Frequent substructure mining - an introduction

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Outline

1. Introduction
2. Frequent itemset mining
3. The Apriori algorithm
4. Abstract problem formulation
5. The Eclat algorithm
6. The FPGrowth algorithm

Frequent substructure mining

- We have a database D of transactions T.
- T can be an arbitrary object.
- For example: itemsets (basket market), time sequences, graphs
- Mining of frequent substructures has exponential complexity (in the worst case)

Frequent itemset mining

Database D:

TID	Transaction
1	$\{1, 2, 3, 4\}$
2	$\{3, 5\}$
3	$\{1, 3, 4\}$
4	$\{1, 2\}$
5	$\{1, 3, 4, 5\}$
6	$\{1, 2, 3, 4, 5\}$

- The problem is to find a set of items (*itemsets*) that occurs in at least p% of *transactions*,
- exponential complexity with respect to the # of items (in the worst case)

Example:

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- are there any correlations among items in D ?

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- Itemset $\{3, 5\}$ occurs in 3 transactions $\Rightarrow$ $Supp(\{3, 5\}, D) = 3$

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- are there any correlations among items in D ?
- Itemset $\{3,5\}$ occurs in 3 transactions $\Rightarrow$ $Supp(\{3,5\},D) = 3$
- *Association rule* $\{3,5\} \rightarrow \{2\}$ in $33.3\overline{3}\%$ of cases $\Rightarrow$ *confidence* $Conf(\{3,5\},\{2\}) = 0.3\overline{3}$

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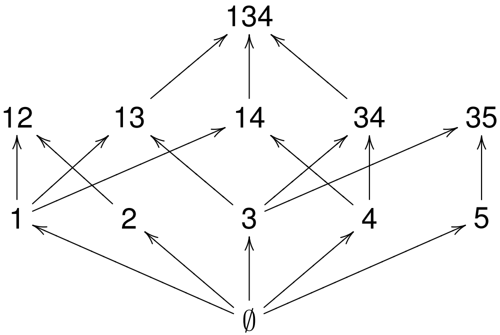
- *Association rule* $\{3, 5\} \rightarrow \{2\}$ in $33.3\overline{3}\%$ of cases $\Rightarrow$ *confidence* $Conf(\{3, 5\}, \{2\}) = 0.3\overline{3}$
- $\Rightarrow$ associations(correlations) among items

Lattice of frequent itemsets for *min_support* $= 3$



$\Rightarrow$ maximal frequent itemsets (MFIs)
$\Rightarrow$ base set of items $B = \{1, 2, 3, 4, 5\}$

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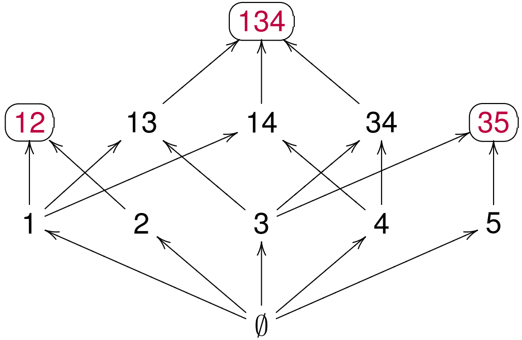

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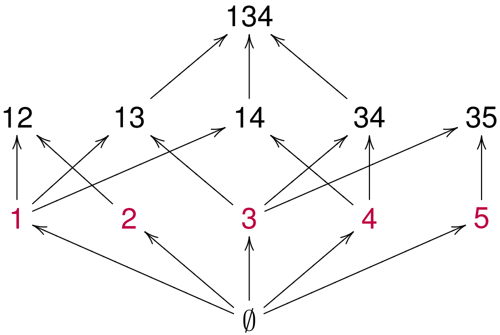


$\Rightarrow$ maximal frequent itemsets (MFIs)

$\Rightarrow$ *base set of items* $B = \{1, 2, 3, 4, 5\}$

General schema of mining association rules

Input: database D, *min_support* and *min_conf*

1. generate frequent itemsets X with $Supp(X) \geq min\_support$ `/* most time consuming part */`
2. generate association rules with confidence $Conf(X) \geq min\_conf$

Algorithms

- The Apriori algorithm: the first and slowest algorithm for generation of frequent itemsets
- The FPGrowth algorithm: based on prefix tree (trie)
- The Eclat algorithm: uses vertical representation of the database

The Apriori algorithm

Lemma (Monotonicity of support)

Let $U \subseteq B$ be an itemset with support $Supp(U)$ in database D. For every superset V of U holds: $Supp(U) \geq Supp(V)$.

Proof.

(By induction)

(i) It is obvious that for an item b_i, $|D| = Supp(\emptyset) \geq Supp(\{b_i\})$.

(ii) If U has support $Supp(U)$, then for arbitrary $b_i \in B - U$ holds: $Supp(U) \geq Supp(U \cup \{b_i\})$, since not all transactions containing U must contain $U \cup \{b_i\}$.

$\square$

The Apriori algorithm contd.

- Based on the monotonicity property of support
- *Generate&test* algorithm
- **The Apriori algorithm can make $k = |B|$ scans of D**

A *candidate* itemset $U, |U| = k$:

- Support of U is unknown
- all $W \subset U, |W| = k - 1$ are frequent, i.e. $Supp(W) \geq min\_support$

From frequent itemsets F_k generate candidates C_{k+1}:

- $f_1, f_2 \in F_k$ such that f_1, f_2 identical in $k - 1$ items;
- $c = \{f_1[j] : j < k\} \cup \{f_1[k], f_2[k]\}$.

The Apriori algorithm contd.

APRIORI(**In:** Database D, **In:** Set B, **In:** Integer *min_support*, **In/Out:** Set F)

$k \leftarrow 1$
$C_k \leftarrow \{\{b_i\} : b_i \in B\}$
while C_k not empty **do**
    COMPUTE-SUPPORT(D, C_k)
    for all $c \in C_k$ **do**
        if $Supp(c) < min\_support$ **then**
            delete c from C_k
        end if
    end for
    $F_k \leftarrow C_k$
    $C_{k+1} \leftarrow$ GENERATE-CANDIDATES(F_k)
    $k \leftarrow k + 1$
end while
return $F_1 \cup F_2 \cup \ldots \cup F_{k-1}$

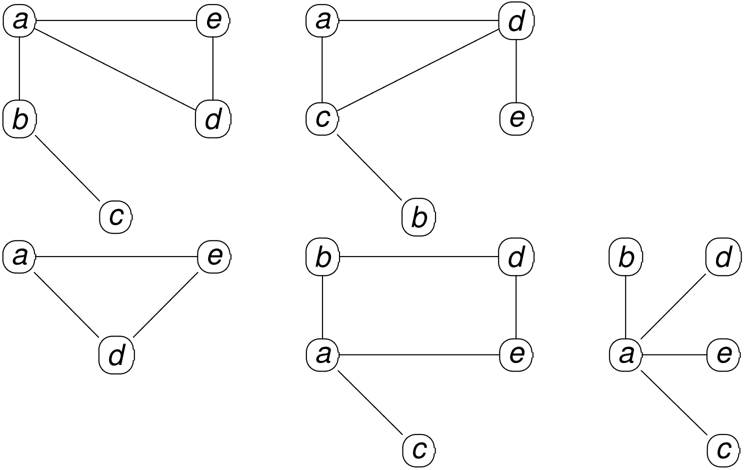
Abstract substructure mining

- A database D, a language $\mathcal{L}$;
- sentences $\varphi, \Phi \in \mathcal{L}$;
- a frequency criterion $q(\varphi) \in \{\text{true}, \text{false}\}$;
- a monotone specialization/generalization relation: $\varphi \preceq \Phi$
- $q(\Phi) = \text{true} \Rightarrow q(\varphi) = \text{true}$

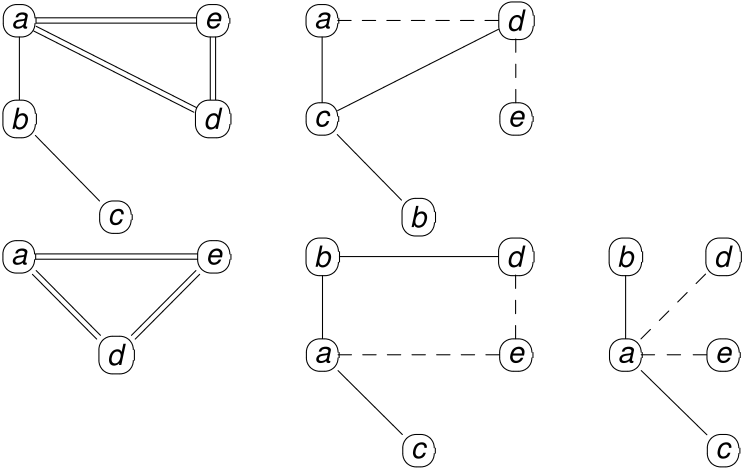
Generalization of the Apriori algorithm

$C_1 \leftarrow \{\varphi \in \mathcal{L} | \text{there is no } \varphi' \text{ such that } \varphi' \prec \varphi\}$
$i \leftarrow 1$
while C_i not empty **do**
    $F_i \leftarrow \{\varphi \in C_i | q(\varphi) = \mathit{true}\}$
    $C_{i+1} \leftarrow \{\varphi \in \mathcal{L} | \forall \varphi' \prec \varphi \text{ we have } \varphi' \in \cup_{j \leq i} F_j\} \setminus \cup_{j \leq i} C_j$
    $i \leftarrow i + 1$
end while
return $F_1 \cup F_2 \cup \ldots \cup F_{k-1}$

Subgraph mining



Subgraph mining



The basic characteristics of the Eclat alg.

- The Eclat algorithm is much quicker then the Apriori algorithm.
- It is a depth-first algorithm $\Rightarrow$ lower memory consumption then the Apriori algorithm.
- Based on the fact that the powerset $\mathcal{P}(B)$ forms a lattice.
- Uses so called prefix-based equivalence classes.
- Uses the vertical representation of the database.

The prefix-based equivalence classes

Definition (equivalence relation)

Let P be a set and $X, Y, Z \in P$ a relation $\equiv$ is called an equivalence relation if the relation is:

1. Reflexive: $X \equiv Y$.
2. Symmetric: if $X \equiv Y$ then $Y \equiv X$.
3. Transitive: if $X \equiv Y$ and $Y \equiv Z$ then $X \equiv Z$.

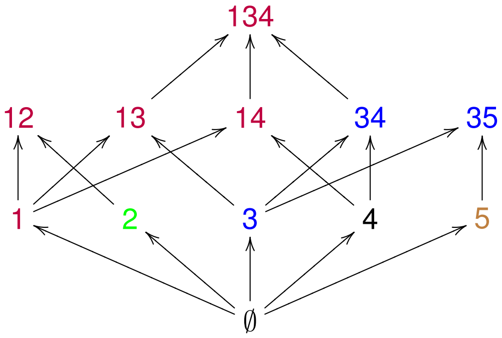
Definition (prefix-based equivalence class)

Let π be a function $\pi : \mathcal{P}(B) \times N \to \mathcal{P}(B)$ such that $\pi(X, l) = X[1 : l]$.
The *prefix-based equivalence* π_l on the lattice $\mathcal{L}$ is defined as follows:
$\forall U, V \subseteq B, U \equiv_{\pi_l} V \Leftrightarrow \pi(U, l) = \pi(V, l)$.

The prefix-based equivalence classes contd.

Lemma

Each equivalence class $[W]_\pi$ induced by the equivalence relation π is a sub-lattice of powerset $\mathcal{P}(B)$.



The vertical representation of a database

Database D:

TID	Transaction
1	$\{1, 2, 3, 4\}$
2	$\{3, 5\}$
3	$\{1, 3, 4\}$
4	$\{1, 2\}$
5	$\{1, 3, 4, 5\}$
6	$\{1, 2, 3, 4, 5\}$

Vertical representation of the database is a set of pairs $\{(b_i, \mathcal{T}(b_i))\}$, where $b_i \in B$ and $\mathcal{T}(b_i)$ is a *transaction list* of item b_i (tidlist in short)

Example:
$(1, \{1, 3, 4, 5, 6\})$
$(2, \{1, 4, 6\})$
$(3, \{1, 2, 3, 5, 6\})$
$(4, \{1, 3, 5, 6\})$
$(5, \{5, 6\})$

Support counting

Support of a set $U \subset B$ can be computed using the tidlists:
$Supp(U) = |\bigcap_{b_i \in U} \mathcal{T}(b_i)|$

- **The Eclat algorithm makes a single scan of D.**
- **The datastructures are processor-cache friendly** (it is just an array of numbers).
- Can be implemented using bitmaps.

itemset	$\{1\}$	$\{2\}$	$\{3\}$	$\{4\}$	$\{5\}$
TID	1	1	1	1	2
	3	4	2	3	5
	4	6	3	5	6
	5		5	6	
	6		6		

Frequent	$\times$	$\times$	$\times$	$\times$	$\times$	$\times$
itemset	$\{1,2\}$	$\{1,3\}$	$\{1,4\}$	$\{1,5\}$	$\{2,3\}$	$\{2,4\}$
TID	1	1	1	5	1	1
	4	3	3	6	6	6
	6	5	5			
		6	6			

		$\times$	$\times$	$\times$
itemset	$\{2,5\}$	$\{3,4\}$	$\{3,5\}$	$\{4,5\}$
TID	6	1	2	5
		3	5	6
		5	6	
		6		

The Eclat algorithm

ECLAT-BOTTOM-UP(**In:** Atoms $\mathcal{A}$, **In:** Itemset P, **Out:** Set F)

```
for all atom a_i ∈ A do
    A_i ← ∅
    for all atom a_j ∈ A, a_i < a_j do
        if |T(P ∪ {a_j})| ≥ min_support then
            A_i ← A_i ∪ {a_j}
            f ← P ∪ {a_j}
            F ← F ∪ f
        end if
    end for
    ECLAT-BOTTOM-UP(A_i, P ∪ {a_i}, F)
end for
```

Optimalizations to the Eclat algorithm

1. The “closed itemset” optimalization
2. Dynamic items ordering
3. The diffsets

Optimalizations – The “closed itemset” optimalization

TID	Transaction
1	{...}
2	{...}
3	{ 1,2 }
4	{ 1,2 }
5	{ 1,2,3,4,5}
6	{ 1,2,3,4,5}

Optimalizations – Dynamic items ordering

Let have a prefix $\Pi = \{\pi_1, \ldots, \pi_k\}, \pi_i \in B$, and extensions $\Sigma = \{\sigma_1, \ldots, \sigma_l\}, \sigma_i \in B$, and $Supp^*(\Pi \cup \{\sigma_1\}) \leq Supp^*(\Pi \cup \{\sigma_2\}) \leq \ldots \leq Supp^*(\Pi \cup \{\sigma_l\})$.
For the prefix Π:

Using the order it follows:

Optimalizations – Dynamic items ordering

Let have a prefix $\Pi = \{\pi_1, \ldots, \pi_k\}, \pi_i \in B$, and extensions $\Sigma = \{\sigma_1, \ldots, \sigma_l\}, \sigma_i \in B$, and $\mathit{Supp}^*(\Pi \cup \{\sigma_1\}) \leq \mathit{Supp}^*(\Pi \cup \{\sigma_2\}) \leq \ldots \leq \mathit{Supp}^*(\Pi \cup \{\sigma_l\})$.
For the prefix Π:

1. consider $\sigma_1, \sigma_2, \ldots, \sigma_l$ as extensions (in that order)

Using the order it follows:

1. the smallest portion of the database gets the largest portion of the search space.

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For the prefix Π:

1. consider $\sigma_1, \sigma_2, \ldots, \sigma_l$ as extensions (in that order)
2. consider $\sigma_l, \sigma_{l-1}, \ldots, \sigma_1$ as extensions (in that order)

Using the order it follows:

1. the smallest portion of the database gets the largest portion of the search space.
2. the largest portion of the database gets the largest portion of the search space.

Optimalizations – The diffsets

Definition

Let $U \subset B$ be an itemset and $i \in B - U$ an item. $\mathcal{T}(U)$ denotes a set of transaction id's. *Difference set* (or diffset in short) is $\mathcal{D}(U \cup \{i\}) = \mathcal{T}(U) - \mathcal{T}(\{i\})$

The support can be computed as:

$$Supp(U \cup \{i\}) = Supp(U) - |\mathcal{D}(U \cup \{i\})|$$

Computation of diffsets:

$$\begin{aligned}
\mathcal{D}(U \cup \{i\} \cup \{j\}) &= \mathcal{T}(U \cup \{i\}) - \mathcal{T}(U \cup \{j\}) \\
&= \mathcal{T}(U \cup \{i\}) - \mathcal{T}(U \cup \{j\}) + \mathcal{T}(U) - \mathcal{T}(U) \\
&= (\mathcal{T}(U) - \mathcal{T}(U \cup \{j\})) - (\mathcal{T}(U) - \mathcal{T}(U \cup \{i\})) \\
&= \mathcal{D}(U \cup \{j\}) - \mathcal{D}(U \cup \{i\})
\end{aligned}$$

The FPGrowth algorithm

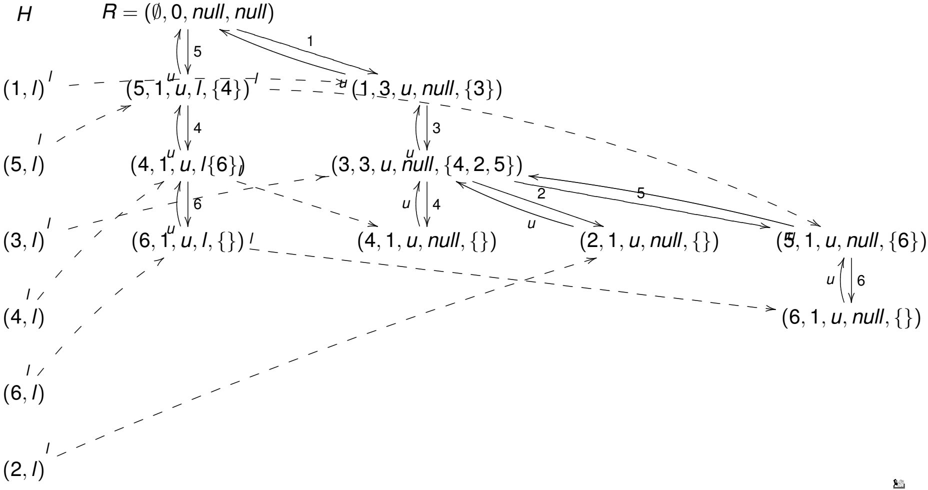
- Very similar to the Eclat algorithm
- the only difference is the used datastructure
- The datastructure (called FPTrie) is a prefix tree with linked nodes

The FPGrowth algorithm - the FPTrie

TID	Transaction
1	$\{1, 3, 4\}$
2	$\{5, 4, 6\}$
3	$\{1, 3, 5, 6\}$
4	$\{1, 3, 2\}$

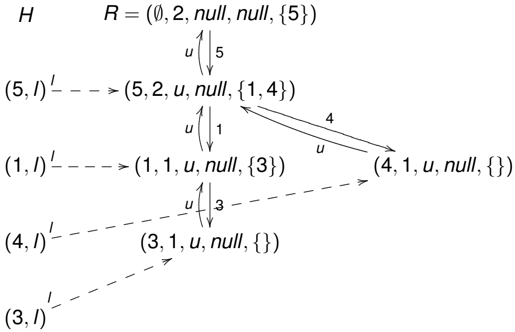
Item	Support
1	3
2	3
3	2
4	2
5	1
6	1

Each node is a tuple (`item, support, upper-link, header-link, children`).



6's conditional tree

Transaction	Support
$\{5, 4\}$	1
$\{5, 3, 1\}$	1



The FPGrowth algorithm

FPGROWTH(**In:** FP-Tree *tree*,**In:** Itemset I)

- **if** *tree* contains only single path P **then**
  - **for all** combination c in path P **do**
    - $s \leftarrow min\{s | i \in c, s = Supp(i)\}$
    - **if** $s \geq min\_support$ **then**
      - generate pattern $c \cup I$ with support s
    - **end if**
  - **end for**
- **else**
  - **for all** a_i in the header of *tree* **do**
    - **if** $Supp(a_i) \geq min\_support$ **then**
      - generate pattern $c = \{a_i\} \cup I$ with support $Supp(a_i)$
    - **end if**
    - construct c's conditional pattern base and
    - then c's conditional **FP-Tree** $tree_c$
    - **if** $Size(tree_c) \neq 0$ **then**
      - FPGROWTH($tree_c, c$)
    - **end if**
  - **end for**
- **end if**