Graph Mining

(In Association Rules: Advanced Concepts and Algorithms)

Mirco Nanni

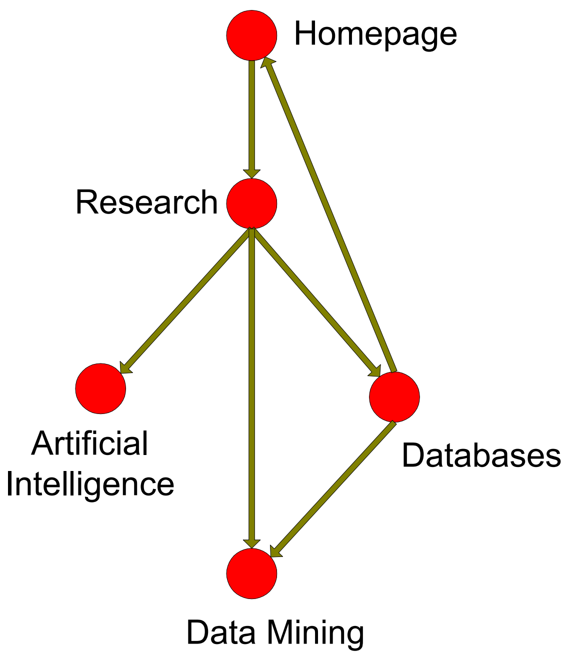
Pisa KDD Lab, ISTI-CNR & Univ. Pisa

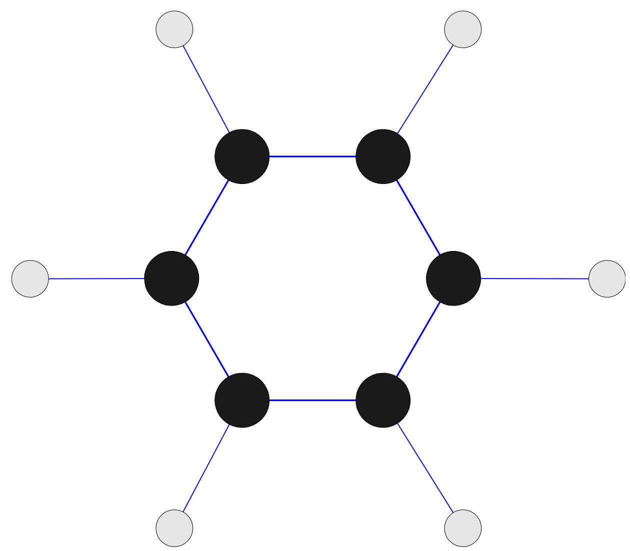
http://kdd.isti.cnr.it/

Slides from “Introduction to Data Mining” (Tan, Steinbach, Kumar)

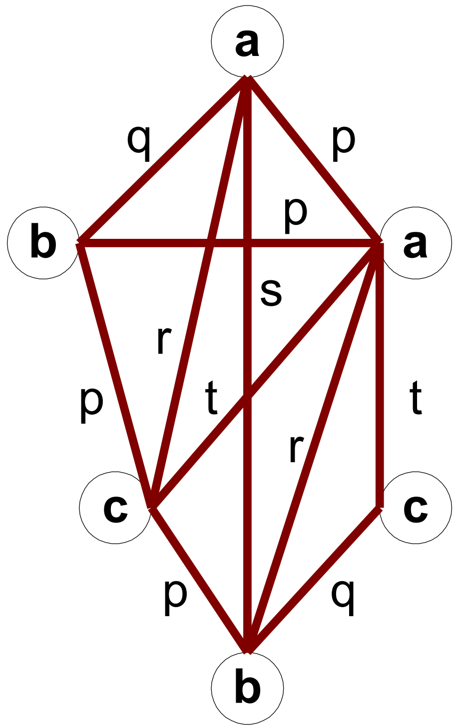
Frequent Subgraph Mining

- Extend association rule mining to finding frequent subgraphs
- Useful for Web Mining, computational chemistry, bioinformatics, spatial data sets, etc

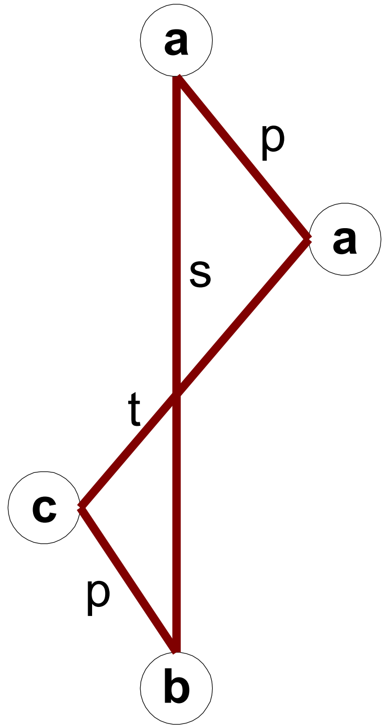




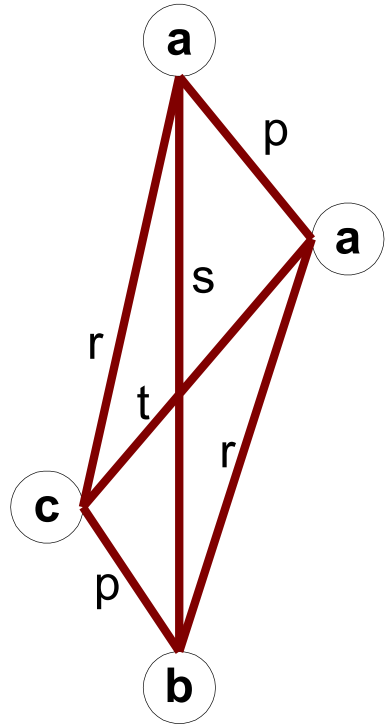
Graph Definitions



(a) Labeled Graph



(b) Subgraph

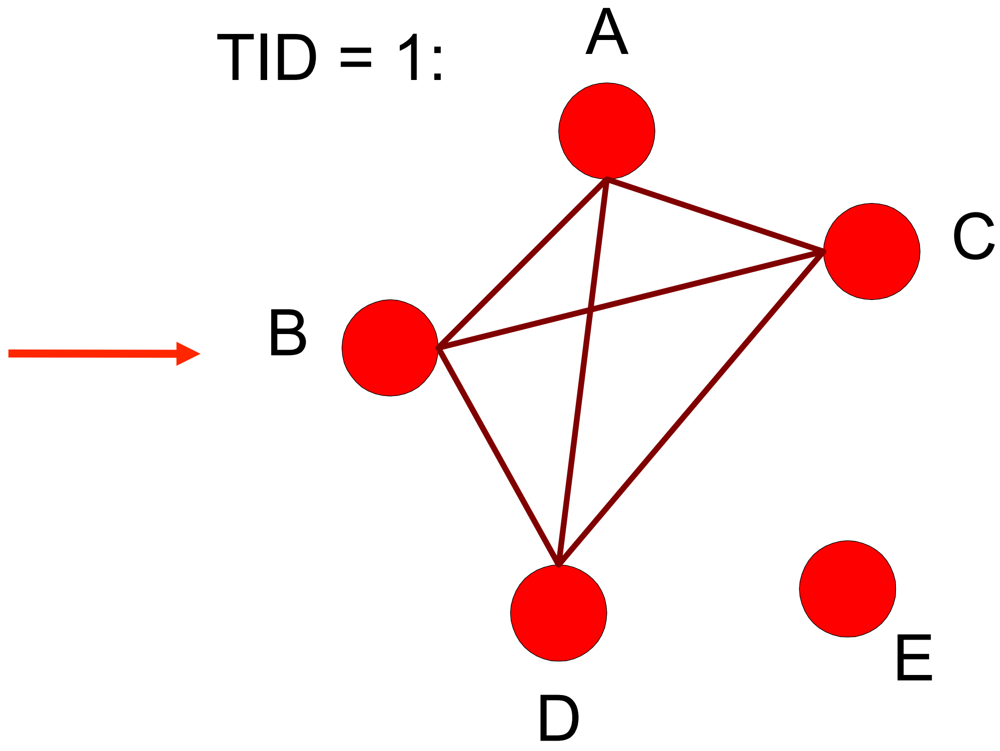


(c) Induced Subgraph

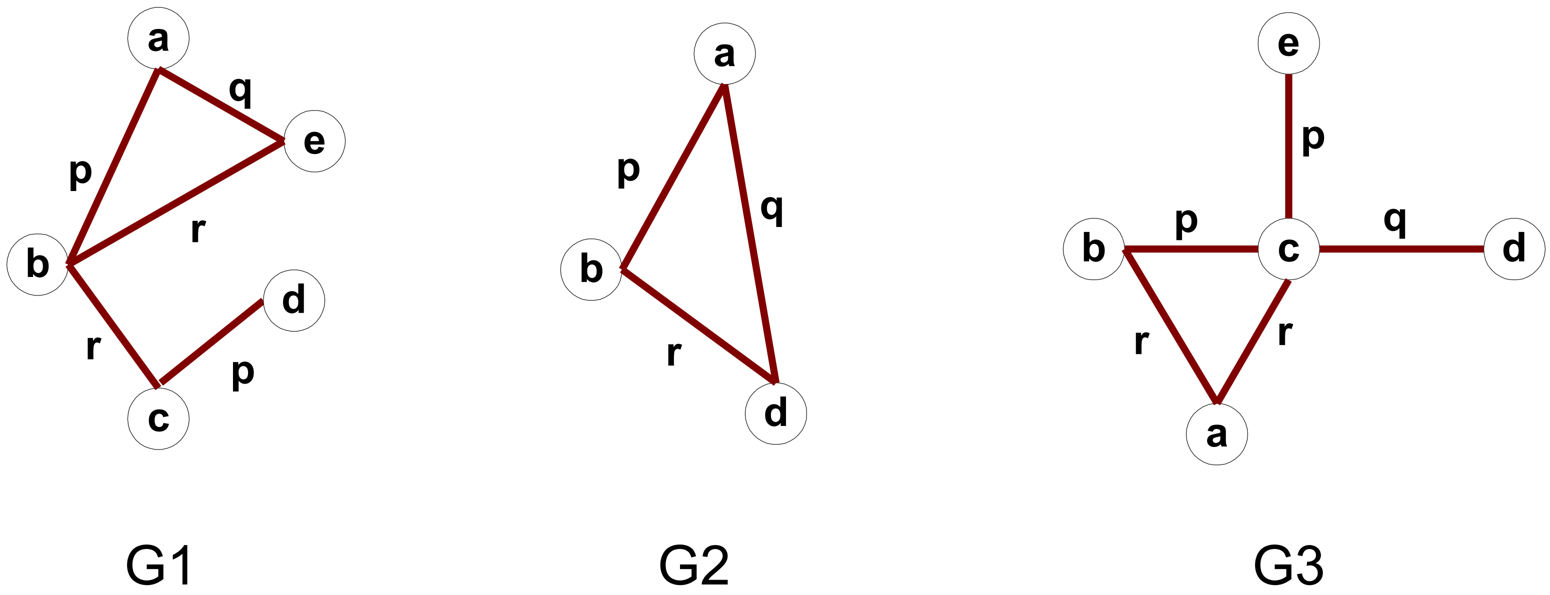
Representing Transactions as Graphs

- Each transaction is a clique of items

Transaction Id	Items
1	{A,B,C,D}
2	{A,B,E}
3	{B,C}
4	{A,B,D,E}
5	{B,C,D}



Representing Graphs as Transactions



	(a,b,p)	(a,b,q)	(a,b,r)	(b,c,p)	(b,c,q)	(b,c,r)	…	(d,e,r)
G1	1	0	0	0	0	1	…	0
G2	1	0	0	0	0	0	…	0
G3	0	0	1	1	0	0	…	0
G3	…	…	…	…	…	…	…	…

Challenges

- Node may contain duplicate labels
- Support and confidence
  - How to define them?
- Additional constraints imposed by pattern structure
  - Support and confidence are not the only constraints
  - Assumption: frequent subgraphs must be connected
- Apriori-like approach:
  - Use frequent k-subgraphs to generate frequent (k+1) subgraphs
    - What is k?

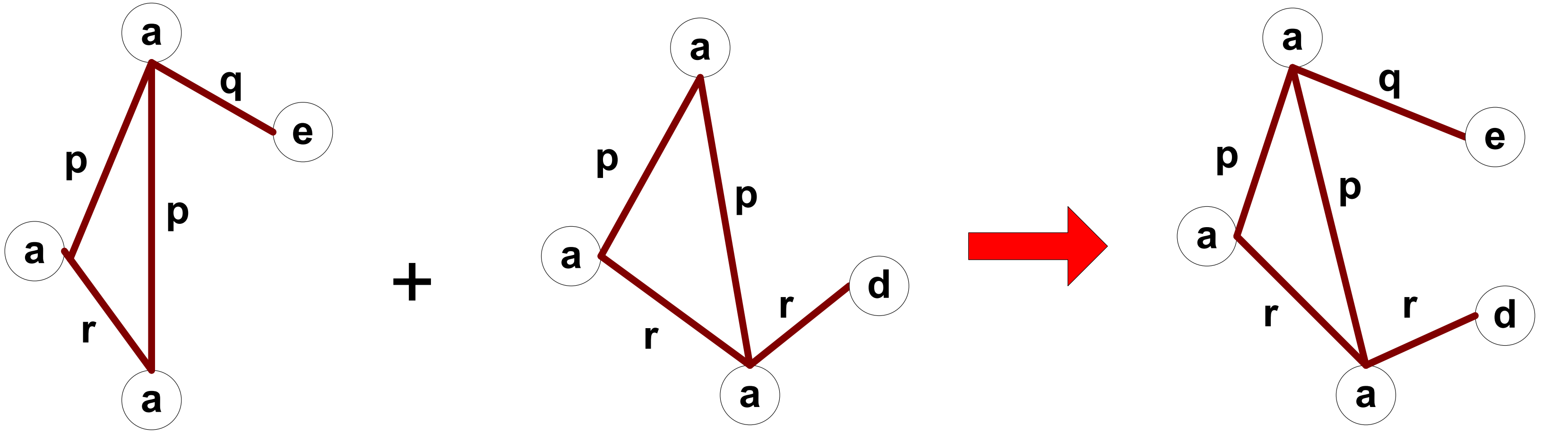
Challenges…

- Support:
  – number of graphs that contain a particular subgraph

- Apriori principle still holds

- Level-wise (Apriori-like) approach:
  – Vertex growing:
    - k is the number of vertices
  – Edge growing:
    - k is the number of edges

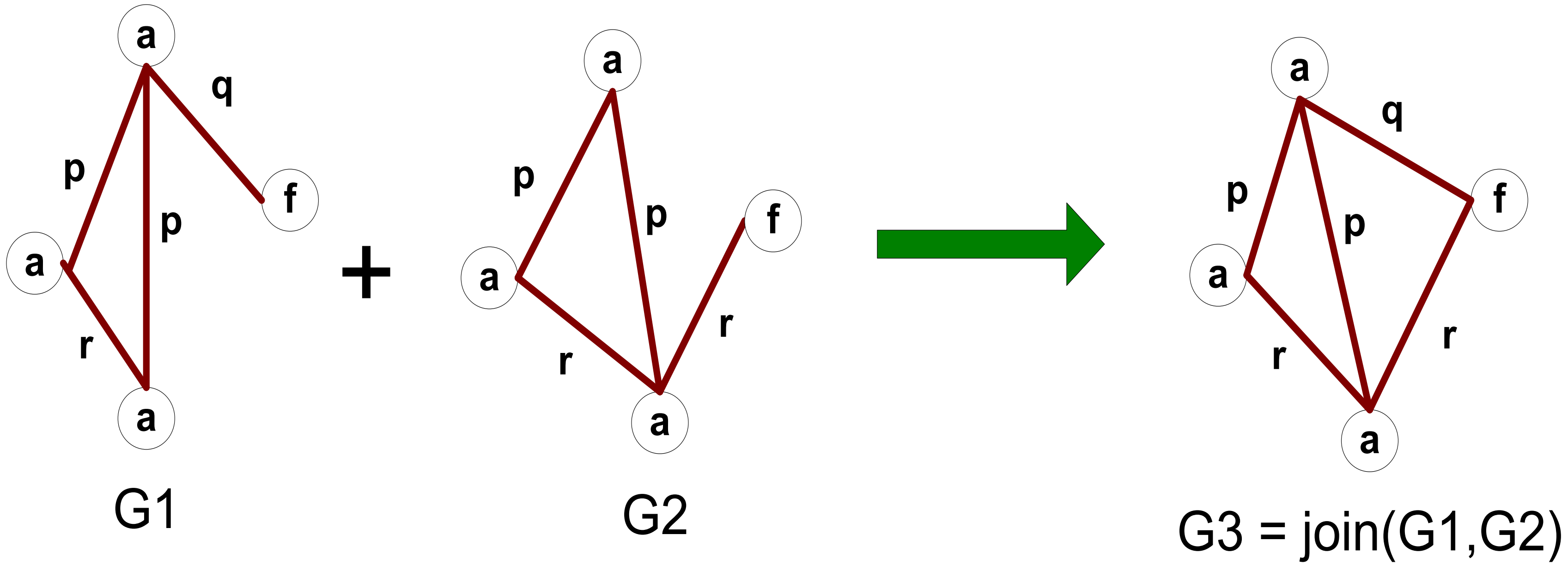
Vertex Growing



G1 G2 G3 = join(G1,G2)

$$M_{G1} = \begin{pmatrix} 0 & p & p & q \\ p & 0 & r & 0 \\ p & r & 0 & 0 \\ q & 0 & 0 & 0 \end{pmatrix} \qquad M_{G2} = \begin{pmatrix} 0 & p & p & 0 \\ p & 0 & r & 0 \\ p & r & 0 & r \\ 0 & 0 & r & 0 \end{pmatrix} \qquad M_{G3} = \begin{pmatrix} 0 & p & p & 0 & q \\ p & 0 & r & 0 & 0 \\ p & r & 0 & r & 0 \\ 0 & 0 & r & 0 & 0 \\ q & 0 & 0 & 0 & 0 \end{pmatrix}$$

Edge Growing

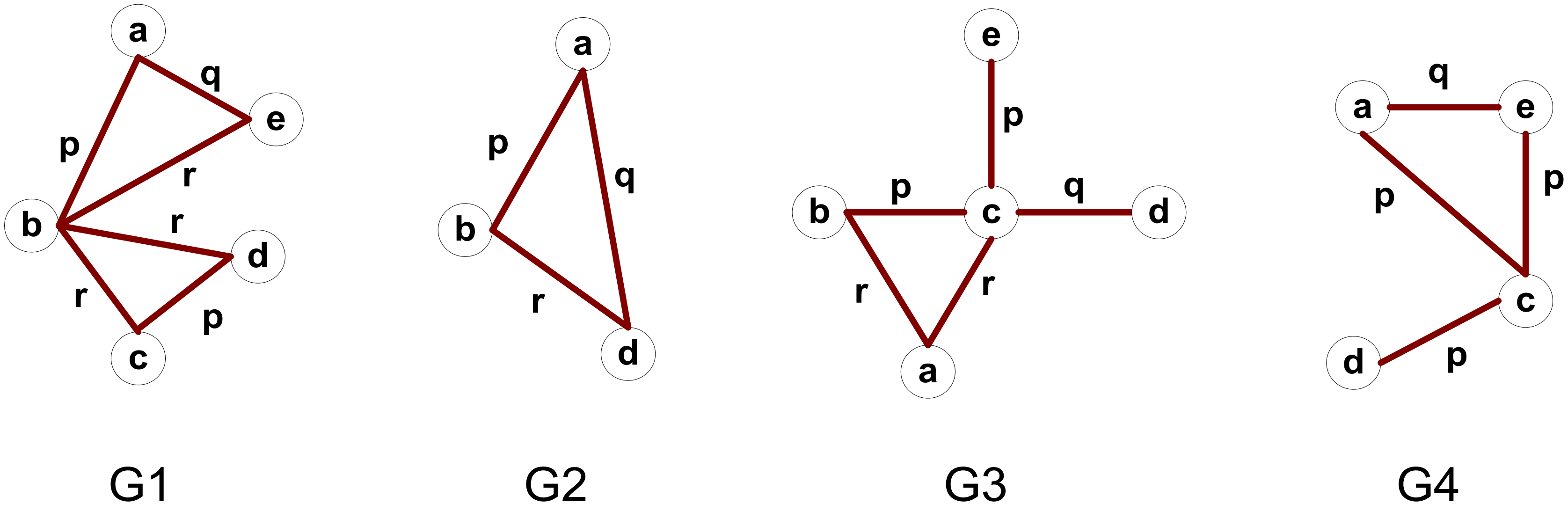


Apriori-like Algorithm

- Find frequent 1-subgraphs
- Repeat
  - Candidate generation
    - Use frequent (*k-1*)-subgraphs to generate candidate *k*-subgraph
  - Candidate pruning
    - Prune candidate subgraphs that contain infrequent (*k-1*)-subgraphs
  - Support counting
    - Count the support of each remaining candidate
  - Eliminate candidate *k*-subgraphs that are infrequent

In practice, it is not as easy. There are many other issues

Example: Dataset

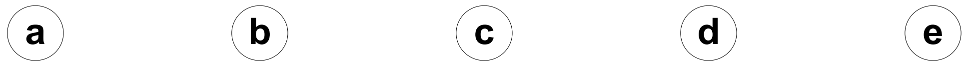


	(a,b,p)	(a,b,q)	(a,b,r)	(b,c,p)	(b,c,q)	(b,c,r)	…	(d,e,r)
G1	1	0	0	0	0	1	…	0
G2	1	0	0	0	0	0	…	0
G3	0	0	1	1	0	0	…	0
G4	0	0	0	0	0	0	…	0

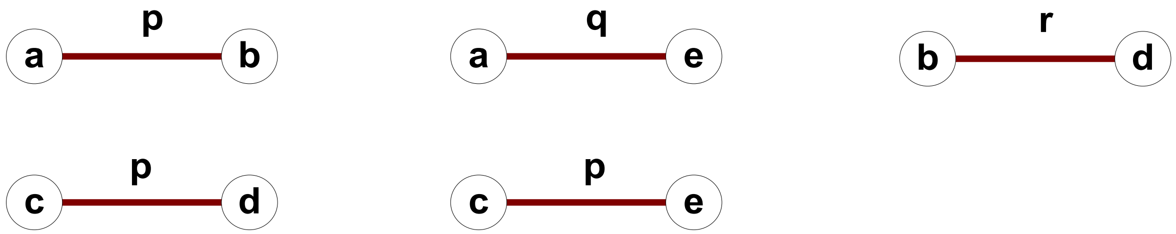
Example

Minimum support count = 2

k=1
Frequent
Subgraphs



k=2
Frequent
Subgraphs



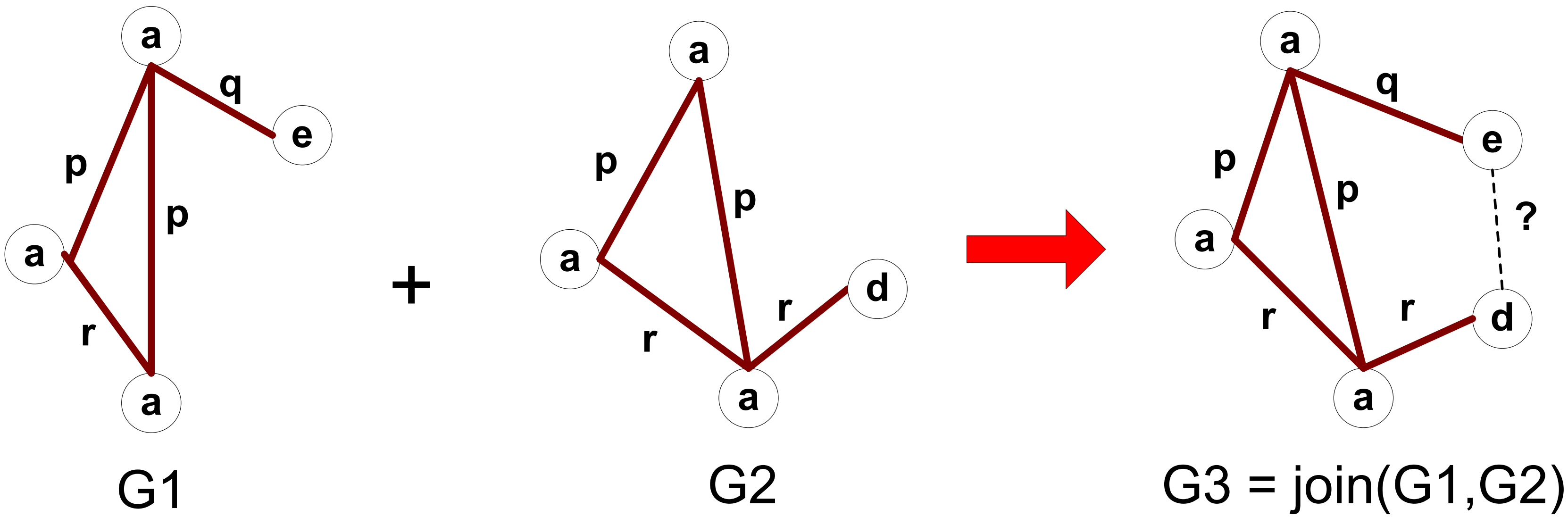
k=3
Candidate
Subgraphs

(Pruned candidate)

Candidate Generation

- In Apriori:
  - Merging two frequent *k*-itemsets will produce a candidate (*k+1*)-itemset
- In frequent subgraph mining (vertex/edge growing)
  - Merging two frequent *k*-subgraphs may produce more than one candidate (*k+1*)-subgraph

Multiplicity of Candidates (Vertex Growing)



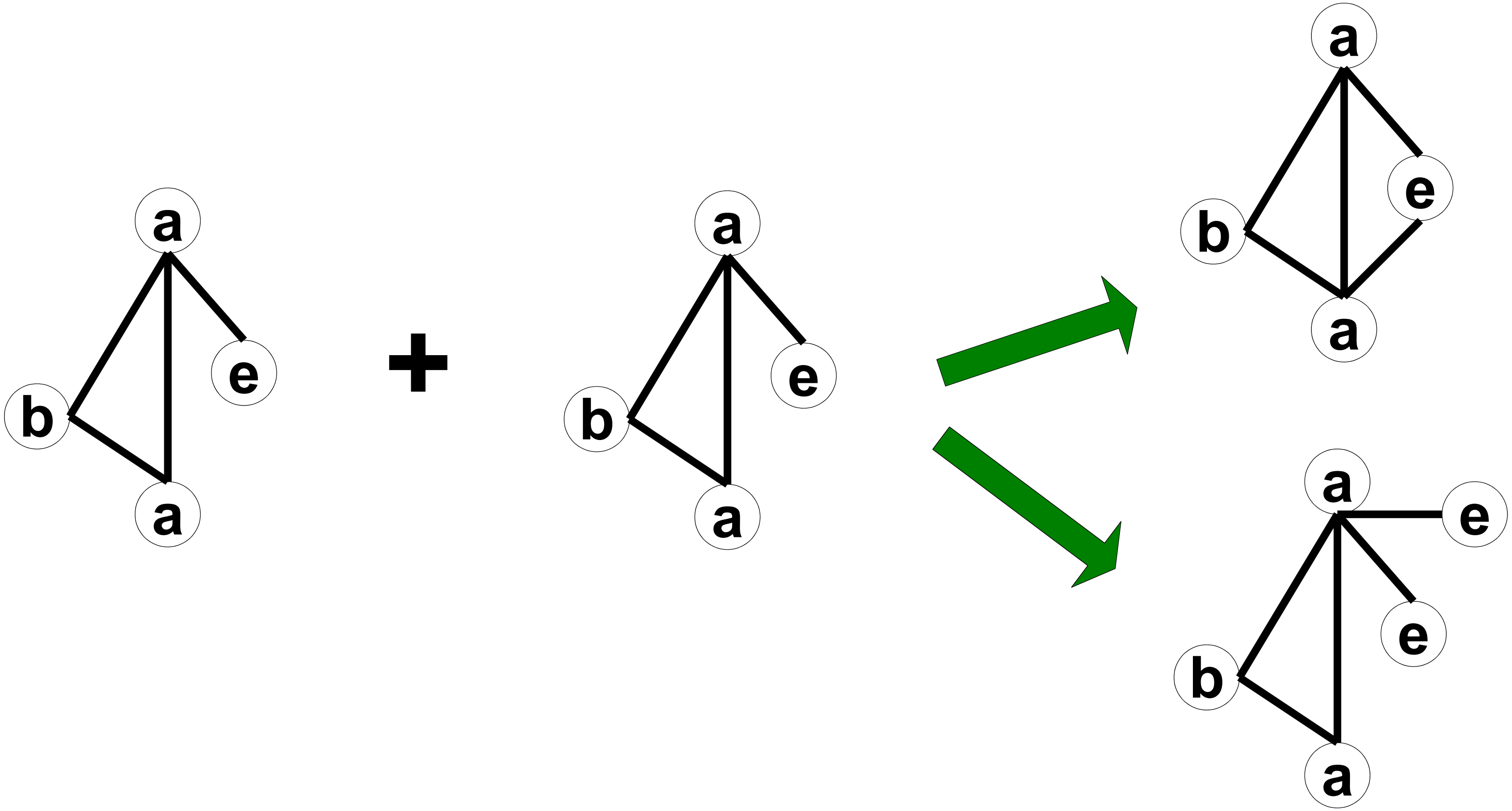
$$M_{G1} = \begin{pmatrix} 0 & p & p & q \\ p & 0 & r & 0 \\ p & r & 0 & 0 \\ q & 0 & 0 & 0 \end{pmatrix}$$

$$M_{G2} = \begin{pmatrix} 0 & p & p & 0 \\ p & 0 & r & 0 \\ p & r & 0 & r \\ 0 & 0 & r & 0 \end{pmatrix}$$

$$M_{G3} = \begin{pmatrix} 0 & p & p & 0 & q \\ p & 0 & r & 0 & 0 \\ p & r & 0 & r & 0 \\ 0 & 0 & r & 0 & ? \\ q & 0 & 0 & ? & 0 \end{pmatrix}$$

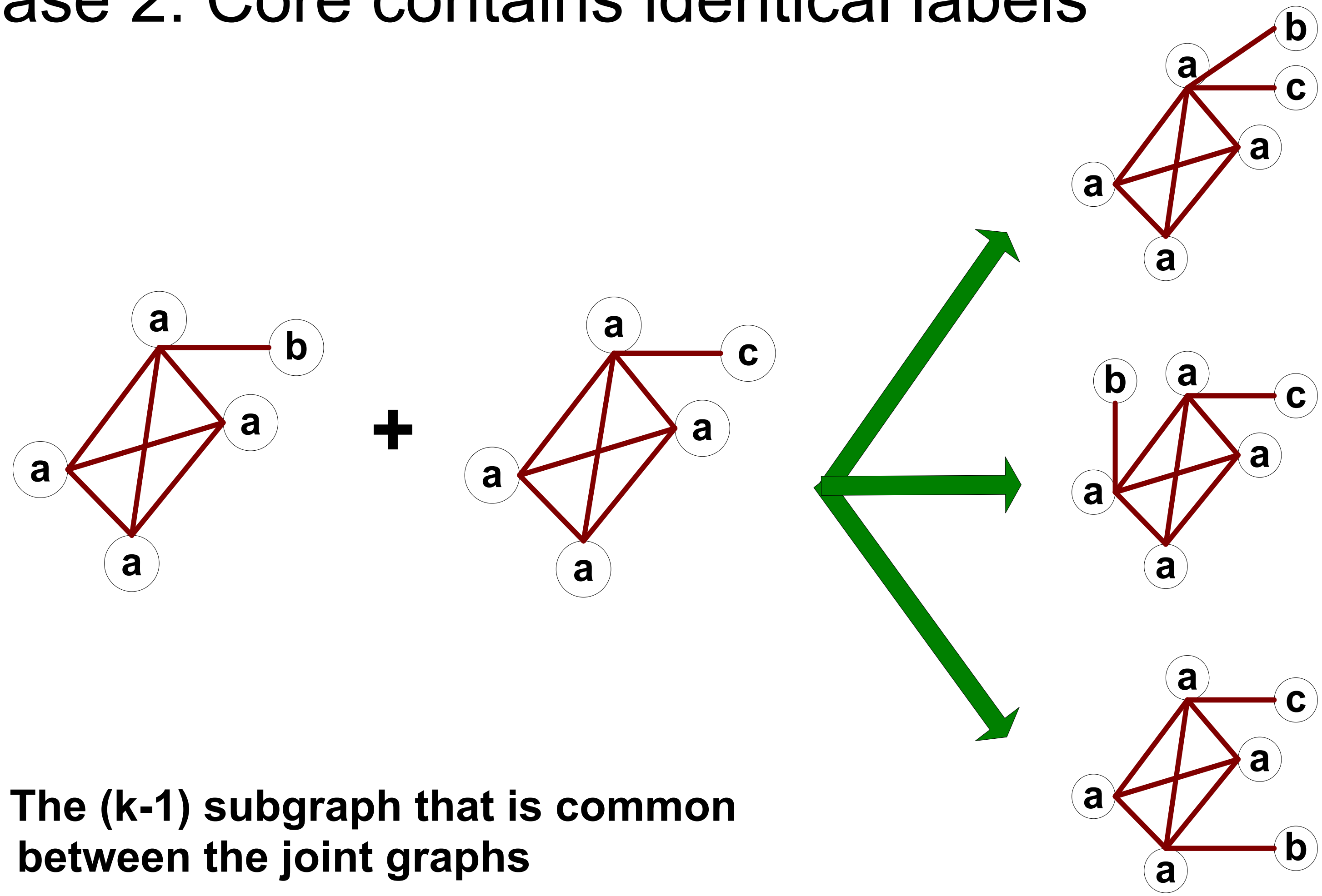
Multiplicity of Candidates (Edge growing)

- Case 1: identical vertex labels



Multiplicity of Candidates (Edge growing)

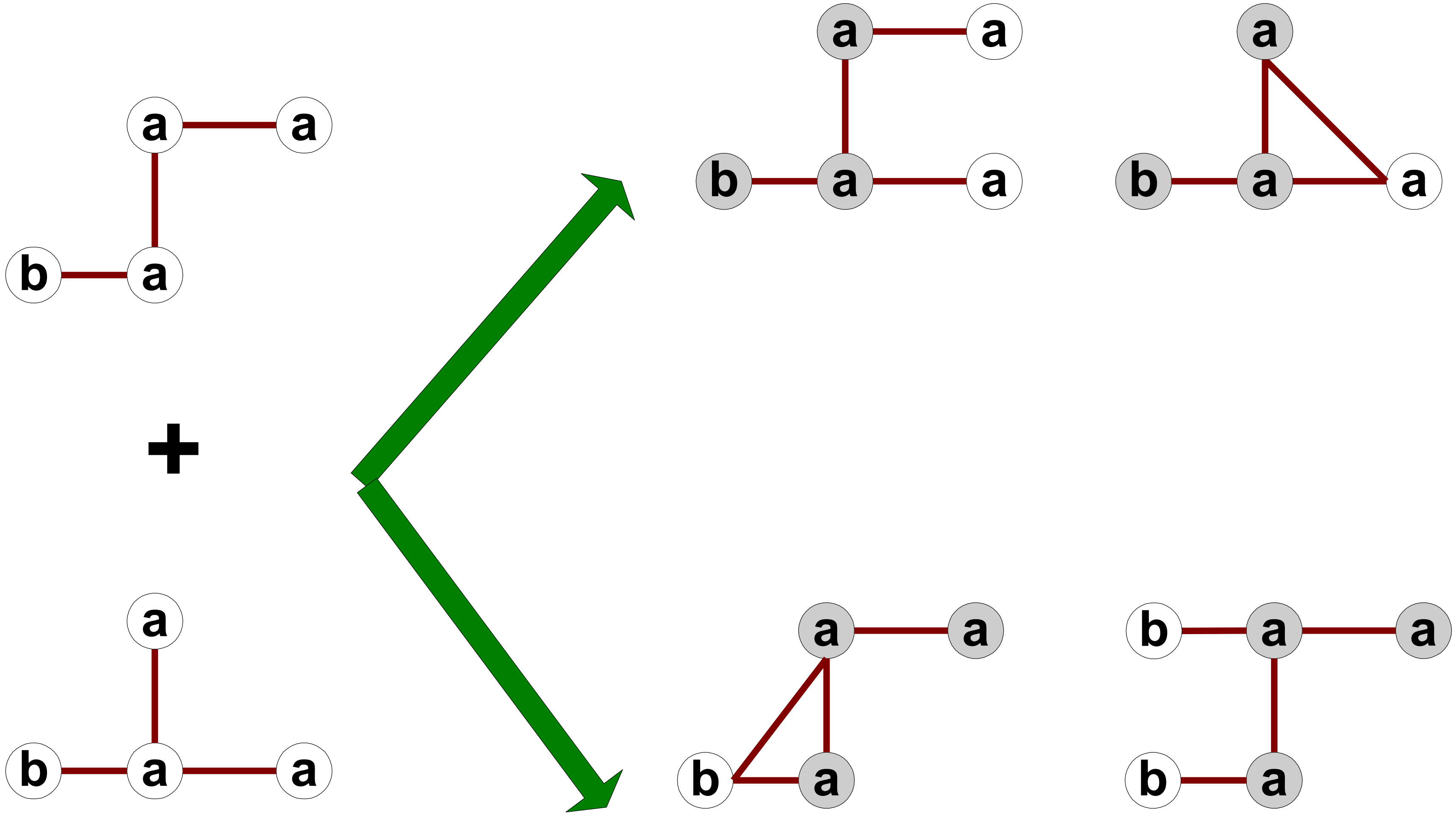
- Case 2: Core contains identical labels



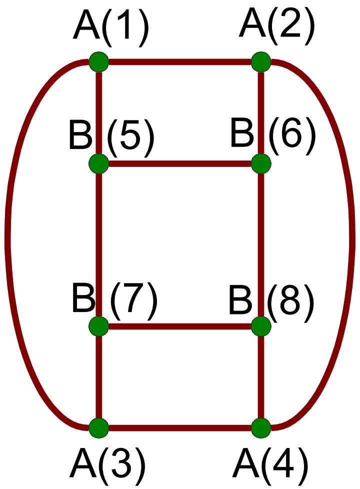
Core: The (k-1) subgraph that is common between the joint graphs

Multiplicity of Candidates (Edge growing)

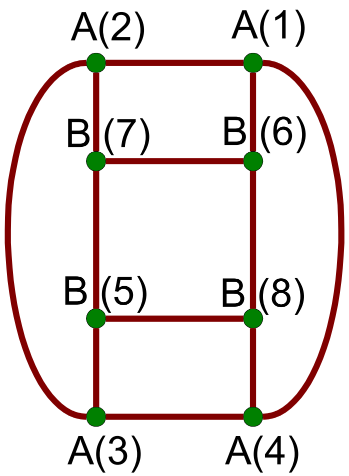
- Case 3: Core multiplicity



Adjacency Matrix Representation



	A(1)	A(2)	A(3)	A(4)	B(5)	B(6)	B(7)	B(8)
A(1)	1	1	1	0	1	0	0	0
A(2)	1	1	0	1	0	1	0	0
A(3)	1	0	1	1	0	0	1	0
A(4)	0	1	1	1	0	0	0	1
B(5)	1	0	0	0	1	1	1	0
B(6)	0	1	0	0	1	1	0	1
B(7)	0	0	1	0	1	0	1	1
B(8)	0	0	0	1	0	1	1	1

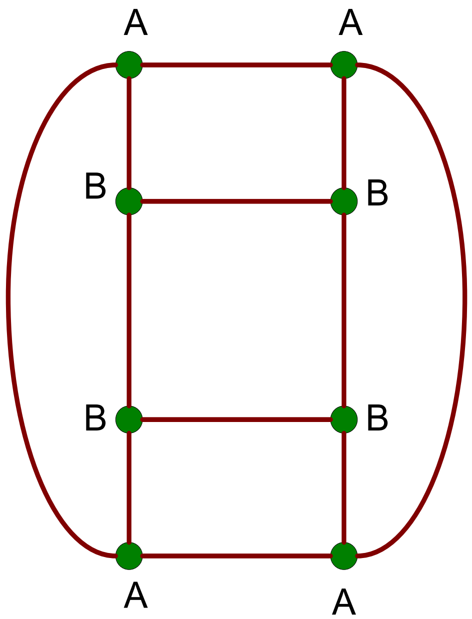


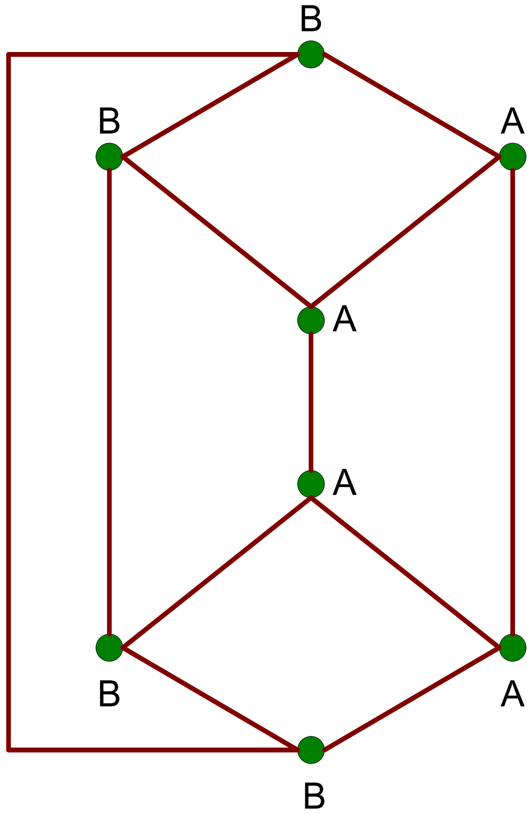
	A(1)	A(2)	A(3)	A(4)	B(5)	B(6)	B(7)	B(8)
A(1)	1	1	0	1	0	1	0	0
A(2)	1	1	1	0	0	0	1	0
A(3)	0	1	1	1	1	0	0	0
A(4)	1	0	1	1	0	0	0	1
B(5)	0	0	1	0	1	0	1	1
B(6)	1	0	0	0	0	1	1	1
B(7)	0	1	0	0	1	1	1	0
B(8)	0	0	0	1	1	1	0	1

- **The same graph can be represented in many ways**

Graph Isomorphism

- A graph is isomorphic if it is topologically equivalent to another graph



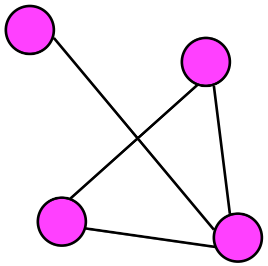


Graph Isomorphism

- Test for graph isomorphism is needed:
  - During candidate generation step, to determine whether a candidate has been generated
  - During candidate pruning step, to check whether its (*k-1*)-subgraphs are frequent
  - During candidate counting, to check whether a candidate is contained within another graph

Graph Isomorphism

- Use canonical labeling to handle isomorphism
  - Map each graph into an ordered string representation (known as its code) such that two isomorphic graphs will be mapped to the same canonical encoding
  - Example:
    - Lexicographically largest adjacency matrix



$$\rightarrow \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} \rightarrow \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

String: 0010001111010110 **Canonical: 0111101011001000**