***** Advanced Machine Learning *****
Association Rule Learning

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Agenda for this Unit

Introduction

What is Association Rule Mining?

- Association rule mining belongs to the category of unsupervised learning.
- Association rules describe frequent co-occurrences in the data (**not necessarily causality!**)
- Examples:
  - Market basket analysis (*Which products are frequently bought together? E. g. Amazon*)
  - Course schedule planning (*Which courses are often attended together?*)
  - Other use cases: Marketing promotions, inventory management, customer relationship management (CRM)
- The general form of a rule is given by:

$$\overbrace{\{a_1, a_2, \ldots, a_n\}}^{\textbf{Antecedent}} \rightarrow \overbrace{\{b_1, b_2, \ldots, b_m\}}^{\textbf{Consequent}} \tag{1}$$

- Example: $\{bread, cheese\} \rightarrow \{wine\}$

Figure 1: Famous example from Amazon

Important Terminology

- Suppose $\mathcal{I}$ is a set of unique items which we have in our portfolio $\mathcal{T} = \{t_1, t_2, \ldots, t_n\}$ is a list of transactions (what customers bought).
- Each transaction $t_i \in \mathcal{T}$ is an element of $\mathfrak{P}(\mathcal{I})$, the power set of $\mathcal{I}$. (**What is a power set?**)
- Example:

Id	Transactions
1	$\{beer, chips, wine\}$
2	$\{beer, chips\}$
3	$\{pizza, wine\}$
4	$\{chips, pizza\}$

Id	*beer*	*chips*	*pizza*	*wine*
1	1	1	0	1
2	1	1	0	0
3	0	0	1	1
4	0	1	1	0

Figure 2: Left: List of transactions (raw), right: List of transactions in binary form

Simplification: We ignore quantities and prices of the items sold.

Item sets

- A collection of k items is called k-item set.
- Example: $\{pizza, wine\}$ is a 2-item set.
- The number of items contained in a transaction t_i is sometimes referred to as the **transaction width** $w(t_i) = |t_i|$.
- An important property of an item set X is the **support count $\boldsymbol{\sigma}$**:

$$\sigma(X) = |\{t_i | X \subseteq t_i \wedge t_i \in \mathcal{T}\}| \tag{2}$$

- **What does the support count tell us?** $\sigma(X)$ refers to the number of transactions X occurs in.

Quality Measures

- *Question:* How to measure the quality of an association rule?
- **Support:**
  - Proportion of examples for which head and body are true.
  - Example $A \rightarrow B$: How many customers bought A and B together?

$$\text{support}(A \rightarrow B) = \text{support}(A \cup B) = \frac{\sigma(A \cup B)}{n} \tag{3}$$

- **Confidence:**
  - Proportion of examples for which the head is true among those for which the body is true.
  - Example: If customers bought A, how likely are they to also buy B?

$$\text{confidence}(A \rightarrow B) = \frac{\text{support}(A \cup B)}{\text{support}(A)} = \frac{\sigma(A \cup B)}{\sigma(A)} \tag{4}$$

- Support: There is a huge number of possible rules, but not all of them are interesting.
  $\Rightarrow$ **Prune (remove) rules with low support.**

- Confidence: The higher the confidence the more reliable is the rule.

- Example:
  - $R = \{bread, cheese\} \rightarrow \{wine\}$
  - $\text{support}(R) = 0.01$ and $\text{confidence}(R) = 0.8$
  - 80 % of all customers who bought bread and cheese also bought red wine.
  - However, only 1 % of the customers bought all three items together.

Apriori

Learning Problem

- The **Apriori algorithm** can be used to find association rules.
- The learning problem can be summarized as follows:

  Given a set of transactions $\mathcal{T}$, find all rules having support $\geqslant s_{min}$ and confidence $\geqslant c_{min}$, where s_{min} and c_{min} are thresholds.

- Obviously, mining all possible rules is super expensive.

$$|\text{rules}| = 3^d - 2^{d+1} + 1 \qquad \text{where} \qquad d \equiv |\mathcal{I}| \tag{5}$$

- Also, rules can be spurious (i. e. patterns may occur by chance and are not systematic).

We have to avoid considering all possible rules! $\Rightarrow$ Employ early pruning.

Early Pruning

- The goal is to generate rules which have high support and high confidence.
- Observation: If an item set is infrequent (does not have sufficient support), calculating the confidence can be omitted.
- As a consequence, all rules which can be generated from this item set do not have to be considered anymore.
- Example for the item set $A = \{beer, diapers, milk\}$:
  - The rules derived from item set A are given below.
  - If we know item set A to be infrequent, we can prune all these rules.
  - There is no need to calculate the confidence for these rules (**decoupling of support and confidence**).

$$\{beer, diapers\} \rightarrow \{milk\} \qquad \{beer, milk\} \rightarrow \{diapers\}$$
$$\{diapers, milk\} \rightarrow \{beer\} \qquad \{beer\} \rightarrow \{diapers, milk\}$$
$$\{milk\} \rightarrow \{beer, diapers\} \qquad \{diapers\} \rightarrow \{beer, milk\}$$

Apriori Algorithm

- The overall algorithm consists of two major steps:

  1. **Frequent item set generation:**
     Find all item sets which have sufficient support (satisfy the support constraint).
  2. **Rule generation:**
     Extract highly confident rules which satisfy the confidence constraint.

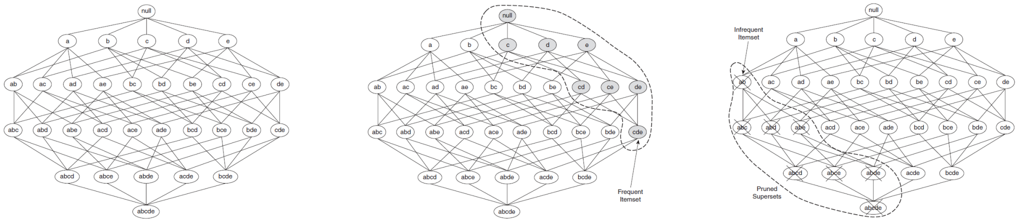
- In the following we will have a closer look at these two steps.

Step 1) Frequent item set generation

- It is possible to enumerate all possible item sets with a lattice $\Rightarrow$ fig. 3.
- A brute force approach could calculate the support for each candidate set and rank them by the result.
- **Problem:** The number of candidate sets grows exponentially with $|\mathcal{I}|$: $2^{|\mathcal{I}|} - 1$ (excluding empty set).
- Example: For $\mathcal{I} = \{a, b, c, d, e\}$, we have 31 possible candidates.
- Therefore, the candidate sets should be generated more efficiently.
- We can make use of the **anti-monotonicity** of the support:
  If an item set is frequent, then all of its subsets must be frequent as well. Also, if an item set is infrequent, then all its supersets must be infrequent too.
- Adding a condition can never increase the support of a rule:

$$A \subseteq B \Longrightarrow \text{support}(A) \geqslant \text{support}(B) \tag{6}$$

- **An item set can only be frequent, if all its subsets are frequent and all supersets of an infrequent item set are also infrequent.**



(a) item set lattice (b) frequent item set (c) infrequent item set

Figure 3: Item set lattice for $\mathcal{I} = \{a, b, c, d, e\}$

1. $k \leftarrow 1$
2. $C_1 \leftarrow \mathcal{I}$
3. **while** $C_k \neq \emptyset$ **do**
   - ▷ $S_k \leftarrow C_k \setminus \{$all infrequent item sets in $C_k\}$
   - ▷ $C_{k+1} \leftarrow$ all sets with $k+1$ elements which can be formed by uniting two item sets in S_k
   - ▷ $C_{k+1} \leftarrow C_{k+1} \setminus \{$item sets, where not all subsets of size k are in $S_k\}$
   - ▷ $S \leftarrow S \cup S_k$
   - ▷ $k \leftarrow k+1$
4. **return** S

The algorithm leaves it open how the candidate set C_{k+1} is generated. How can this be done efficiently?

- Requirements for efficient candidate generation:
  - We have to avoid producing too many candidates.
  - At the same time we have to ensure that all frequent item sets are found (**completeness**)
  - We don't want to produce duplicates (**efficiency**)
- The Apriori algorithm uses the following method:
  - Merge a pair of k-item sets only if their first $k-1$ items are identical.

$$A = \{a_1, a_2, \ldots, a_k\} \qquad\qquad B = \{b_1, b_2, \ldots, b_k\} \tag{7}$$

  - Merge A and B, if $a_j = b_j \ (j = 1, 2, \ldots, k-1) \wedge a_k \neq b_k$
  - Example:
    - ▷ $A = \{bread, milk, pizza\}$, $B = \{bread, milk, wine\}$
    - ▷ A and B are merged into $\{bread, milk, pizza, wine\}$.
  - This method still requires pruning non-frequent item sets.
  - **Important: The item sets have to be in lexicographic order.**

Let's calculate the frequent item sets from the introductory example ($s_{min} = 0.25$):

Id	*beer*	*chips*	*pizza*	*wine*
1	1	1	0	1
2	1	1	0	0
3	0	0	1	1
4	0	1	1	0

$$C_1 = \{\{beer\}, \{chips\}, \{pizza\}, \{wine\}\}$$
$$S_1 = \{\{beer\}, \{chips\}, \{pizza\}, \{wine\}\}$$
$$C_2 = \{\{beer, chips\}, \{beer, pizza\}, \{beer, wine\}, \{chips, pizza\}, \{chips, wine\}, \{pizza, wine\}\}$$
$$S_2 = \{\{beer, chips\}, \{beer, wine\}, \{chips, pizza\}, \{chips, wine\}, \{pizza, wine\}\}$$
$$C_3 = \{\{beer, chips, wine\}, \{chips, pizza, wine\}\}$$
$$S_3 = \{\{beer, chips, wine\}\}$$
$$C_4 = \emptyset$$
$$S = \bigcup_{k=1}^{3} S_k$$

- The search space for frequent item sets can be structured using the subset relationship.
- **Border:**
  - The border ⇒ fig. 4 consists of all item sets for which...
    - ▷ ...all subsets are frequent and...
    - ▷ ...no superset is frequent.
  - **Positive border:** Elements of the border which are frequent.
  - **Negative border:** Elements of the border which are infrequent.

Frequent item sets = positive border plus all subsets of border elements

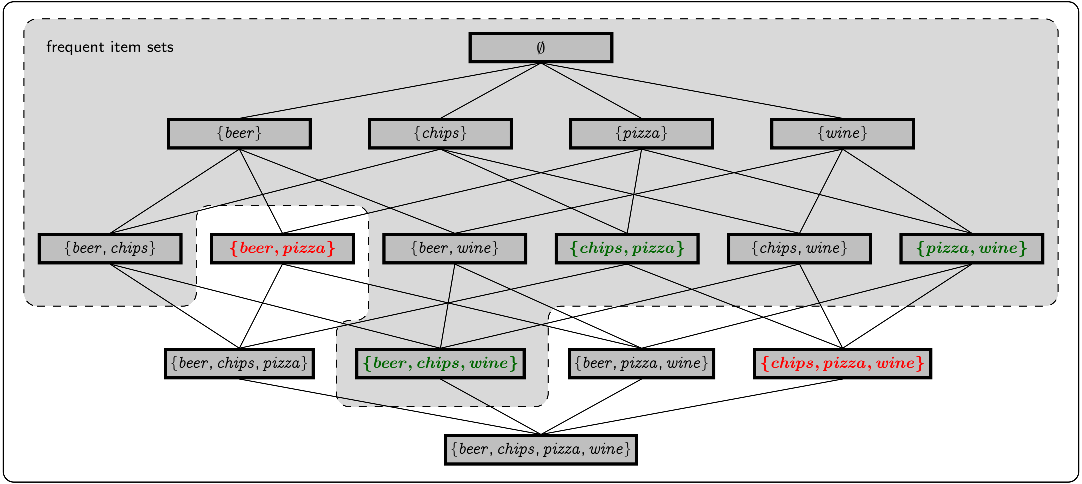


Figure 4: Border for the example above

Step 2) Generation of association rules

- The frequent item sets can now be used to generate association rules.
- For each frequent k-item set X, there are $2^k - 2$ possible association rules (without $X \to \emptyset$ and $\emptyset \to X$) of the general form ⇒ fig. 5:

$$A \to B \qquad \text{with} \qquad A \cup B = X \wedge A \cap B = \emptyset \tag{8}$$

- Calculate the confidence for the rules and check whether they fulfill the confidence constraint.
- We can also define **anti-monotonicity** for the confidence:
  If a rule is not confident, moving conditions from body to head results in rules which are also not confident.

$$\text{confidence}(A \to B \cup C) \leqslant \text{confidence}(A \cup B \to C) \tag{9}$$

- This circumstance can again be used for pruning the search space!

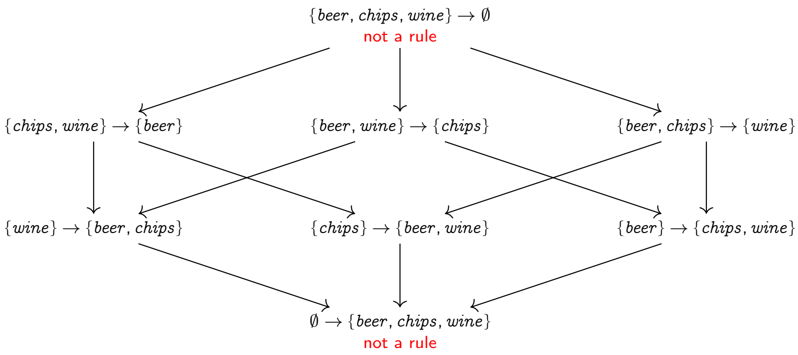


Figure 5: Search space for association rules (frequent item set $\{beer, chips, wine\}$)

Let's make a full example for the Apriori algorithm ($s_{min} = 0.5$, $c_{min} = 1.0$):

Id	*bread*	*butter*	*coffee*	*milk*	*sugar*
1	1	1	0	0	1
2	0	0	1	1	1
3	1	0	1	1	1
4	0	0	1	1	0

$$
\begin{aligned}
C_1 &= \{\{bread\}, \{butter\}, \{coffee\}, \{milk\}, \{sugar\}\} \\
S_1 &= \{\{bread\}, \{coffee\}, \{milk\}, \{sugar\}\} \\
C_2 &= \{\{bread, coffee\}, \{bread, milk\}, \{bread, sugar\}, \{coffee, milk\}, \{coffee, sugar\}, \{milk, sugar\}\} \\
S_2 &= \{\{bread, sugar\}, \{coffee, milk\}, \{coffee, sugar\}, \{milk, sugar\}\} \\
C_3 &= \{\{coffee, milk, sugar\}\} \\
S_3 &= \{\{coffee, milk, sugar\}\} \\
C_4 &= \emptyset \\
S &= \bigcup_{k=1}^{3} S_k
\end{aligned}
$$

- Rules with $c_{min} = 1.0$:

$\{bread\} \rightarrow \{sugar\}$	$s = 0.50$	$c = 1.00$
$\{milk\} \rightarrow \{coffee\}$	$s = 0.75$	$c = 1.00$
$\{coffee\} \rightarrow \{milk\}$	$s = 0.75$	$c = 1.00$
$\{milk, sugar\} \rightarrow \{coffee\}$	$s = 0.50$	$c = 1.00$
$\{sugar, coffee\} \rightarrow \{milk\}$	$s = 0.50$	$c = 1.00$

- Other rules are either not frequent enough and are filtered out in step 1;
  e. g. $\{butter\} \rightarrow \{bread, sugar\}$; $(s = 0.25, c = 1.0)$...

- ...or not confident enough and filtered out in step 2;
  e. g. $\{milk, coffee\} \rightarrow \{sugar\}$; $(s = 0.5, c = 0.67))$

Miscellaneous

Interestingness

- **Problem:** There might still be way too many rules.
- Assume the following two rules:

$$R_1 = A \cup B \to C \qquad\qquad R_2 = A \to C \tag{10}$$

- Filter out R_1, if the rule is...
  - ...*trivial* (R_2 covers the same examples)
  - ...*unproductive* (R_2 has equal or higher confidence)
  - ...*insignificant* (Confidence of R_2 is not significantly worse)
- Filter by **interestingness** (*How can we measure interestingness?*)

- Support and confidence are not sufficient to capture whether a rule is interesting or not.
- A rule may have high support and confidence, but still may not be interesting.
- Example:
  - Consider the rule: $\{diapers\} \rightarrow \{beer\}$; $c = 0.90$
  - 90 % of all customers who buy diapers also buy beer.
  - Sounds like and interesting association rule.
  - **But:** If we know, that 90 % of all customers buy beer, this rule is not interesting anymore.

Lift, Leverage and Conviction

- Consider rule $R = A \rightarrow B$
- **Lift:** Rule R is interesting, if $\text{lift}(R) \gg 1$.

$$\text{lift}(A \rightarrow B) = \frac{\text{support}(A \rightarrow B)}{\text{support}(A) \cdot \text{support}(B)} \tag{11}$$

- **Leverage:** Rule R is interesting, if $\text{leverage}(R) \gg 0$.

$$\text{leverage}(A \rightarrow B) = \text{support}(A \rightarrow B) - \text{support}(A) \cdot \text{support}(B) \tag{12}$$

- **Conviction:** Expected ratio that A occurs without B (incorrect prediction of R).

$$\text{conviction}(A \rightarrow B) = \frac{1 - \text{support}(B)}{1 - \text{confidence}(A \rightarrow B)} \tag{13}$$