CI-6227 Data Mining

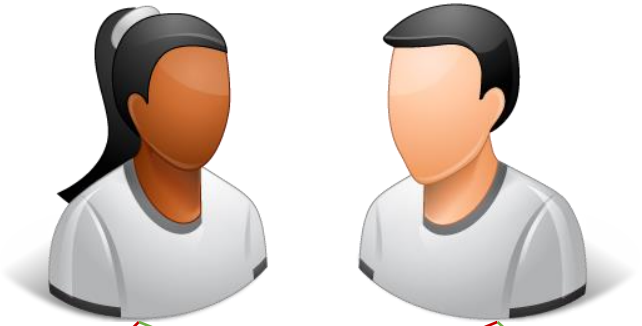
Lecture 6

Association Rules: Advanced Concepts and Algorithms

Asymmetric Binary Attributes

If the values of a binary attribute are not equally important, the binary attribute is called **asymmetric**.

Usually, denotes presence or absence of something.



Works as a data analyst?

Do they have something in common?

NO **YES**

Continuous and Categorical Attributes

How to apply association analysis formulation to attributes that are NOT **asymmetric binary variables?**

Session Id	Country	Session Length (sec)	Number of Web Pages viewed	Gender	Browser	OS
1	USA	982	8	Male	IE	Win
2	China	811	10	Female	Chrome	Win
3	USA	2125	45	Female	Firefox	Mac
4	Germany	596	4	Male	IE	Linux
5	Australia	123	9	Male	Firefox	Win
…	…	…	…	…	…	…

Example of Association Rule:

(Browser=Firefox) ∧ (OS=Mac) → (Session Length < 45sec) ∧ (No. of Pages < 2)

Handling Categorical Attributes

- Transform categorical attribute into asymmetric binary variables
- Introduce a new "item" for each distinct attribute-value pair
  - *Example*: replace "Browser" attribute with
    - Browser is Internet Explorer
    - Browser is Firefox
    - Browser is Chrome

Session Id	Country	Session Length (sec)	Number of Web Pages viewed	Gender	Browser is IE	Browser is Firefox	Browser is Chrome	OS
…	…	…	…	…	…	…	…	…

Handling Categorical Attributes

- Potential Issues
  - What if attribute has many possible values
    - Example: attribute *country* has more than 200 possible values
    - Many of the attribute values may have very low support
      - *Potential solution*: Aggregate the low-support attribute values
  - What if distribution of attribute values is highly skewed
    - Example: 90% of the visitors have OS=Win
    - Most of the items will be associated with (OS=Win) item
      - *Potential solution*: drop the highly frequent items

Handling Continuous Attributes

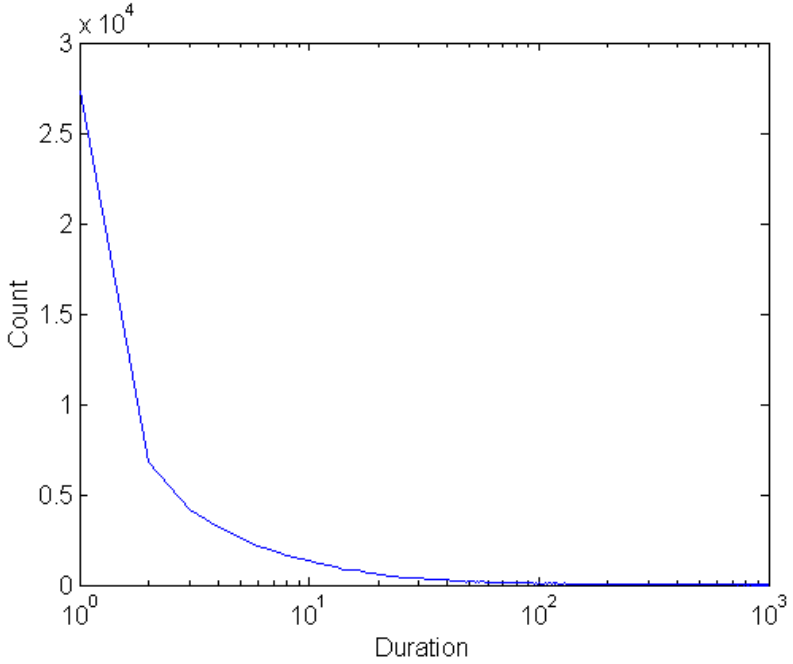
- Different kinds of rules:
  - Age$\in$[21,35) $\wedge$ Salary$\in$[70k,120k) $\rightarrow$ Buy
  - Salary$\in$[70k,120k) $\wedge$ Buy $\rightarrow$ Age: μ=28, σ=4

- Different methods:
  - Discretization-based
  - Statistics-based
  - Non-discretization based
    - minApriori

Handling Continuous Attributes

Approach 1: Discretization

- Equal-width binning
- Equal-depth (equal-freq) binning
- Clustering



Discretization Issues

- Size of the discretized intervals affect support & confidence

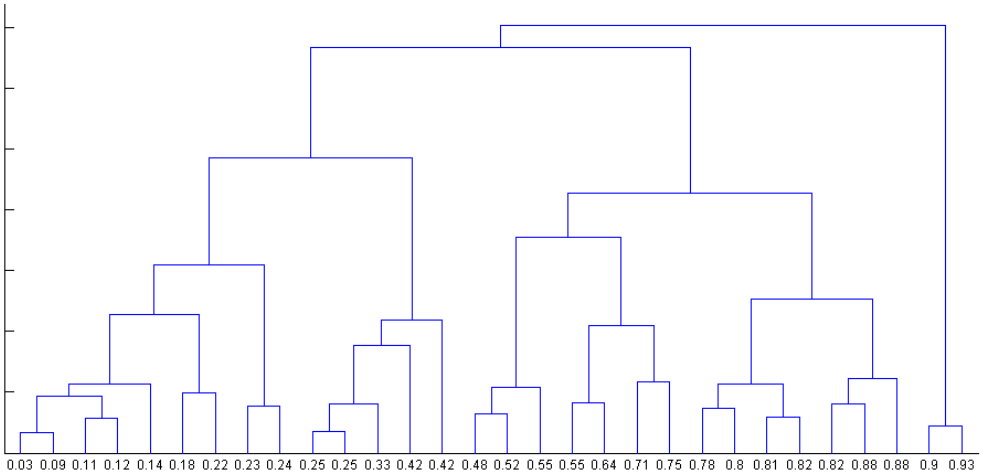
  {Refund = No, (Income = $51,250)} → {Cheat = No}
  {Refund = No, (60k ≤ Income ≤ 80k)} → {Cheat = No}
  {Refund = No, (0k ≤ Income ≤ 1bn)} → {Cheat = No}

  - If intervals too small
    - may not have enough support
  - If intervals too large
    - may not have enough confidence

- *Potential solution*: use all possible intervals

Discretization Issues

- Execution time
  - If intervals contain n values, there are on average $O(n^2)$ possible ranges



- Too many rules

{Refund = No, (Income = $51,250)} → {Cheat = No}
{Refund = No, (5**1**k ≤ Income ≤ 52k)} → {Cheat = No}
{Refund = No, (5**0**k ≤ Income ≤ 52k)} → {Cheat = No}

Statistics-based Methods

- Example:

$$\text{Browser=Chrome} \wedge \text{OS=Mac} \rightarrow \text{Age: } \mu=23$$

- Rule consequent consists of a continuous variable, characterized by their statistics
  - —mean, median, standard deviation, *etc*.
- Approach:
  - —Withhold the target variable from the rest of the data
  - —Apply existing frequent itemset generation on the rest of the data
  - —For each frequent itemset, compute the descriptive statistics for the corresponding target variable
    - Frequent itemset becomes a rule by introducing the target variable as rule consequent
  - —Apply statistical test to determine interestingness of the rule

Statistics-based Methods

- How to determine whether an association rule is *interesting*?
  - Compare the statistics for segment of population covered by the rule vs. segment of population not covered by the rule:
    - $A \Rightarrow B: \mu$ versus $\bar{A} \Rightarrow B: \mu'$

$$Z = \frac{\mu' - \mu - \Delta}{\sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}}$$

  - Statistical hypothesis testing:
    - Null hypothesis $H_0: \mu' = \mu + \Delta$
    - Alternative hypothesis $H_1: \mu' > \mu + \Delta$
    - $Z \sim N(0,1)$ under null hypothesis

Statistics-based Methods

- *Example*:

r: Browser=Chrome $\wedge$ OS=Mac $\rightarrow$ Age: μ=23

  - Rule is interesting if difference between μ and μ' is greater than 5 years (i.e., $\Delta = 5$)
  - For r, suppose: $n_1 = 50, s_1 = 3.5$
  - For r' (complement): $n_2 = 250, s_2 = 6.5$

$$Z = \frac{\mu' - \mu - \Delta}{\sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}} = \frac{30 - 23 - 5}{\sqrt{\frac{3.5^2}{50} + \frac{6.5^2}{250}}} = 3.11$$

  - For 1-sided test at 95% confidence level, critical Z-value for rejecting null hypothesis is 1.64.
  - Since Z is greater than 1.64, r is an interesting rule

Min-Apriori (Han *et al.*, 1997)

- Document-term matrix:

DId	W1	W2	W3	W4	W5
D1	2	2	0	0	1
D2	0	0	1	2	2
D3	2	3	0	0	0
D4	0	0	1	0	1
D5	1	1	1	0	2

- *Example*:
  - W1 and W2 tends to appear together in the same document

Min-Apriori

- Data contains only continuous attributes of the same "type"
  - e.g., frequency of words in a document

DId	W1	W2	W3	W4	W5
D1	2	2	0	0	1
D2	0	0	1	2	2
D3	2	3	0	0	0
D4	0	0	1	0	1
D5	1	1	1	0	2

- *Potential solutions*:
  - Convert into 0/1 matrix and then apply existing algorithms
    - lose word frequency information
  - Discretization does not apply as users want association among words not ranges of word frequencies:

    $\texttt{data} \wedge \texttt{mining}$ *vs.* $\texttt{data} \in [1,4] \wedge \texttt{mining} \in [2,3]$

Min-Apriori

- How to determine the support of a word?
  - —If we simply sum up its frequency, support count will be greater than total number of documents!
    - Normalize the word vectors — e.g., using L_1 norm
    - Each word has a support of 1.0

DId	W1	W2	W3	W4	W5
D1	2	2	0	0	1
D2	0	0	1	2	2
D3	2	3	0	0	0
D4	0	0	1	0	1
D5	1	1	1	0	2

Normalize

DId	W1	W2	W3	W4	W5
D1	0.4	0.33	0	0	0.17
D2	0	0	0.33	1.00	0.33
D3	0.4	0.5	0	0	0
D4	0	0	0.33	0	0.17
D5	0.2	0.17	0.33	0	0.33

Min-Apriori

- New definition of support:

Normalized frequency of word j in document i

$$\sup(C) = \sum_{i \in T} \min_{j \in C} D(i, j)$$

Across all documents

Across all words in C

DId	W1	W2	W3	W4	W5
D1	0.4	0.33	**0**	0	0.17
D2	**0**	**0**	0.33	1.00	0.33
D3	0.4	0.5	**0**	0	0
D4	**0**	**0**	0.33	0	0.17
D5	0.2	**0.17**	0.33	0	0.33

Example:

$$\sup(W1, W2, W3) = 0 + 0 + 0 + 0 + 0.17 = 0.17$$

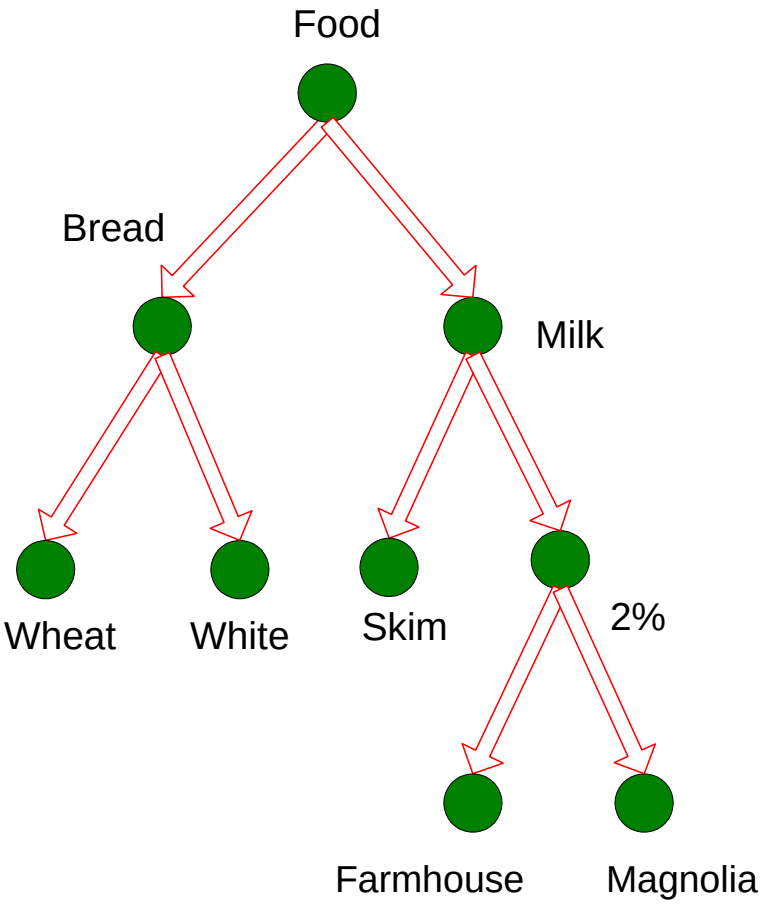
Anti-monotone Property of Support

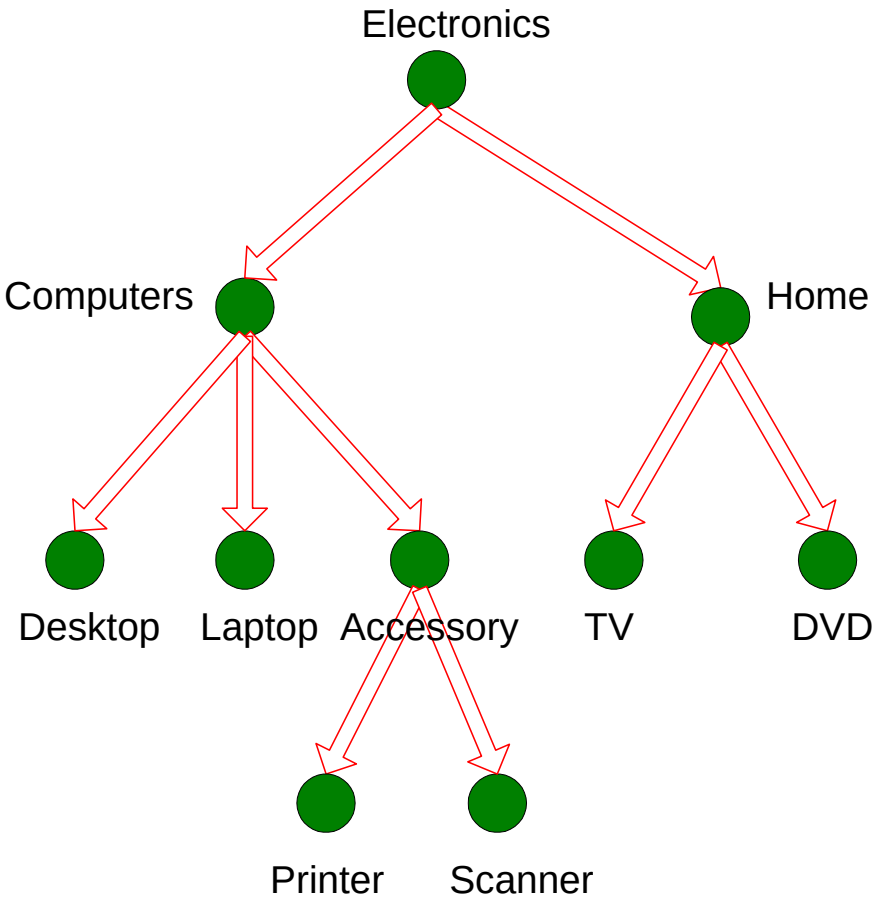
DId	W1	W2	W3	W4	W5
D1	0.4	0.33	0	0	0.17
D2	0	0	0.33	1.00	0.33
D3	0.4	0.5	0	0	0
D4	0	0	0.33	0	0.17
D5	0.2	0.17	0.33	0	0.33

Example:

$$\sup(W1) = 0.4 + 0 + 0.4 + 0 + 0.2 = 1$$
$$\sup(W1, W2) = 0.33 + 0 + 0.4 + 0 + 0.17 = 0.9$$
$$\sup(W1, W2, W3) = 0 + 0 + 0 + 0 + 0.17 = 0.17$$

Multi-level Association Rules





Multi-level Association Rules

- Why should we incorporate concept hierarchy?
  - Rules at lower levels may not have enough support to appear in any frequent itemsets
  - Rules at lower levels of the hierarchy are overly specific
    - E.g., *skim* milk $\rightarrow$ *white* bread,
      2% milk $\rightarrow$ *wheat* bread,
      skim milk $\rightarrow$ *wheat* bread, *etc*.

    indicate general association between *milk* and *bread*

Multi-level Association Rules

- How do *support* and *confidence* vary as we traverse the concept hierarchy?
  - If X is the parent item for both X1 and X2, then $\sigma(X) \leq \sigma(X1) + \sigma(X2)$
  - If $\sigma(X1 \cup Y1) \geq$ minsup,
    and X is parent of X1, Y is parent of Y1
    then $\sigma(X \cup Y1) \geq$ minsup, $\sigma(X1 \cup Y) \geq$ minsup
    $\sigma(X \cup Y) \geq$ minsup
  - If conf(X1 $\Rightarrow$ Y1) ≥ minconf,
    then conf(X1 $\Rightarrow$ Y) ≥ minconf

Multi-level Association Rules

- Approach 1:
  - Extend current association rule formulation by augmenting each transaction with higher level items

  Original Transaction: {skim milk, wheat bread}

  Augmented Transaction:

  {skim milk, wheat bread, milk, bread, food}

- Issues:
  - Items that reside at higher levels have much higher support counts
    - If support threshold is low, too many frequent patterns involving items from the higher levels
  - Increased dimensionality of the data
  - Redundant rules (although, easy to eliminate)

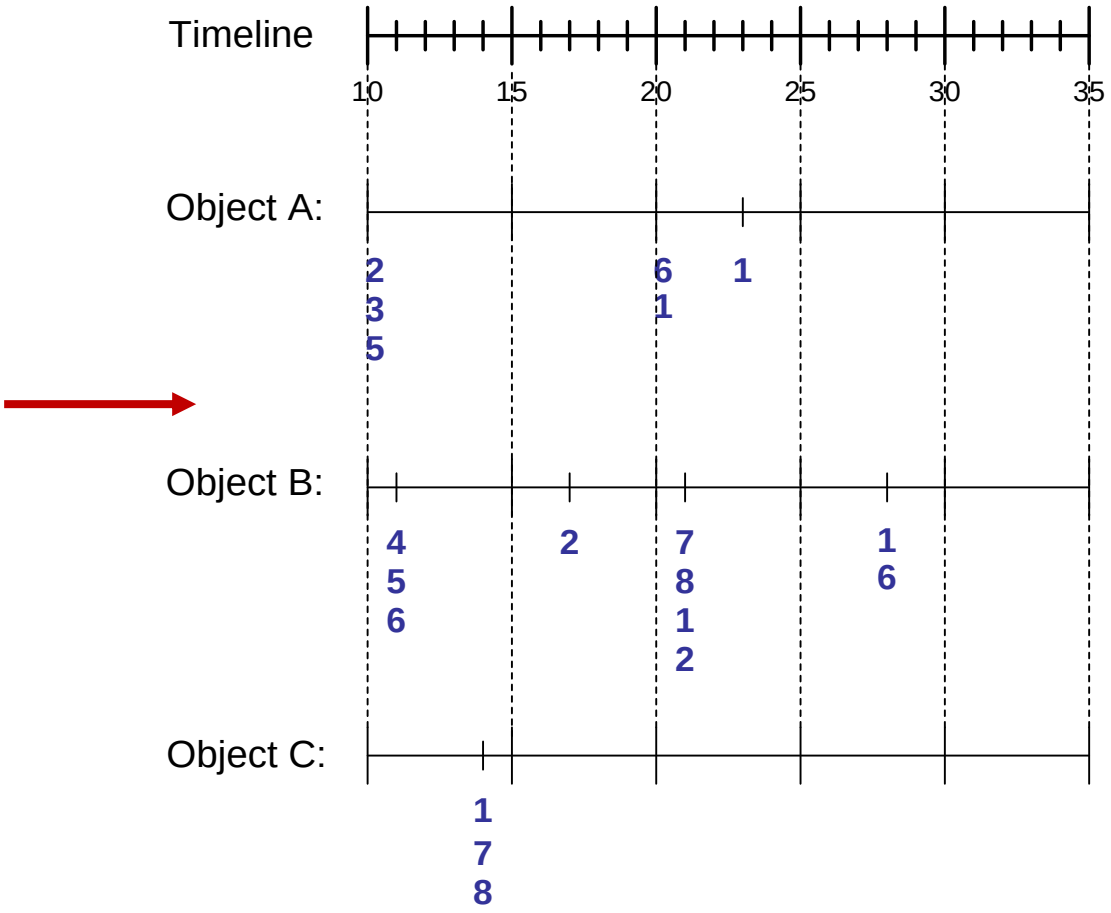
Multi-level Association Rules

- Approach 2:
  - Generate frequent patterns at highest level first
  - Then, generate frequent patterns at the next highest level, and so on
- Issues:
  - I/O requirements will increase dramatically because we need to perform more passes over the data
  - May miss some potentially interesting cross-level association patterns

Sequence Data

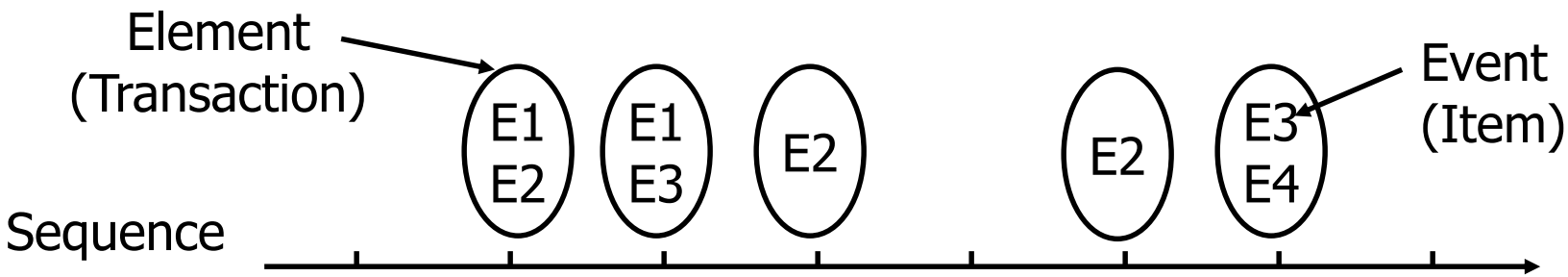
Sequence Database:

Object	Timestamp	Events
A	10	2, 3, 5
A	20	6, 1
A	23	1
B	11	4, 5, 6
B	17	2
B	21	7, 8, 1, 2
B	28	1, 6
C	14	1, 7, 8



Examples of Sequence Data

Sequence Database	Sequence	Element (Transaction)	Event (Item)
Customer	Purchase history of a given customer	A set of items bought by a customer at day d	Books, diary products, CDs, etc
Web Data	Browsing activity of a particular Web visitor	A collection of files viewed by a Web visitor in a session	Pages URLs
Event data	History of events generated by a given sensor	Events generated by a sensor at time t	Specific messages generated by sensors
Genome sequences	DNA sequence of a particular species	An element of the DNA sequence	Bases A,T,G,C



Formal Definition of a Sequence

- A sequence is an ordered list of **elements** (transactions)

$$s = < e_1\ e_2\ e_3 >$$

  - Each element contains a collection of **events** (items)

$$e_i = \{i_1, i_2, \ldots, i_k\}$$

  - Each element is attributed to a specific time or location

- Length of a sequence, $|s|$, is given by the number of **elements** of the sequence

- A k-sequence is a sequence that contains k **events** (items)

Examples of Sequence

- Web sequence:

  < {Homepage} {Electronics} {Digital Cameras}
  {Canon Digital Camera} {Shopping Cart} {Order Confirmation}
  {Return to Shopping} >

- Sequence of initiating events causing the nuclear accident at Three-Mile Island:
  (http://stellar-one.com/nuclear/staff_reports/summary_SOE_the_initiating_event.htm)

  < {clogged resin} {outlet valve closure} {loss of feedwater}
  {condenser polisher outlet valve shut} {booster pumps trip}
  {main waterpump trips} {main turbine trips}
  {reactor pressure increases} >

- Sequence of books checked out at a library:

  < {Fellowship of the Ring, The Two Towers} {Return of the King} >

Formal Definition of a Subsequence

A sequence $< a_1\ a_2\ \ldots\ a_n >$ is **contained** in another sequence $< b_1\ b_2\ \ldots\ b_m >$ $(m \geq n)$ if there exist integers $i_1 < i_2 < \cdots < i_n$ such that $a_1 \subseteq b_{i_1}$, $a_2 \subseteq b_{i_2}$, …, $a_n \subseteq b_{i_n}$

Data sequence	Subsequence	Contain?
< {2,4} {3,5,6} {8} >	< {2} {3,5} >	Yes
< {1,2} {3,4} >	< {1} {2} >	No
< {2,4} {2,4} {2,5} >	< {2} {5} >	Yes

- The **support** of a subsequence w is defined as the fraction of data sequences that contain w
- A **sequential pattern** is a **frequent** subsequence (i.e., a subsequence whose support is $\geq$ *minsup*)

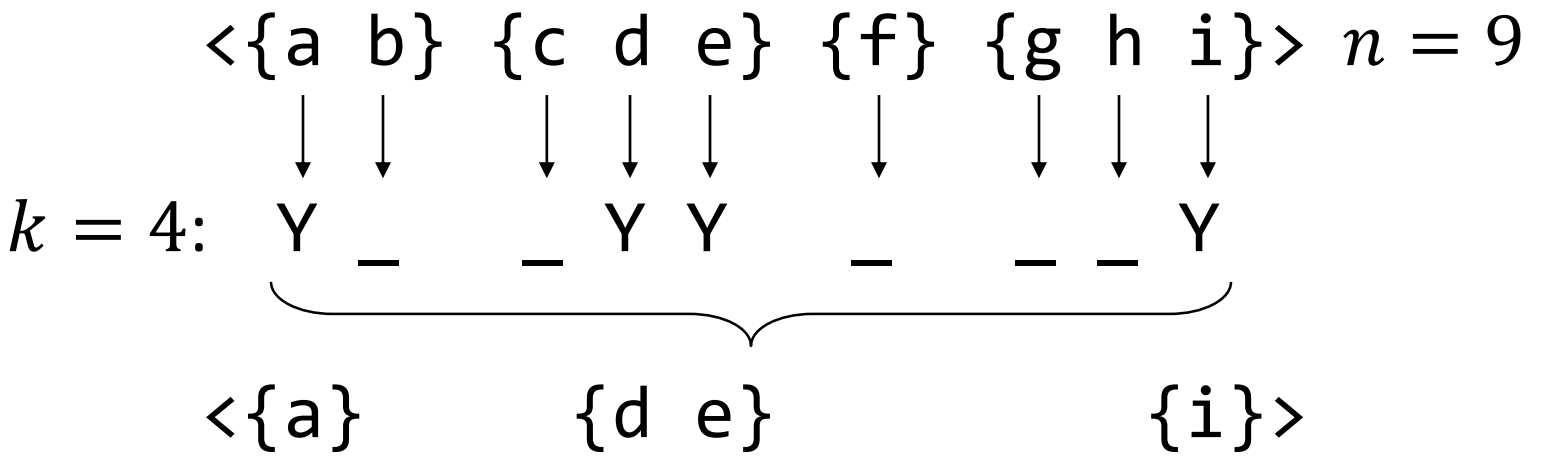
Sequential Pattern Mining: Definition

- Given:
  - a database of sequences
  - a user-specified minimum support threshold, *minsup*
- Task:
  - Find all subsequences with support $\geq$ *minsup*

Sequential Pattern Mining: Challenge

- Given a sequence: <{a b} {c d e} {f} {g h i}>
  - Examples of subsequences:
    <{a} {c d} {f} {g} >, < {c d e} >, < {b} {g} >, etc.

- How many k-subsequences can be extracted from a given n-sequence?



Sequential Pattern Mining: Example

Object	Timestamp	Events
A	1	1,2,4
A	2	2,3
A	3	5
B	1	1,2
B	2	2,3,4
C	1	1, 2
C	2	2,3,4
C	3	2,4,5
D	1	2
D	2	3, 4
D	3	4, 5
E	1	1, 3
E	2	2, 4, 5

Minsup = 50%

Examples of Frequent Subsequences:

< {1,2} >	s=60%
< {2,3} >	s=60%
< {2,4}>	s=80%
< {3} {5}>	s=80%
< {1} {2} >	s=80%
< {2} {2} >	s=60%
< {1} {2,3} >	s=60%
< {2} {2,3} >	s=60%
< {1,2} {2,3} >	s=60%

Extracting Sequential Patterns

- Given n events: $i_1, i_2, i_3, \ldots, i_n$

- Candidate 1-subsequences:

  $\langle\{i_1\}\rangle, \langle\{i_2\}\rangle, \langle\{i_3\}\rangle, \ldots, \langle\{i_n\}\rangle$

- Candidate 2-subsequences:

  $\langle\{i_1, i_2\}\rangle, \langle\{i_1, i_3\}\rangle, \ldots, \langle\{i_1\}\ \{i_1\}\rangle, \langle\{i_1\}\ \{i_2\}\rangle, \ldots, \langle\{i_{n-1}\}\ \{i_n\}\rangle$

- Candidate 3-subsequences:

  $\langle\{i_1, i_2, i_3\}\rangle, \langle\{i_1, i_2, i_4\}\rangle, \ldots, \langle\{i_1, i_2\}\ \{i_1\}\rangle, \langle\{i_1, i_2\}\ \{i_2\}\rangle, \ldots,$
  $\langle\{i_1\}\ \{i_1, i_2\}\rangle, \langle\{i_1\}\ \{i_1, i_3\}\rangle, \ldots, \langle\{i_1\}\ \{i_1\}\ \{i_1\}\rangle, \langle\{i_1\}\ \{i_1\}\ \{i_2\}\rangle,$
  …

Generalized Sequential Pattern (GSP)

- **Step 1**:
  - Make the first pass over the sequence database D to yield all the 1-element frequent sequences
- **Step 2**:

  Repeat until no new frequent sequences are found
  - **Candidate Generation**:
    - Merge pairs of frequent subsequences found in the $(k-1)^{th}$ pass to generate candidate sequences that contain k items
  - **Candidate Pruning**:
    - Prune candidate k-sequences that contain infrequent $(k-1)$-subsequences
  - **Support Counting**:
    - Make a new pass over the sequence database D to find the support for these candidate sequences
  - **Candidate Elimination**:
    - Eliminate candidate k-sequences whose actual support is less than *minsup*

Candidate Generation

- Base case ($k = 2$):
  - —Merging two frequent 1-sequences <{i_1}> and <{i_2}> will produce two candidate 2-sequences: <{i_1} {i_2}> and <{i_1 i_2}>
- General case ($k > 2$):
  - —A frequent $(k-1)$-sequence w_1 is merged with another frequent $(k-1)$-sequence w_2 to produce a candidate k-sequence if the subsequence obtained by removing the first event in w_1 is the same as the subsequence obtained by removing the last event in w_2
    - The resulting candidate after merging is given by the sequence w_1 extended with the last event of w_2
      - If the last two events in w_2 belong to the same element, then the last event in w_2 becomes part of the last element in w_1
      - Otherwise, the last event in w_2 becomes a separate element appended to the end of w_1

Candidate Generation Examples

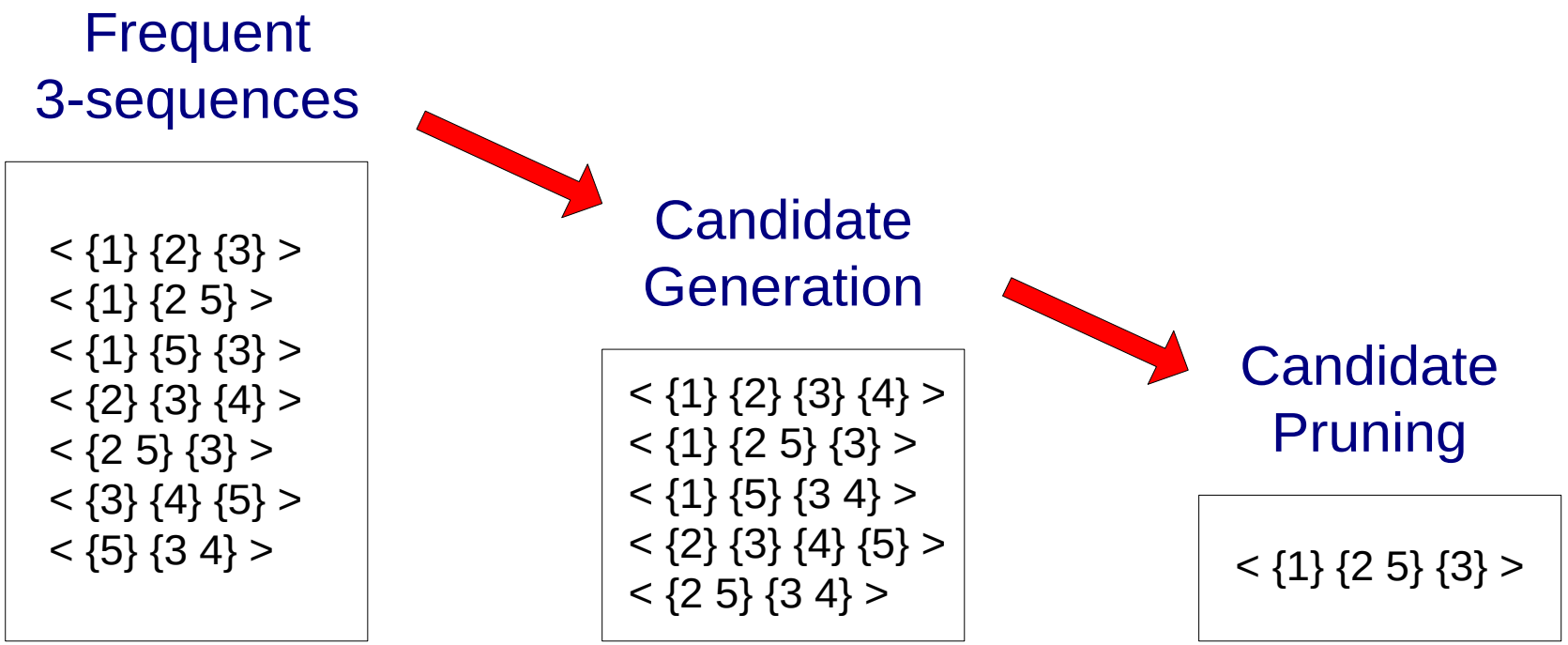
- Merging the sequences
  w_1=<{1} {2 3} {4}> and w_2 =<{2 3} {4 5}>
  will produce the candidate sequence < {1} {2 3} {4 5}> because the last two events in w_2 (4 and 5) belong to the same element

- Merging the sequences
  w_1=<{1} {2 3} {4}> and w_2 =<{2 3} {4} {5}>
  will produce the candidate sequence < {1} {2 3} {4} {5}> because the last two events in w_2 (4 and 5) do not belong to the same element

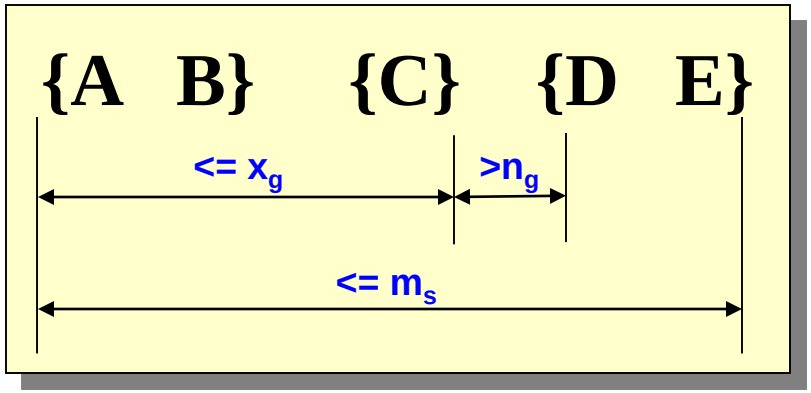
- We do not have to merge the sequences
  w_1 =<{1} {2} {3}> and w_2 =<{1} {2 5}>
  to produce the candidate <{1} {2 5} {3}> because if the latter is a viable candidate, then it can be obtained by merging w_2 with <{2 5} {3}>

  The procedure is *complete*

GSP Example


Frequent
3-sequences
< {1} {2} {3} >
< {1} {2 5} >
< {1} {5} {3} >
< {2} {3} {4} >
< {2 5} {3} >
< {3} {4} {5} >
< {5} {3 4} >
Candidate
Generation
< {1} {2} {3} {4} >
< {1} {2 5} {3} >
< {1} {5} {3 4} >
< {2} {3} {4} {5} >
< {2 5} {3 4} >
Candidate
Pruning
< {1} {2 5} {3} >

Timing Constraints (I)



x_g: max-gap

n_g: min-gap

m_s: maximum span

x_g = 2, n_g = 0, m_s= 4

Data sequence	Subsequence	Contain?
< {2,4} {3,5,6} {4,7} {4,5} {8} >	< {6} {5} >	Yes
< {1} {2} {3} {4} {5}>	< {1} {4} >	No
< {1} {2,3} {3,4} {4,5}>	< {2} {3} {5} >	Yes
< {1,2} {3} {2,3} {3,4} {2,4} {4,5}>	< {1,2} {5} >	No

Mining Sequential Patterns with Timing Constraints

- Approach 1:
  - Mine sequential patterns without timing constraints
  - Postprocess the discovered patterns

- Approach 2:
  - Modify GSP to directly prune candidates that violate timing constraints
  - Question:
    - Does Apriori principle still hold?

Apriori Principle for Sequence Data

Object	Timestamp	Events
A	1	1,2,4
A	2	2,3
A	3	5
B	1	1,2
B	2	2,3,4
C	1	1, 2
C	2	2,3,4
C	3	2,4,5
D	1	2
D	2	3, 4
D	3	4, 5
E	1	1, 3
E	2	2, 4, 5

Suppose:

x_g = 1 (max-gap)

n_g = 0 (min-gap)

m_s = 5 (maximum span)

minsup = 60%

<{2} {5}> support = 40%

but

<{2} {3} {5}> support = 60%

Problem exists because of max-gap constraint

No such problem if max-gap is infinite

Contiguous Subsequences

- s is a **contiguous subsequence** of

$$w = \langle e_1\ e_2\ \ldots\ e_k \rangle$$

if any of the following conditions hold:

1. s is obtained from w by deleting an item from either e_1 or e_k
2. s is obtained from w by deleting an item from any element e_i that contains more than 2 items
3. s is a contiguous subsequence of s' and s' is a contiguous subsequence of w (recursive definition)

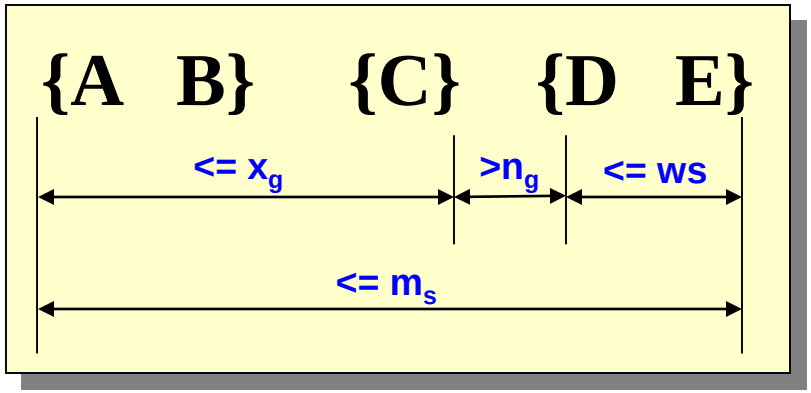
- Examples: s = < {1} {2} >
  - —is a contiguous subsequence of
    <{1} {2 3}>, <{1 2} {2} {3}>, and <{3 4} {1 2} {2 3} {4}>
  - —is not a contiguous subsequence of
    <{1} {3} {2}> and <{1, 2} {1} {3} {2}>

Modified Candidate Pruning Step

Modified Apriori: if a k-sequence is frequent, all of its contiguous $(k-1)$-subsequences must be frequent

- Without maxgap constraint:
  - A candidate k-sequence is pruned if at least one of its $(k-1)$-subsequences is infrequent
- With maxgap constraint:
  - A candidate k-sequence is pruned if at least one of its **contiguous** $(k-1)$-subsequences is infrequent

Timing Constraints (II)



x_g: max-gap

n_g: min-gap

ws: window size

m_s: maximum span

x_g = 2, n_g = 0, ws = 1, m_s= 5

Data sequence	Subsequence	Contain?
< {3,4} {4} {5} {6,7} {8} >	< {3,4,6} {8} >	No
< {1} {2} {3} {4} {5}>	< {1,2} {3} >	Yes
< {1,2} {2,3} {3,4} {4,5}>	< {1,2} {3,4} >	Yes

Modified Support Counting Step

- Given a candidate pattern: <{a, c}>

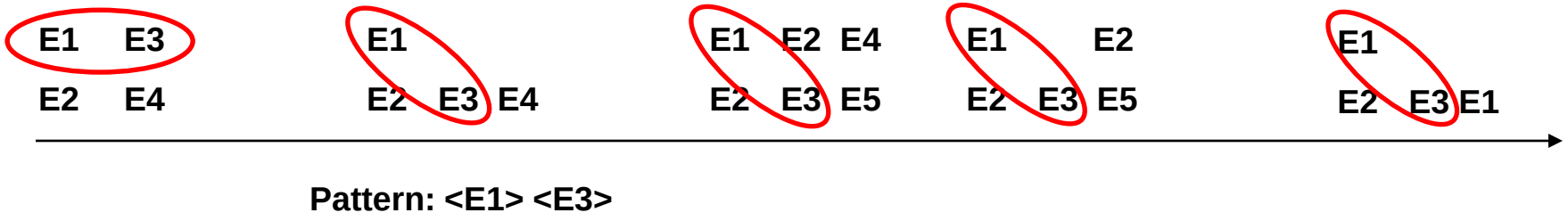
  Any data sequences that contain

  <… {a c} …>,
  <… {a} … {c}…> (where time({c}) – time({a}) ≤ ws)
  <… {c} … {a} …> (where time({a}) – time({c}) ≤ ws)

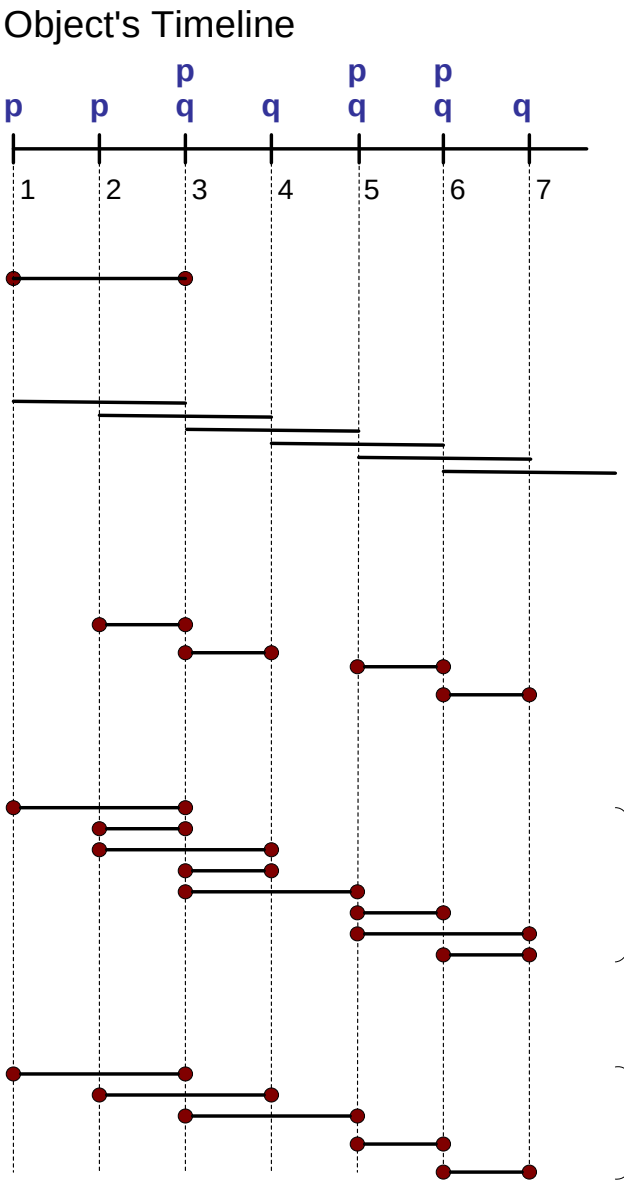
  Will contribute to the support count of candidate pattern

Another Formulation

- In some domains, we may have only one very long time series
  - Example:
    - monitoring network traffic events for attacks
    - monitoring telecommunication alarm signals
- Goal is to find frequent sequences of events in the time series
  - This problem is also known as *frequent episode mining*



General Support Counting Schemes



Sequence: (p) (q)

Method	Support Count
COBJ	1
CWIN	6
CMINWIN	4
CDIST_O	8
CDIST	5

Assume:

x_g = 2 (max-gap)

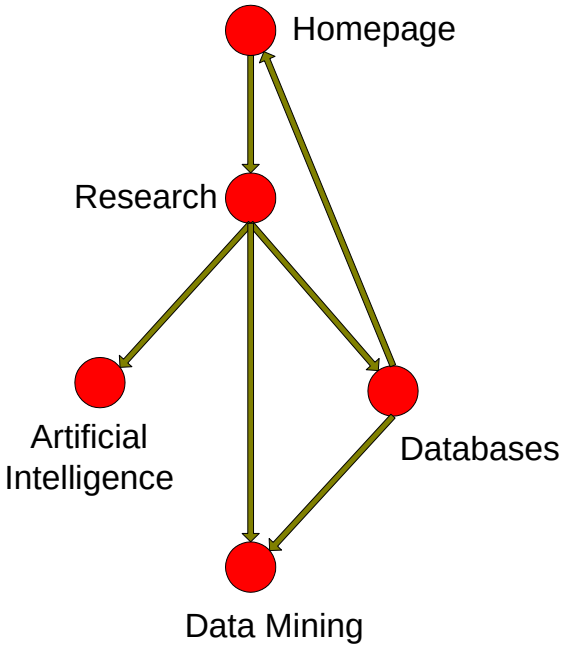
n_g = 0 (min-gap)

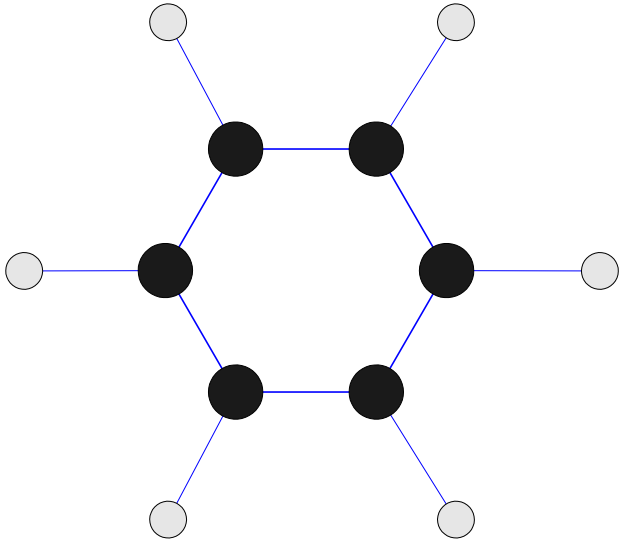
ws = 0 (window size)

m_s = 2 (maximum span)

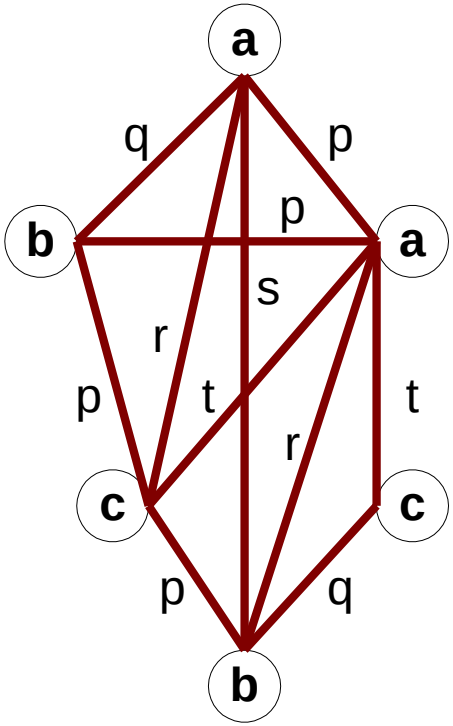
Frequent Subgraph Mining

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

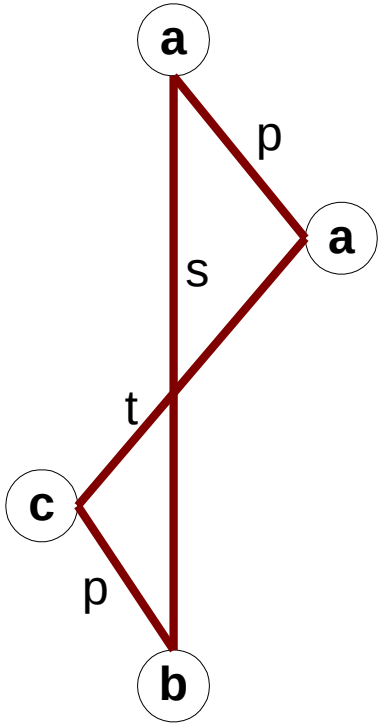




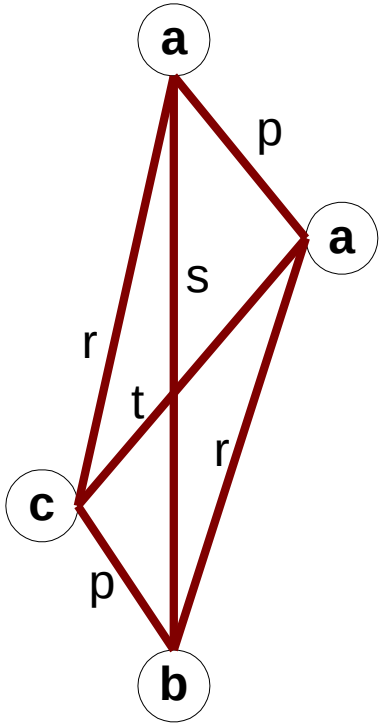
Graph Definitions



(a) Labeled Graph



(b) Subgraph

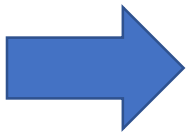


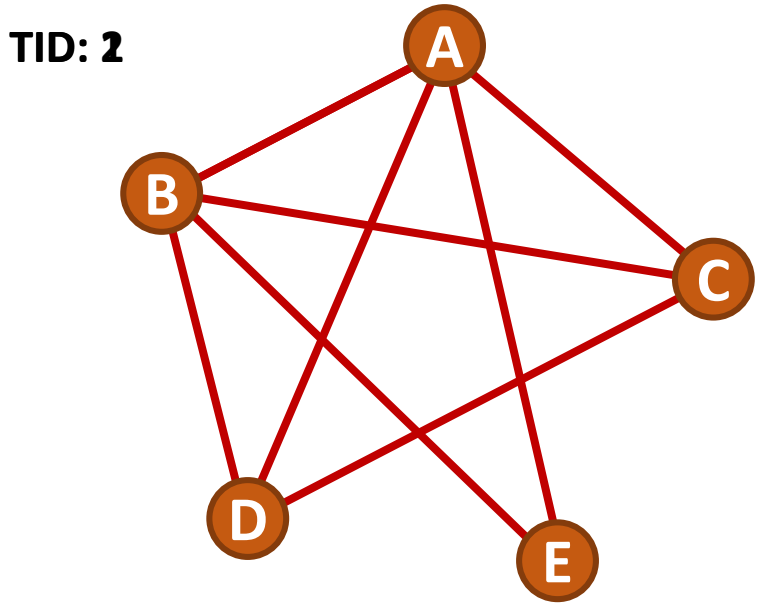
(c) Induced Subgraph

Representing Transactions as Graphs

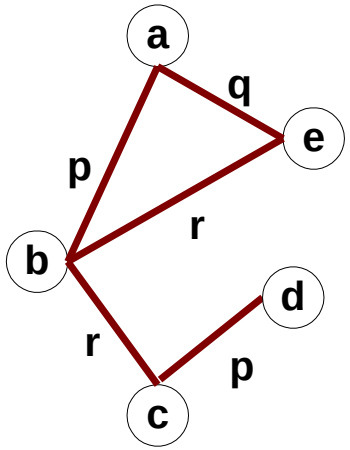
- Each transaction is a clique of items

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

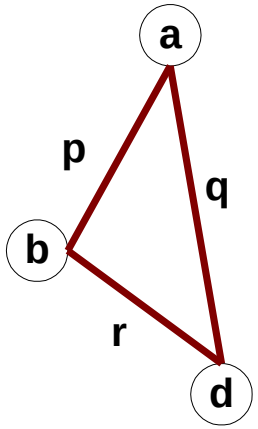




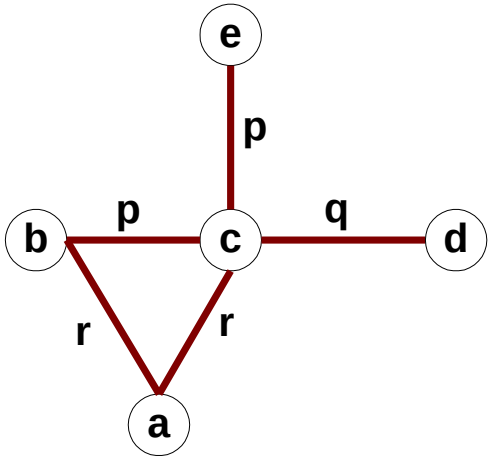
Representing Graphs as Transactions



G1



G2



G3

	(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	…	…	…	…	…	…	…	…

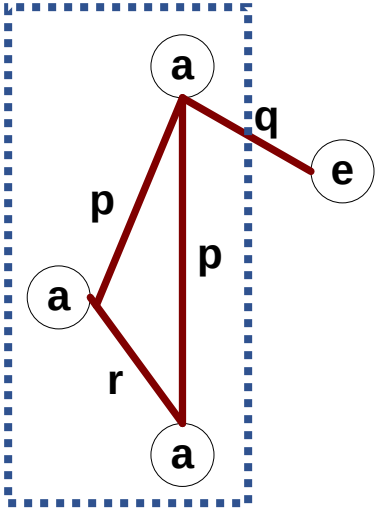
Challenges

- 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…

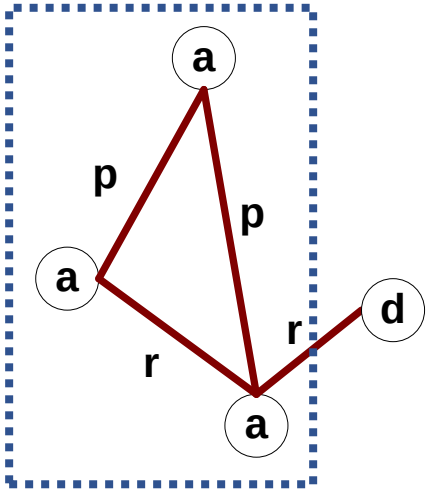
- Support:
  - number of graphs that contain a particular subgraph
- Apriori principle still holds
- Level-wise (Apriori-like) approach:
  - Vertex growing:
    - k is the number of vertices
  - Edge growing:
    - k is the number of edges

Vertex Growing

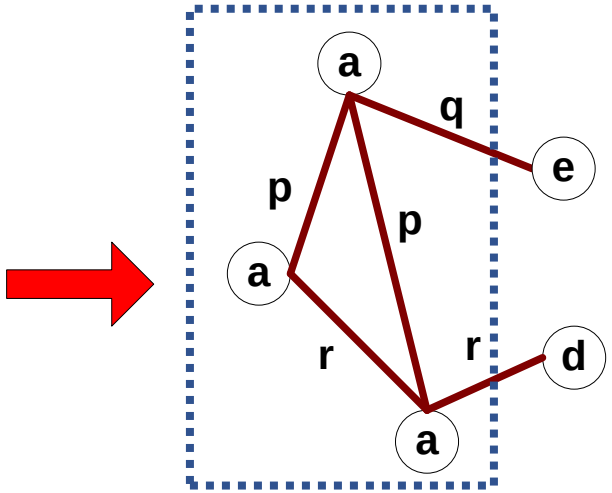


G1

+



G2



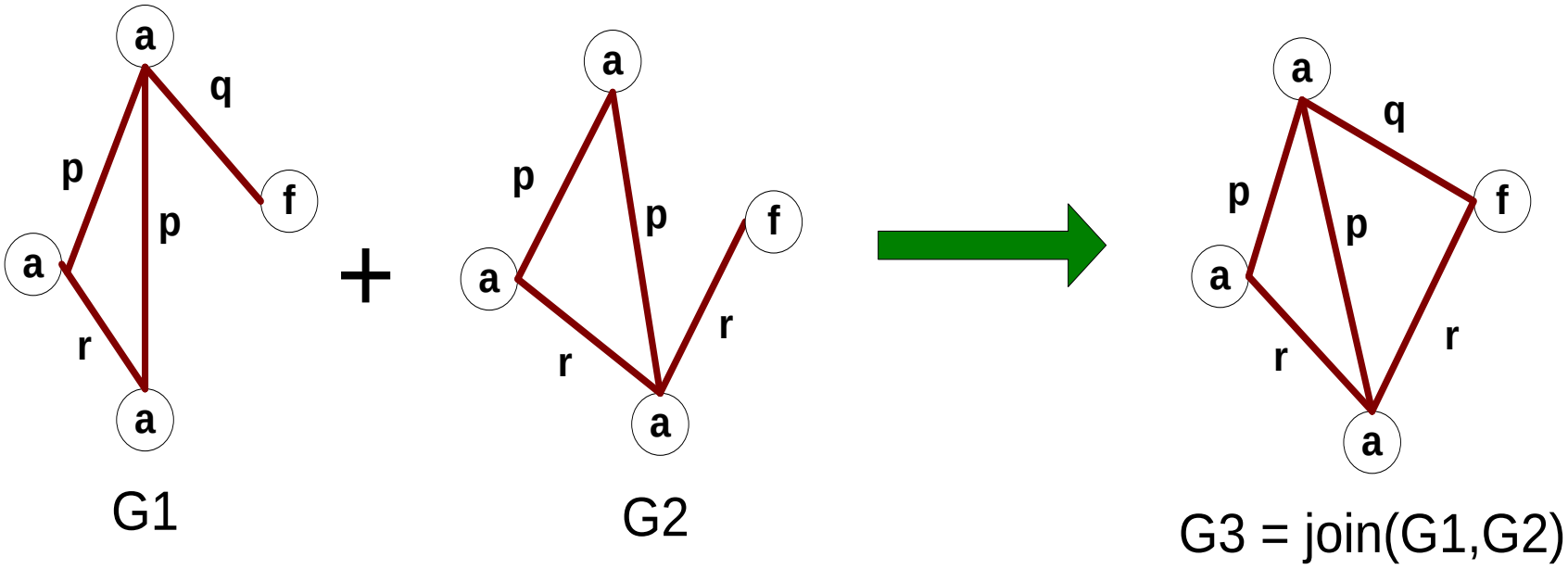
G3 = join(G1,G2)

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

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

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

Edge Growing

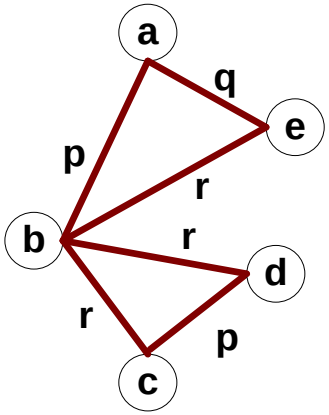


Apriori-like Algorithm

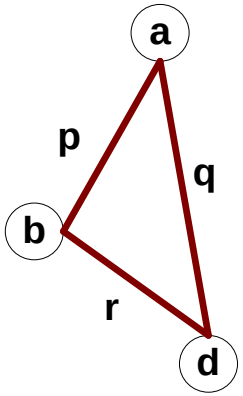
- Find frequent 1-subgraphs
- Repeat
  - Candidate generation
    - Use frequent $(k-1)$-subgraphs to generate candidate k-subgraph
  - Candidate pruning
    - Prune candidate subgraphs that contain infrequent $(k-1)$-subgraphs
  - Support counting
    - Count the support of each remaining candidate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

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

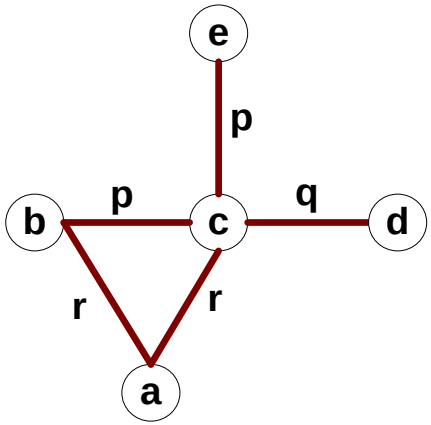
Example: Dataset



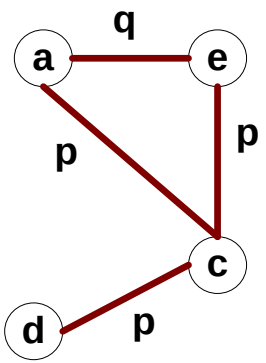
G1



G2



G3



G4

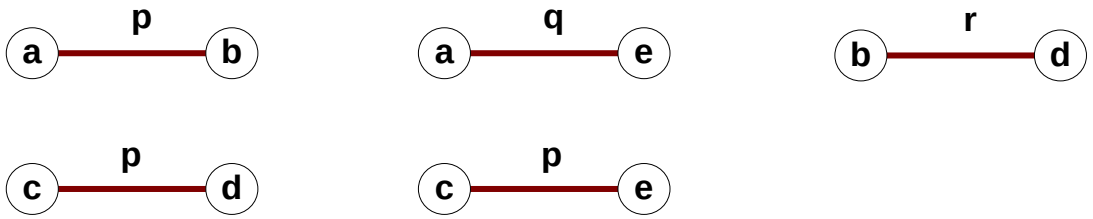
	(a,b,p)	(a,b,q)	(a,b,r)	(b,c,p)	(b,c,q)	(b,c,r)	…	(d,e,r)
G1	1	0	0	0	0	1	…	0
G2	1	0	0	0	0	0	…	0
G3	0	0	1	1	0	0	…	0
G4	0	0	0	0	0	0	…	0

Example

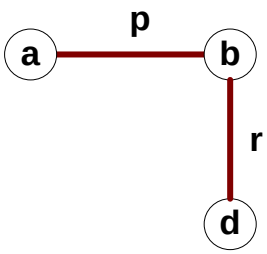
Minimum support count = 2

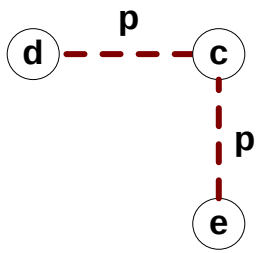
k=1
Frequent
Subgraphs

k=2
Frequent
Subgraphs



k=3
Candidate
Subgraphs



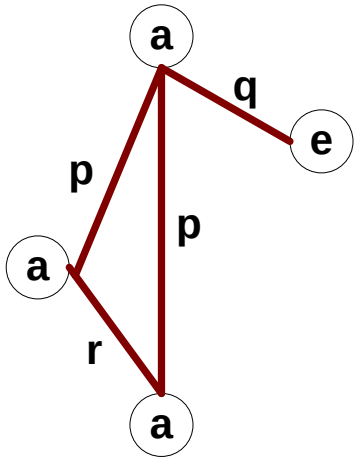


(Pruned candidate)

Candidate Generation

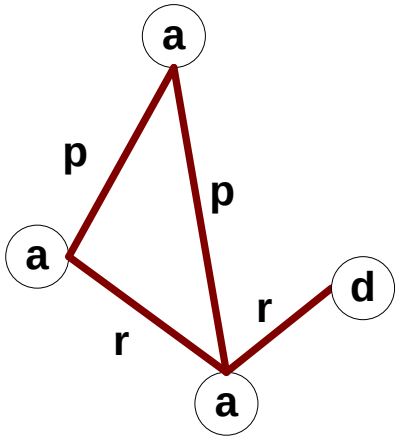
- In Apriori:
  - Merging two frequent k-itemsets will produce a candidate $(k+1)$-itemset
- In frequent subgraph mining (vertex/edge growing)
  - Merging two frequent k-subgraphs may produce more than one candidate $(k+1)$-subgraph

Multiplicity of Candidates (Vertex Growing)

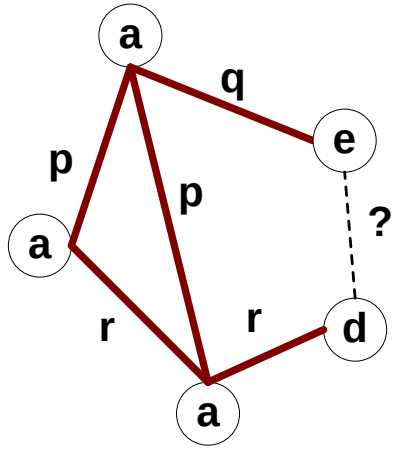


G1

+



G2

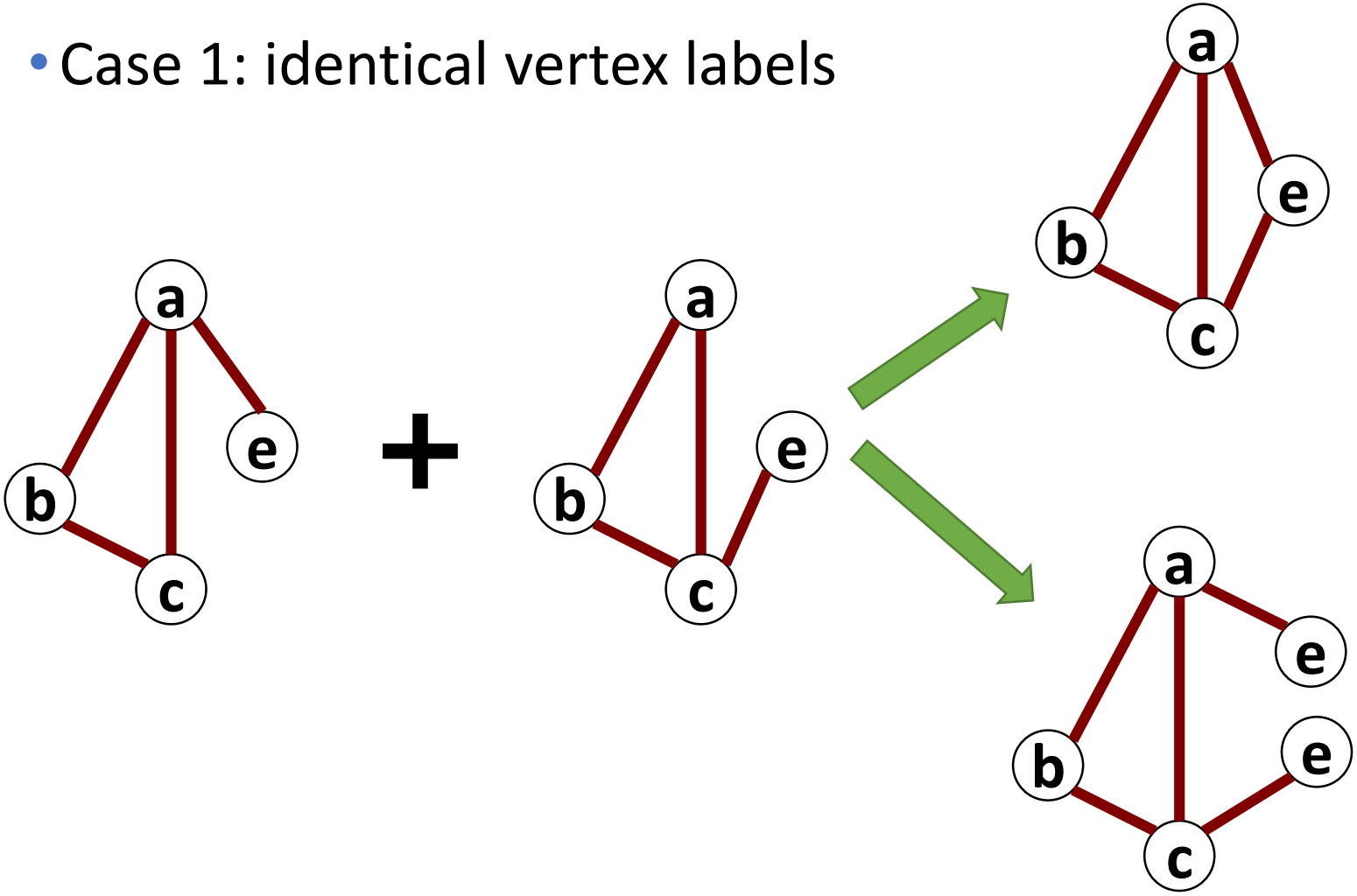


G3 = join(G1,G2)

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

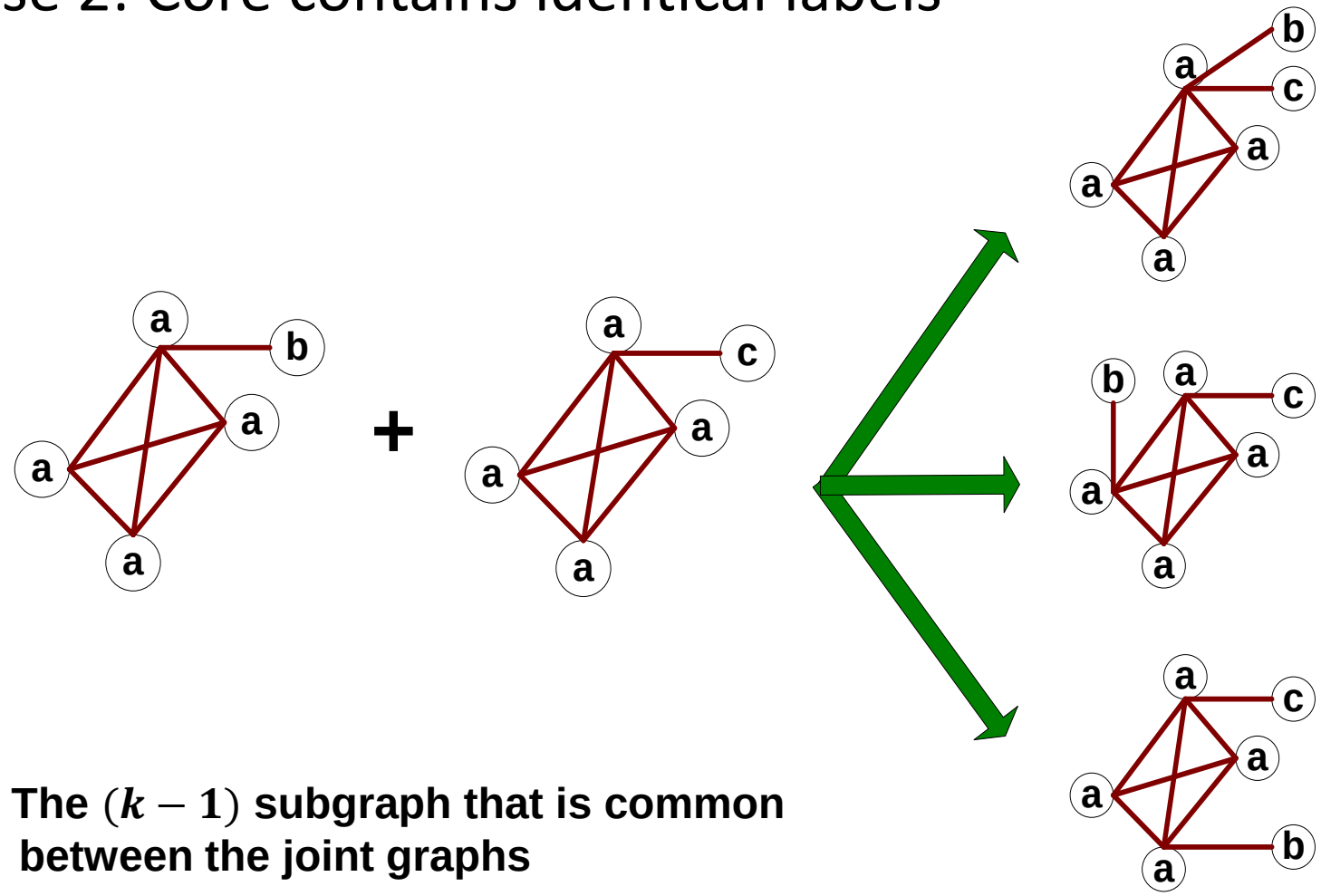
Multiplicity of Candidates (Edge growing)

- Case 1: identical vertex labels



Multiplicity of Candidates (Edge growing)

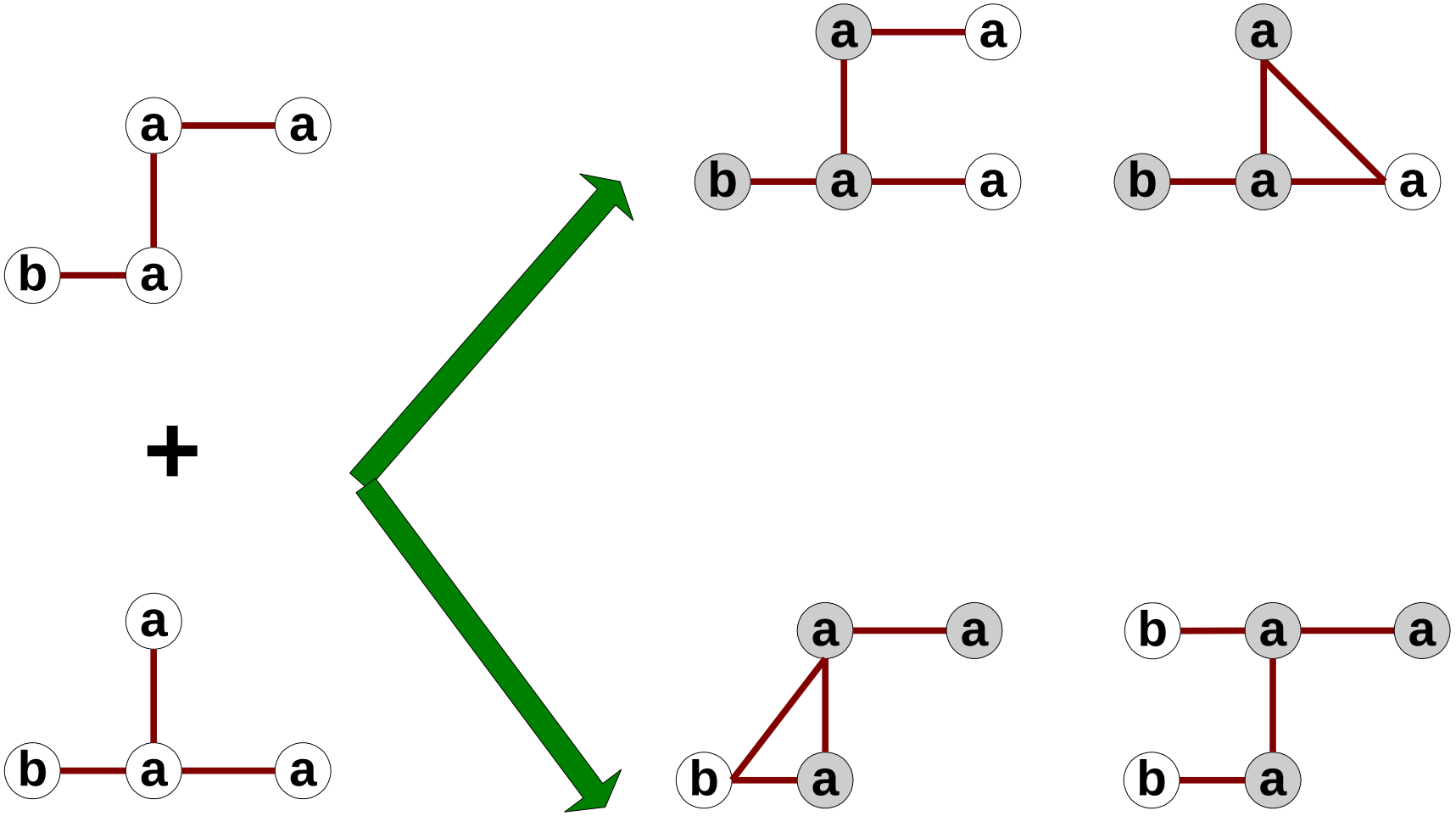
- Case 2: Core contains identical labels



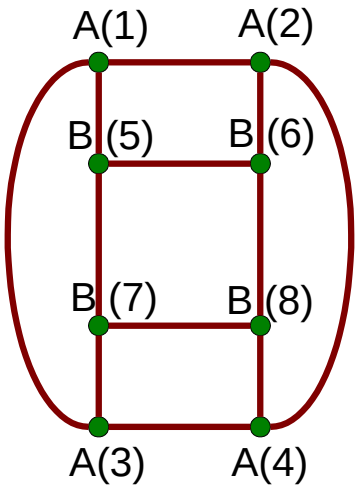
Core: The $(k-1)$ subgraph that is common between the joint graphs

Multiplicity of Candidates (Edge growing)

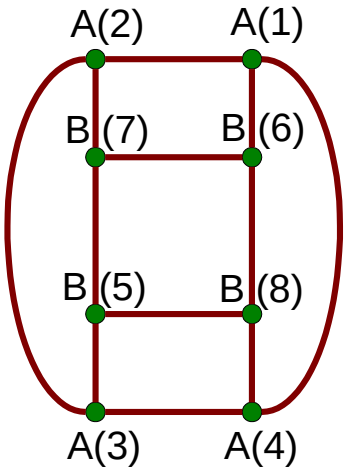
- Case 3: Core multiplicity



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

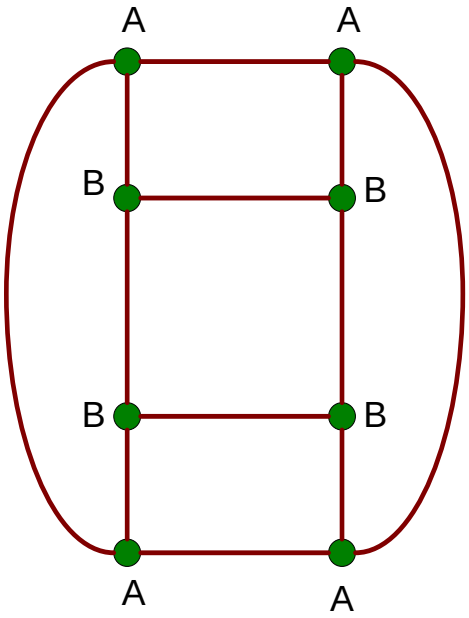


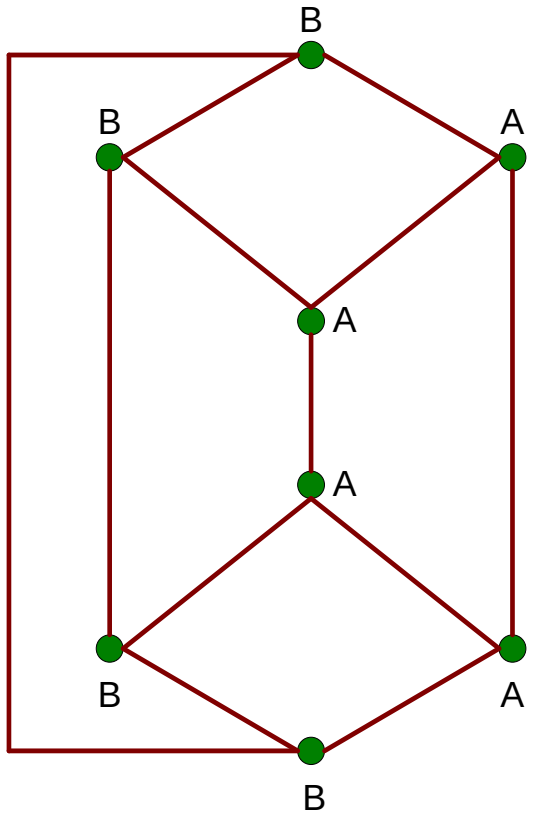
	A(1)	A(2)	A(3)	A(4)	B(5)	B(6)	B(7)	B(8)
A(1)	1	1	0	1	0	1	0	0
A(2)	1	1	1	0	0	0	1	0
A(3)	0	1	1	1	1	0	0	0
A(4)	1	0	1	1	0	0	0	1
B(5)	0	0	1	0	1	0	1	1
B(6)	1	0	0	0	0	1	1	1
B(7)	0	1	0	0	1	1	1	0
B(8)	0	0	0	1	1	1	0	1

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

Graph Isomorphism

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



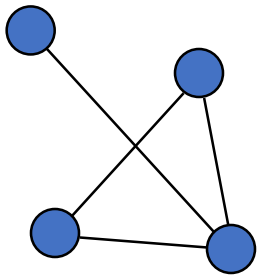


Graph Isomorphism

- 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



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

String: 0010001111010110 **Canonical: 0111101011001000**