# "Association mining-2" 

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## Continuous and Categorical Attributes

How to apply association analysis formulation to non-asymmetric binary variables, like "Buy", or continuous like "Session length", or categorical like "Country"?

| Session <br> Id | Country | Session <br> Length <br> $(\mathbf{s e c})$ | Number of <br> Web Pages <br> viewed | Gender | Browser <br> Type | Buy |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | USA | 982 | 8 | Male | IE | No |
| 2 | China | 811 | 10 | Female | Netscape | No |
| 3 | USA | 2125 | 45 | Female | Mozilla | Yes |
| 4 | Germany | 596 | 4 | Male | IE | Yes |
| 5 | Australia | 123 | 9 | Male | Mozilla | No |
| $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ |

Example of Association Rule:
$\{$ Number of Pages $\in[5,10) \wedge($ Browser=Mozilla $)\} \rightarrow\{$ Buy $=$ No $\}$

## Handling Categorical Attributes

- Transform categorical attribute into asymmetric binary variables
- Introduce a new "item" for each distinct attribute-value pair
- Example: replace Browser Type attribute with
- Browser Type = Internet Explorer
- Browser Type = Mozilla
- Browser Type = Netscape


## Handling Categorical Attributes

- Potential Issues
- What if an 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: $95 \%$ of the visitors have Buy = No
- Most of the items will be associated with (Buy=No) item
- Potential solution: drop the highly frequent items, since these items, like "Buy=No", should be associated with every itemset returned


## Handling Continuous Attributes

- Different kinds of rules:
- Age $\in[21,35) \wedge$ Salary $\in[70 k, 120 k) \rightarrow$ Buy
- Salary $\in[70 k, 120 k) \wedge$ Buy $\rightarrow$ Age $(\mu=28, \sigma=4)$
- Different methods:
- Discretization-based
- Statistics-based
- Non-discretization based
- minApriori


## Handling Continuous Attributes

- Use discretization
- Unsupervised:
- Equal-width binning
- Equal-depth binning
- Clustering


Attribute values, v

| Class | $\mathrm{V}_{1}$ | $\mathrm{~V}_{2}$ | $\mathrm{~V}_{3}$ | $\mathrm{~V}_{4}$ | $\mathrm{~V}_{5}$ | $\mathrm{~V}_{6}$ | $\mathrm{~V}_{7}$ | $\mathrm{~V}_{8}$ | $\mathrm{~V}_{9}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Anomalous | 0 | 0 | 20 | 10 | 20 | 0 | 0 | 0 | 0 |
| Normal | 150 | 100 | 0 | 0 | 0 | 100 | 100 | 150 | 100 |
| bin $_{1}$ | $\underbrace{}_{\text {bin }_{2}}$ |  |  |  |  |  |  |  |  |

## Discretization Issues

- Size of the discretized intervals affect support \& confidence

$$
\begin{aligned}
& \{\text { Refund }=\text { No, }(\text { Income }=\$ 51,250)\} \rightarrow\{\text { Cheat }=\text { No }\} \\
& \{\text { Refund }=\text { No },(60 \mathrm{~K} \leq \text { Income } \leq 80 \mathrm{~K})\} \rightarrow\{\text { Cheat }=\text { No }\} \\
& \{\text { Refund }=\text { No },(0 \mathrm{~K} \leq \text { Income } \leq 1 \mathrm{~B})\} \rightarrow\{\text { Cheat }=\text { No }\}
\end{aligned}
$$

- If intervals too small
- may not have enough support
- If intervals too large
- may not have enough confidence
- Potential solution: use all possible intervals with small supports
- Expensive and too many rules
$\{$ Refund $=$ No, $($ Income $=\$ 51,250)\} \rightarrow\{$ Cheat $=$ No $\}$
$\{$ Refund $=$ No, $(51 \mathrm{~K} \leq$ Income $\leq 52 \mathrm{~K})\} \rightarrow\{$ Cheat $=$ No $\}$
$\{$ Refund $=$ No, $(50 \mathrm{~K} \leq$ Income $\leq 60 \mathrm{~K})\} \rightarrow\{$ Cheat $=$ No $\}$


## Min-Apriori

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

| TID | 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 |

- Convert into 0/1 matrix and then apply existing algorithms
- lose word frequency information
- Discretization does not apply properly, as users want association among words not ranges of words (like the following rule)

$$
\{(2 \leq \mathrm{W} 2 \leq 3)\} \rightarrow\{\mathrm{W} 1=2\}
$$

## Non-discretization methods: <br> Min-Apriori (Han et al.)

Document-term matrix, where each entry is the (normalized) frequency count of a word in a document:

Example:

| CID | Wi | 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 |

W1 and W2 tend to appear together in the same document

## 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!
- Solution
- Normalize the word vectors (by column)
- Each word has an overall support equals to 1.0

| TID | 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 |$\xrightarrow{\text { Normaize }}$


| TID | W1 | W2 | W3 | W4 | W5 |
| :--- | :--- | :--- | :--- | :--- | :--- |
| D1 | 0.40 | 0.33 | 0.00 | 0.00 | 0.17 |
| D2 | 0.00 | 0.00 | 0.33 | 1.00 | 0.33 |
| D3 | 0.40 | 0.50 | 0.00 | 0.00 | 0.00 |
| D4 | 0.00 | 0.00 | 0.33 | 0.00 | 0.17 |
| D5 | 0.20 | 0.17 | 0.33 | 0.00 | 0.33 |

## Min-Apriori

- New definition of support:

$$
\sup (C)=\sum_{i=1} \min _{j \in C} D(i, j)
$$

| TID | W1 | W2 | W3 | W4 | W5 |
| :--- | :--- | :--- | :--- | :--- | :--- |
| D1 | 0.40 | 0.33 | 0.00 | 0.00 | 0.17 |
| D2 | 0.00 | 0.00 | 0.33 | 1.00 | 0.33 |
| D3 | 0.40 | 0.50 | 0.00 | 0.00 | 0.00 |
| D4 | 0.00 | 0.00 | 0.33 | 0.00 | 0.17 |
| D5 | 0.20 | 0.17 | 0.33 | 0.00 | 0.33 |

Example:
Sup(W1,W2,W3)
$=0+0+0+0+0.17$
$=0.17$

## Anti-monotone property of Support

| TID | W1 | W2 | W3 | W4 | W5 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| D1 | 0.40 | 0.33 | 0.00 | 0.00 | 0.17 |
| D2 | 0.00 | 0.00 | 0.33 | 1.00 | 0.33 |
| D3 | 0.40 | 0.50 | 0.00 | 0.00 | 0.00 |
| D4 | 0.00 | 0.00 | 0.33 | 0.00 | 0.17 |
| D5 | 0.20 | 0.17 | 0.33 | 0.00 | 0.33 |

Example (anti-monotone support):
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



- In market basket analysis, the concept hierarchy becomes an item taxonomy
- Edges are "is-a" relationships
- Directed Acyclic Graph
- Parent-Child Ancestor-Descendant


## 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. are indicative of association between milk and bread

## Multi-level Association Rules

- Approach 1:
- Extend current association rule formulation by augmenting each transaction with higher level items, and then apply standard Apriori algorithm

Original Transaction, with items at the lowest level of the hierarchy: \{skim milk, wheat bread\}
Augmented Transaction, adding the ancestors: \{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
- Easily remove redundant itemsets like: \{skim milk, milk, food\}


## 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, by reducing the support threshold
- 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 | $1,8,7$ |



Element composed of multiple events/items, i.e., each record is a transaction associated with

## Examples of Sequence Data

| Sequence <br> Database | Sequence | Element <br> (Transaction) | Event <br> (Item) |
| :--- | :--- | :--- | :--- |
| Customer | Purchase history of a given <br> customer | A set of items bought by <br> a customer at time t | Books, diary products, <br> CDs, etc |
| Web Data | Browsing activity of a <br> particular Web visitor | A collection of files <br> viewed by a Web visitor <br> after a single mouse click | Home page, index <br> page, contact info, etc |
| Event data | History of events generated <br> by a given sensor | Events triggered by a <br> sensor at time t | Types of alarms <br> generated by sensors |
| Genome <br> sequences | DNA sequence of a <br> particular species | An element of the DNA <br> sequence | Bases A,T,G,C |



## Examples of Mined Sequences

- 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 3mile 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 Sequence

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

$$
s=\left\langle\mathbf{e}_{1} \mathbf{e}_{2} \mathbf{e}_{3} \ldots\right\rangle
$$

- Each element contains a collection of events (items)

$$
e_{i}=\left\{i_{1}, i_{2}, \ldots, i_{k}\right\}
$$

- Each element is attributed to a specific time (even location)
- Length of a sequence, |s|, is given by the number of elements/transactions in the sequence
- A k-sequence is a sequence that globally contains k events (items)


## 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 $\mathrm{i}_{1}<\mathrm{i}_{2}<\ldots<\mathrm{i}_{\mathrm{n}}$ such that $a_{1} \subseteq b_{i 1}, a_{2} \subseteq b_{i 2}, \ldots, a_{n} \subseteq b_{\text {in }}$

The timestamps associated with the transactions are not shown Contajned

| subsequence | DAJA sequence | Contajned <br> $\langle(3)(45)(8)\rangle$ <br> $\langle(3)(5)\rangle$$\quad\langle(7)(38)(9)(456)(8)\rangle$ |  | $\mathbf{Y}$ |
| :---: | :---: | :---: | :---: | :---: |
| $\langle(3)(5)\rangle$ | $\langle(35)\rangle$ | N |  |  |
|  | $\langle(35)(35)(345)\rangle$ | $\mathbf{Y}$ |  |  |

- The support of a subsequence wis defined as the fraction of input data sequences that contain w
- Note that a sequence can be contained in a given "data sequence" in different ways (see the last example)
- A sequential pattern is frequent if it is a subsequence of $\sigma$ input sequences ( $\sigma=$ support of the pattern), and $\sigma \geq$ 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: < $\{\mathrm{ab}\}\{\mathrm{c} d \mathrm{e}\}\{\mathrm{f}\}\{\mathrm{gh} \mathrm{i}\}$
- Examples of subsequences:

$$
<\{a\}\{c d\}\{f\}\{g\}>,<\{c d e\}>,<\{b\}\{g\}>, \text { etc. }
$$

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


Answer :

$$
\binom{n}{k}=\binom{9}{4}=126
$$

## Sequential Pattern Mining: Example

| customes <br> Id | fansaction fne | Items Boyght |
| :---: | :---: | :---: |
| 1 | June 25,93 | 30 |
| 1 | June 30,93 | 90 |
| 2 | June 10,93 | 10,20 |
| 2 | June 15,93 | 30 |
| 2 | June 20,93 | $40,60,70$ |
| 3 | June 25,93 | $30,50,70$ |
| 4 | June 25,93 | 30 |
| 4 | June 30,93 | 40,70 |
| 4 | July 25,93 | 90 |
| 5 | June 12,93 | 90 |



MinSupp $=40 \%$, i.e. 2 customers of 5:
<30><90> (supported by 1,4)
<30><40,70> (supported by 2,4) <10 $20><30>$ Infrequent

## 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:

| $<\{1,2\}>$ | $\mathrm{s}=60 \%$ |
| :--- | :--- |
| $<\{2,3\}>$ | $\mathrm{s}=60 \%$ |
| $<\{2,4\}>$ | $\mathrm{s}=80 \%$ |
| $<\{3\}\{5\}>$ | $\mathrm{s}=80 \%$ |
| $<\{1\}\{2\}>$ | $\mathrm{s}=80 \%$ |
| $<\{2\}\{2\}>$ | $\mathrm{s}=60 \%$ |
| $<\{1\}\{2,3\}>$ | $\mathrm{s}=60 \%$ |
| $<\{2\}\{2,3\}>$ | $\mathrm{s}=60 \%$ |
| $<\{1,2\}\{2,3\}>$ | $\mathrm{s}=60 \%$ |

## Extracting Sequential Patterns

- Given $\mathbf{n}$ events: $\mathbf{i}_{1}, \mathbf{i}_{2}, \mathbf{i}_{3}, \ldots, \mathbf{i}_{\mathrm{n}}$
- Candidate 1-subsequences:

$$
\left.<\left\{i_{1}\right\}>,\left\langle\left\{i_{2}\right\}\right\rangle,<\left\{i_{3}\right\}\right\rangle, \ldots,\left\langle\left\{i_{n}\right\}\right\rangle
$$

- Candidate 2-subsequences:

$$
<\left\{i_{1}, i_{2}\right\}>,<\left\{i_{1}, i_{3}\right\}>, \ldots,<\left\{i_{1}\right\}\left\{i_{1}\right\}>,<\left\{i_{1}\right\}\left\{i_{2}\right\}>, \ldots,<\left\{i_{n-1}\right\}\left\{i_{n}\right\}>
$$

- Candidate 3-subsequences:

$$
\begin{aligned}
& <\left\{i_{1}, i_{2}, i_{3}\right\}>,<\left\{i_{1}, i_{2}, i_{4}\right\}>, \ldots,<\left\{i_{1}, i_{2}\right\}\left\{i_{1}\right\}>,<\left\{i_{1}, i_{2}\right\}\left\{i_{2}\right\}>, \ldots \\
& <\left\{i_{1}\right\}\left\{i_{1}, i_{2}\right\}>,<\left\{i_{1}\right\}\left\{i_{1}, i_{3}\right\}>, \ldots,<\left\{i_{1}\right\}\left\{i_{1}\right\}\left\{i_{1}\right\}>,<\left\{i_{1}\right\}\left\{i_{1}\right\}\left\{i_{2}\right\}>, \ldots
\end{aligned}
$$

## 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 < $\left\{i_{1}\right\}>$ and $<\left\{i_{2}\right\}>$ will produce two candidate 2-sequences: < $\left\{i_{1}\right\}\left\{i_{2}\right\}>$ and $<\left\{i_{1} i_{2}\right\}>$
- General case ( $\mathrm{k}>2$ ):
- 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 $\mathrm{w}_{1}$ is the same as the subsequence obtained by removing the last event in $\mathbf{w}_{2}$ (suffix of $\mathbf{w}_{1}=$ prefix of $\mathbf{w}_{2}$ )
- 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 (in red the common portion) $w_{1}=<\{1\}\{23\}\{4\}>$ and $w_{2}=<\{23\}\{45\}>$ will produce the candidate sequence < \{1\} \{2 3\} \{45\}> because the last two events in $\mathbf{w}_{2}(4$ and 5$)$ belong to the same element
- Merging the sequences (in red the common portion) $w_{1}=<\{1\}\{23\}\{4\}>$ and $w_{2}=<\{23\}\{4\}\{5\}>$ will produce the candidate sequence < \{1\} \{2 3\} \{4\} \{5\}> because the last two events in $\mathbf{w}_{2}(4$ and 5$)$ do not belong to the same element


## GSP Example

## Frequent

 3 -sequences$$
\begin{aligned}
& <\{1\}\{2\}\{3\}> \\
& <\{1\}\{25\}> \\
& <\{1\}\{5\}\{3\}> \\
& <\{2\}\{3\}\{4\}> \\
& <\{25\}\{3 \gg \\
& <\{3\}\{4\}\{5\}> \\
& <\{5\}\{34\}>
\end{aligned}
$$

$$
\begin{aligned}
& \text { Candidate } \\
& \begin{array}{l}
\text { Generation }
\end{array} \\
& \begin{array}{ll}
<\{1\}\{2\}\{3\}\{4\}> \\
<\{1\}\{25\}\{3\}> \\
<\{1\}\{5\}\{34\}> \\
<\{2\} & \text { Candidate } \\
<\{25\}\{4\}\{5\}> & \text { Pruning }
\end{array} \\
& <254\}>
\end{aligned}
$$

## Timing Constraints (I)


$x_{g}:$ max-gap
$n_{g}:$ min-gap
$w_{s}:$ window size
$m_{s}:$ maximum span

$$
x_{g}=2, n_{g}=0, w_{s}=1, m_{s}=5
$$

| 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


## Frequent Subgraph Mining

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



## Graph representation of entities

| Application | Graphs | Vertices | Edges |
| :--- | :--- | :--- | :--- |
| Web mining | Web browsing <br> patterns | Web pages | Hyperlinks between <br> pages |
| Computational <br> chemistry | Structure of <br> chemical <br> compounds | Atoms or ions | Bond between <br> atoms or ions |
| Sematic Web | Collection of XML <br> documents | XML elements | Parent-child <br> relationships <br> between elements |
| Bioinformatics | Protein structures | Amino acids | Contact residue |
| Network computing | Computer networks | Computer and <br> servers | Interconnections <br> between machines |

## Graph Definitions


(a) Labeled Graph
(b) Subgraph

## Frequent Subgraph Mining

## Computing the Subgraph Support


$\mathrm{G}_{3}$
Subgraph $\mathrm{g}_{1}$

support $=80 \%$
Subgraph $\mathrm{g}_{2}$

support = 60\%
Subgraph $\mathrm{g}_{3}$

support $=40 \%$

## Representing Transactions as (unlabeled) Graphs

- Each transaction is a clique of items
TID = 1:

| Transaction <br> 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

|  | $(\mathrm{a}, \mathrm{b}, \mathrm{p})$ | $(\mathrm{a}, \mathrm{b}, \mathrm{q})$ | $(\mathrm{a}, \mathrm{b}, \mathrm{r})$ | $(\mathrm{b}, \mathrm{c}, \mathrm{p})$ | $(\mathrm{b}, \mathrm{c}, \mathrm{q})$ | $(\mathrm{b}, \mathrm{c}, \mathrm{r})$ | $\ldots$ | $(\mathrm{d}, \mathrm{e}, \mathrm{r})$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| G1 | 1 | 0 | 0 | 0 | 0 | 1 | $\ldots$ | 0 |
| G2 | 1 | 0 | 0 | 0 | 0 | 0 | $\ldots$ | 0 |
| G3 | 0 | 0 | 1 | 1 | 0 | 0 | $\ldots$ | 0 |
| G3 | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ |

## Challenges

- Nodes 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



## 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

|  | $(\mathrm{a}, \mathrm{b}, \mathrm{p})$ | $(\mathrm{a}, \mathrm{b}, \mathrm{q})$ | $(\mathrm{a}, \mathrm{b}, \mathrm{r})$ | $(\mathrm{b}, \mathrm{c}, \mathrm{p})$ | $(\mathrm{b}, \mathrm{c}, \mathrm{q})$ | $(\mathrm{b}, \mathrm{c}, \mathrm{r})$ | $\ldots$ | $(\mathrm{d}, \mathrm{e}, \mathrm{r})$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| G1 | 1 | 0 | 0 | 0 | 0 | 1 | $\ldots$ | 0 |
| G2 | 1 | 0 | 0 | 0 | 0 | 0 | $\ldots$ | 0 |
| G3 | 0 | 0 | 1 | 1 | 0 | 0 | $\ldots$ | 0 |
| G4 | 0 | 0 | 0 | 0 | 0 | 0 | $\ldots$ | 0 |

## Example

Minimum support count $=2$
$\mathrm{k}=1$
Frequent
(a) b
d e Subgraphs
$\mathrm{k}=2$


Frequent Subgraphs

k=3
Candidate Subgraphs

(Pruned candidate)

## Candidate Generation

- In Apriori:
- Merging two frequent $\boldsymbol{k}$-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

$\mathrm{G} 3=\mathrm{join}(\mathrm{G} 1, \mathrm{G} 2)$
$M_{\sigma 1}=\left(\begin{array}{llll}0 & p & p & q \\ p & 0 & r & 0 \\ p & r & 0 & 0 \\ q & 0 & 0 & 0\end{array}\right)$

$$
M_{\sigma 2}=\left(\begin{array}{llll}
0 & p & p & 0 \\
p & 0 & r & 0 \\
p & r & 0 & r \\
0 & 0 & r & 0
\end{array}\right)
$$

$$
M_{c 3}=\left(\begin{array}{ccccc}
0 & p & p & 0 & q \\
p & 0 & r & 0 & 0 \\
p & r & 0 & r & 0 \\
0 & 0 & r & 0 & ? \\
q & 0 & 0 & ? & 0
\end{array}\right)
$$

## Multiplicity of Candidates (Edge growing)

- Case 1: identical vertex labels



## Multiplicity of Candidates (Edge growing)

- Case 2: Core contains identical labels


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


## Multiplicity of Candidates (Edge growing)

- Case 3: Core multiplicity



## Graph Isomorphism

- A graph $G$ is isomorphic to a graph $H$, if it is topologically equivalent to $H$
- There exists a bijection between the vertex sets of the two graph

$$
f: V(G) \rightarrow V(H)
$$

such that any two vertices $u$ and $v$ of $G$ are adjacent in $G$ if and only if $f(u)$ and $f(v)$ are adjacent in $H$.


## Graph Isomorphism

- Test for graph isomorphism is needed:
- During candidate generation step, to determine whether a candidate has been already 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
- Find the permutations of the vertices so that the adjacency matrix is lexicographically maximized when read off from left to right, one row at a time



## 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 |

It is sufficient to consider the string representation (canonical encoding) of the upper triangular matrix

