Lecture 2

Association rules

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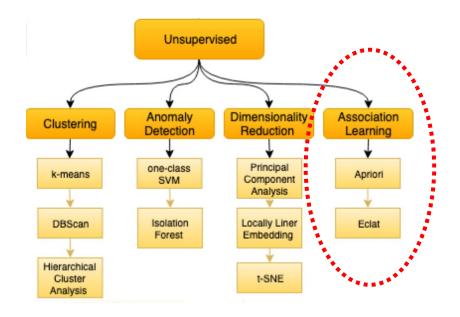
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Unsupervised learning

Experience: objects for which **no class labels** have been given

<u>Performance:</u> typically concerns the ability to output useful **characterizations**(or groupings) of objects





Problem 1:
Mining
Frequent Itemsets

Problem 2:
Mining
Association Rules



Problem 1: Mining frequent itemsets

Given a set of transactions D, find combinations of items that occur frequently

Market-Basket transactions

TID	Items
1	Bread, Milk
2	Bread, Diaper, Beer, Eggs
3	Milk, Diaper, Beer, Coke
4	Bread, Milk, Diaper, Beer
5	Bread, Milk, Diaper, Coke

Examples of *frequent* **itemsets**

```
{Diaper, Beer},
{Milk, Bread},
{Beer, Bread, Milk}
```



Problem 2: Mining Association Rules

• Given a set of transactions **D**, find rules that will predict the occurrence of an item (or a set of items) based on the occurrences of other items in the transaction

Market-Basket transactions

TID	Items
1	Bread, Milk
2	Bread, Diaper, Beer, Eggs
3	Milk, Diaper, Beer, Coke
4	Bread, Milk, Diaper, Beer
5	Bread, Milk, Diaper, Coke

Examples of *association rules*

```
{Diaper} \rightarrow {Beer},

{Milk, Bread} \rightarrow {Diaper, Coke},

{Beer, Bread} \rightarrow {Milk}
```



Why do we want to find frequent itemsets?

Find all combinations of items that occur together



o e.g., in placement of items in a store ©



- Frequent itemsets are only positive combinations (we do not report combinations that do not occur frequently together)
- Frequent itemsets aim at providing a summary of the data



Definitions

Itemset

- A set of one or more items
 - e.g.: {Milk, Bread, Diaper}
- k-itemset
 - An itemset that contains k items
- Absolute Support
 - Number of transactions in which an itemset appears
 - o e.g., $\sigma(\{Milk, Bread, Diaper\}) = 2$
- Relative Support
 - Fraction of the transactions in which an itemset appears
 - e.g., s({Milk, Bread, Diaper}) = 2/5
- Frequent Itemset
 - An itemset whose relative support is greater than or equal to a minsup threshold

TID	Items
1	Bread, Milk
2	Bread, Diaper, Beer, Eggs
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Mining frequent itemsets

Task

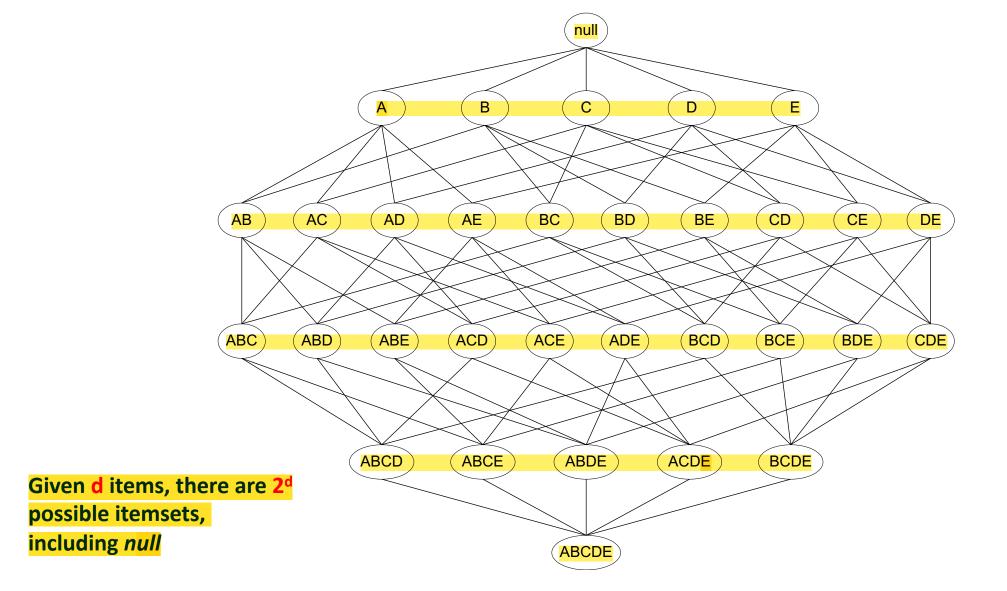
Given a transaction database **D** and a **minsup** threshold, find all frequent itemsets and the frequency of each set in this collection

Stated differently:

Count the number of times combinations of attributes occur in the data. If the count of a combination is above *minsup*, report it

Recall: The input is a transaction database D where every transaction consists of a subset of items from some universe I

How many itemsets are there?





Brute-force algorithm for finding all frequent itemsets?

- Generate all possible itemsets (lattice of itemsets)
 - Start with 1-itemsets, 2-itemsets, ..., d-itemsets

- Compute the frequency of each itemset from the data
 - Count in how many transactions each itemset occurs
- If the support of an itemset is above minsup report it as a frequent itemset



Brute-force algorithm for finding all frequent itemsets?

- Complexity?
 - Match every candidate against each transaction
 - For M candidates and N transactions, the complexity is approximately O(NM)
 - Expensive since M = 2^d !!!





Speeding-up the brute-force algorithm

- Reduce the number of candidates (M)
 - Complete search: M=2^d
 - Use pruning techniques to reduce M
- Reduce the number of comparisons (NM)
 - Use efficient data structures to store the candidates or transactions
 - No need to match every candidate against every transaction
- Reduce the number of transactions (N)
 - Reduce the size of N as the size of itemsets increases
 - Use vertical-partitioning of the data to apply the mining algorithms



Reduce the number of candidates

- Apriori principle (Main observation):
 - If an itemset is frequent, then all of its subsets must also be frequent
- Apriori principle holds due to the following property of the support measure:

$$\forall X, Y : (X \subseteq Y) \Rightarrow s(X) \ge s(Y)$$

- The support of an itemset never exceeds the support of its subsets
- This is known as the anti-monotone property of support



Example

TID	Items
1	Bread, Milk
2	Bread, Diaper, Beer, Eggs
3	Milk, Diaper, Beer, Coke
4	Bread, Milk, Diaper, Beer
5	Bread, Milk, Diaper, Coke

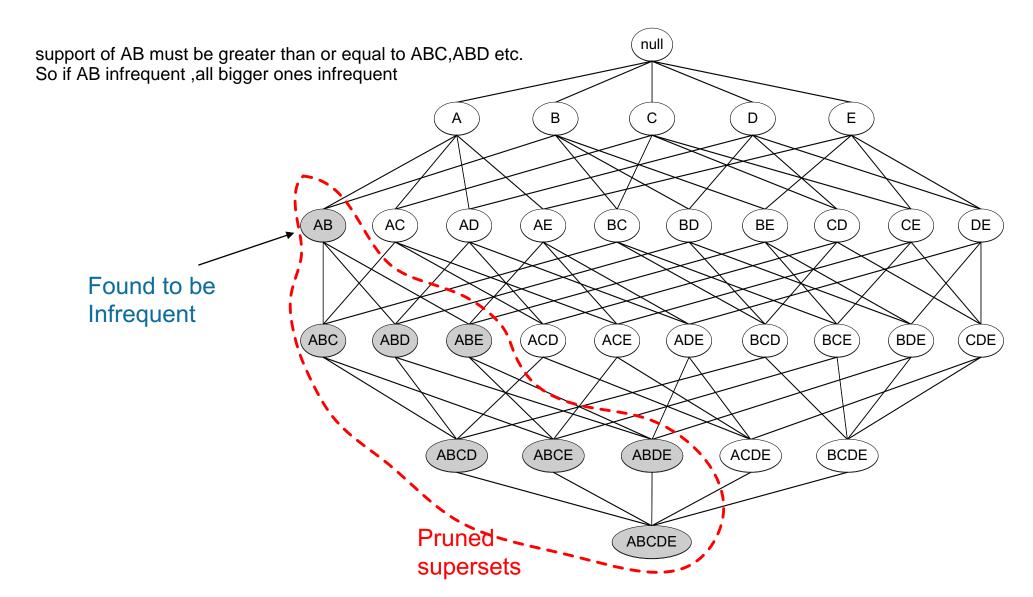
$$\forall X, Y : (X \subseteq Y) \Rightarrow s(X) \ge s(Y)$$

itemset infrequent all supersets also infrequent

- The support of an itemset never exceeds the support of its subsets
- This is known as the anti-monotone property of support



Illustrating the Apriori principle





The Apriori algorithm [Agrawal&Srikant 1994]

```
C<sub>k</sub>: Candidate itemsets of size k
L<sub>k</sub>: Frequent itemsets of size k
L<sub>1</sub> = {frequent 1-itemsets};
for (k = 1; L_k != \emptyset; k++)
 C_{k+1} = GenerateCandidates(L_k)
  for each transaction t in the database do
         increment count of candidates in C_{k+1} that are contained in t
  endfor
  L_{k+1} = candidates in C_{k+1} with support \geq minsup
endfor
return \bigcup_k L_k;
```



C_{k+1} = GenerateCandidates()

- Assume the items in L_k are listed in an order (e.g., alphabetical)
- Step 1: self-joining L_k (IN SQL)

```
insert into C_{k+1}

select p.item_1, p.item_2, ..., p.item_k, q.item_k

from L_k p, L_k q

where p.item_1 = q.item_1, ..., p.item_{k-1} = q.item_{k-1} and p.item_k < q.item_k
```

$$p = \{item_1, item_2, ..., item_{k-1}, item_k\}$$

$$q = \{item_1, item_2, ..., item_{k-1}, item_k\}$$

candidate = { $item_1$, $item_2$, ..., $item_{k-1}$, $item_k$, $item_k$ }



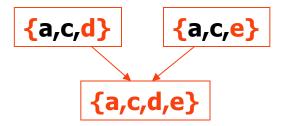
Example of Candidate Generation

- *k*=3
- L_3 ={abc, abd, acd, ace, bcd}
- $C_4 = ?$



Example of Candidate Generation

- *k*=3
- $L_3 = \{ \underline{ab}c, \underline{ab}d, \underline{ac}d, \underline{ac}e, bcd \}$
- *Self-joining*: L_3*L_3
 - o **abcd** from **abc** and **abd**
 - o acde from acd and ace





C_{k+1} = GenerateCandidates()

- Assume the items in L_k are listed in an order (e.g., alphabetical)
- Step 2: pruning

```
for all itemsets c in C_{k+1} do

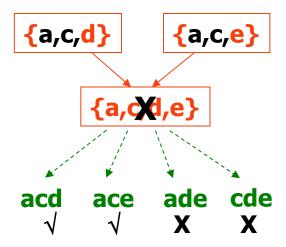
for all k-subsets s of c do

if (s is not in L_k) then delete c from C_{k+1}
```



Example of Candidate Pruning

- $L_3 = \{\underline{abc}, \underline{abd}, \underline{acd}, \underline{ace}, \underline{bcd}\}$
- *Self-joining*: L_3*L_3
 - o **abcd** from **abc** and **abd**
 - o acde from acd and ace
- Pruning
 - o acde is removed because ade is not in L₃
- *C*₄={abcd}





Discussion of the Apriori algorithm

- Much faster than the Brute-force algorithm
 - It avoids checking all elements in the lattice
- The running time is in the worst case O(2^d)
 - Pruning really prunes in practice
- It makes multiple passes over the dataset
 - One pass for every level k
- Multiple passes over the dataset are inefficient when we have thousands of candidates and millions of transactions

Implementations

Lots of them around

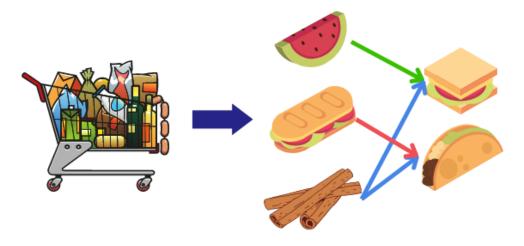
See, for example, the web page of Bart Goethals:
 http://www.adrem.ua.ac.be/~goethals/software/



 Typical input format: each row lists the items (using item id's) that appear in every row



Association Rule Learning



"93% of people who purchased item A also purchased item B"



Association Rules

Let D be a database of transactions, e.g.,

TID	Items	
1	A, B, C	
2	A, C	
3	A, D	
4	B, E, F	

- Let I be the set of items that appear in the database, e.g., I={A,B,C,D,E,F}
- A rule is defined by $X \rightarrow Y$, where $X \subset I$, $Y \subset I$, and $X \cap Y = \emptyset$
 - e.g., {B,C} → {A} is a rule



Definitions

Association Rule

- An implication expression of the form X → Y, where X and Y are non-overlapping itemsets
 - Example: {Milk, Diaper} → {Beer}

Rule Evaluation Metrics

- Support (s)
 - Fraction of transactions that contain both X and Y
- Confidence (c)
 - Measures how often items in Y appear in transactions that also contain X

$$c = \frac{\sigma(X, Y)}{\sigma(X)}$$

Example:

TID	Items
1	Bread, Milk
2	Bread, Diaper, Beer, Eggs
3	Milk, Diaper, Beer, Coke
4	Bread, Milk, Diaper, Beer
5	Bread, Milk, Diaper, Coke

 $\{Milk, Diaper\} \rightarrow \{Beer\}$

$$s = \frac{\sigma(\text{Milk, Diaper,Beer})}{|D|} = \frac{2}{5} = 0.4$$

$$c = \frac{\sigma(\text{Milk, Diaper, Beer})}{\sigma(\text{Milk, Diaper})} = \frac{2}{3} = 0.67$$

Mining association rules

• Task:

Given a set of transactions **D**, the goal of association rule mining is to find all rules having:

- o support ≥ *minsup* threshold
- confidence ≥ minconf threshold



Brute-force algorithm for association-rule mining

- List all possible association rules
- Compute the support and confidence for each rule
- Prune rules that fail the minsup and minconf thresholds

⇒ Computationally prohibitive!



A faster solution...

TID	Items
1	Bread, Milk
2	Bread, Diaper, Beer, Eggs
3	Milk, Diaper, Beer, Coke
4	Bread, Milk, Diaper, Beer
5	Bread, Milk, Diaper, Coke

Example of Rules:

```
{Milk, Diaper} \rightarrow {Beer} (s=0.4, c=0.67)

{Milk, Beer} \rightarrow {Diaper} (s=0.4, c=1.0)

{Diaper, Beer} \rightarrow {Milk} (s=0.4, c=0.67)

{Beer} \rightarrow {Milk, Diaper} (s=0.4, c=0.67)

{Diaper} \rightarrow {Milk, Beer} (s=0.4, c=0.5)

{Milk} \rightarrow {Diaper, Beer} (s=0.4, c=0.5)
```

Observations:

- All the above rules are binary partitions of the same itemset:
 {Milk, Diaper, Beer}
- Rules originating from the same itemset have identical support but can have different confidence
- Thus, we may decouple the support and confidence requirements



A faster solution...

- Two-step approach:
 - Frequent Itemset Generation

Generate all itemsets whose support ≥ *minsup*

solved

Rule Generation

Generate high-confidence rules from each frequent itemset, where each rule is a binary partition of a frequent itemset



Rule Generation – Naive algorithm

- Given a frequent itemset X, find all non-empty subsets $y \subset X$ such that $y \to X y$ satisfies the minimum confidence requirement
- If X = {A,B,C,D} is a frequent itemset, the candidate rules are:

$$ABC \rightarrow D$$
, $ABD \rightarrow C$, $ACD \rightarrow B$, $BCD \rightarrow A$, $A \rightarrow BCD$, $B \rightarrow ACD$, $C \rightarrow ABD$, $D \rightarrow ABC$, $AB \rightarrow CD$, $AC \rightarrow BD$, $AD \rightarrow BC$, $BC \rightarrow AD$, $BD \rightarrow AC$, $CD \rightarrow AB$

• If |X| = k, then there are $2^k - 2$ candidate association rules (ignoring $L \to \emptyset$ and $\emptyset \to L$)



Efficient rule generation

- How to efficiently generate rules from frequent itemsets?
 - In general, confidence does not have an anti-monotone property
 - $c(ABC \rightarrow D)$ can be larger or smaller than $c(AB \rightarrow D)$
 - But the confidence of rules generated from the same itemset has an anti-monotone property
 - Example: X = {A,B,C,D}:

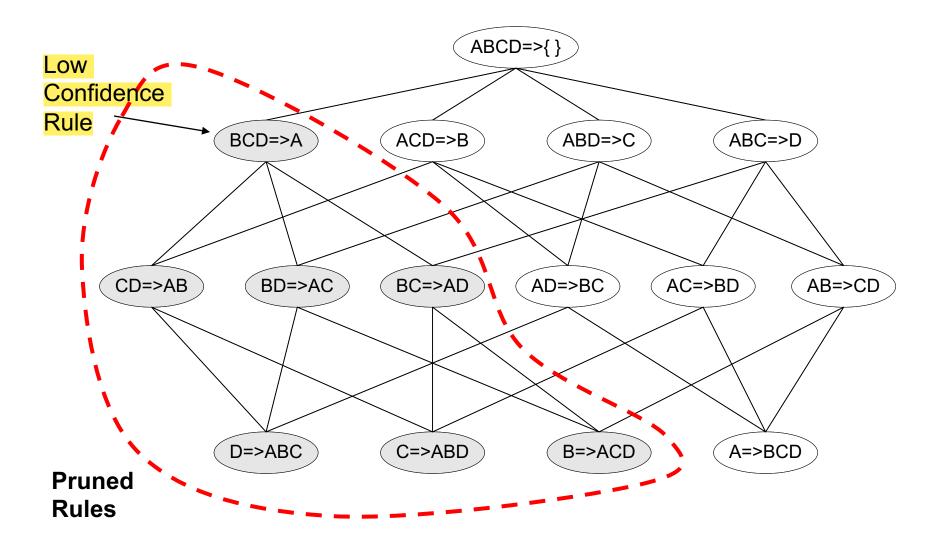
$$c(ABC \rightarrow D) \ge c(AB \rightarrow CD) \ge c(A \rightarrow BCD)$$

$$c(ABC->D) = \frac{\sigma(\{A,B,C,D\})}{\sigma(\{A,B,C\})}$$

Confidence is anti-monotone w.r.t. number of items on the Right-Hand-Side of the rule



Rule Generation for Apriori Algorithm





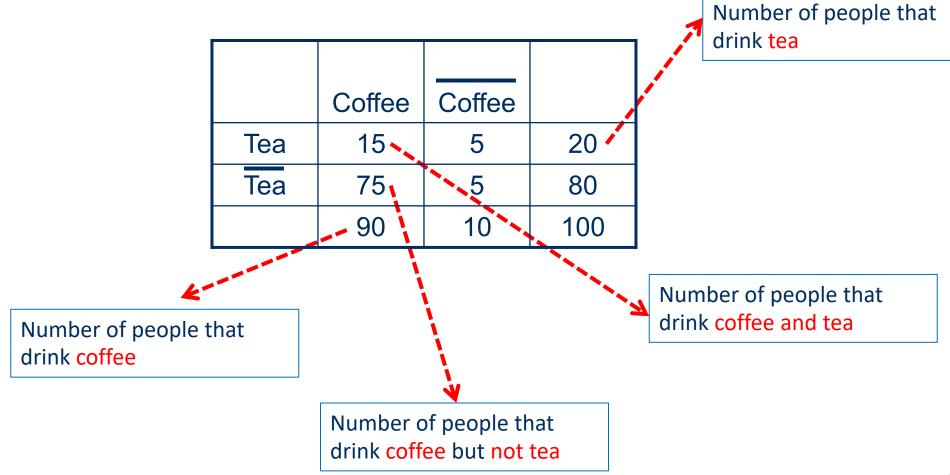
Other interestingness measures

- Lift
- Cosine
- All-confidence
- Leverage

• ...



Drawback of Confidence





Drawback of Confidence

	Coffee	Coffee	
Tea	15	5	20
Tea	75	5	80
	90	10	100

Association Rule: Tea → Coffee

• Confidence:
$$P(Coffee | Tea) = \frac{15}{20} = 0.75$$
, but $P(Coffee) = \frac{90}{100} = 0.9$

- Although confidence is high, the rule is misleading
- o someone buying tea is less likely to buy coffee than someone for whom we have no information



$$\circ$$
 $P(Coffee | Tea) = 0.9375$

Lift of a Rule

Given association rule
$$X \to Y$$
: $lift(X \to Y) = \frac{P(X,Y)}{P(X)P(Y)} = \frac{conf(X \to Y)}{P(Y)} = \frac{|X,Y|n}{|X||Y|}$

- If P(X,Y) = P(X) P(Y), then $lift(X \rightarrow Y) = 1$
 - o means that the occurrences of X and Y in the same transaction are independent events, i.e., X and Y are not correlated, and the rule is meaningless!
- $lift(X \rightarrow Y) = k > 1$
 - means that X and Y are dependent so that if X occurs, then Y is k times more likely to occur than expected
- $lift(X \rightarrow Y) = k < 1$
 - means that the occurrence of X prevents the occurrence of Y, i.e., Y is k times less likely to occur than expected



Example: Lift/Interest

	Coffee	Coffee	
Tea	15	5	20
Tea	75	5	80
	90	10	100

Association Rule: Tea → Coffee

Confidence:
$$P(Coffee | Tea) = \frac{15}{20} = 0.75$$
, but $P(Coffee) = \frac{90}{100} = 0.9$

 \Rightarrow Lift = 0.75 / 0.9= 0.8333 (< 1, thus it is negatively associated)

⇒ therefore, coffee occurs less than expected when tea also occurs



Too many frequent itemsets

• If $\{a_1, ..., a_{100}\}$ is a frequent itemset, then there are

$$\binom{100}{1} + \binom{100}{2} + \ldots + \binom{100}{100} = 2^{100} - 1$$

1.27*10³⁰ frequent sub-patterns!

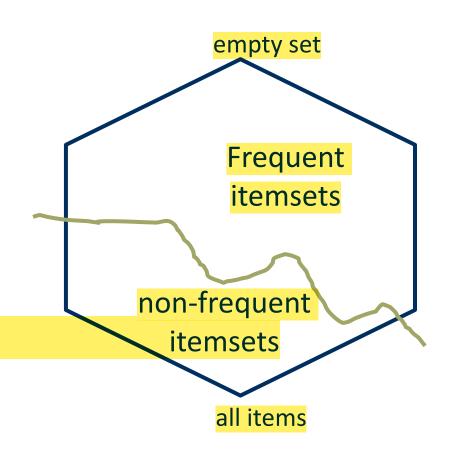
There should be some more condensed way to describe the data



Frequent itemsets maybe too many to be helpful

- If there are many & large frequent itemsets,
 enumerating all of them is costly!
- We may be interested in finding the boundary frequent patterns

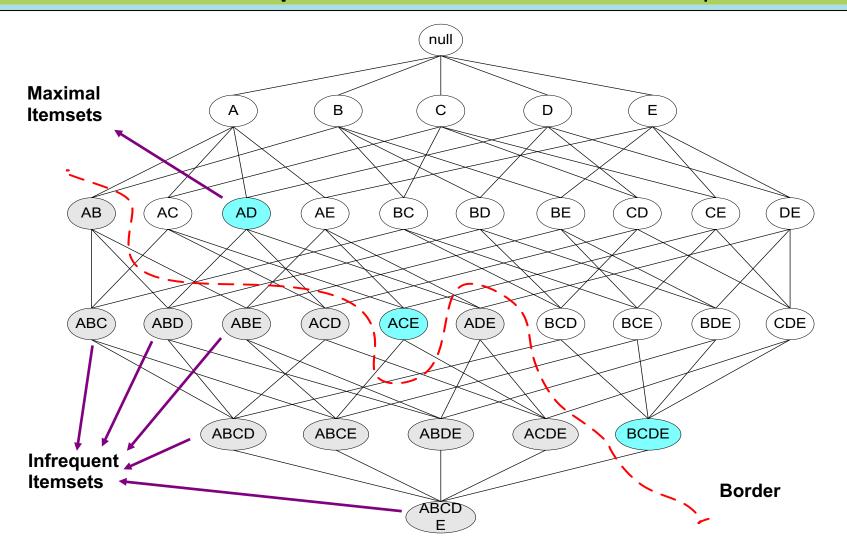
Question: Is there a good definition of such boundary?





Maximal frequent itemsets

An itemset is maximal frequent if none of its immediate supersets is frequent





Descriptive power of maximal patterns

 Knowing the set of all maximal patterns allows us to reconstruct the set of all frequent itemsets!!

We can only reconstruct the set, not the actual frequencies



An itemset is **closed** if **none of its immediate supersets** has the same support as the itemset

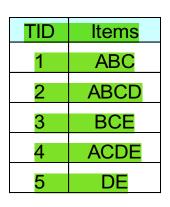
TID	Items
1	{A,B}
2	$\{B,C,D\}$
3	${A,B,C,D}$
4	${A,B,D}$
5	$\{A,B,C,D\}$

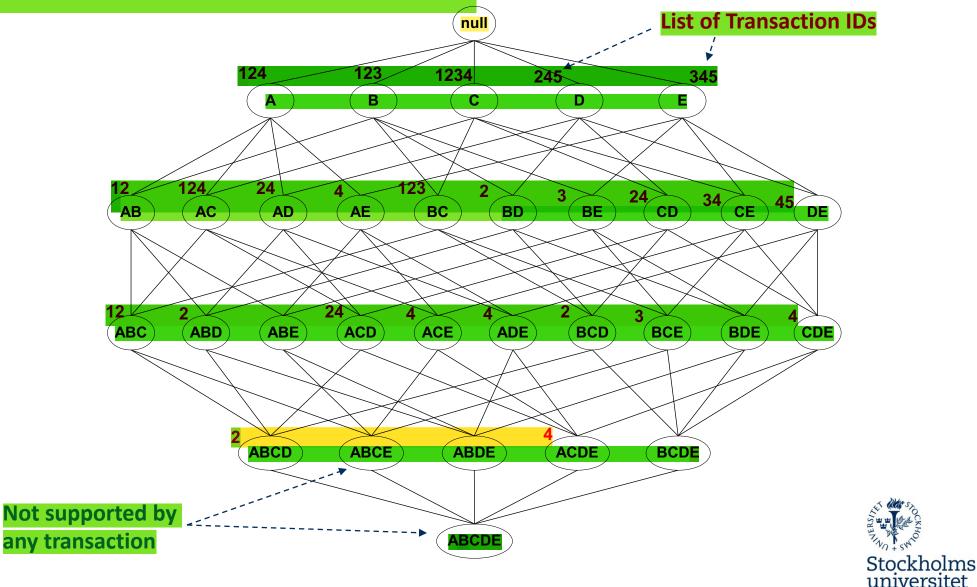
Itemset	Support
{A}	4
{B}	5
{C}	3
{D}	4
{A,B}	4
{A,C}	2
{A,D}	3
{B,C}	3
{B,D}	4
{C,D}	3

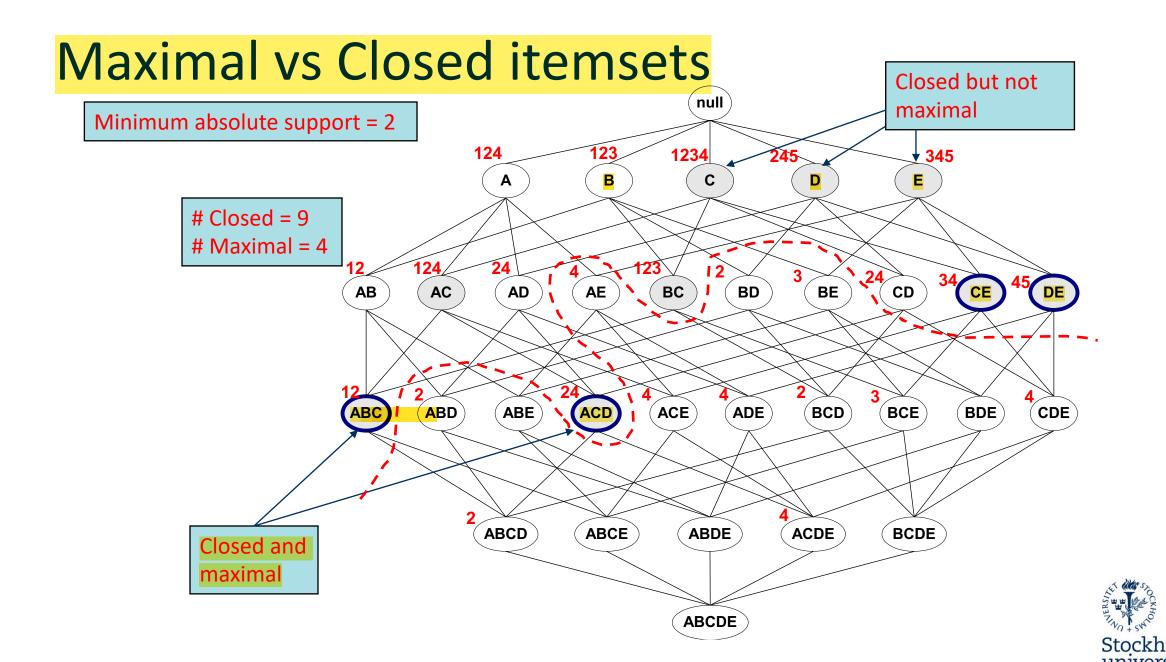
Itemset	Support
$\{A,B,C\}$	2
$\{A,B,D\}$	3
{A,C,D}	2
{B,C,D}	3
$\{A,B,C,D\}$	2



Maximal vs Closed itemsets







Why are closed itemsets interesting?

- Closed patterns and their frequencies alone are a sufficient representation of all the frequencies of all frequent patterns
- **Proof:** Assume a frequent itemset **X**:
 - o X is closed $\rightarrow s(X)$ is known
 - ∴ X is not closed →
 s(X) = max {s(Y) | Y is closed and X subset of Y}



An itemset is **closed** if **none of its immediate supersets** has the same support as the itemset

TID	Items
1	{A,B}
2	$\{B,C,D\}$
3	$\{A,B,C,D\}$
4	$\{A,B,D\}$
5	$\{A,B,C,D\}$

Itemset	Support
{A}	?
{B}	5
{C}	?
{D}	?
{A,B}	4
{A,C}	?
{A,D}	?
{B,C}	3
{B,D}	4
{C,D}	3

Itemset	Support
{A,B,C}	2
{A,B,D}	3
{A,C,D}	2
{B,C,D}	3
{A,B,C,D}	2



An itemset is **closed** if **none of its immediate supersets** has the same support as the itemset

TID	Items
1	{A,B}
2	$\{B,C,D\}$
3	$\{A,B,C,D\}$
4	$\{A,B,D\}$
5	$\{A,B,C,D\}$

Itemset	Support
{A}	?
{B}	5
{C}	?
{D}	?
{A,B}	4
{A,C}	?
{A,D}	?
{B,C}	3
{B,D}	4
{C,D}	3

Itemset	Support
{A,B,C}	2
{A,B,D}	3
{A,C,D}	2
{B,C,D}	3
{A,B,C,D}	2



An itemset is **closed** if **none of its immediate supersets** has the same support as the itemset

TID	Items
1	{A,B}
2	{B,C,D}
3	$\{A,B,C,D\}$
4	{A,B,D}
5	$\{A,B,C,D\}$

Itemset	Support
{A}	?
{B}	5
{C}	3
{D}	?
{A,B}	4
{A,C}	?
{A,D}	?
{B,C}	3
{B,D}	4
{C,D}	3

Itemset	Support
{A,B,C}	2
{A,B,D}	3
{A,C,D}	2
{B,C,D}	3
{A,B,C,D}	2



An itemset is **closed** if **none of its immediate supersets** has the same support as the itemset

TID	Items	
1	{A,B}	
2	$\{B,C,D\}$	
3	$\{A,B,C,D\}$	
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5	$\{A,B,C,D\}$	

Itemset	Support
{A}	?
{B}	5
{C}	3
{D}	?
{A,B}	4
{A,C}	?
{A,D}	?
{B,C}	3
{B,D}	4
{C,D}	3

Itemset	Support
{A,B,C}	2
{A,B,D}	3
{A,C,D}	2
{B,C,D}	3
{A,B,C,D}	2



An itemset is **closed** if **none of its immediate supersets** has the same support as the itemset

TID	Items	
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2	$\{B,C,D\}$	
3	$\{A,B,C,D\}$	
4	{A,B,D}	
5	$\{A,B,C,D\}$	

Itemset	Support
{A}	?
{B}	5
{C}	3
{D}	4
{A,B}	4
{A,C}	?
{A,D}	?
{B,C}	3
{B,D}	4
{C,D}	3

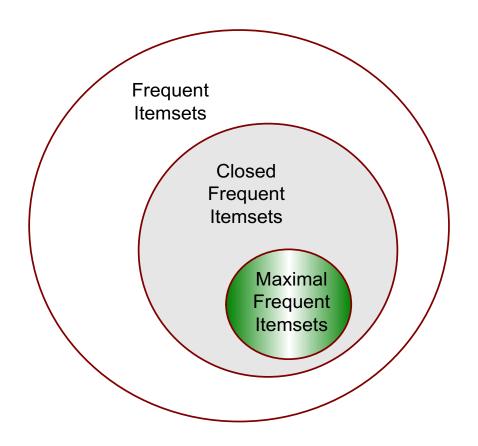
Itemset	Support
{A,B,C}	2
{A,B,D}	3
{A,C,D}	2
{B,C,D}	3
{A,B,C,D}	2



Maximal vs Closed itemsets

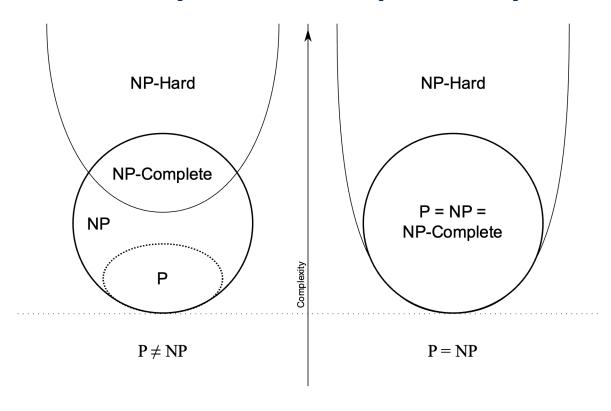
- Knowing all maximal patterns (and their frequencies) allows us to reconstruct the set of frequent itemsets
- Knowing all closed patterns and their frequencies allows us to reconstruct the set of all frequent itemsets and their frequencies
- The problems of finding the set of frequent itemsets, maximal itemsets, and closed itemsets are all NP-hard

Proof?





Back to the theory of complexity



NP: a solution can be verified in polynomial time

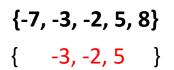
NP-hard: every NP problem can be reduced to it in polynomial time (the problem can be used as a subroutine to solve any NP problem)

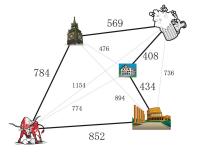
NP-complete: the problem is in NP and it is NP-hard

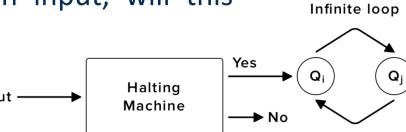


Examples of NP-hard problems

- Subset sum: given a set of integers is there a non-empty set of those integers that adds up to zero?
- Traveling salesman: given a set of cities and the distances between the cities, what is the possible shortest route visiting each and every city (once) and returning to the starting city?
- Halting problem: given a program and an input, will this program run for ever?





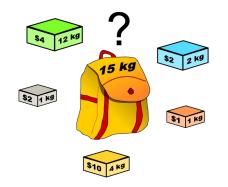




Examples of NP-complete problems

- Boolean satisfiability (SAT): given a boolean formula, is there a configuration of the variables that satisfies it?
- Knapsack problem: given a set of items, each having a value and a weight, find the subset of items so that the weight is at most W (minimized) and the total value is at least V (maximized)
- Vertex cover: given a graph, find a set of at most k vertices so that each and every edge in the graph is incident to at least one of these vertices
- Maximum Clique: given a graph, find the largest complete subgraph of size at most k

 $(x OR y OR z) AND (x OR \overline{y} OR z) AND$ $(x OR y OR \overline{z}) AND (x OR \overline{y} OR \overline{z}) AND$ $(\overline{x} OR y OR z) AND (\overline{x} OR \overline{y} OR \overline{z})$







Proving NP-hardness

- Not always easy
- But sometimes easier than you think
- To prove that problem T is NP-hard:
 - find a known NP-hard problem L
 - reduce L to T in polynomial time: show that all instances of L can be solved by solving T, which
 is done by mapping L to T in polynomial time
 - since L is NP-hard, T cannot be solved faster than that...hence it is also NP-hard
- If we can also verify any solution to T in polynomial time, then T is in NP; hence T is also NP-complete



Maximal frequent itemset mining

- Use the set-cover problem formulation!
 - universe of m elements $U = \{U_1, ..., U_m\}$: each U_i is a frequent itemset
 - set of \mathbf{n} sets $\mathbf{S} = \{\mathbf{S}_1,...,\mathbf{S}_n\}$: each \mathbf{S}_i contains all itemsets covered by a given frequent itemset X, i.e., all subsets of X

Formulation:

- Problem A: find the smallest collection of sets in S such that all elements in U are covered (set cover)
- equivalent to Problem B: find the smallest collection of itemsets each covering a set of frequent itemsets, so that all frequent itemsets are covered (maximal itemsets)
- so...if we can solve Problem B we can also solve all instances of Problem A
- since A is known to be NP-hard, then B is also NP-hard



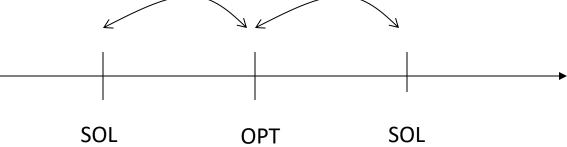
Approximation algorithms

For an NP-hard problem, we cannot compute an optimal solution in polynomial time

The key of designing a polynomial time approximation algorithm is to obtain a good (lower or upper) bound to the optimal solution

- OPT: value of an optimal solution
- **SOL:** value of the solution that our algorithm returns

The general strategy (for an optimization problem) is:



 $f \cdot \mathsf{OPT} \leq \mathsf{SOL} \leq \mathsf{OPT}$, if $\mathsf{f} < \mathsf{1}$

Maximization Problem: maximize some cost function

OPT \leq SOL \leq $f \cdot$ OPT, if f > 1

Minimization Problem: minimize some cost function



Approximation for set cover

The greedy algorithm for set cover has an approximation factor of:

f = |s_{max}| s_{max}: the size of the largest set

Proof: From CLR "Introduction to Algorithms"

The set cover cannot be approximated with a factor better than $O(log |s_{max}|)$





Best-collection problem

- Universe of m elements U = {U₁,...,U_m}
- A set of n sets $S = \{S_1, ..., S_n\}$ such that they cover the universe
- Question: Find a collection C consisting of k sets from S such that

 $f(C) = |U_{c \in C}c|$ is maximized

f: the number of elements in U that are covered by C

The best-collection problem is NP-hard



Greedy approximation algorithm for the best-collection problem

- C = {}
- for every set s in S and not in C compute the gain of s:

$$g(s) = f(C \cup \{s\}) - f(C)$$

- Select the set s with the maximum gain
- C = C U {s}
- Repeat until C has k elements

The *greedy* algorithm for the best-collection problem has the following approximation factor:

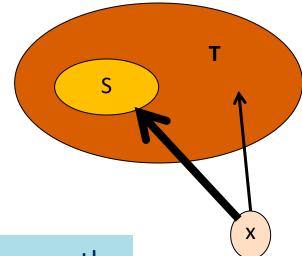
$$F = (e-1)/e = 0.6321$$



Submodular functions

- A function f (defined on sets of some universe) is submodular if
 - for all sets S, T, such that S is subset of T and x any element in the universe
 - $f(S \cup \{x\}) f(S) \ge f(T \cup \{x\}) f(T)$

adding an element to a smaller subset will have a higher gain than adding it to a superset



Theorem: For **all maximization** problems where the optimization function is **submodular**, the **greedy** algorithm has the following approximation factor

$$F = (e-1)/e = 0.6321$$



Today...

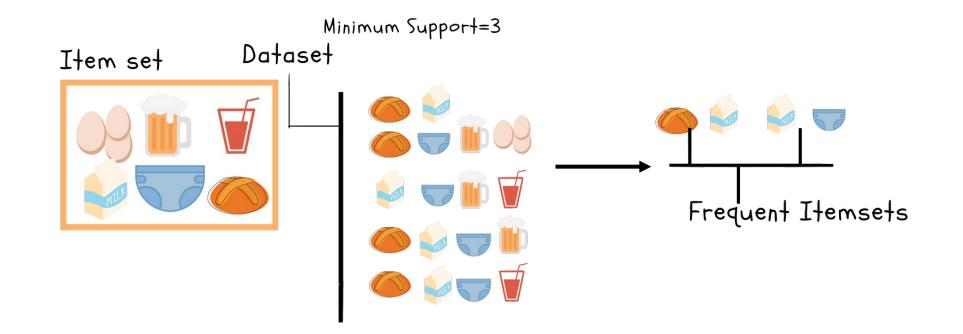
What is **Itemset Mining**?

What is the **Apriori Principle**?

How do we use the **Apriori Algorithm**?

The importance of Maximal and Closed Itemsets

The set cover problem and Approximation Algorithms





TODOs



Reading:

Main course book: Chapter 3.5

Extra Material



Lab 0

Recommended to complete the lab before the end of the week



Quiz 1



Coming up next week



Lecture 3 – Dimensionality Reduction



Thursday

Lecture 4 – Clustering I

Lab 1 – Data Exploration



