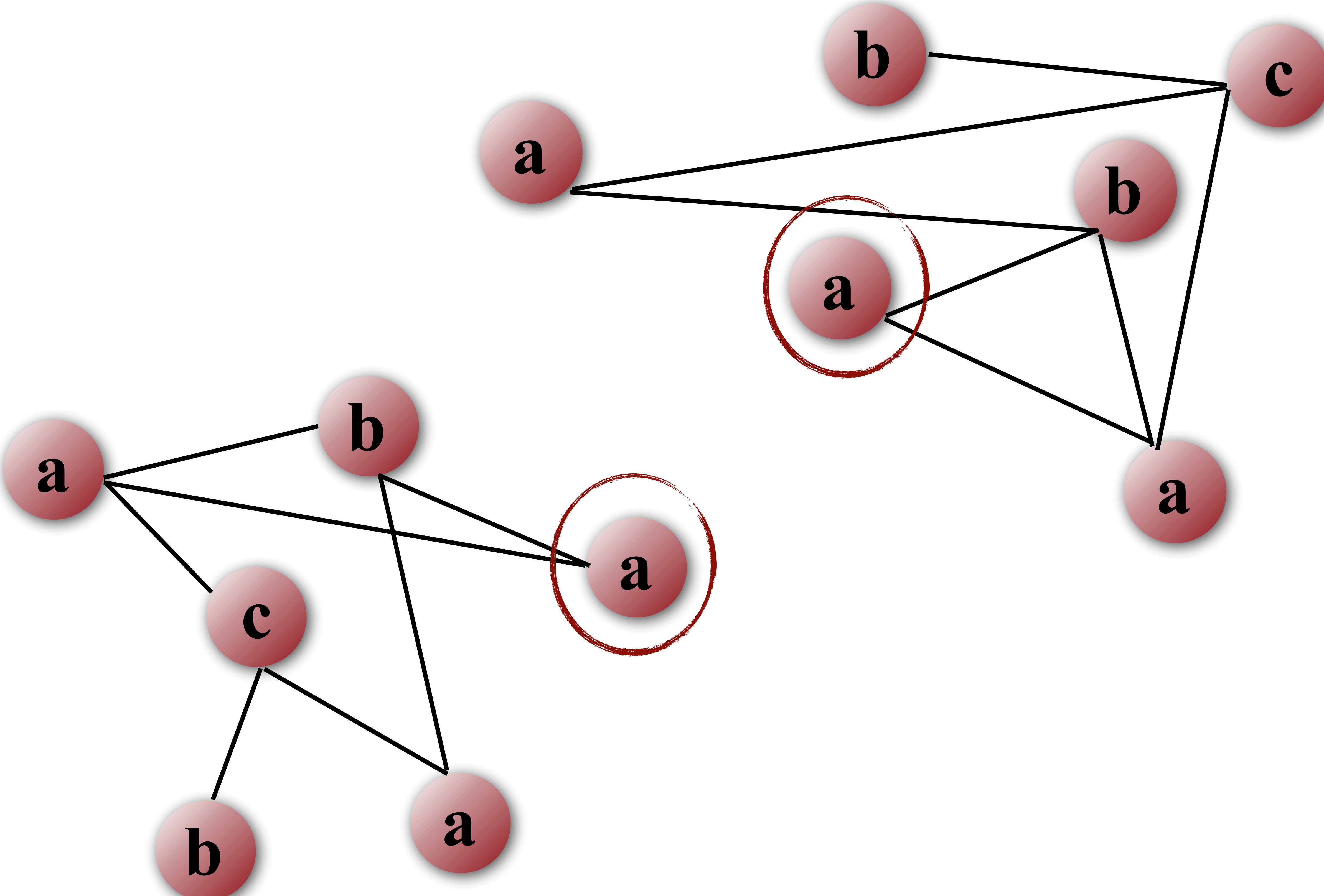

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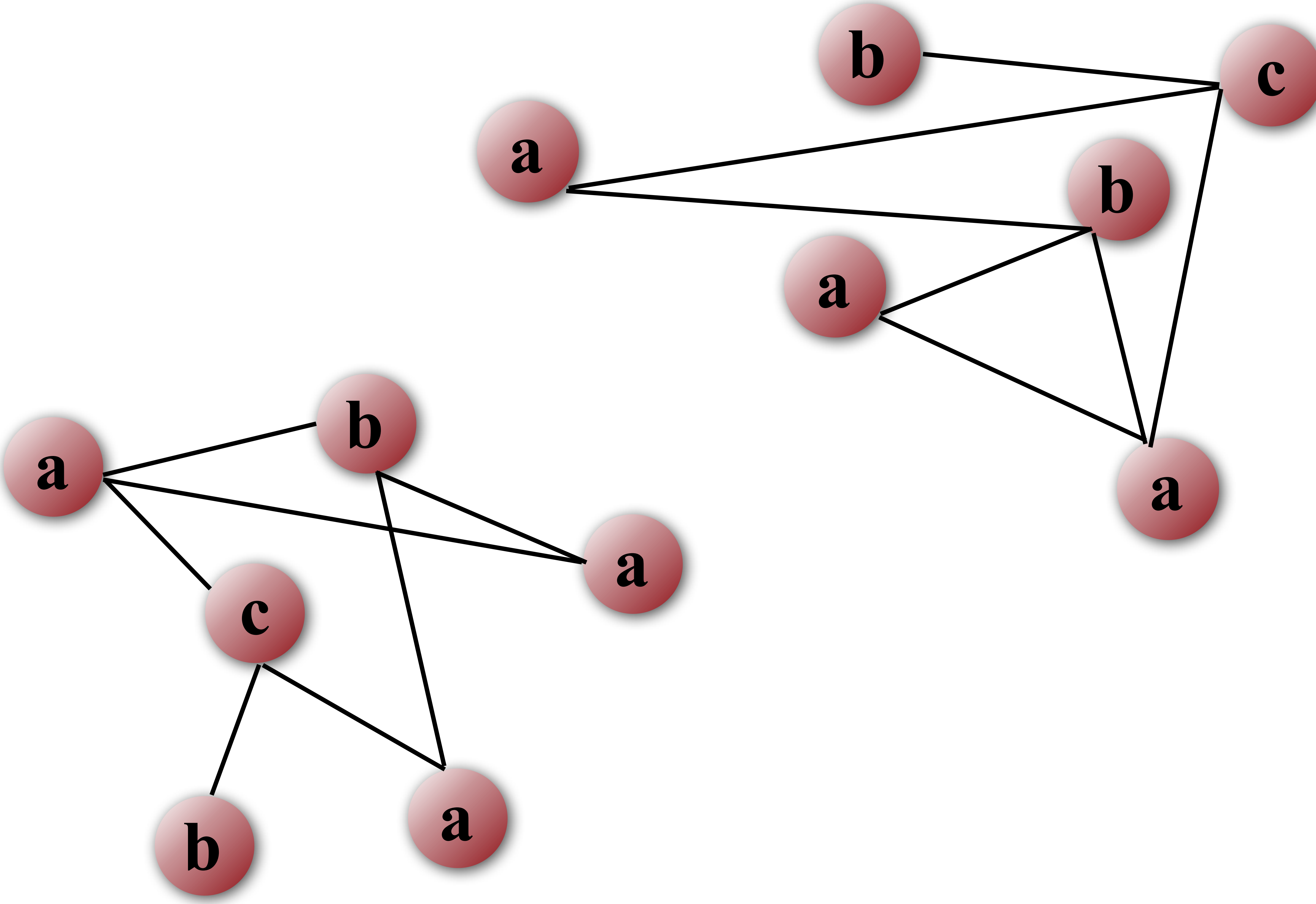
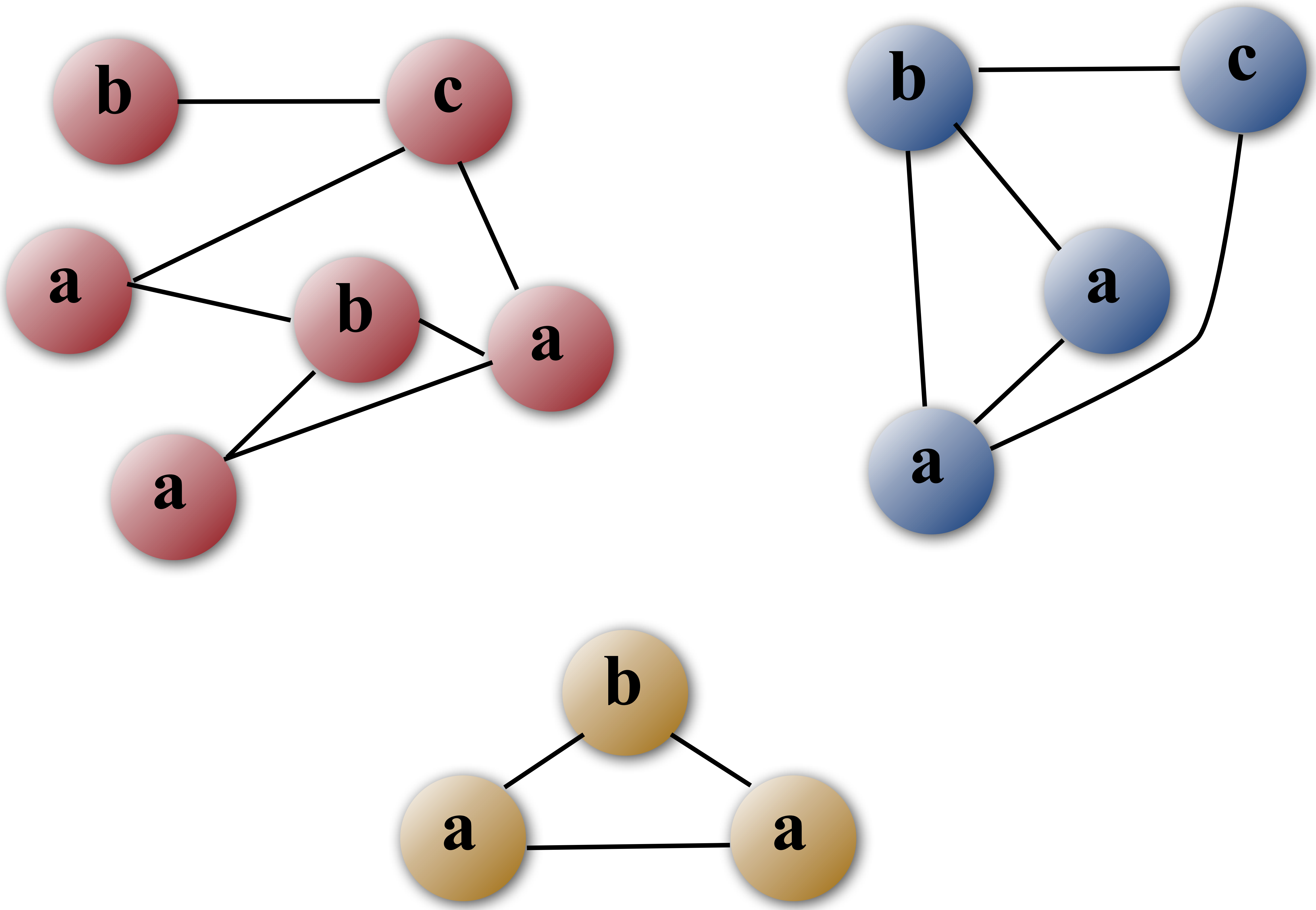


Frequent Subgraph Mining

- Given a set D of n graphs and a minimum support parameter *minsup*, find all connected graphs that are subgraph isomorphic to at least *minsup* graphs in D
  - Enormously complex problem
  - For graphs that have m vertices there are
    - $2^{O(m^2)}$ subgraphs (not all are connected)
  - If we have s labels for vertices and edges we have
    - $O\left((2s)^{O(m^2)}\right)$ labelings of the different graphs
  - Counting the support means solving multiple NP-hard problems

An Example



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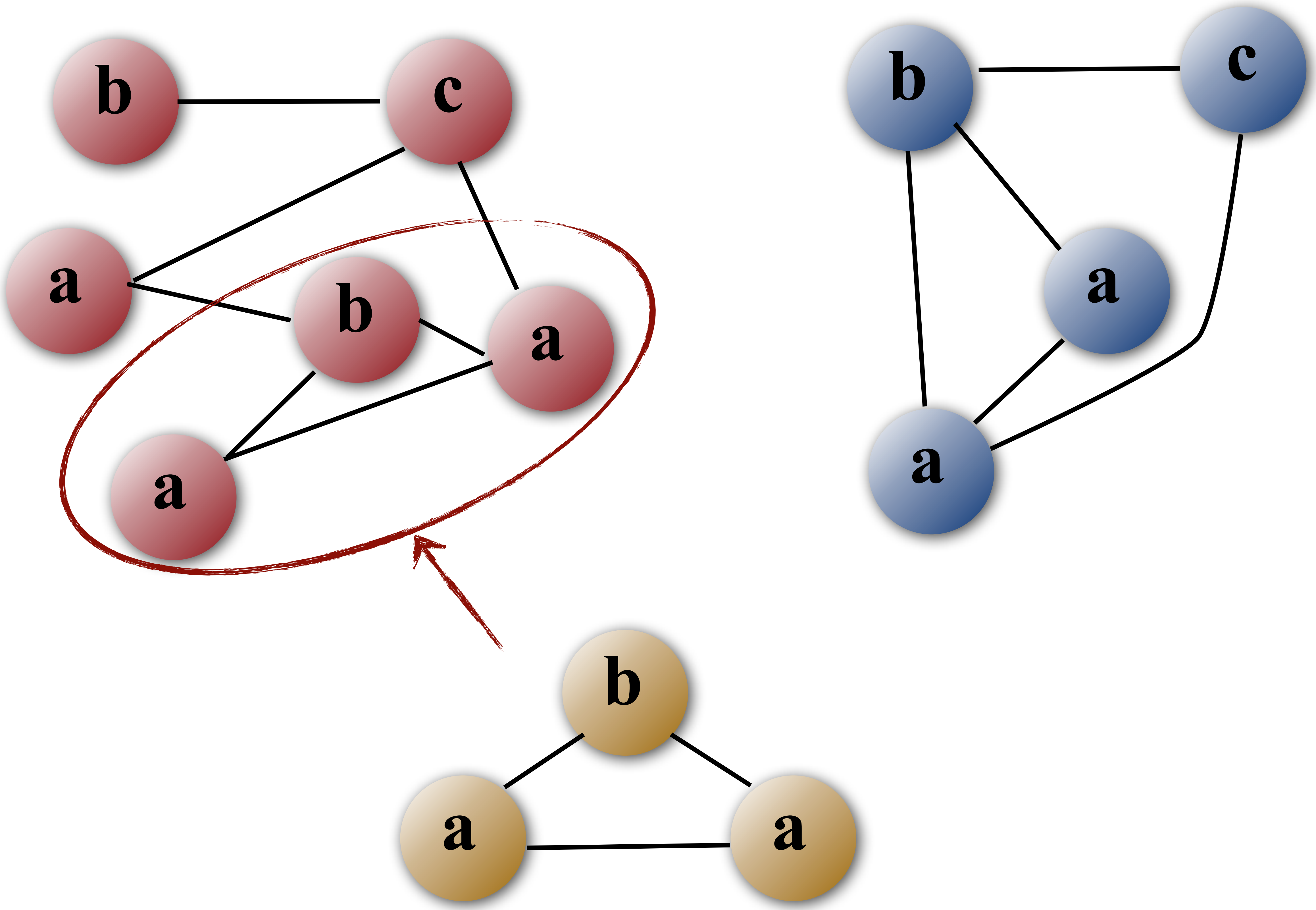

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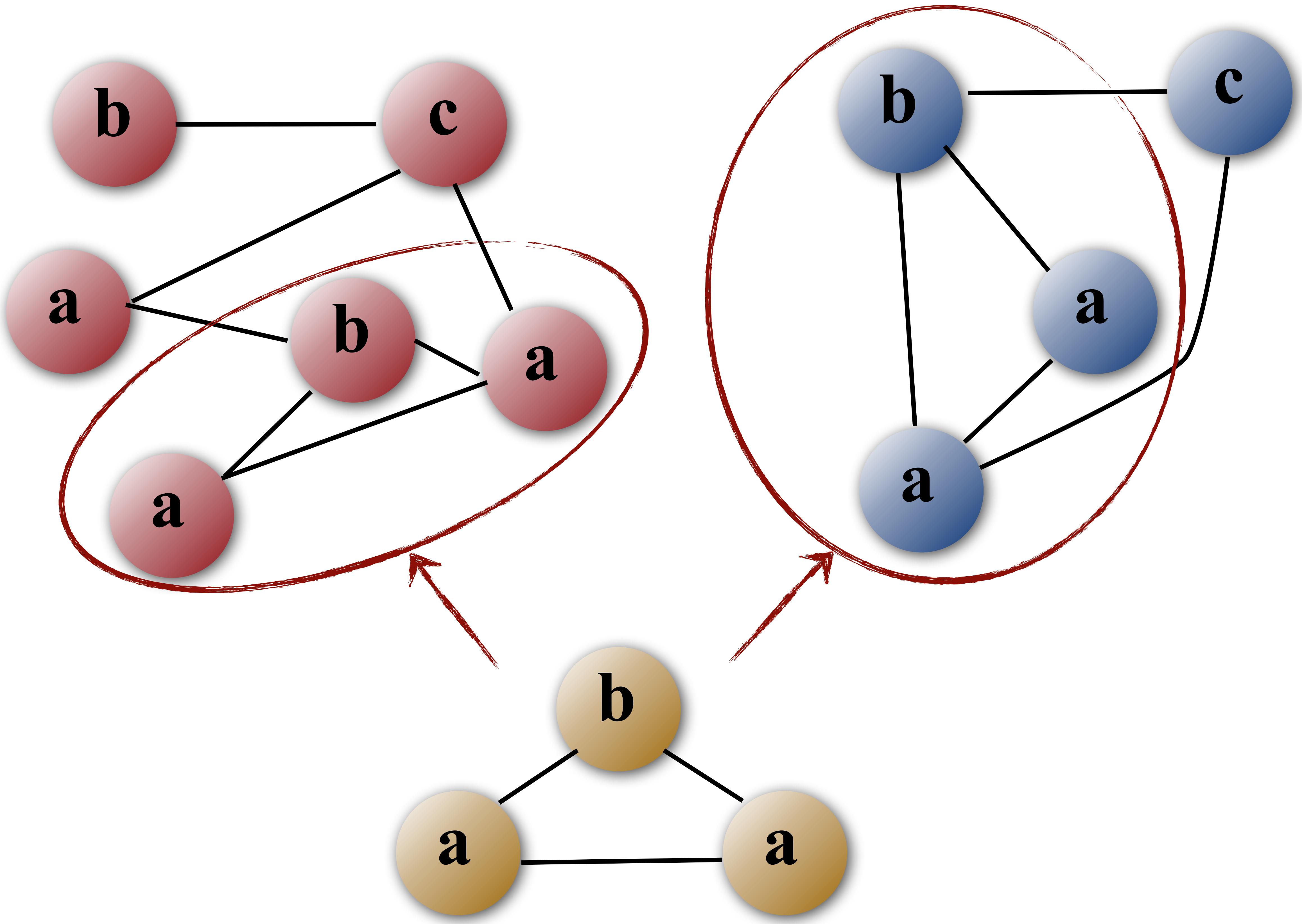


Apriori-Based Graph Mining (AGM)

- Subgraph frequency follows downwards closedness property
  - A supergraph cannot be frequent unless its subgraph is
- Idea: generate all k-vertex graphs that are supergraphs of k–1 vertex frequent graphs and check frequency
- Two problems:
  - How to generate the graphs
  - How to check the frequency
- Idea: do the generation based on adjacency matrices

Inokuchi, Washio & Motoda 2000

Matrices and Codes

- In *labelled adjacency matrix* we have
  - Vertex labels in the diagonal
  - Edge labels in off-diagonal (or 0 if no edges)
- The *code* of the the adjacency matrix $\boldsymbol{X}$ is the lower-left triangular submatrix listed in row-major order
  - $x_{1,1}x_{2,1}x_{2,2}x_{3,1}\ldots x_{k,1}\ldots x_{k,k}\ldots x_{n,n}$
- The adjacency matrices can be sorted using the standard lexicographical order in their codes

Joining Two Subgraphs

- Assume we have two frequent subgraphs of *k* vertices whose adjacency matrices agree on the first *k–1* edges

$$X_k = \begin{pmatrix} X_{k-1} & \boldsymbol{x}_1 \\ \boldsymbol{x}_2^T & x_{kk} \end{pmatrix}, Y_k = \begin{pmatrix} X_{k-1} & \boldsymbol{y}_1 \\ \boldsymbol{y}_2^T & y_{kk} \end{pmatrix}$$

- We can do the join as follows

$$Z_{k+1} = \begin{pmatrix} X_{k-1} & \boldsymbol{x}_1 & \boldsymbol{y}_1 \\ \boldsymbol{x}_2^T & x_{kk} & z_{k,k+1} \\ \boldsymbol{y}_2^T & z_{k+1,k} & y_{kk} \end{pmatrix} = \left(\begin{array}{cc|c} \multicolumn{2}{c|}{X_k} & \begin{array}{c}\boldsymbol{y}_1 \\ z_{k,k+1}\end{array} \\ \hline \boldsymbol{y}_2^T & z_{k+1,k} & y_{kk} \end{array}\right)$$

  - $z_{k+1,k} = z_{k,k+1}$ assumes all possible edge labels
    - One matrix for each possibility

Avoiding Redundancy

- The two adjacency matrices are joined only if code($\boldsymbol{X}_k$) ≤ code($\boldsymbol{Y}_k$) ("normal order")
- We need to confirm that all subgraphs of the resulting (k +1)-vertex matrix are frequent
  - We need to consider the normal-order generated k-vertex subgraphs
    - The algorithm only stores normal-order generated graphs
  - They are generated by re-generating the k-vertex subgraph from singletons in normal order
    - Process is called *normalization* and can compute the normal forms of all subgraphs
  - Normalization can be expressed as a row and column permutations: $\boldsymbol{X}_n = \boldsymbol{P}^T\boldsymbol{X}\boldsymbol{P}$

Canonical Forms

- Isomorphic graphs can have many different normal forms
- Given a set $NF(G)$ of all normal forms representing graphs isomorphic to G, the *canonical form* of G is the adjacency matrix $\boldsymbol{X}_c$ that has the minimum code in $NF(G)$

$$\boldsymbol{X}_c = \arg\min \{code(X) : X \in NF(G)\}$$

- Given an adjacency matrix $\boldsymbol{X}$, its normal form is $\boldsymbol{X}_n = \boldsymbol{P}^T\boldsymbol{X}\boldsymbol{P}$ for some permutation matrix $\boldsymbol{P}$, and its canonical form $\boldsymbol{X}_c$ is $\boldsymbol{Q}^T\boldsymbol{P}^T\boldsymbol{X}\boldsymbol{P}\boldsymbol{Q}$ for some permutation matrix $\boldsymbol{Q}$

Finding Canonical Forms

- Let $\boldsymbol{X}$ be an adjacency matrix of $k+1$ vertices
  - Let $\boldsymbol{Y}$ be $\boldsymbol{X}$ with vertex m removed
  - Let $\boldsymbol{P}$ be the permutation of $\boldsymbol{Y}$ to its normal form and $\boldsymbol{Q}$ the permutation of $\boldsymbol{P}^T\boldsymbol{Y}\boldsymbol{P}$ to the canonical form
    - We assume we have already computed them
  - We compute candidate $\boldsymbol{P}'$ and $\boldsymbol{Q}'$ for $\boldsymbol{X}$ by
    - $\boldsymbol{Q}'$ is like $\boldsymbol{Q}$ but bottom-right corner is 1
    - p'_{ij} is
      - p_{ij} if $i < m$ and $j \neq k$
      - $p_{i-1,j}$ if $i > m$ and $j \neq k$
      - 1 if $i = m$ and $j = k$
      - 0 otherwise
  - Final $\boldsymbol{P}'$ and $\boldsymbol{Q}'$ are found by trying all candidates and selecting the ones that give the lowest code

The Algorithm

- Start with frequent graphs of 1 vertex
- **while** there are frequent graphs left
  - Join two frequent (k–1)-vertex graphs
  - Check the resulting graphs subgraphs are frequent
    - If not, **continue**
  - Compute the canonical form of the graph
    - If this canonical form has already been studied, **continue**
  - Compare the canonical form with the canonical forms of the k-vertex subgraphs of the graphs in D
    - If the graph is frequent, keep, otherwise discard
- **return** all frequent subgraphs

The gSpan Algorithm

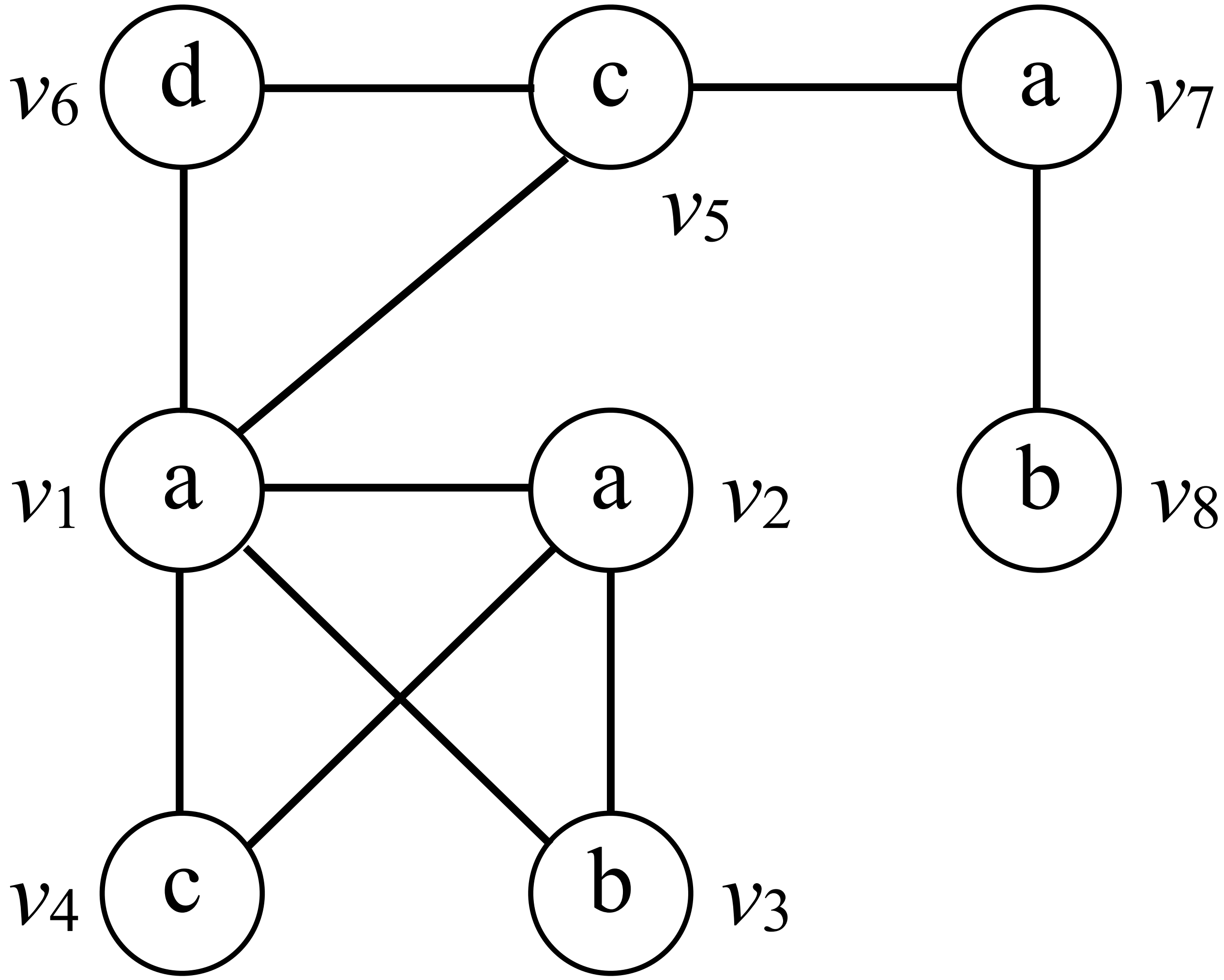
- We can improve the running time of frequent subgraph mining by either
  - Making the frequency check faster
    - Lots of efforts in faster isomorphism checking but only little progress
  - Creating less candidates that need to be checked
    - Level-wise algorithms (like AGM) generate huge numbers of candidates
    - Each must be checked with for isomorphism with others
- The gSpan (graph-based Substructure pattern mining) algorithm replaces the level-wise approach with a depth-first approach

Yan & Han 2002; Z&M Ch. 11

Depth-First Spanning Tree

- A dept-first spanning (DFS) tree of a graph *G*
  - Is a connected tree
  - Contains all the vertices of *G*
  - Is build in depth-first order
    - Selection between the siblings is e.g. based on the vertex index
- Edges of the DFS tree are *forward edges*
- Edges not in the DFS tree are *backward edges*
- A *rightmost path* in the DFS tree is the path travels from the root to the *rightmost vertex* by always taking the rightmost child (last-added)

An Example



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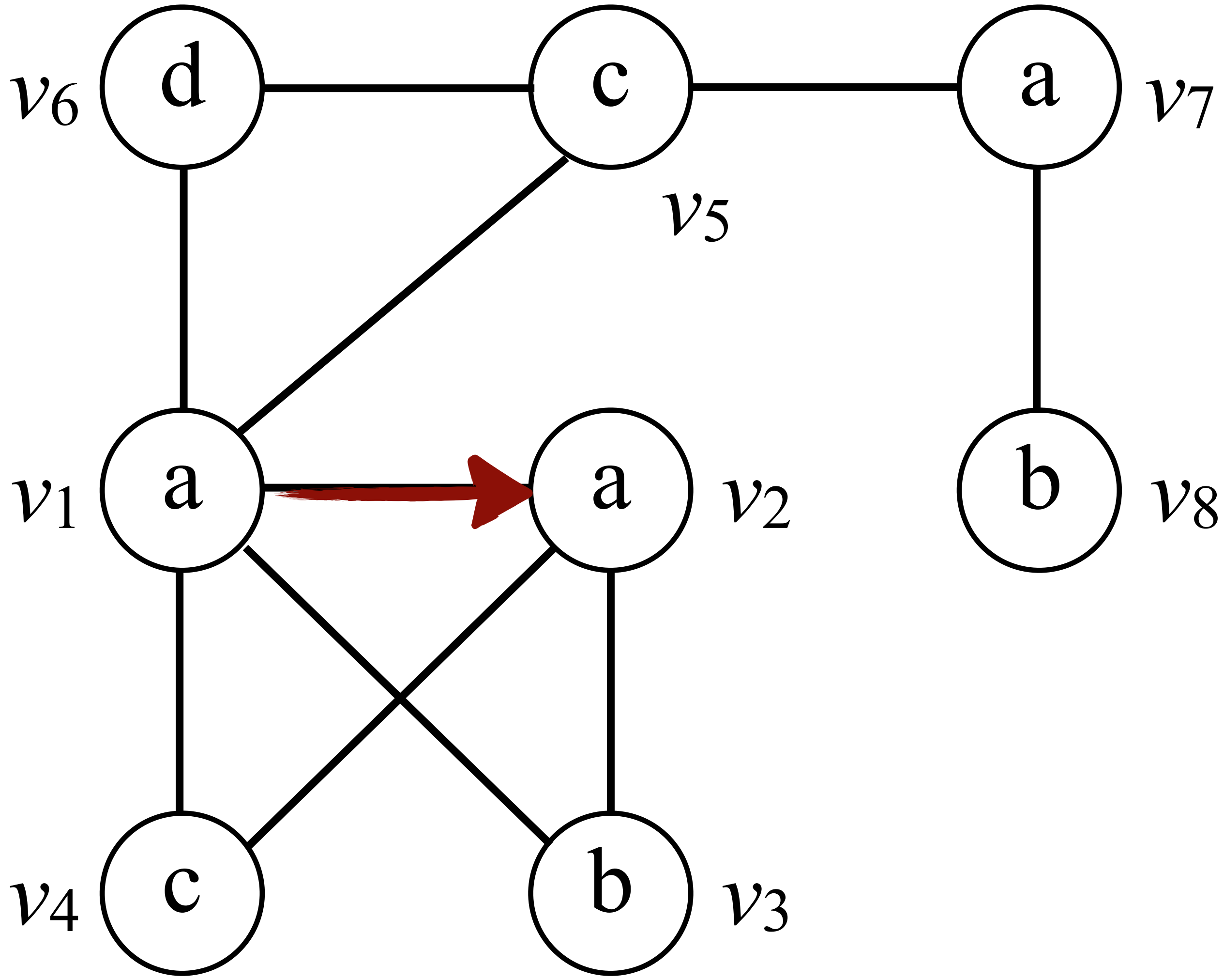

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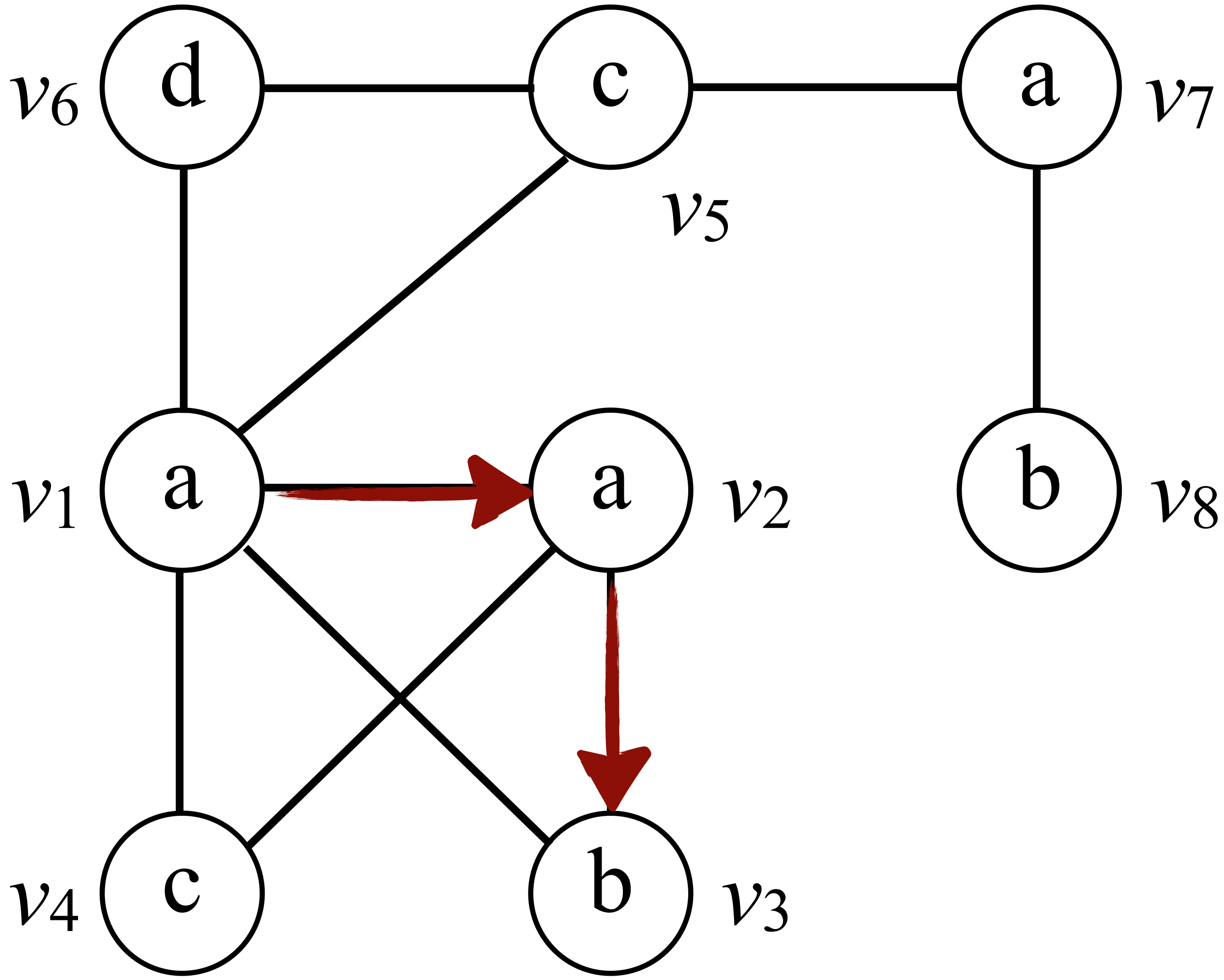

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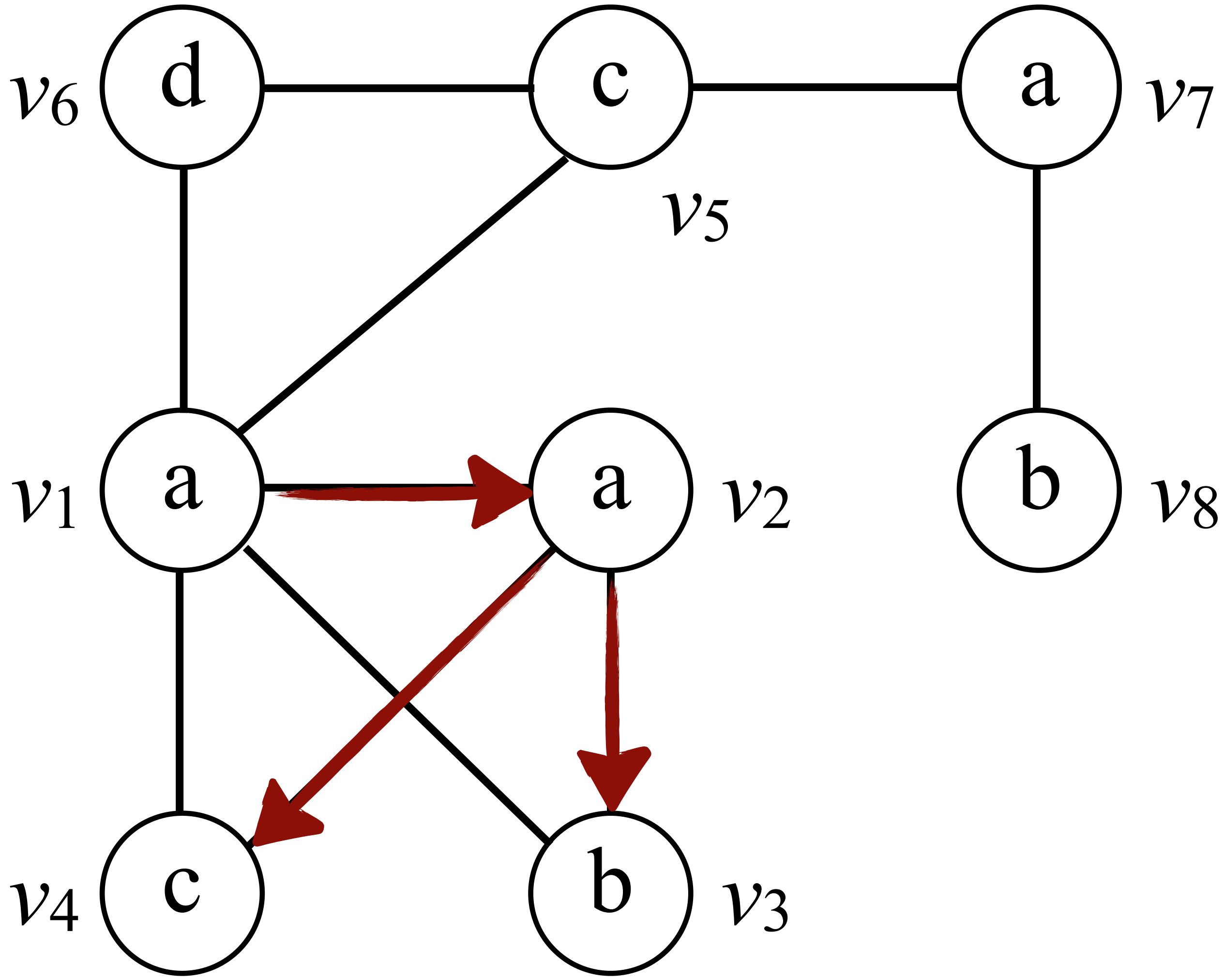

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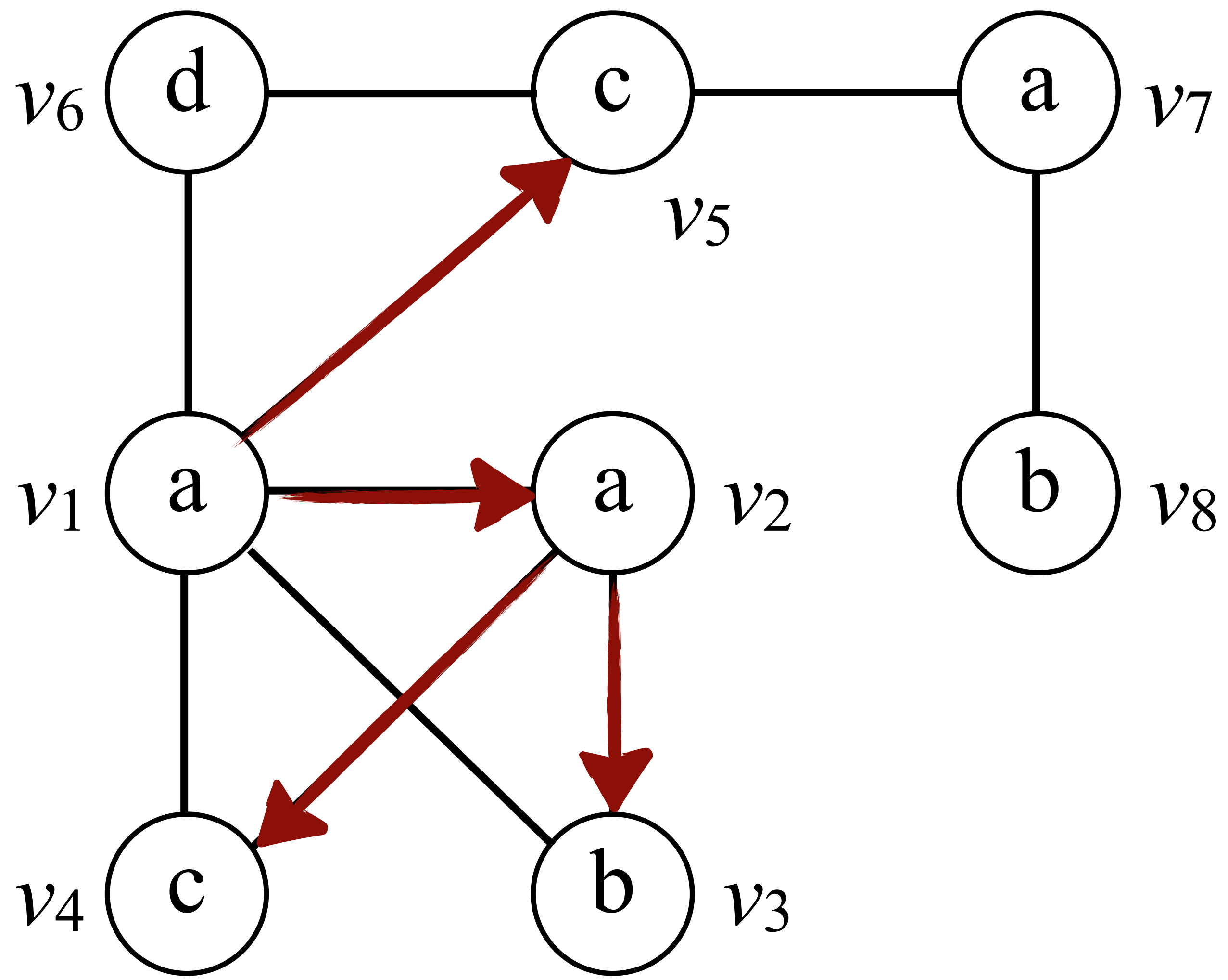

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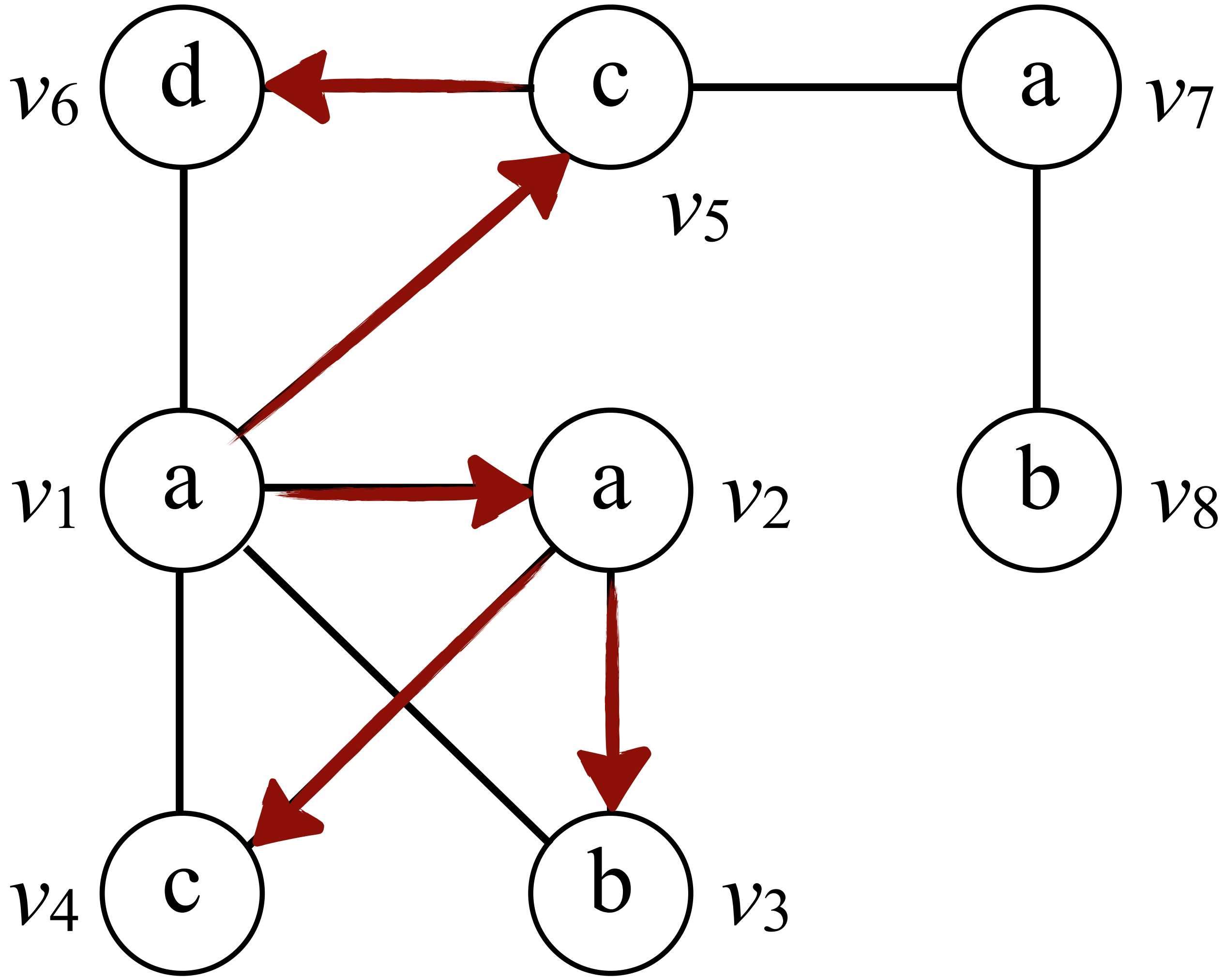

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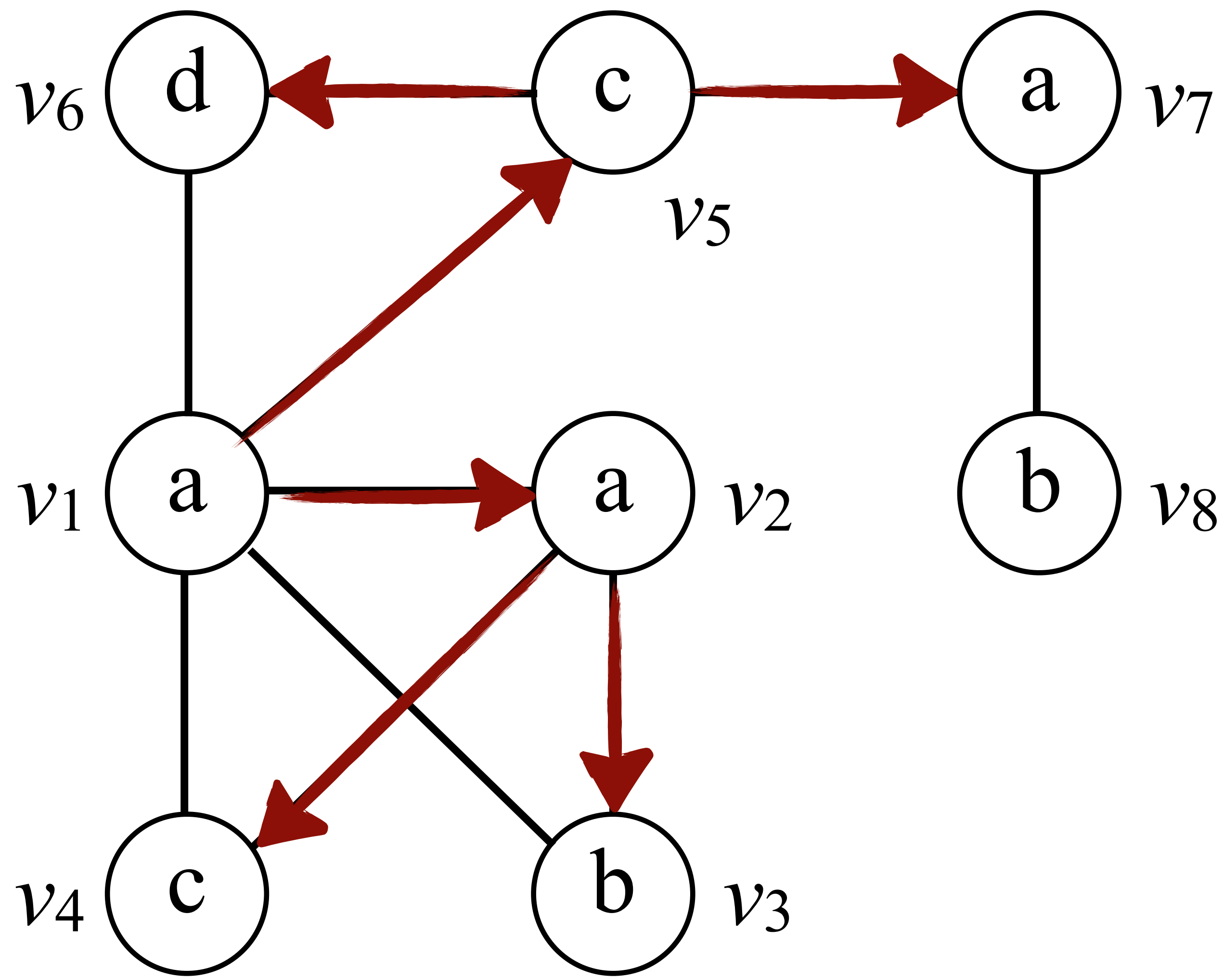

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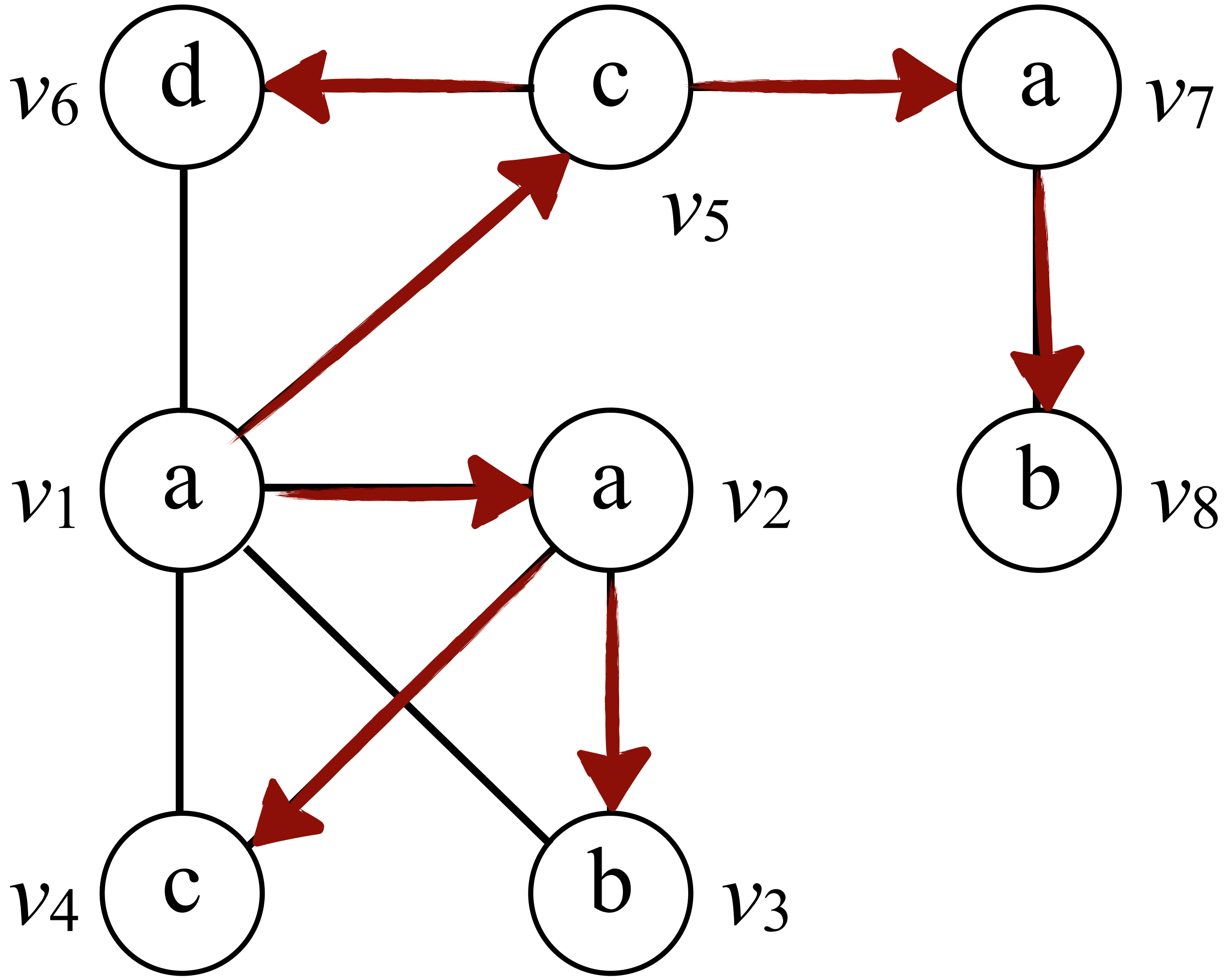
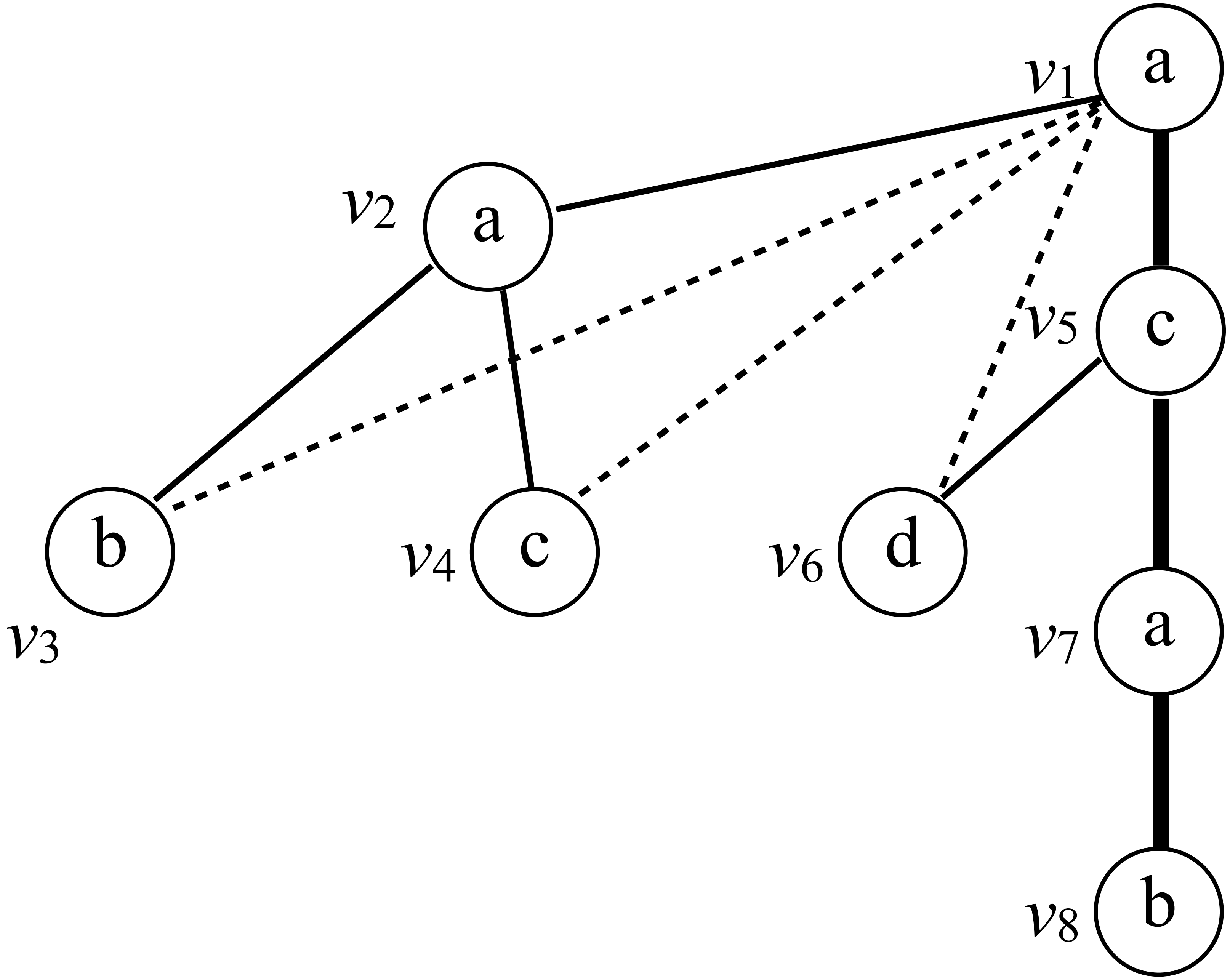


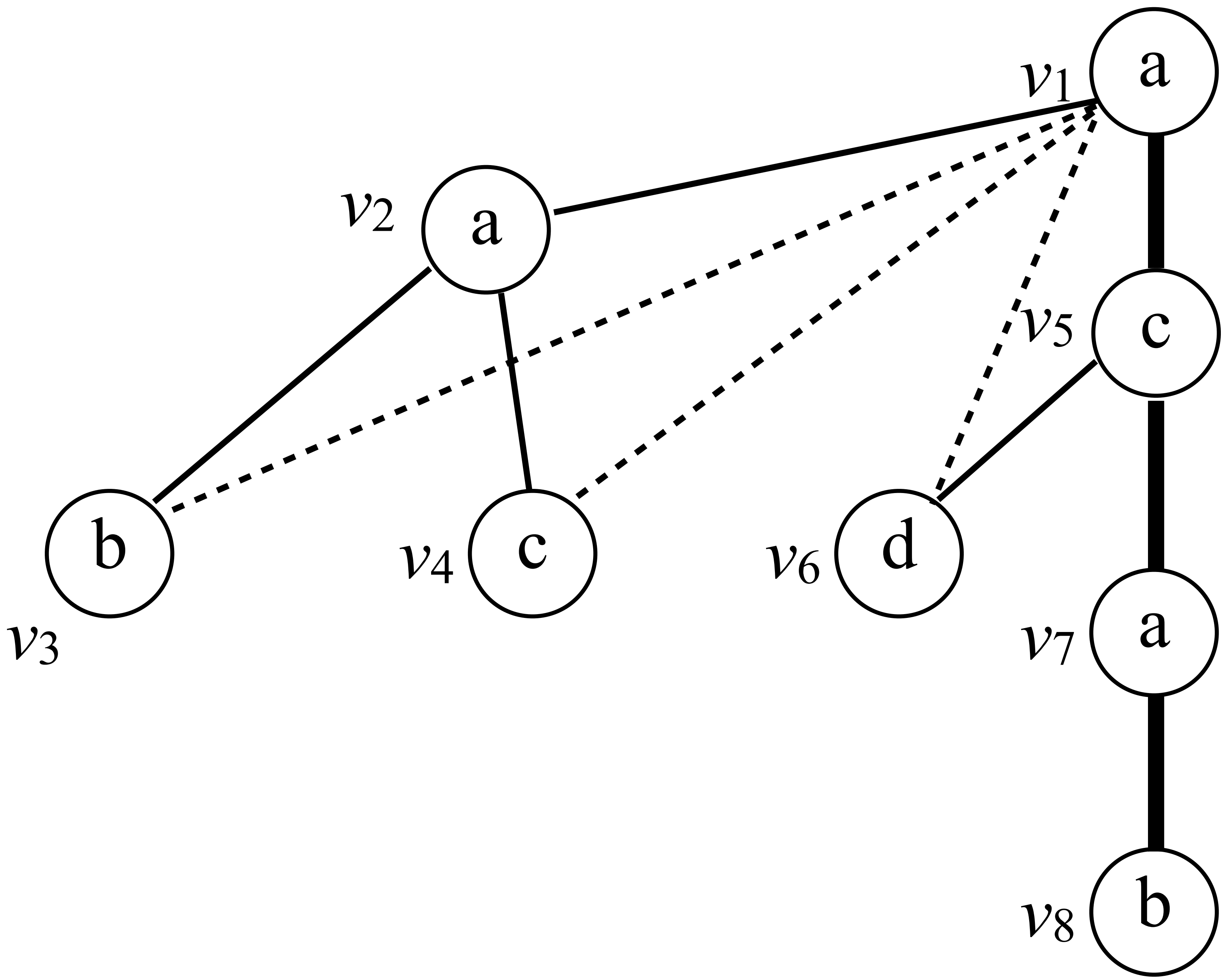
The DFS Tree



Generating Candidates from DFS Tree

- Given graph G, we extend it *only* from the vertices in the rightmost path
  - We can add backwards edges from the rightmost vertex to some other vertex in the rightmost path
  - We can add a forward edge from any vertex in the rightmost path
    - This increases the number of vertices by 1
- The order of generating the candidates is
  - First backward extensions
    - First to root, then to root's child, …
  - Then forward extensions
    - First from the leaf, then from leaf's father, …

An Example



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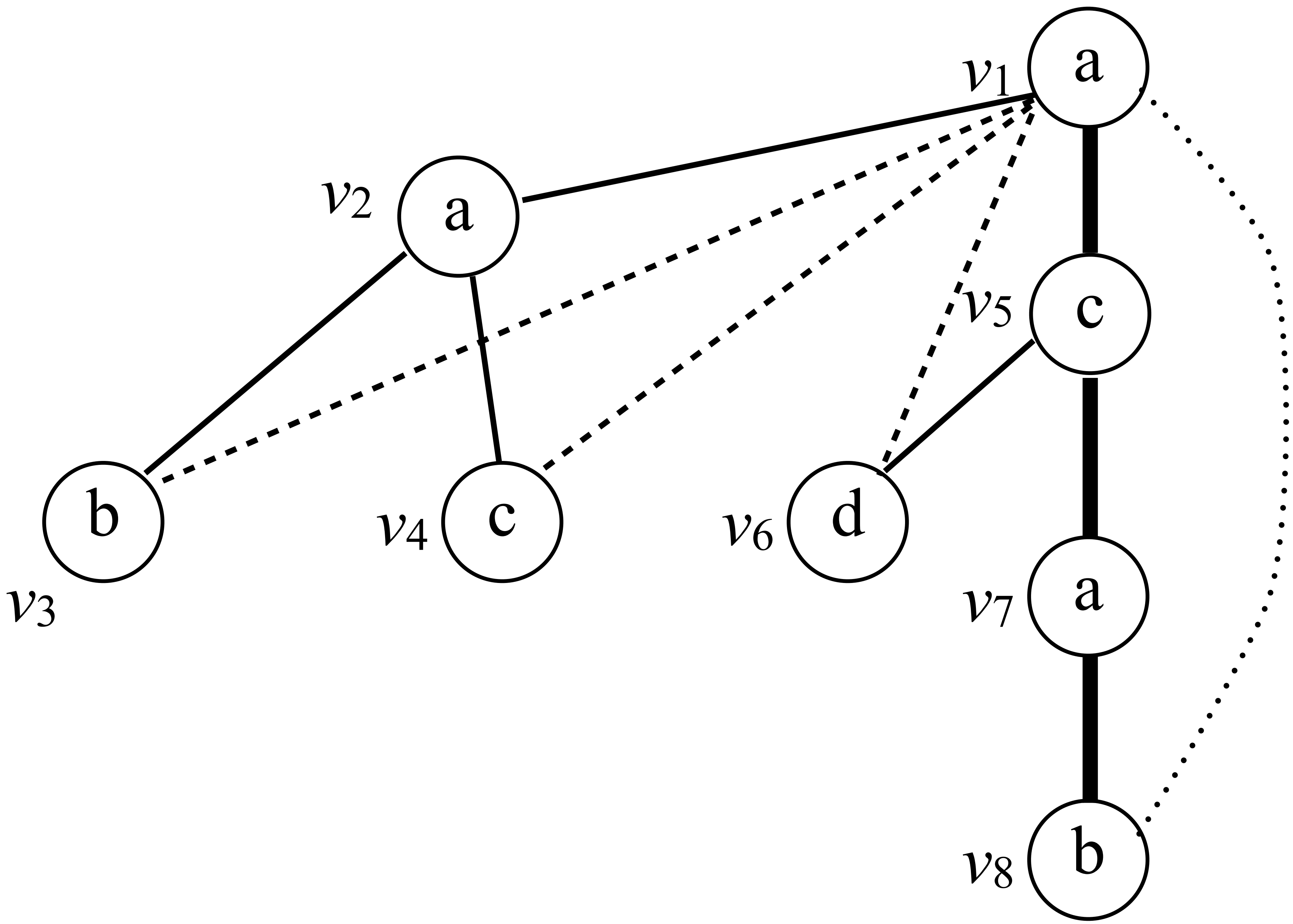

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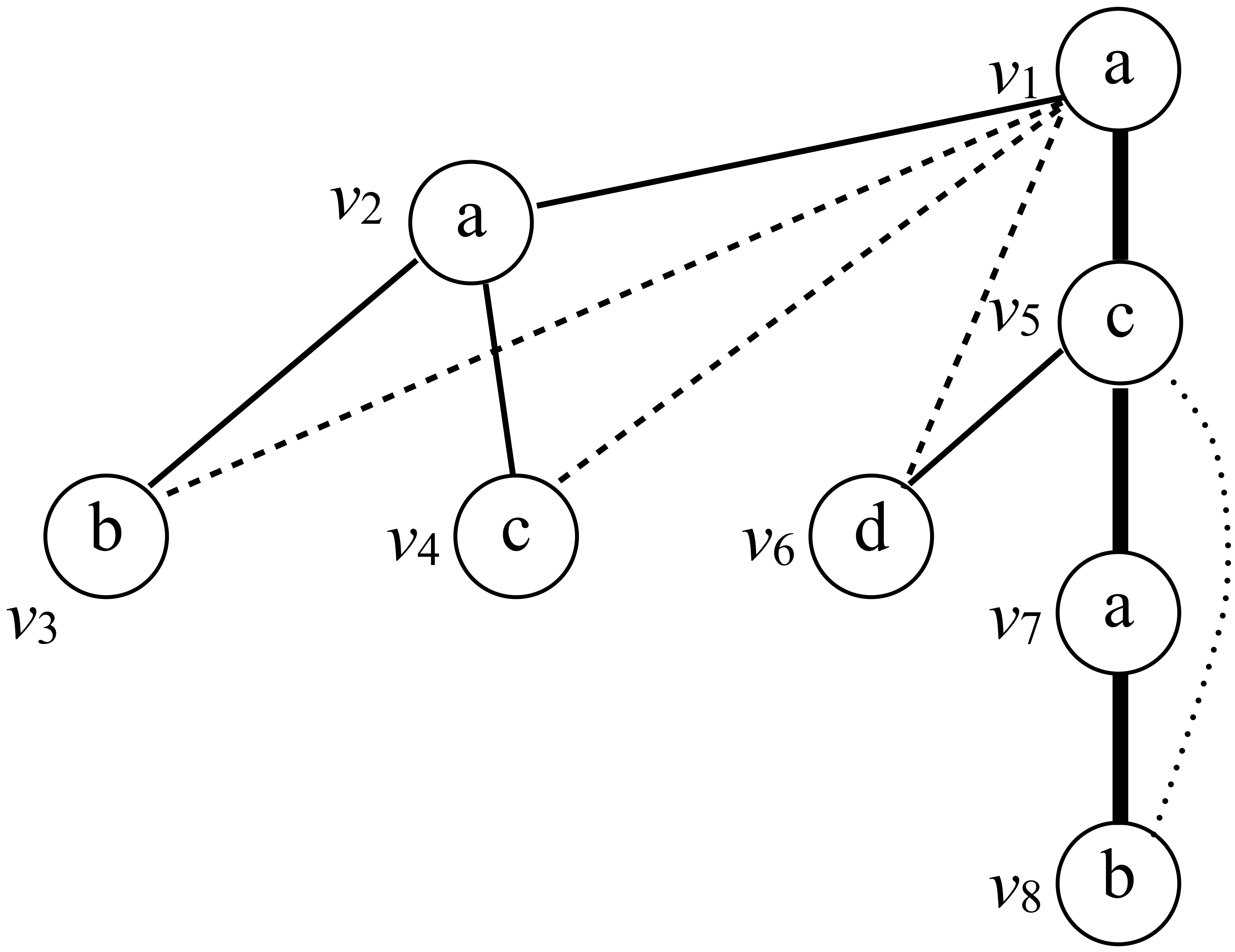

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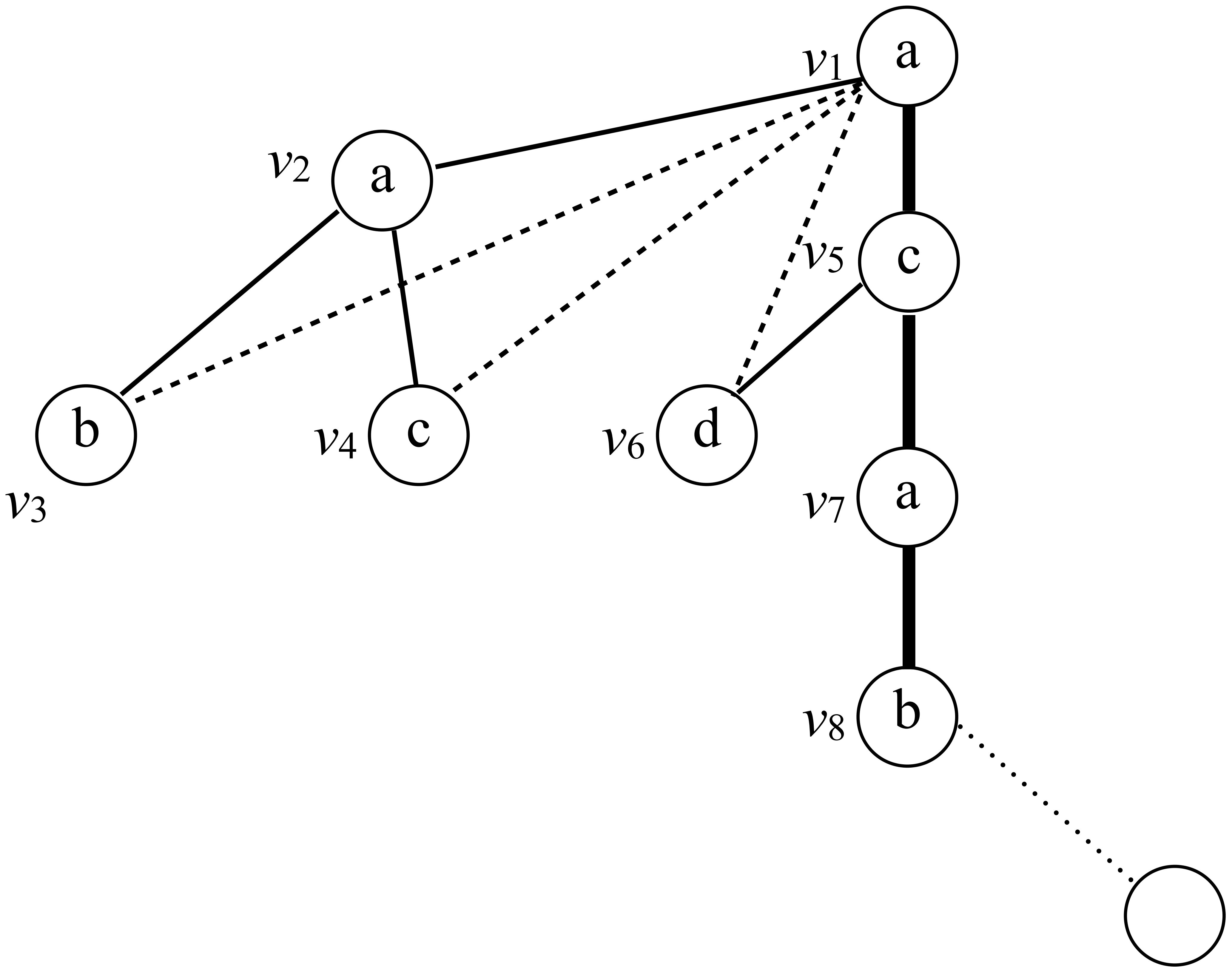

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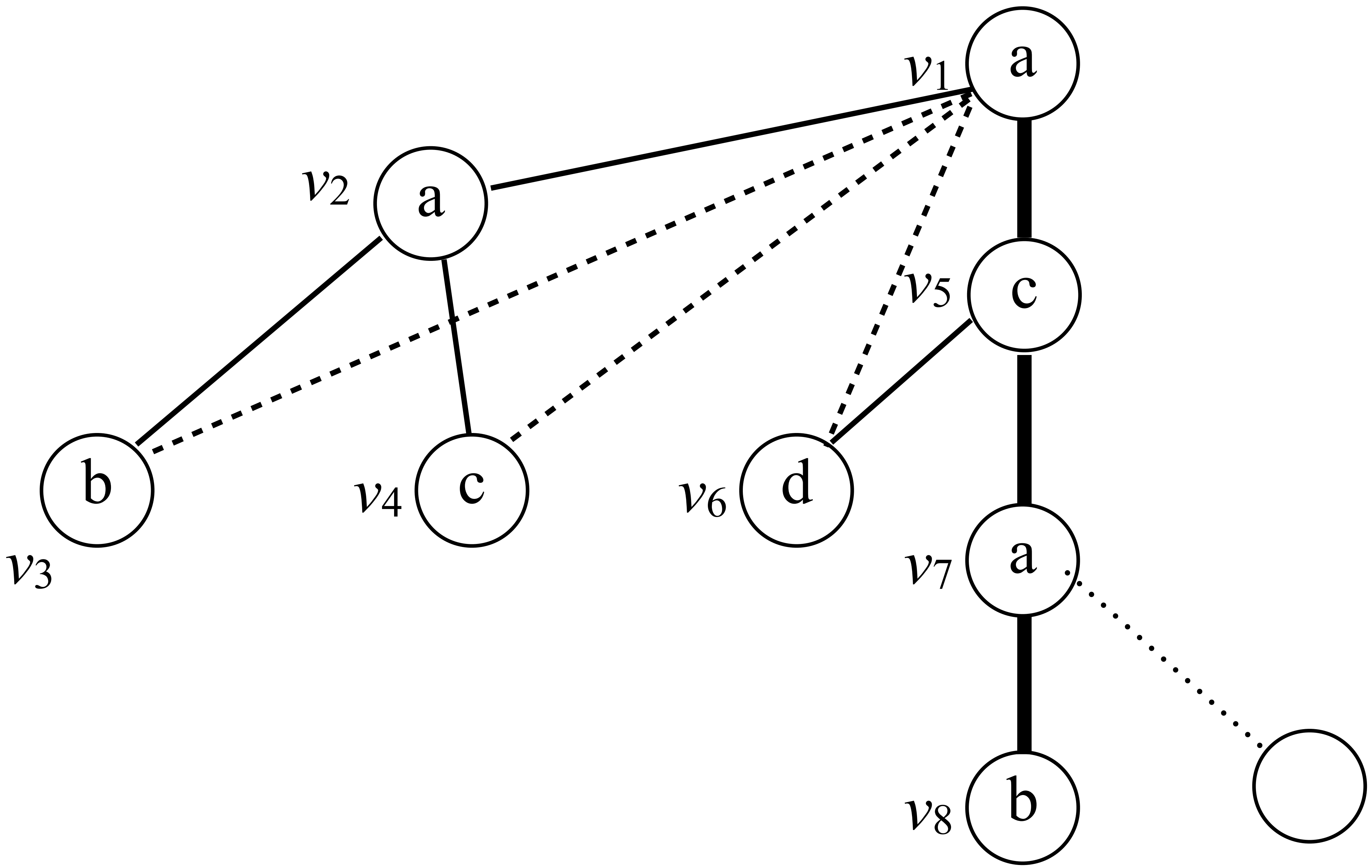

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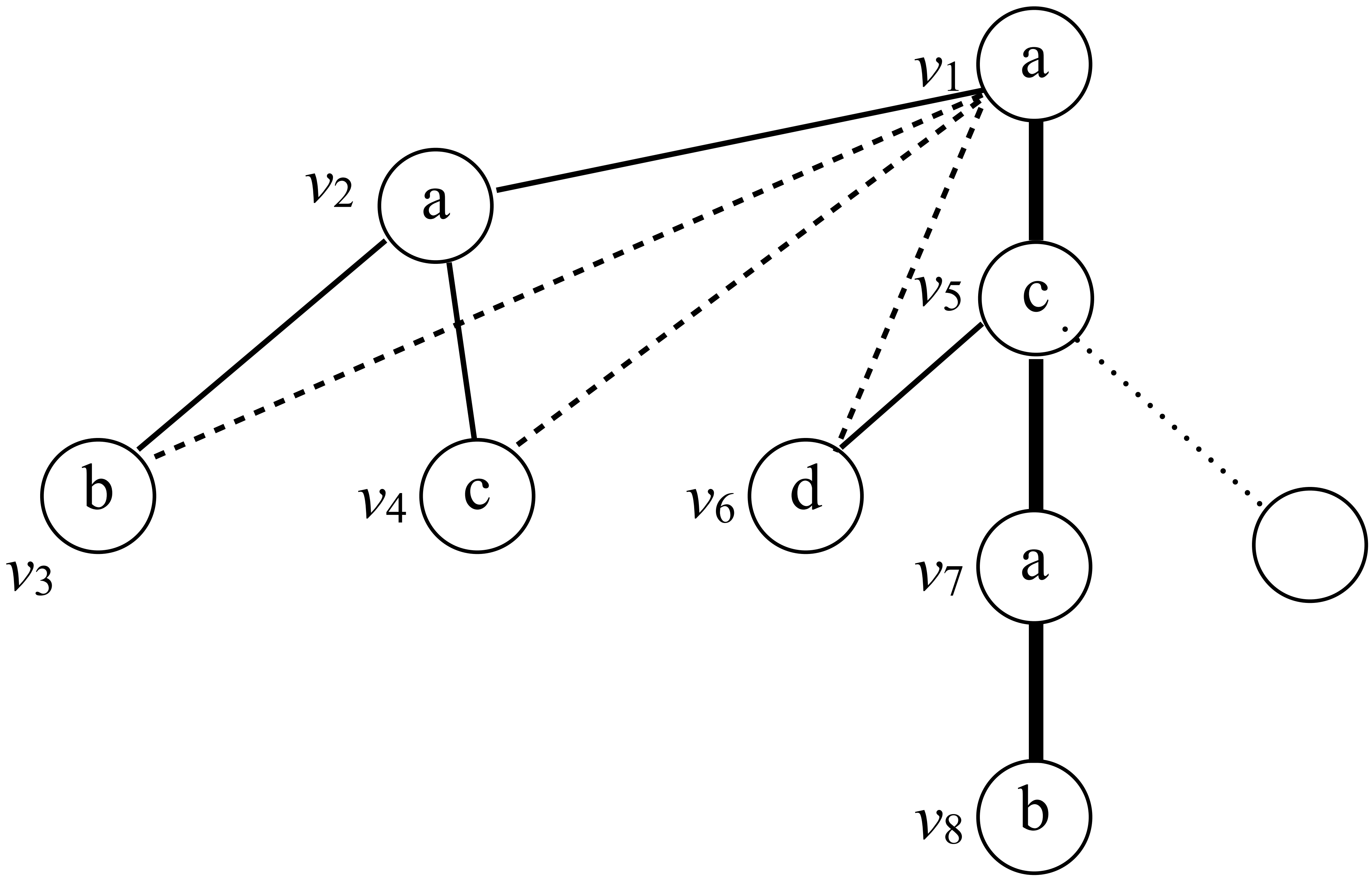

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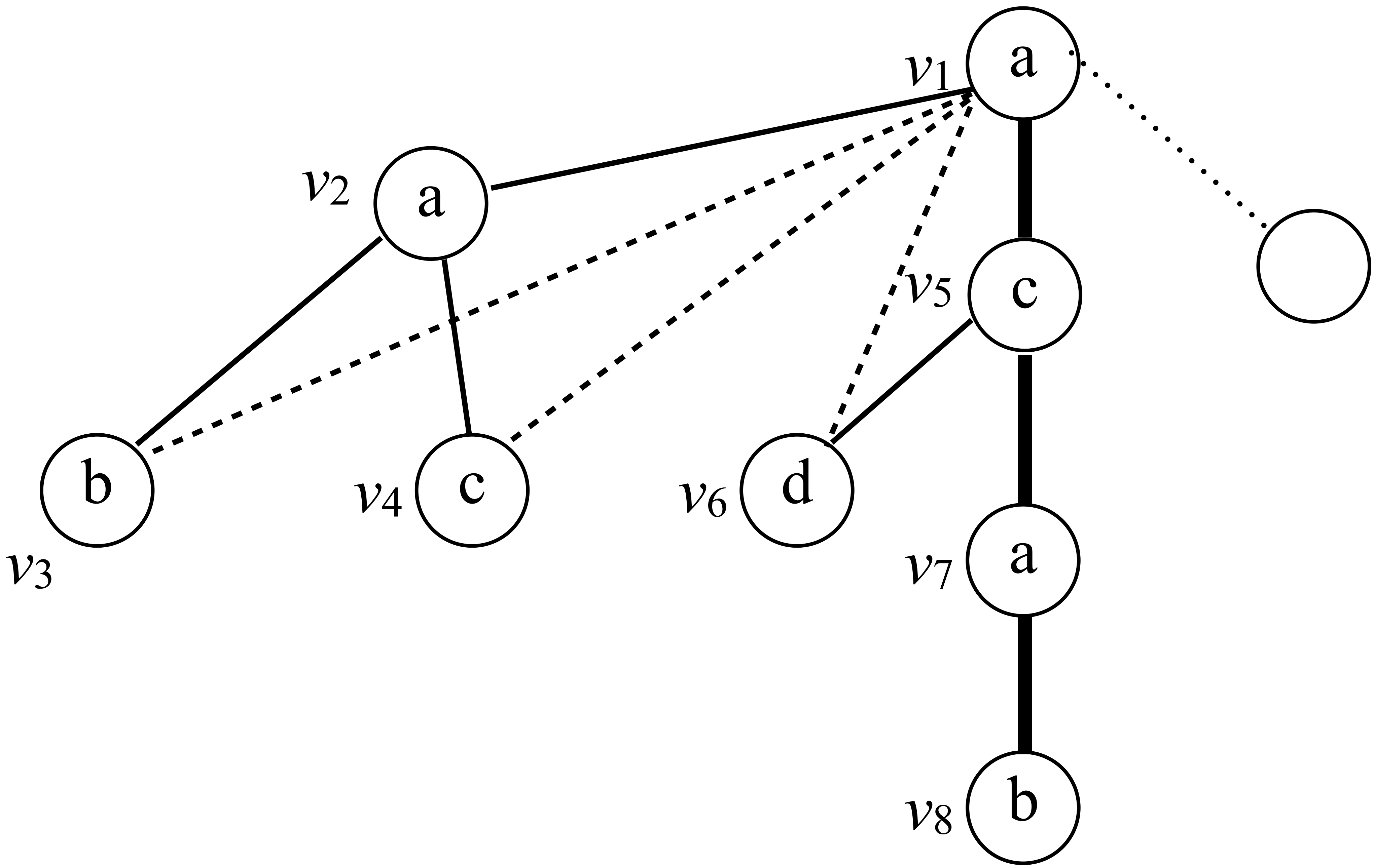


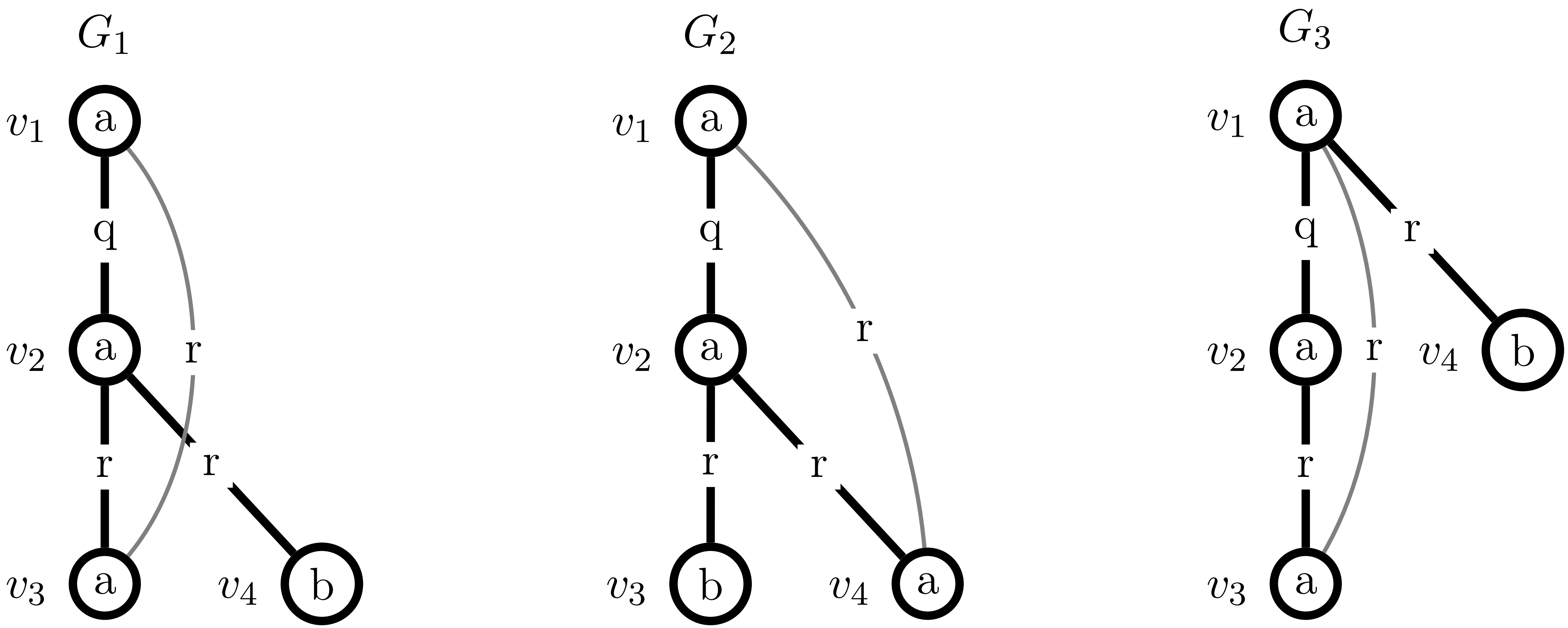
DFS Codes and their Orders

- A *DFS code* is a sequence of tuples of type $\langle v_i, v_j, L(v_i), L(v_j), L(v_i, v_j)\rangle$
  - Tuples are given in DFS order
    - Backwards edges are listed before forward edges
- A DFS code is *canonical* if it is the smallest of the codes in the ordering
  - $\langle v_i, v_j, L(v_i), L(v_j), L(v_i, v_j)\rangle < \langle v_x, v_y, L(v_x), L(v_y), L(v_x, v_y)\rangle$ if
    - $\langle v_i, v_j\rangle <_e \langle v_x, v_y\rangle$; or
    - $\langle v_i, v_j\rangle = \langle v_x, v_y\rangle$ and $\langle L(v_i), L(v_j), L(v_i, v_j)\rangle <_l \langle L(v_x), L(v_y), L(v_x, v_y)\rangle$
  - The ordering of the label tuples is the lexicographical ordering

Ordering the Edges

- Let $e_{ij} = \langle v_i, v_j \rangle$ and $e_{xy} = \langle v_x, v_y \rangle$
- $e_{ij} <_e e_{xy}$ if
  - If e_{ij} and e_{xy} are forward edges, then
    - $j < y$; or
    - $j = y$ and $i > x$
  - If e_{ij} and e_{xy} are backward edges, then
    - $i < x$; or
    - $i = x$ and $j < y$
  - If e_{ij} is forward and e_{xy} is backward, then $i < y$
  - If e_{ij} is backward and e_{xy} is forward, then $j \leq x$

Example



$$
\begin{aligned}
t_{11} &= \langle v_1, v_2, a, a, q \rangle \\
t_{12} &= \langle v_2, v_3, a, a, r \rangle \\
t_{13} &= \langle v_3, v_1, a, a, r \rangle \\
t_{14} &= \langle v_2, v_4, a, b, r \rangle
\end{aligned}
$$

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\begin{aligned}
t_{21} &= \langle v_1, v_2, a, a, q \rangle \\
t_{22} &= \langle v_2, v_3, a, b, r \rangle \\
t_{23} &= \langle v_2, v_4, a, a, r \rangle \\
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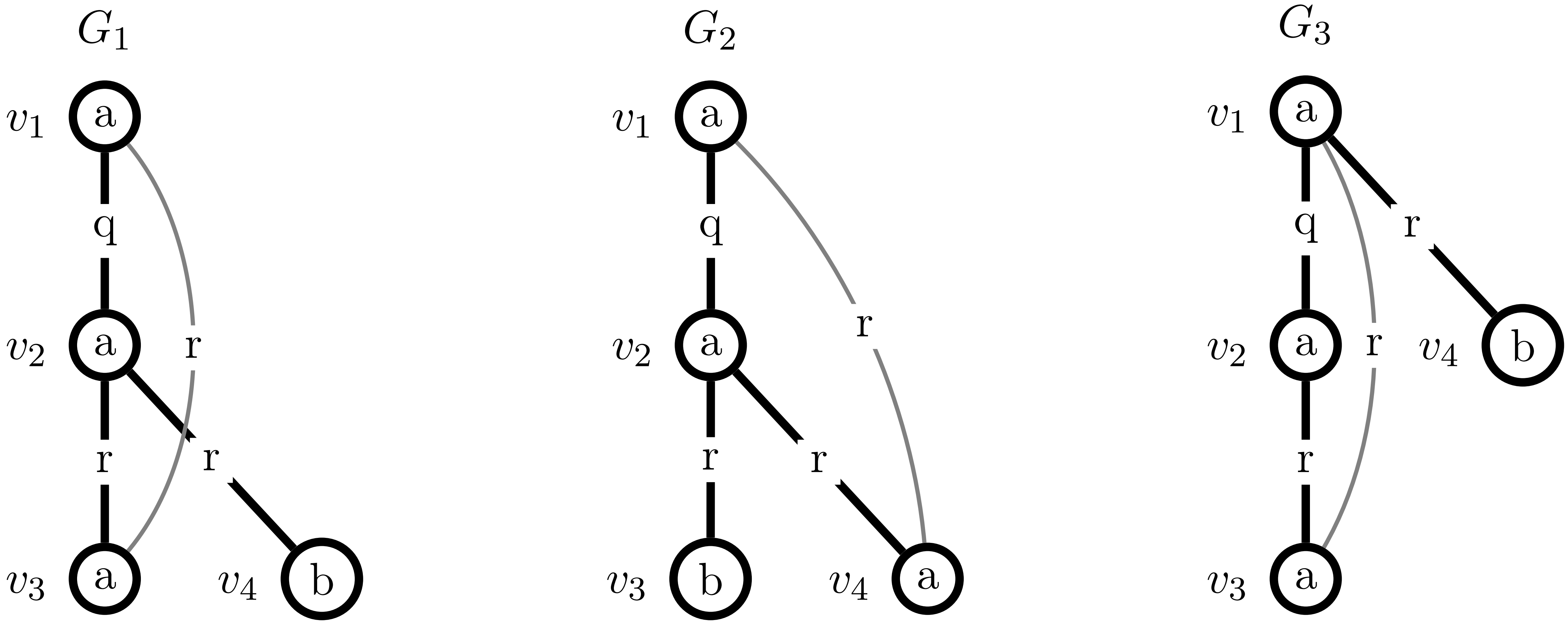
Example



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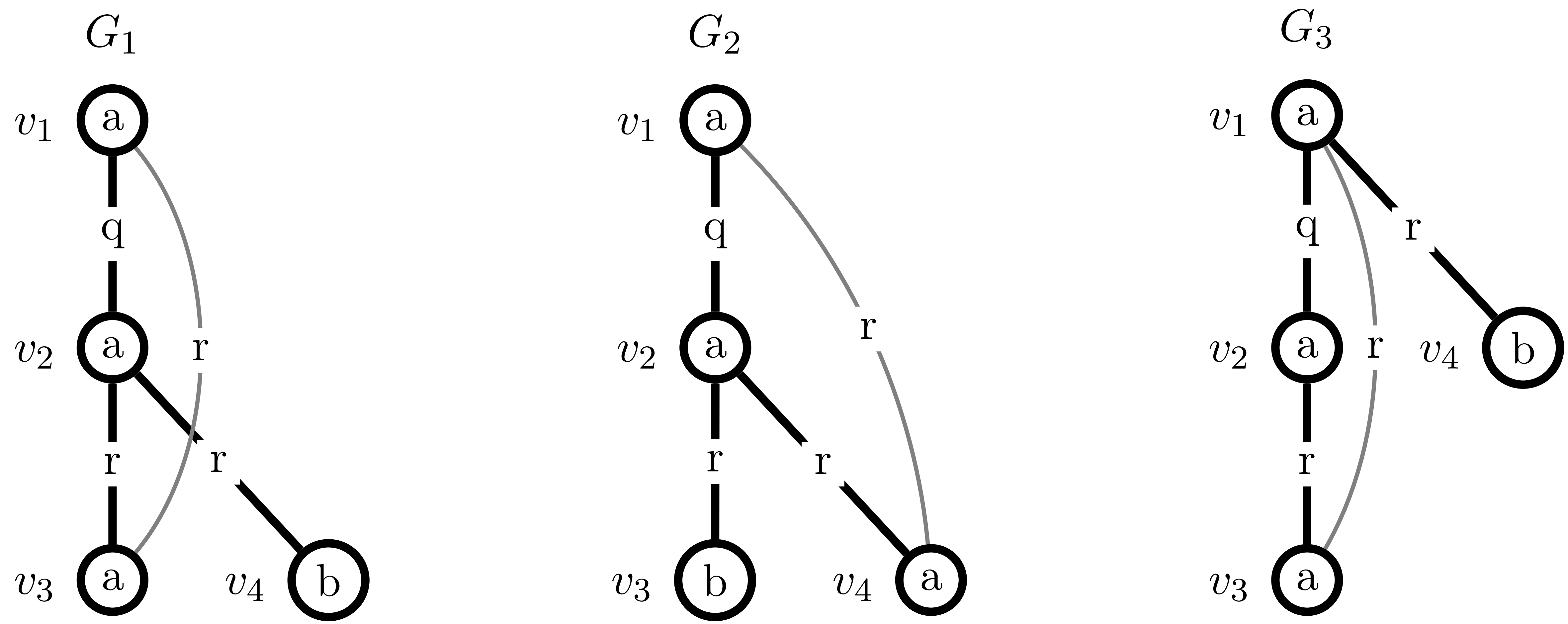
First rows are identical

Example



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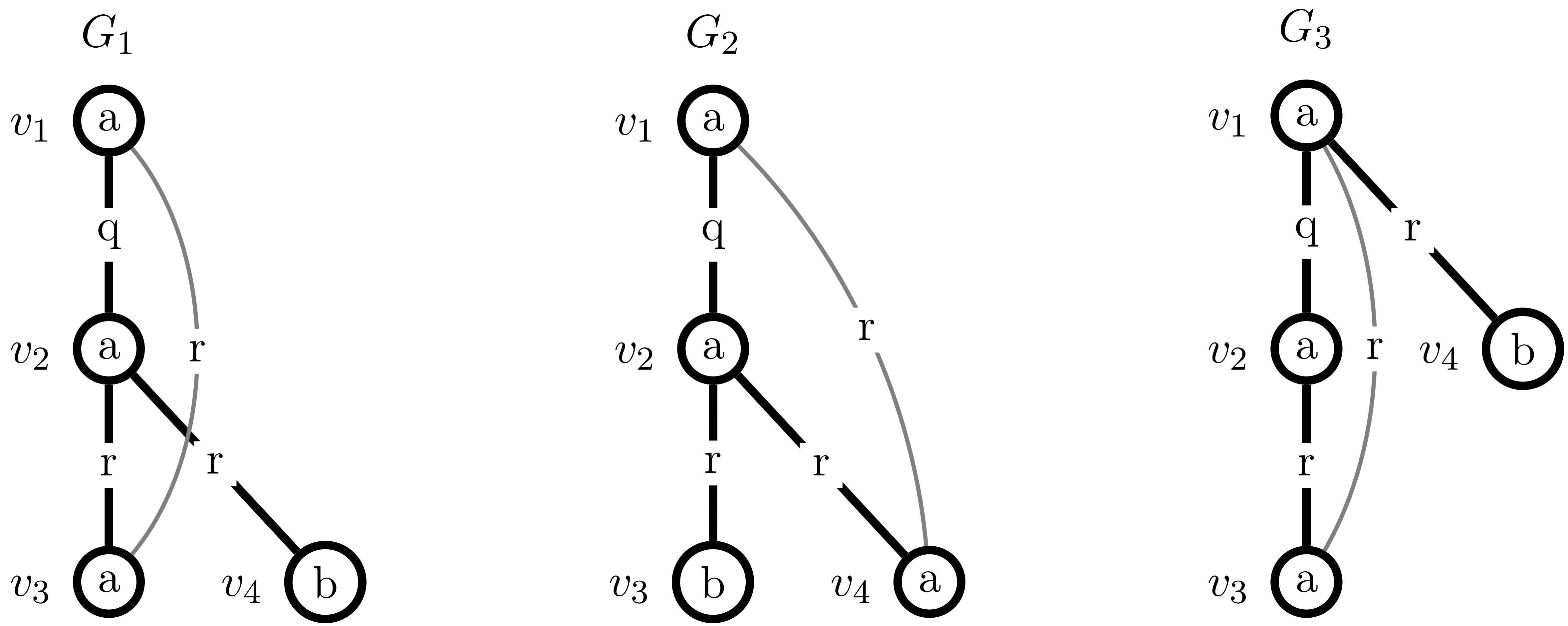
In second row, G_2 is bigger in labels' order

Example



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Last rows are forward edges and 4 = 4 but 2 > 1 $\Rightarrow$ G_1 is smallest

Building the Candidates

- The candidates are build in a *DFS code tree*
  - A DFS code **a** is an *ancestor* of DFS code **b** if **a** is a proper prefix of **b**
  - The siblings in the tree follow the DFS code order
- A graph can be frequent only if all of the graph representing its ancestors in the DFS tree are frequent
- The DFS tree contains all the canonical codes for all the subgraphs of the graphs in the data
  - But not all of the vertices in the code tree correspond to canonical codes
- We will (implicitly) traverse this tree

The Algorithm

- `gSpan`:
  - **for each** frequent 1-edge graphs
    - **call** `subgrm` to grow all nodes in the code tree rooted in this 1-edge graph
    - remove this edge from the graph
- `subgrm`
  - **if** the code is not canonical, return
  - Add this graph to the set of frequent graphs
  - Create each super-graph with one more edge and compute its frequency
  - **call** `subgrm` with each frequent super-graph