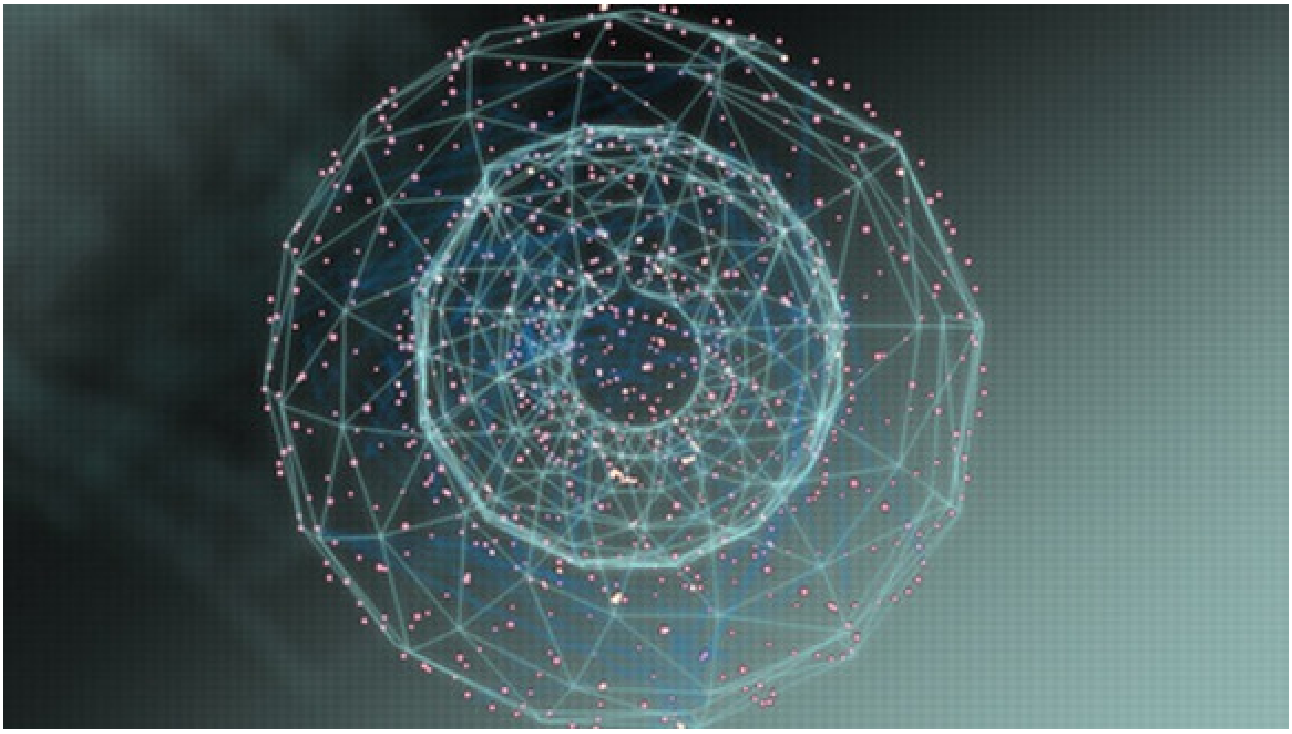
PATTERN DISCOVERY
IN
DATA MINING

Concepts and challenges in pattern discovery and analysis.
Pattern evaluation, mining and classification

Course author:

JIAWEI HAN



University of Illinois at Urbana-Champaign
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2015

Contents

1 Lecture 2: Pattern Discovery Basic Concepts

1.1 Frequent Itemsets (Patterns)

X = itemset

- **(absolute) support (count) of X:** Frequency or the number of occurrences of an itemset X
- **(relative) support, s:** The fraction of transactions that contains X (i.e., the probability that a transaction contains X)
- An itemset X is **frequent** if the support of X is no less than a $minsup$ threshold (denoted as σ): $sup(X) \geqslant \sigma$.

1.2 Association Rules

Association rules: $X \to Y(s, c)$:

- **Support** (s): the probability that a transaction contains $X \cup Y$:

$$\mathrm{sup}(X \to Y) = \mathrm{P}(X \cup Y)$$

- **Confidence** (c): the conditional probability that a transaction containing X also contains Y:

$$c = \mathrm{P}(Y \mid X) = \frac{sup(X \cup Y)}{sup(X)}$$

1.3 Expressing Patterns in Compressed Form

Definition. Closed patterns: *A pattern (itemset) X is closed if X is frequent, and there exists no super-pattern $Y \supset X$, with the same support as X.*

Closed pattern is a lossless compression of frequent patterns.

Definition. Max-patterns: *A pattern X is a max-pattern if X is frequent and there exists no frequent super-pattern $Y \supset X$.*

Max-pattern is a lossy compression!

1.4 Recommended readings

- R. Agrawal, T. Imielinski, and A. Swami, «Mining association rules between sets of items in large databases», in Proc. of SIGMOD'93
- R. J. Bayardo, «Efficiently mining long patterns from databases», in Proc. of SIGMOD'98
- N. Pasquier, Y. Bastide, R. Taouil, and L. Lakhal, «Discovering frequent closed itemsets for association rules», in Proc. of ICDT'99
- J. Han, H. Cheng, D. Xin, and X. Yan, «Frequent Pattern Mining: Current Status and Future Directions», Data Mining and Knowledge Discovery, 15(1): 55-86, 2007

2 Lecture 3. Efficient Pattern Mining Methods

2.1 The Downward Closure Property of Frequent Patterns

The downward closure (also called «Apriori») property of frequent patterns: **Any subset of a frequent itemset must be frequent**. Apriori pruning principle: **If there is any itemset which is infrequent, its superset should not even be generated!**

Scalable mining Methods: Three major approaches

- Level-wise, join-based approach: Apriori (2.2)
- Vertical data format approach: Eclat (2.4)
- Frequent pattern projection and growth: FPgrowth (2.5)

2.2 The Apriori Algorithm

2.2.1 Algorithm pseudocode

C_k: Candidate itemset of size k
F_k : Frequent itemset of size k
TDB = transactional database

Algorithm 1 The Apriori Algorithm

```
k := 1
F_k := frequent items                                   # frequent 1-itemset
while F_k ≠ ∅ do
    C_{k+1} := candidates generated from F_k            # candidate generation
    Derives F_{k+1} by counting candidates in C_{k+1} with respect to TDB at minsup
    k := k + 1
end while
return ∪_k F_k                                  # return F_k generated at each level
```

2.2.2 How to generate candidates?

- Step1: self-joining F_k
- Step2: pruning

Algorithm 2 Step1: self-joining F_k

```
insert into C_k
select p.item_1, p.item_2, ..., p.item_{k-1}, q.item_{k-1}
from F_{k-1} as p, F_{k-1} as q
where p.item_1= q.item_1, ..., p.item_{k-2} = q.item_{k-2}, p.item_{k-1} < q.item_{k-1}
```

Algorithm 3 Step2: pruning

```
for all itemsets c in C_k do
   for all (k-1) subsets s of c do
      if s is not in F_k-1 then
         delete c from C_k
      end if
   end for
end for
```

2.3 Extensions or Improvements of Apriori

- Reduce passes of transaction database scans
  - Partitioning
  - Dynamic itemset counting
- Shrink the number of candidates
  - Hashing
  - Pruning by support lower bounding
  - Sampling
- Exploring special data structures
  - Tree projection
  - H-miner
  - Hypecube decomposition

2.3.1 Partitioning

Theorem. *Any itemset that is potentially frequent in TDB must be frequent in at least one of the partitions of TDB*

Method: Scan Database Only Twice:

- Scan 1: Partition database (how?) and find local frequent patterns
- Scan 2: Consolidate global frequent patterns (how to?)

2.3.2 Direct Hashing and Pruning (DHP)

Observation: *A k-itemset whose corresponding hashing bucket count is below the threshold cannot be frequent*

2.4 Vertical Data Format

ECLAT - Equivalence Class Transformation
Frequent patterns are derived based on vertical intersections. To accelerate data mining you can use **diffset**: only keep track of differences of tids.

2.5 A Pattern Growth Approach

FP-tree - frequent pattern tree

TID	Items in the Transaction	Ordered, frequent items
100	$\{f, a, c, d, g, i, m, p\}$	$\{f, c, a, m, p\}$
200	$\{a, b, c, f, l, m, o\}$	$\{f, c, a, b, m\}$
300	$\{b, f, h, j, o, w\}$	$\{f, b\}$
400	$\{b, c, k, s, p\}$	$\{c, b, p\}$
500	$\{a, f, c, e, l, p, m, n\}$	$\{f, c, a, m, p\}$

Figure 1: Transational DB

Header Table

Item	Frequency	header
f	4	
c	4	
a	3	
b	3	
m	3	
p	3	

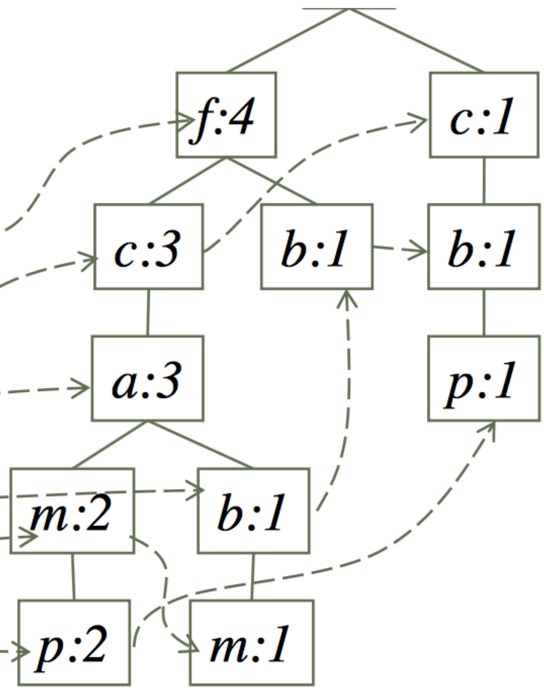


Figure 2: FP-tree

2.6 CLOSET+: Mining Closed Itemsets by Pattern-Growth

Itemset merging: *If Y appears in every occurrence of X, then Y is merged with X*

2.7 Recommended readings

- R. Agrawal and R. Srikant, «Fast algorithms for mining association rules», VLDB'94
- A. Savasere, E. Omiecinski, and S. Navathe, «An efficient algorithm for mining association rules in large databases», VLDB'95
- J. S. Park, M. S. Chen, and P. S. Yu, «An effective hash-based algorithm for mining association rules», SIGMOD'95

- S. Sarawagi, S. Thomas, and R. Agrawal, «Integrating association rule mining with relational database systems: Alternatives and implications», SIGMOD'98
- M. J. Zaki, S. Parthasarathy, M. Ogihara, and W. Li, «Parallel algorithm for discovery of association rules», Data Mining and Knowledge Discovery, 1997
- J. Han, J. Pei, and Y. Yin, «Mining frequent patterns without candidate generation», SIGMOD'00
- M. J. ZakiandHsiao, «CHARM: An Efficient Algorithm for Closed Itemset Mining», SDM'02
- J. Wang, J. Han, and J. Pei, «CLOSET+: Searching for the Best Strategies for Mining Frequent Closed Itemsets», KDD'03
- C. C. Aggarwal, M.A., Bhuiyan, M. A. Hasan, «Frequent Pattern Mining Algorithms: A Survey», in Aggarwal and Han (eds.): Frequent Pattern Mining, Springer, 2014

3 Lecture 4: Pattern Evaluation

3.1 Interestingness Measures: Lift and χ^2

3.1.1 Interestingness Measure: Lift

Lift - measure of dependent/correlated events:

$$\text{lift}(B, C) = \frac{c(B \to C)}{s(C)} = \frac{s(B \cup C)}{s(B) \times s(C)}$$

Lift(B, C) may tell how B and C are correlated:

- $\text{Lift}(B, C) = 1$: B and C are independent
- $\text{Lift}(B, C) > 1$: positively correlated
- $\text{Lift}(B, C) < 1$: negatively correlated

3.1.2 Interestingness Measure: χ^2

$$\chi^2 = \sum \frac{(Observed - Expected)^2}{Expected}$$

General rules:

- $\chi^2 = 0$: independent
- $\chi^2 > 0$: correlated, either positive or negative, so it needs additional test

Too many null transactions may lead to invalid correlation result!

3.2 Null Invariance Measures

$$\text{AllConf}(A, B) = \frac{s(A \cup B)}{\max\{s(A), s(B)\}}$$
$$\text{Jaccard}(A, B) = \frac{s(A \cup B)}{s(A) + s(B) - s(A \cup B)}$$
$$\text{Cosine}(A, B) = \frac{s(A \cup B)}{\sqrt{s(A) \times s(B)}}$$
$$\text{Kulczynsky}(A, B) = \frac{1}{2}\left(\frac{s(A \cup B)}{s(A)} + \frac{s(A \cup B)}{s(B)}\right)$$
$$\text{MacConf}(A, B) = \max\left\{\frac{s(A)}{s(A \cup B)}, \frac{s(B)}{s(A \cup B)}\right\}$$

3.3 Imbalance Ratio

IR (Imbalance Ratio): measure the imbalance of two itemsets A and B in rule implications:

$$\text{IR}(A, B) = \frac{|s(A) - s(B)|}{s(A) + s(B) - s(A \cup B)}$$

Kulczynski and Imbalance Ratio (IR) together present a clear picture

3.4 Recommended Readings

- C. C. Aggarwal and P. S. Yu. A New Framework for Itemset Generation. PODS'98
- S. Brin, R. Motwani, and C. Silverstein. Beyond market basket: Generalizing association rules to correlations. SIGMOD'97
- M. Klemettinen, H. Mannila, P. Ronkainen, H. Toivonen, and A. I. Verkamo. Finding interesting rules from large sets of discovered association rules. CIKM'94
- E. Omiecinski. Alternative Interest Measures for Mining Associations. TKDE'03
- P.-N. Tan, V. Kumar, and J. Srivastava. Selecting the Right Interestingness Measure for Association Patterns. KDD'02
- T. Wu, Y. Chen and J. Han, Re-Examination of Interestingness Measures in Pattern Mining: A Unified Framework, Data Mining and Knowledge Discovery, 21(3):371-397, 2010

4 Lecture 4: Mining Diverse Patterns

4.1 Mining Multi-Level Associations

Items often form hierarchies. How to set min-support thresholds? **Level-reduced min-support**: items at the lower level are expected to have lower support.

Efficient mining: **shared** multi-level mining. Use the lowest min-support to pass down the set of candidates.

Redundancy[1] filtering: some rules may be redundant due to «ancestor»[2] relationships between items. A rule is **redundant** if:

- its support is close to the «expected» value, according to its «ancestor» rule
- it has a similar confidence as its «ancestor».

It is necessary to have customized min-support settings for different kinds of items: group-based «individualized» min-support.

4.2 Mining Multi-Dimensional Associations

Rules can be single-dimensional or multi-dimensional:

- Single-dimentional:

$$\text{buys}(X, \text{«milk»}) \Rightarrow \text{buys}(X, \text{«bread»})$$

- Inter-dimension association rule:

$$\text{age}(X, \text{«18-25»}) \wedge \text{occupation}(X, \text{«student»}) \Rightarrow \text{buys}(X, \text{«coke»})$$

- Hybrid-dimension association rules:

$$\text{age}(X, \text{«18-25»}) \wedge \text{buys}(X, \text{«popcorn»}) \Rightarrow \text{buys}(X, \text{«coke»})$$

Attributes can be categorical or numerical

4.3 Mining Quantitative Associations

Methods:

- Static discretization based on predefined concept hierarchies
- Dynamic discretization based on data distribution
- Clustering: distance-based association
- Deviation analysis

4.4 Mining Negative Correlations

- Rare patterns = very low support but interesting
- Negative patterns = negatively correlated, unlikely to happen together

A support-based definition: if itemsets A and B are both frequent but rarely occur together, i.e., $\text{sup}(A \cup B) << \text{sup}(A) \times \text{sup}(B)$ then A and B are negatively correlated.

The support-based definition is not null-invariant!

A Kulczynski measure-based definition: if itemsets A and B are frequent but $\frac{P(A|B)+P(B|A)}{2} < \varepsilon$, where ε is a negative pattern threshold, then A and B are negatively correlated.

[1]Redundancy - избыточность
[2]Ancestor – предок

4.5 Mining Compressed Patterns

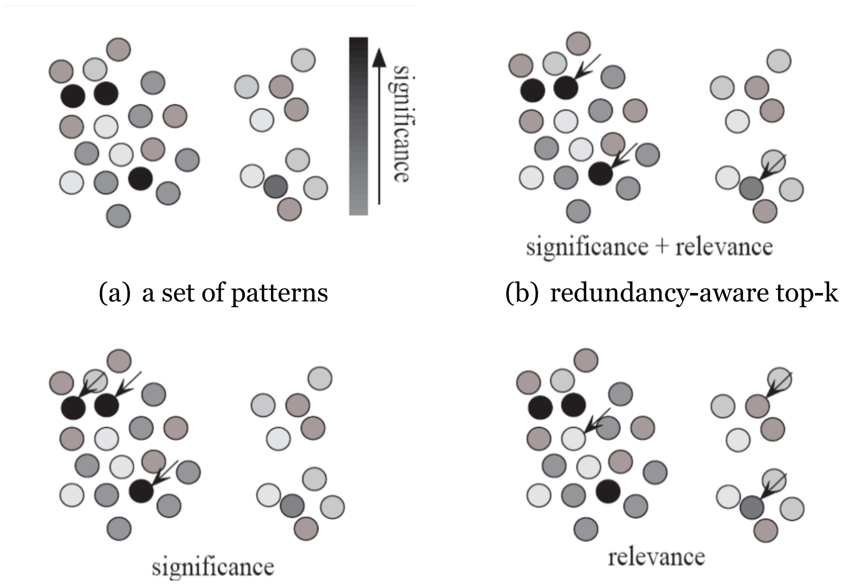
4.5.1 Mining Compressed Patterns

Pattern distance measure:

$$Dist(P_1, P_2) = 1 - \frac{|T(P_1) \cap T(P_2)|}{|T(P_1) \cup T(P_2)|}$$

δ-clustering. For each pattern P, find all patterns which can be expressed by P and whose distance to P is within δ (δ-cover). All patterns in the cluster can be represented by P = compressed patterns.[3]

4.5.2 Redundancy-Aware Top-k Patterns



(a) a set of patterns (b) redundancy-aware top-k

(c) traditional top-k (d) summarization

Figure 3: Desired patterns: high significance & low redundancy

Use **MMS (Maximal Marginal Significance)** for measuring the combined significance of a pattern set.[4]

4.6 Mining Colossal Patterns

4.6.1 Pattern-Fusion

Pattern fusion strategy: fuse small patterns together in one step to generate new pattern candidates of significant sizes.

Subpatterns α_1 to α_k cluster tightly around the colossal pattern α by sharing a similar support. Such subpatterns are **core patterns** of α. A colossal pattern can be generated by merging a set of core patterns.

[3]Method for efficient, direct mining of compressed frequent patterns: Xin et al., VLDB'05.
[4]Xin et al., Extracting Redundancy-Aware Top-K Patterns, KDD'06.

4.6.2 Robustness of Colossal Patterns

Definition. For a frequent pattern α, a subpattern β is a **τ-core pattern** of α if β shares a similar support set with α, i.e.,

$$\frac{|D_\alpha|}{|D_\beta|} \geqslant \tau, 0 < \tau \leqslant 1,$$

where τ is called the **core ratio**.

Definition. $(\mathrm{d}, \boldsymbol{\tau})$**-robustness**[5]: a pattern α is (d, τ)-robust if d is the maximum number of items that can be removed from α for the resulting pattern to remain a τ-core pattern of α:

$$d = \max_{\beta}\{|\alpha| - |\beta| \mid \beta \subseteq \alpha, \text{ and } \beta \text{ is a } \tau\text{-core pattern of } \alpha\}$$

For a pattern α let C_α be the set of all its core patterns for a specified τ:

$$C_\alpha = \{\beta \mid \beta \subseteq \alpha, \frac{|D_\alpha|}{|D_\beta|} \geqslant \tau\}$$

Theorem. *For a (d, τ)-robust pattern α:*

$$|C_\alpha| \geqslant 2^d$$

Robustness of Colossal Patterns: a colossal pattern tends to have much more core patterns than small patterns. Such core patterns can be clustered together to form «dense balls» based on pattern distance defined by

$$Dist(\alpha, \beta) = 1 - \frac{|D_\alpha \cap D_\beta|}{|D_\alpha \cup D_\beta|}$$

Theorem. *For two patterns $\beta_1, \beta_2 \in C_\alpha$*

$$Dist(\beta_1, \beta_2) \leqslant r(\tau), \textit{ where } r(\tau) = 1 - \frac{1}{2/\tau - 1}$$

4.6.3 The Pattern-Fusion Algorithm

- Initialization (Creating initial pool): Use an existing algorithm to mine all frequent patterns up to a small size, e.g., 3
- Iteration (Iterative Pattern Fusion):
  - At each iteration, K seed patterns are randomly picked from the current pattern pool
  - For each seed pattern thus picked, we find all the patterns within a bounding ball centered at the seed pattern
  - All these patterns found are fused together to generate a set of super-patterns
  - All the super-patterns thus generated form a new pool for the next iteration
- Termination: when the current pool contains no more than K patterns at the beginning of an iteration

[5]Robustness - прочность

4.7 Recommended Readings

- R. Srikant and R. Agrawal, «Mining generalized association rules», VLDB'95
- Y. Aumann and Y. Lindell, «A Statistical Theory for Quantitative Association Rules», KDD'99
- D. Xin, J. Han, X. Yan and H. Cheng, «On Compressing Frequent Patterns», Knowledge and Data Engineering, 60(1): 5-29, 2007
- D. Xin, H. Cheng, X. Yan, and J. Han, «Extracting Redundancy-Aware Top-K Patterns», KDD'06
- F. Zhu, X. Yan, J. Han, P. S. Yu, and H. Cheng, «Mining Colossal Frequent Patterns by Core Pattern Fusion», ICDE'07
- J. Han, H. Cheng, D. Xin, and X. Yan, «Frequent Pattern Mining: Current Status and Future Directions», Data Mining and Knowledge Discovery, 15(1): 55-86, 2007

5 Constraint-Based Pattern Mining

5.1 Meta-Rule Guided Mining

In general, (meta) rules can be in the form of

$$P_1 \wedge P_2 \wedge ... \wedge P_l \Rightarrow Q_1 \wedge Q_2 \wedge ... \wedge Q_r$$

Method to find meta-rules:

- Find frequent (l + r) predicates (based on min-support)
- Push constraints deeply when possible into the mining process
- Also, push min_conf, min_correlation, and other measures as early as possible (measures acting as constraints)

5.2 Kinds of Constraints

- Pattern space pruning constraints
  - Anti-monotonic: If constraint c is violated, its further mining can be terminated
  - Monotonic: If c is satisfied, no need to check c again
  - Succinct[6]: if the constraint c can be enforced by directly manipulating the data
  - Convertible: c can be converted to monotonic or anti-monotonic if items can be properly ordered in processing
- Data space pruning constraints
  - Data succinct: Data space can be pruned at the initial pattern mining process
  - Data anti-monotonic: If a transaction t does not satisfy c, then t can be pruned to reduce data processing effort

Anti-monotonic constraints have more pruning power than monotonic constraints.

[6]Succinct - краткий

5.2.1 Pattern space pruning constraints

Constraint c is **anti-monotone**: if an itemset S violates constraint **c**, so does any of its superset. That is, mining on itemset S can be terminated. For example, constraint $\sup(S) \geqslant \sigma$ is anti-monotone.

A constraint c is **monotone**: if an itemset S satisfies the constraint **c**, so does any of its superset. That is, we do not need to check **c** in subsequent mining. For example, constraints $\text{sum}(S.price) \geqslant v$ or $\min(S.price) \leqslant v$ are monotone.

5.2.2 Data space pruning constraints

A constraint **c** is **data anti-monotone**: if a data entry **t** cannot satisfy a pattern **p** under constraint **c**, **t** cannot satisfy **p**'s superset either. That's why, data entry **t** can be pruned.

Succinctness: if the constraint **c** can be enforced by directly manipulating the data.

Convertible constraints: convert tough[7] constraints into (anti-)monotone by proper ordering of items in transactions. For example, ordering items in value-descending order makes the constraint $\text{avg}(S.profit) > 20$ anti-monotone *if the patterns grow in the right order*.

5.3 Recommended Readings

- R. Srikant, Q. Vu, and R. Agrawal, «Mining association rules with item constraints», KDD'97
- R. Ng, L.V.S. Lakshmanan, J. Han & A. Pang, Exploratory mining and pruning optimizations of constrained association rules», SIGMOD'98
- G. Grahne, L. Lakshmanan, and X. Wang, «Efficient mining of constrained correlated sets», ICDE'00
- J. Pei, J. Han, and L. V. S. Lakshmanan, «Mining Frequent Itemsets with Convertible Constraints», ICDE'01
- J. Pei, J. Han, and W. Wang, «Mining Sequential Patterns with Constraints in Large Databases», CIKM'02
- F. Bonchi, F. Giannotti, A. Mazzanti, and D. Pedreschi, «ExAnte: Anticipated Data Reduction in Constrained Pattern Mining», PKDD'03
- F. Zhu, X. Yan, J. Han, and P. S. Yu, «gPrune: A Constraint Pushing Framework for Graph Pattern Mining», PAKDD'07

6 Sequential Pattern Mining

6.1 Sequential Pattern

Sequence $\rightarrow$ Element $\rightarrow$ Item or Event (items within an element are unordered)

[7] Tough - жесткий

The Apriori property still holds: if a subsequence s_1 is infrequent, none of s_1's super-sequences can be frequent.

Algorithms:

- Generalized Sequential Patterns: **GSP**
- Vertical format-based mining: **SPADE**
- Pattern-growth methods: **PrefixSpan**
- Mining closed sequential patterns: **CloSpan**

6.2 GSP: Apriori-Based Sequential Pattern Mining

Algorithm 4 GSP

```
k = 1
repeat
    find length=k frequent sequences
    Apriori: remove candidates with sup < min_sup
    length=k frequent sequences ⇒ length=(k+1) candidate sequences
    k = k + 1
until no frequent sequences or candidates
```

6.3 SPADE: Sequential Pattern Mining in Vertical Data Format

SPADE = **S**equential **P**attern **D**iscovery using **E**quivalent Class

SID	Sequence
1	<a(abc)(ac)d(cf)>
2	<(ad)c(bc)(ae)>
3	<(ef)(ab)(df)cb>
4	<eg(af)cbc>

min_sup = 2

Figure 4: A sequence database

SID	EID	Items
1	1	a
1	2	abc
1	3	ac
1	4	d
1	5	cf
2	1	ad
2	2	c
2	3	bc
2	4	ae
3	1	ef
3	2	ab
3	3	df
3	4	c
3	5	b
4	1	e
4	2	g
4	3	af
4	4	c
4	5	b
4	6	c

a		b		...
SID	EID	SID	EID	...
1	1	1	2	
1	2	2	3	
1	3	3	2	
2	1	3	5	
2	4	4	5	
3	2			
4	3			

ab			ba		
SID	EID (a)	EID(b)	SID	EID (b)	EID(a)
1	1	2	1	2	3
2	1	3	2	3	4
3	2	5			
4	3	5			

aba				...
SID	EID (a)	EID(b)	EID(a)	...
1	1	2	3	
2	1	3	4	

Figure 5: SPADE algorithm

6.4 PrefixSpan: A Pattern-Growth Approach

PrefixSpan = Prefix-projected Sequential pattern mining

SID	Sequence
10	<a(abc)(ac)d(cf)>
20	<(ad)c(bc)(ae)>
30	<(ef)(ab)(df)cb>
40	<eg(af)cbc>

Prefix	Suffix (Projection)
<a>	<(abc)(ac)d(cf)>
<aa>	<(_bc)(ac)d(cf)>
<ab>	<(_c)(ac)d(cf)>

Figure 6: SPADE algorithm

PrefixSpan Mining: Prefix Projections

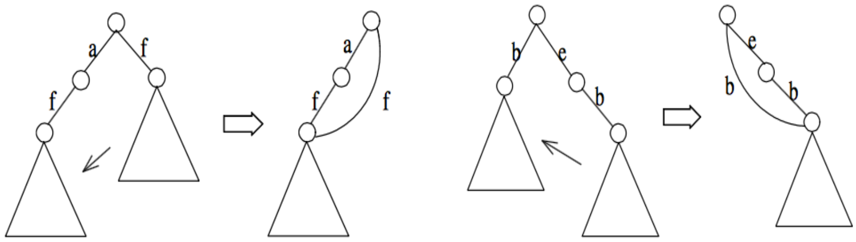
- Step 1: Find length-1 sequential patterns: <a>, <b>, etc.
- Step 2: Divide search space and mine each projected DB: <a>-projected DB, <b>-projected DB, etc.

6.5 CloSpan: Mining Closed Sequential Patterns

Definition. A closed sequential pattern α: there exists no superpattern β such that β and α have the same support:

$$CS = \{\alpha \mid \alpha \in FS \text{ and } \nexists \beta \in FS, \text{ such that } \alpha \subseteq \beta \text{ and } sup(\alpha) = sup(\beta)\}$$

CloSpan is based on this property: if $s \supset s_1$ then s is closed only if two project DBs have the same size. So redundant search space can be pruned using **Backward Subpattern** and **Backward Superpattern** pruning.



(a) backward sub-pattern (b) backward super-pattern

Figure 7: CloSpan pruning algorithm

6.6 Constraint-Based Sequential-Pattern Mining

- **Anti-monotonic**: If S violates c, the super-sequences of S also violate c
- **Monotonic**: If S satisfies c, the super-sequences of S also do so
- **Data anti-monotonic**: If a sequence s1 with respect to S violates c3, s1 can be removed
- **Succinct**: Enforce constraint c by explicitly manipulating data
- **Convertible**: Projection based on the sorted value not in sequence order

6.6.1 Timing-Based Constraints

- **Order constraint**: Some items must happen before the other. Anti-monotonic: constraint-violating sub-patterns pruned
- **Min-gap/max-gap constraint**: Confines two elements in a pattern. Succinct: enforced directly during pattern growth
- **Max-span constraint**: Maximum allowed time difference between the 1st and the last elements in the pattern. Succinct: enforced directly when the 1st element is determined
- **Window size constraint**: Time window allows a group of consecutive elements of a data-sequence to be merged and treated as a single element as long as their timestamps are within the user-specified window-size.

6.7 Recommended Readings

- M. N. Garofalakis, R. Rastogi, K. Shim: Mining Sequential Patterns with Regular Expression Constraints. IEEE Trans. Knowl. Data Eng. 14(3), 2002

- H. Mannila, H. Toivonen, and A. I. Verkamo, "Discovery of frequent episodes in event sequences", Data Mining and Knowledge Discovery, 1997
- J. Pei, J. Han, B. Mortazavi-Asl, J. Wang, H. Pinto, Q. Chen, U. Dayal, and M.-C. Hsu, "Mining Sequential Patterns by Pattern-Growth: The PrefixSpan Approach", IEEE TKDE, 16(10), 2004
- J. Pei, J. Han, and W. Wang, "Constraint-based sequential pattern mining: the pattern-growth methods", J. Int. Inf. Sys., 28(2), 2007
- R. Srikant and R. Agrawal, "Mining sequential patterns: Generalizations and performance improvements", EDBT'96
- X. Yan, J. Han, and R. Afshar, "CloSpan: Mining Closed Sequential Patterns in Large Datasets", SDM'03
- M. Zaki, "SPADE: An Efficient Algorithm for Mining Frequent Sequences", Machine Learning, 2001

7 Lecture 8. Graph Pattern Mining

7.1 Frequent (Sub)Graph Patterns

Given a labeled graph dataset $D = \{G_1, G_2, ..., G_n\}$, the supporting graph set of a subgraph g is $D_g = \{G_i \mid g \subseteq G_i, G_i \in D\}$:

$$support(g) = |D_g| / |D|$$

A (sub)graph g is frequent if $support(g) \geqslant min\_sup$.

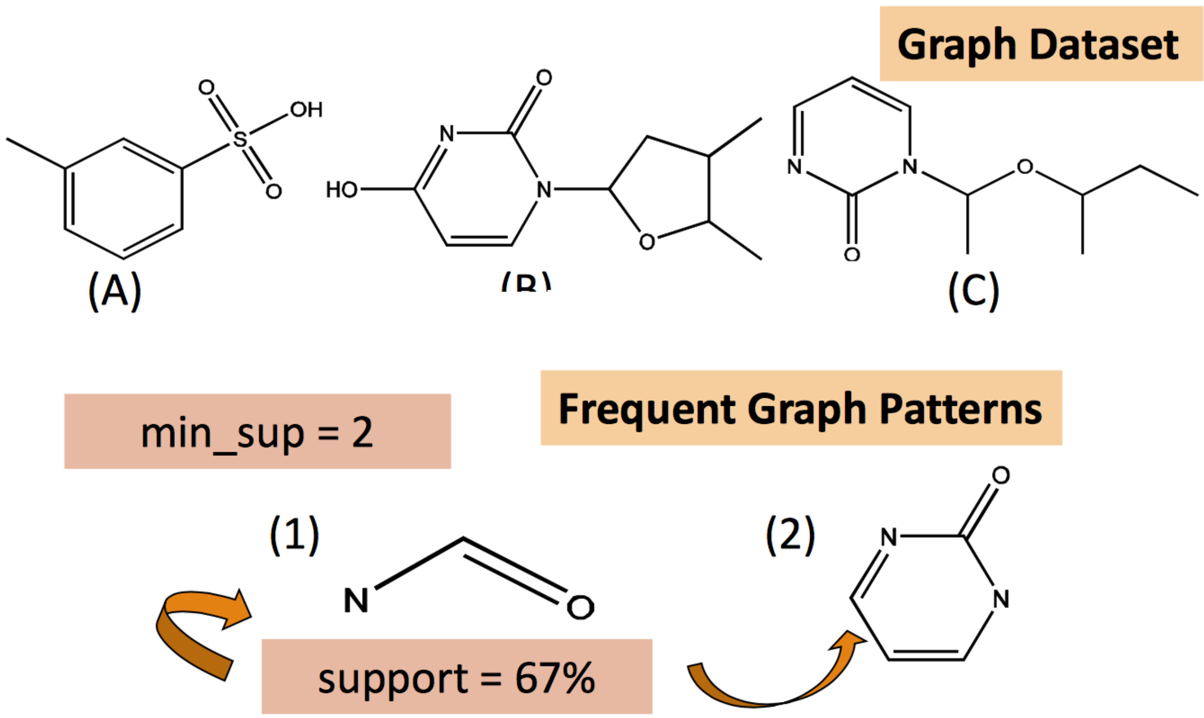


Figure 8: Example: Chemical structures

7.2 Apriori-Based Approach

The Apriori property (anti-monotonicity): a size-k subgraph is frequent if and only if all of its subgraphs are frequent.

Candidate generation: a candidate size-(k+1) edge/vertex subgraph is generated if its corresponding two k-edge/vertex subgraphs are frequent:

- AGM - Generating new graphs with one more vertex
- FSG - Generating new graphs with one more edge (more efficient)

Iterative mining process: Candidate-generation $\rightarrow$ candidate pruning $\rightarrow$ support counting $\rightarrow$ candidate elimination.

7.3 gSPAN: Graph Pattern Growth

Depth-first growth of subgraphs from k-edge to (k+1)-edge, then (k+2)-edge subgraphs generates many duplicate subgraphs.

Right-most path extension in subgraph pattern growth reduces generation of duplicate subgraphs: *take the path from root to the right-most leaf (choose the vertex with the smallest index at each step)*. The Enumeration of graphs using right-most path extension is complete.

DFS Code: flatten a graph into a sequence using depth-first search

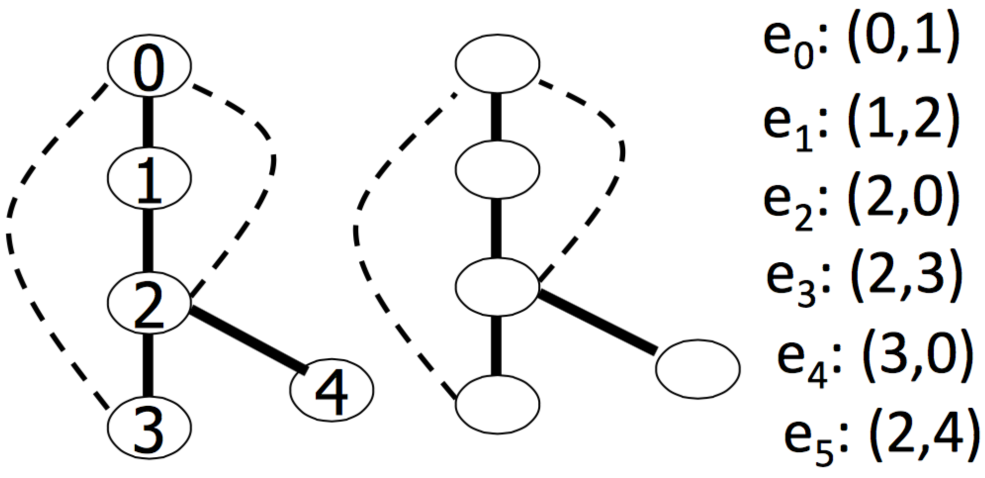


Figure 9: gSPAN

7.4 Mining Closed Graph Patterns

A frequent graph G is closed if there exists no supergraph of G that carries the same support as G.

CloseGraph algorithm: mining closed graph patterns by extending gSpan. Suppose G and G_1 are frequent, and G is a subgraph of G_1. If in any part of the graph in the dataset where G occurs, G_1 also occurs, then we need not grow G (except some special, subtle cases), since *none of G's children will be closed except those of G_1*.

7.5 gIndex: A Graph Indexing Method

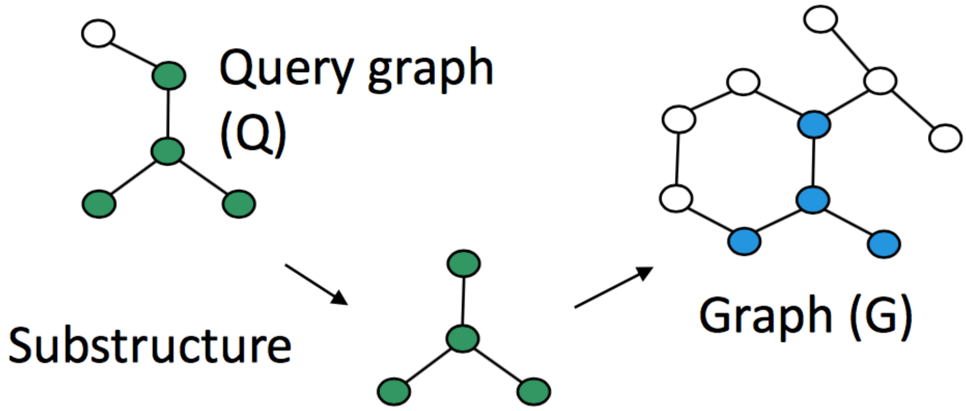


Figure 10: Graph query

- use frequent substructures for indexing
- discriminative substructures: reduce index size by removing similar (not discriminative) substructures from the index

Definition. Fragment x is **discriminative** with respect to feature set F if $D_x \ll \bigcap_{f \in F \wedge f \subseteq x} D_f$, where D_x is the set of graphs containing x.

Selection: Given a set of indexing features $f_1, f_2, ..f_n$, and a new structure x (x should be either redundant or discriminative), the extra indexing power is measured by occurrence probability

$$Pr(x \mid f_1, f_2, ...f_n) = \frac{\left|\bigcap_{f \in F \wedge f \subseteq x} D_f\right|}{|D_x|}$$

When $Pr(x \mid f_1, f_2, ...f_n) \ll 1$, x is a discriminative structure and should be included in the index.

7.6 SpiderMine: Mining Top-K Large Structural Patterns in a Massive Network

SpiderMine: mine top-K largest frequent substructure patterns whose diameter is bounded by $_{Dmax}$ with a probability at least $1 - \varepsilon$. General idea: large patterns are composed of a number of small components («spiders») which will eventually connect together after some rounds of pattern growth.

An r-spider is a frequent graph pattern P such that there exists a vertex u of P, and all other vertices of P are within distance r from u.

The SpiderMine Algorithm

- Mine the set S of all the r-spiders
- Randomly draw M r-spiders

- Grow these M r-spiders for $t = D_{max}/2$ iterations, and merge two patterns whenever possible
- Discard unmerged patterns
- Continue to grow the remaining ones to maximum size
- Return the top-K largest ones in the result

SpiderMine general ideas:

- Small patterns are much less likely to be hit in the random draw
- Even if a small pattern is hit, it is even less likely to be hit multiple times
- The larger the pattern, the greater the chance it is hit and saved

7.7 Recommended Readings

- C. Borgelt and M. R. Berthold, «Mining molecular fragments: Finding relevant substructures of molecules», ICDM'02
- J. Huan, W. Wang, and J. Prins. «Efficient mining of frequent subgraph in the presence of isomorphism», ICDM'03
- A. Inokuchi, T. Washio, and H. Motoda. «An apriori-based algorithm for mining frequent substructures from graph data», PKDD'00
- M. Kuramochi and G. Karypis. «Frequent subgraph discovery», ICDM'01
- S. Nijssen and J. Kok. A quickstart in frequent structure mining can make a difference. KDD'04
- N. Vanetik, E. Gudes, and S. E. Shimony. «Computing frequent graph patterns from semistructured data», ICDM'02
- X. Yan and J. Han, «gSpan: Graph-Based Substructure Pattern Mining», ICDM'02
- X. Yan and J. Han, «CloseGraph: Mining Closed Frequent Graph Patterns», KDD'03
- X. Yan, P. S. Yu, and J. Han, «Graph Indexing: A Frequent Structure-based Approach», SIGMOD'04
- F. Zhu, Q. Qu, D. Lo, X. Yan, J. Han, and P. S. Yu, «Mining Top-K Large Structural Patterns in a Massive Network», VLDB'11

8 Lecture 9. Pattern-Based Classification

8.1 Classification: Basic Concepts

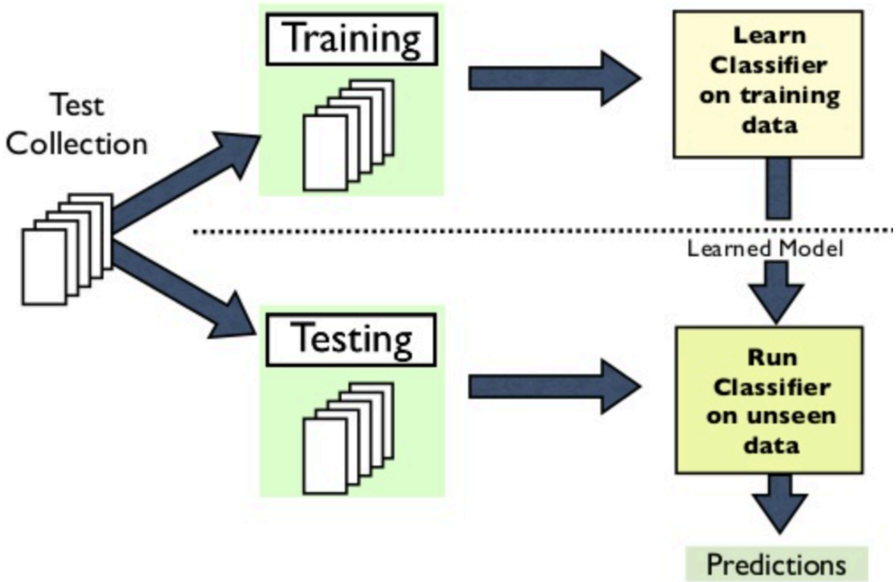


Figure 11: Classification

Typical Classification Methods:

- Support Vector Machines
- Decision Tree
- Neural Network
- Bayesian Network

8.2 Pattern-based classification methods

- CBA [Liu, Hsu & Ma, KDD'98]: Use high-conf., high-support class association rules to build classifiers
- Emerging patterns [Dong & Li, KDD'99]: Patterns whose support changes significantly between the two classes
- CMAR [Li, Han & Pei, ICDM'01]: Multiple rules in prediction
- CPAR [Yin & Han, SDM'03]: Beam search on multiple prediction rules
- RCBT [Cong et al., SIGMOD'05]: Build classifier based on mining top-k covering rule groups with row enumeration (for high-dimensional data)
- Lazy classifier [Veloso, Meira & Zaki, ICDM'06]: For a test t, project training data D on t, mine rules from D_t , predict on the best rule
- Discriminative pattern-based classification [Cheng et al., ICDE'07]

8.3 CBA: Classification Based on Associations

- Mine high-confidence, high-support class association rules
- LHS: conjunctions of attribute-value pairs); RHS: class labels
  $p_1 \wedge p_2 ... \wedge p_l \to [A_{class-label} = C]$
- Rank rules in descending order of confidence and support
- Classification: Apply the first rule that matches a test case; otherwise apply the default rule

8.4 CMAR: Classification Based on Multiple Association Rules

Rule pruning whenever a rule is inserted into the tree:

- Given two rules, R_1 and R_2, if the antecedent[8] of R_1 is more general than that of R_2 and $conf(R_1) \geqslant conf(R_2)$, then prune R_2
- Prunes rules for which the rule antecedent and class label are not positively correlated, based on the χ^2 test of statistical significance

Classification based on generated/pruned rules:

- If only one rule satisfies tuple X, assign the class label of the rule
- If a ruleset S satisfies X
  - Divide S into groups according to class labels
  - Use a weighted χ^2 measure to find the strongest group of rules, based on the statistical correlation of rules within a group
  - Assign X the class label of the strongest group

8.5 Discriminative Pattern-Based Classification

Principle: Mining discriminative frequent patterns as high-quality features and then apply any classifier.
Framework (**PatClass**):

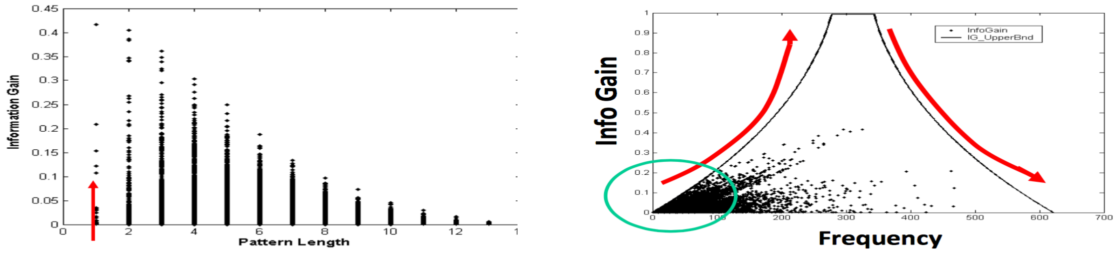
- Feature construction by **frequent itemset mining**
- Feature selection (e.g., using **Maximal Marginal Relevance (MMR)**)
  - Select **discriminative features** (i.e., that are relevant but minimally similar to the previously selected ones)
  - Remove redundant or closely correlated features
- Model learning: apply a general classifier, such as SVM or C4.5, to build a classification model

[8] Antecedent - предшественник

8.5.1 On the Power of Discriminative Patterns

K-itemsets are often more informative than single features (1-itemsets) in classification. Computation on real datasets shows: the discriminative power of k-itemsets (for $k > 1$ but often $\leqslant 10$) is higher than that of single features.

Computation on real datasets shows: pattern frequency (but not too frequent) is strongly tied with the discriminative power (information gain). Information gain upper bound monotonically increases with pattern frequency.



(a) IG vs. Pattern Length (b) IG vs. Frequency

Figure 12: Information Gain

Information gain formula:

$$IG(C \mid X) = H(C) - H(C \mid X), \text{ where}$$
$$H(C) = -\sum_{i=1}^{m} p_i \log_2(p_i) \text{ - entropy of given data}$$
$$H(C \mid X) = \sum_{j} P(X = x_j) H(Y \mid X = x_j) \text{ - conditional entropy of study focus}$$

8.6 DDPMine: Direct Mining of Discriminative Patterns

General methodology:

- Input: A set of training instances D and a set of features F
- Iteratively perform feature selection based on the **«sequential coverage»** paradigm
  - Select the feature fi with the highest discriminative power
  - Remove instances Di from D covered by the selected feature fi

Implementation:

- Integration of **branch-and-bound search** with FP-growth mining
- Iteratively eliminate training instances and **progressively shrink the FP-tree**

8.6.1 Branch-and-Bound Search

- The discriminative power (information gain) of a low frequency pattern is upper bounded by a small value
- During FPGrowth mining we record the most discriminative itemset discovered so far and its information gain value g_{best}

- Before constructing a conditional FP-tree, we first estimate the upper bound of information gain based on the conditional DB
- If the upper bound value $\leqslant g_{best}$, skip this conditional FP-tree and its subsequent trees

8.7 Recommended Readings

- H. Cheng, X. Yan, J. Han & C.-W. Hsu, Discriminative Frequent Pattern Analysis for Effective Classification, ICDE'07
- H. Cheng, X. Yan, J. Han & P. S. Yu, Direct Discriminative Pattern Mining for Effective Classification, ICDE'08
- G. Cong, K. Tan, A. Tung & X. Xu. Mining Top-k Covering Rule Groups for Gene Expression Data, SIGMOD'05
- M. Deshpande, M. Kuramochi, N. Wale & G. Karypis. Frequent Substructure-based Approaches for Classifying Chemical Compounds, TKDE'05
- G. Dong & J. Li. Efficient Mining of Emerging Patterns: Discovering Trends and Differences, KDD'99
- W. Fan, K. Zhang, H. Cheng, J. Gao, X. Yan, J. Han, P. S. Yu & O. Verscheure. Direct Mining of Discriminative and Essential Graphical and Itemset Features via Model-based Search Tree, KDD'08
- W. Li, J. Han & J. Pei. CMAR: Accurate and Efficient Classification based on Multiple Class-association Rules, ICDM'01
- B. Liu, W. Hsu & Y. Ma. Integrating Classification and Association Rule Mining, KDD'98
- J. Wang and G. Karypis. HARMONY: Efficiently Mining the Best Rules for Classification, SDM'05
- X. Yin & J. Han. CPAR: Classification Based on Predictive Association Rules, SDM'03