## Deep of Enumeration Algorithms

# Implementation and Data-Driven Speeding Up

- Motivation and situation
- Frequent itemset mining
- Maximal clique enumeration

## Enumeration is Already Efficient

• Enumeration algorithms we have seen are output polynomial time, linear in output size in particular

• On the other hand, enumeration algorithms output exponentially many solutions, so we might think that the problem sizes are usually small (up to 100)

...so, "input size is constant" would be valid and thus enumeration algorithms are optimal. ("less than 100" is constant) this would be true in "theoretical sense"

• ...however, there exist other kinds of applications

# **Big Data Applications**

• In practice, enumeration is widely used in data mining / data engineering area

frequent pattern mining, candidate enumeration, community mining, feasible solution enumeration...

- In such areas, input data is often big data
- Indeed, #solutions is small, often O(n) to O(n2) thus, actually "tractable large-scale problems"

## Why #Solutions is Small?

- ...#solutions seem to easily increase to exponential, however...
  - + if exponentially many solutions, many solutions are similar, thus quite redundant
  - + We don't want to have such many solutions! they are intractable (too long time for post process)
  - + Even though #solutions is huge, the modeling was bad, from the beginning

**Ex)** #Maximal cliques in the large sparse graphs are not huge, but #independent sets (no vertex pair is connected) are extremely huge

## **Constant Time Enumeration**

- ...so, enumeration should take short time per solution in particular, constant time for each
- However, handling big data in constant in an iteration is hard we need techniques to compute without looking the whole data
- + data structure for dynamic computation, data compression to unify the operation, ancestor-processing for reducing descendants...
- Further, engineering techniques help the improvements
  - + memory saving
  - + make the computation fitting to the architecture

See the techniques in itemset mining and clique enumeration

# **3-1** Frequent Itemset (LCM)

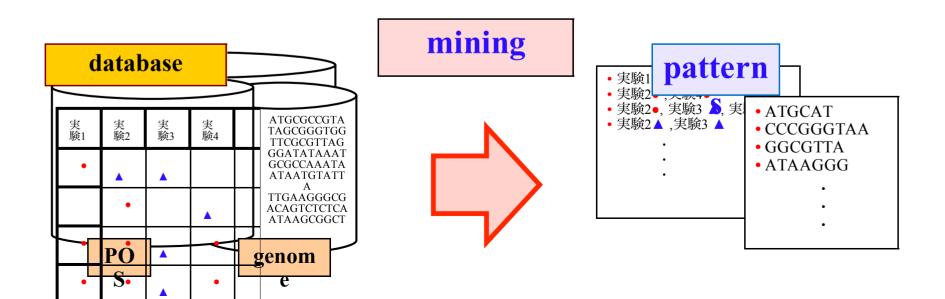
## Frequent Pattern Mining

• Problem of enumerating all frequently appearing patterns in big data

(pattern = itemsets, item sequence, short string, subgraphs,...)

- Nowadays, one of the fundamental problems in data mining
- Many applications, many algorithms, many researches

High Speed Algorithms are important

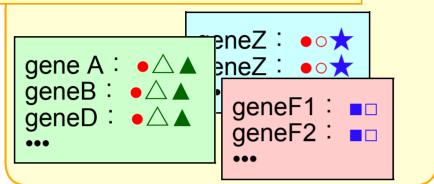


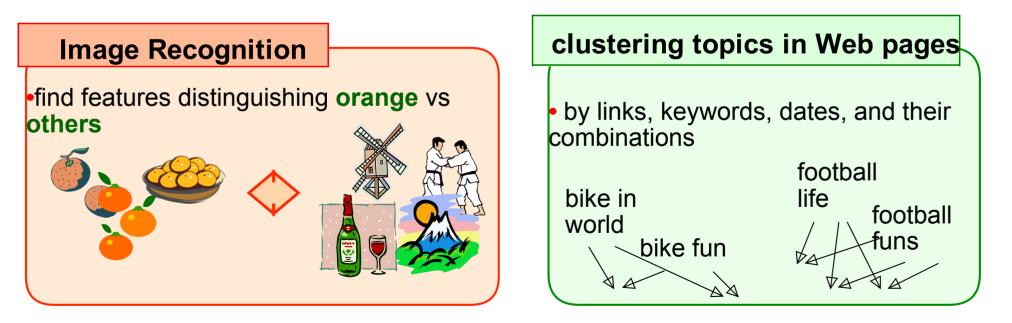
# **Applications of Pattern Mining**

#### **Market Data**

Books & coffee are frequently sold together
Male coming at Night tends to purchase foods with bit higher prices...

#### automatic classification



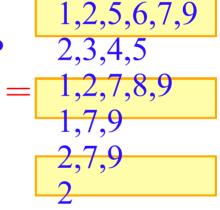


### Fundamental, thus applicable to vatious areas

### **Transaction Database**

• A database D such that each transaction (record) T is a subset of itemset E, i.e.,  $\forall T \in D, T \subseteq E$ 

For itemset P, occurrence of P: a transaction of D including P occurrence set of P (Occ(P)): set of occurrences of P frequency of P (frq(P)): cardinality of Occ(P) D =



$$= \begin{array}{c} \mathbf{Occ}(\{1,2\}) \\ \{ \{1,2,5,6,7,9\}, \\ \{1,2,7,8,9\} \} \end{array}$$

 $Occ(\{2,7,9\}) = \{\{1,2,5,6,7,9\}, \\ \{1,2,7,8,9\}, \\ \{2,7,9\}\}\}$ 

## Frequent Itemset

frequent itemset: an itemset included in at least σ transactions of D
 (a set whose frequency is at least σ) (σ is given, and called
 minimum support)

**Ex**) itemsets included in at least 3 transactions in **D** 

$$D = \begin{array}{c} 1,2,5,6,7,9\\ 2,3,4,5\\ 1,2,7,8,9\\ 1,7,9\\ 2,7,9\\ 2 \end{array}$$

included in at least 3 {1} {2} {7} {9} {1,7} {1,9} {2,7} {2,9} {7,9} {1,7,9} {2,7,9}

Frequent itemset mining is to enumerate all frequent itemsets of the given database and minimum support σ

# Backtracking Algorithm

• Set of frequent itemsets is monotone (any subset of a frequent itemset is also frequent) backtrack algorithm is applicable

**Backtrack** (**P**) O(|D|)**1.** output **P 2.** for each e > tail of P (m ximum item in P)if  $P \cup e$  is frequent then call Backtrack ( $P \cup e$ ) + #recursive calls = #frequent itemsets 1,3,4 2,3,4 + a recursive call (iteration) takes time (**n**- (tail of **P**))×(time for frequency counting) 2,3 2,4 3,4 .3 1,4 **O(n|D|)** per solution is too long

## Shorten "Time for One Solution"

- Time per solution is polynomial, but too long
- Each **PUe** needs to compute its frequency

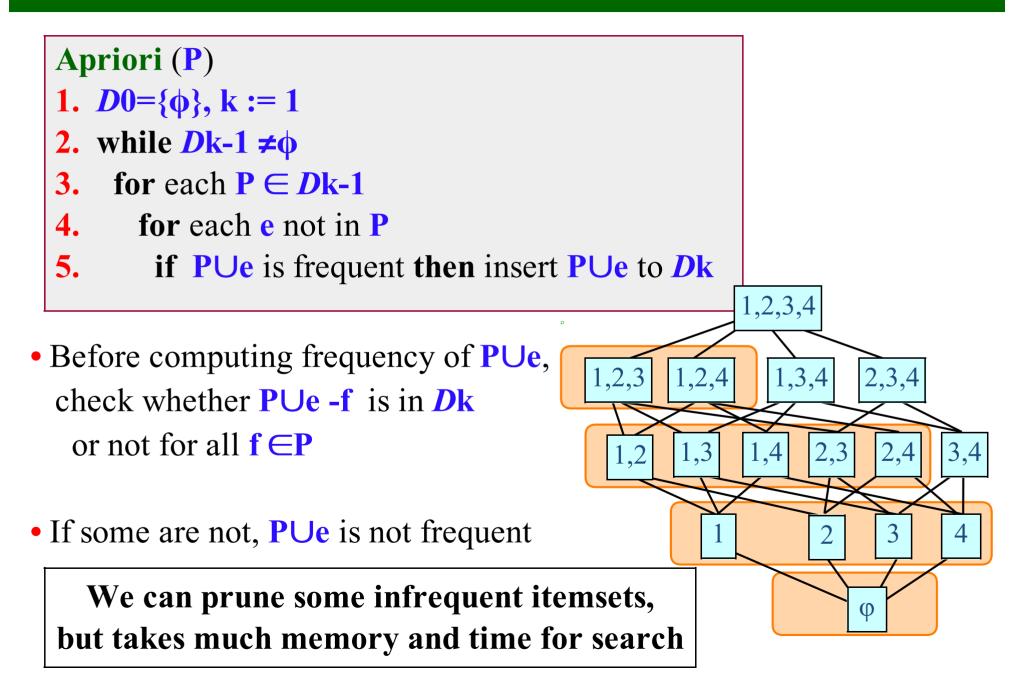
+ Simply, check each transaction includes PUe or not worst case: linear time in the database size average: max{ #transactions, frq(P)×|P| }

+ Constructing efficient index, such as binary tree, is very difficult, for inclusion relation

1,2,5,6,7,9 2,3,4,5 1,2,7,8,9 1,7,9 2,7,9 2

Algorithm for fast computation is needed

## (a) Breadth-first Search



# (b) Using Bit Operations

• Represent each transaction/itemset by a bit sequence

{1,3,7,8,9} [101000111]
{1,2,4,7,9} [110100101]
[100000101]

Intersection can be computed by AND operation (64 bits can be computed at once!) Also, memory efficient, if the database is dense On the other hand, very bad for sparse database

But, incompatible with the database reduction, explained later

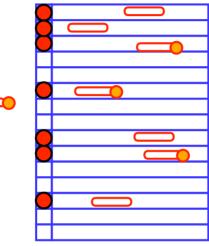
## (c) Down Project

 Any occurrence of PUe includes P ( included in Occ(P)) to find transactions including PUe , we have to see only transactions in Occ(P)

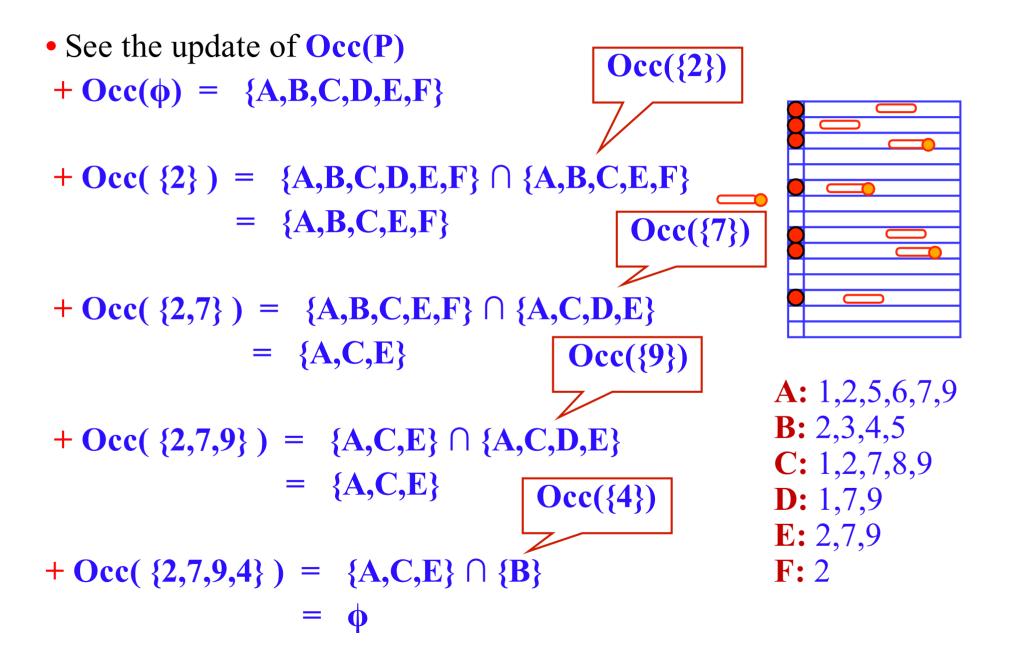
• **T**∈ **Occ(P**) is included in **Occ(PUe)** if and only if **T** includes **e** 

• By computing Occ(PUe) from Occ(P), we do not have to scan the whole database

Computation time is reduced much



## Example: Down Project



## Intersection Efficiently

•  $T \in Occ(P)$  is included in  $Occ(P \cup e)$  if and only if T includes e

**Occ(PUe)** is the intersection of **Occ(P)** and **Occ({e})** 

• Taking the intersection of two itemsets can be done by scanning the itemsets simultaneously in the increasing order of items (itemsets have to be sorted)

 $\{1, 3, 7, 8, 9\}$   $\cap \{1, 2, 4, 7, 9\}$  $= \{1, 7, 9\}$ 

Linear time in #scanned items sum of their sizes

# Using Delivery

- Taking intersection for all **e** at once, fast computation is available
- **1.** Set empty bucket for each item
- **2.** For each transaction **T** in **Occ(P)**,
  - + Insert T to the buckets of all item e included in T

After the execution, the bucket of **e** becomes **Occ(PUe)** 

**Delivery** (**P**)

- **1. bucket[e] := \ophi** for all **e**
- **2.** for each  $T \in P$

```
A: 1,2,5,6,7,9
B: 2,3,4,5
C: 1,2,7,8,9
D: 1,7,9 
E: 2,7,9
F: 2
```

```
1: A,C,D
2: A,B,C,E,F
3: B
4: B
5: A,B
6: A
7: A,C,D,E
8: C
9: A,C,D,E
```

## Time for Delivery

**Delivery** (P)

- **1.** jump :=  $\phi$ , bucket[e] :=  $\phi$  for all e
- **2.** for each  $T \in P$
- **3.** for each  $e \in T$ , e > tail(P)
- 4. **if bucket[e] = \phi then** insert **e** to **jump**
- 5. insert T to bucket[e]
- 6. end for
- 7. end for

```
• Comp. time is ΣT∈Occ(P) |{e | e∈T, e > tail(P)}|
```

• Computation time is reduced by sorting the items in each transaction, in the initialization

```
A: 1,2,5,6,7,9
B: 2,3,4,5
C: 1,2,7,8,9
D: 1,7,9
E: 2,7,9
F: 2
```

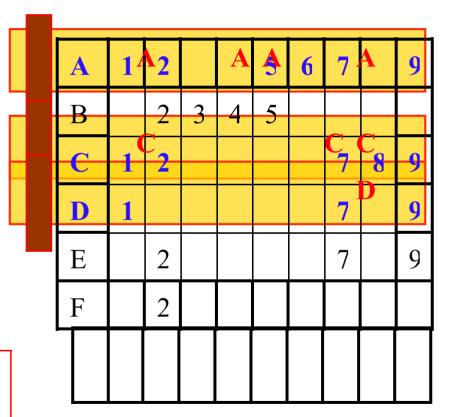
# Delivery

### • Compute the denotations of $P \cup \{i\}$ for all *i*'s at once,

 $\mathbf{D} = \begin{array}{c} 1,2,5,6,7,9\\ 2,3,4,5\\ 1,2,7,8,9\\ 1,7,9\\ 2,7,9\\ 2 \end{array}$ 

Check the frequency for all items to be added in linear time of the database size

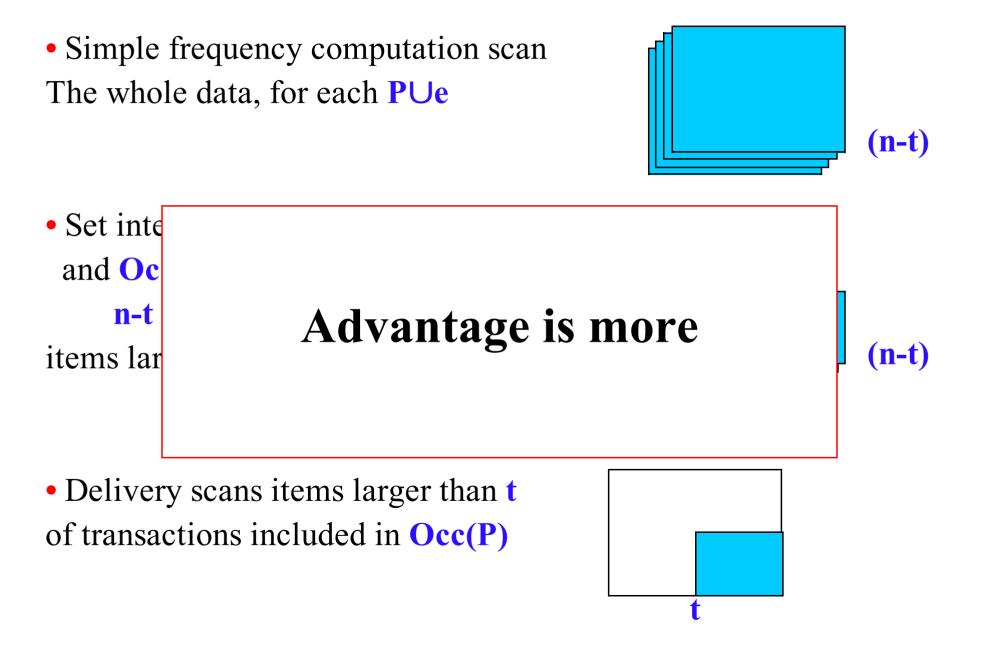
 $\{1,7\}$ 



Generating the recursive calls in reverse

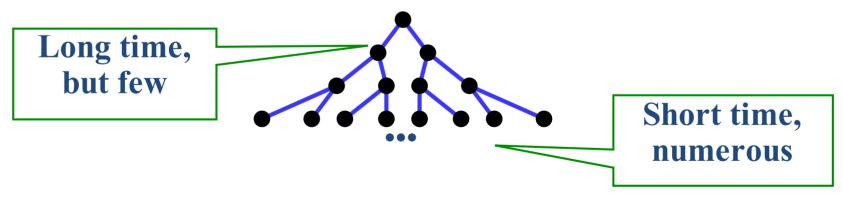
direction, we can re-use the memory

## Intuitive Image of Iteration Cost



## **Bottom-wideness**

- In the deep levels of the recursion, frequency of **P** is small Time for delivery is also short
- Backtrack generates several recursive calls in each iteration Recursion tree spreads exponentially, as going down Computation time is dominated by the bottom-level exponentially many iterations



Almost all iterations takes short time In total, average time per iteration is also short

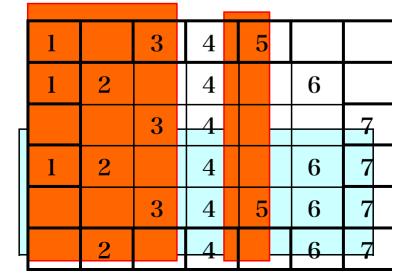
# Even for Large Support

 When σ is large, |Occ(P)| is large in bottom levels Bottom-wideness doesn't work

Speed up bottom levels by database reduction
(1) delete items smaller than added item most recently
(2) delete items infrequent in the database induced by Occ(P) (they never be added to the solution, in the recursive calls)
(3) unify the identical transactions

• In real data, usually the size of reduced database is constant, in bottom levels

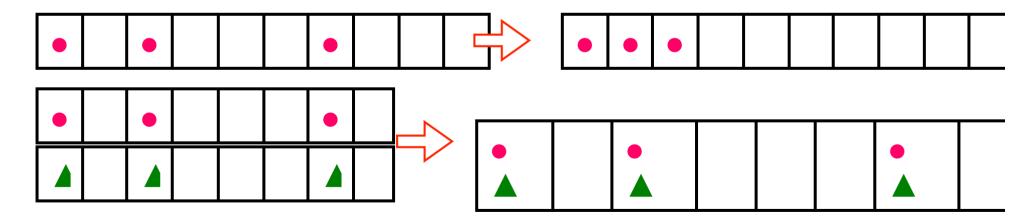
#### fast as much as small $\sigma$



# Synergy with Cache

- Efficient implementation needs "hit/miss ratio" of cache
  - open the loops
  - change memory allocation

```
for i=1 to n { x[i]=0; }
for i=1 to n step 3 { x[i]=0; x[i+1]=0; x[i+2]=0; }
```

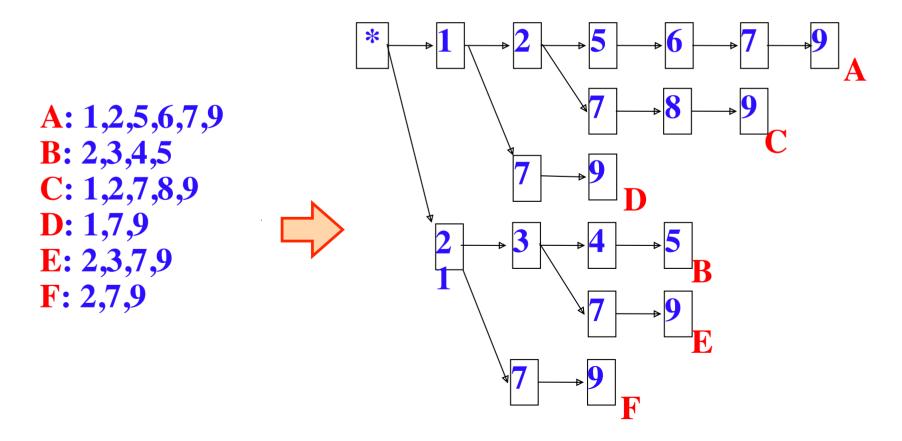


By database reduction, memory for deeper levels fits cache Bottom-wideness implies "cache hits almost all accesses"

## Compression by Trie/Prefix Tree

• Regarding each transaction as a string, we can use trie / prefix tree to store the transactions, to save memory usage

Orthogonal to delivery, shorten the time to scan (disadvantage is overhead, for its representations)



# 3-2 Result of Competition

## Competition: FIMI04

- FIMI: Frequent Itemset Mining Implementations
- + A satellite workshop of ICDM (International Conference on Data Mining). Competition on implementations for frequnet/closed/maximal frequent itemsets enumeration
   FIMI 04 is the second, and the last
- The first has 15, the second has 8 submissions

### **Rule and Regulation:**

- + Read data file, and output all solutions to a file
- + Time/memory are evaluated by time/memuse command
- + direct CPU operations (such as pipeline control) are forbidden

## Environment : FIMI04

• CPU, memory: Pentium4 3.2GHz、1GB RAM OS, Language, compiler: Linux, C, gcc

• dataset:

- + real-world data: sparse, many items
- + machine learning repository: dense, few items, structured
- + synthetic data: sparse, many items, random
- + dense real-world data: very dense, few items

### LCM ver.2 (Uno, Arimura, Kiyomi) won the Award

### Award and Prize

Second International Workshop on Frequent Itemset Mining Implementations in conjunction with the fourth IEEE International Conference on Data Mining

#### **BEST IMPLEMENTATION AWAF**

granted to

"LCM v.2: Efficient Mining Algorithms for Frequent/Closed/Maxima Takeaki Uno, Masashi Kiyomi and Hiroki Arimura

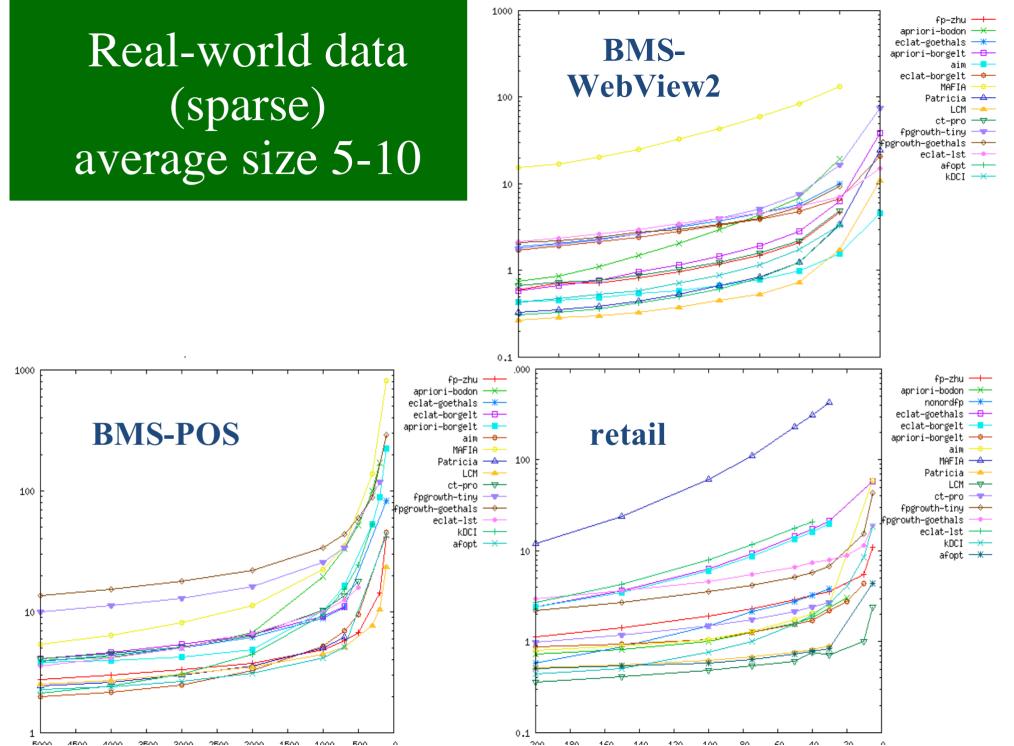
1st November 2004, Brighton, UK

Roberto Bayardo

Bart Goethals Moha

Mohammed J. Za

Prize is {beer, nappy} the "Most Frequent Itemset"

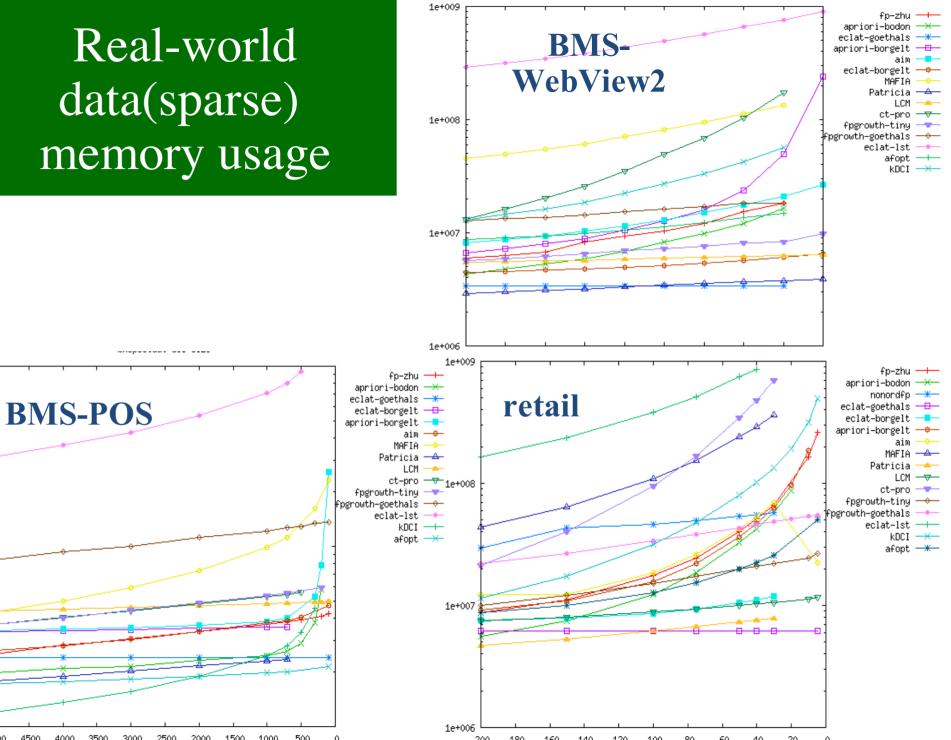


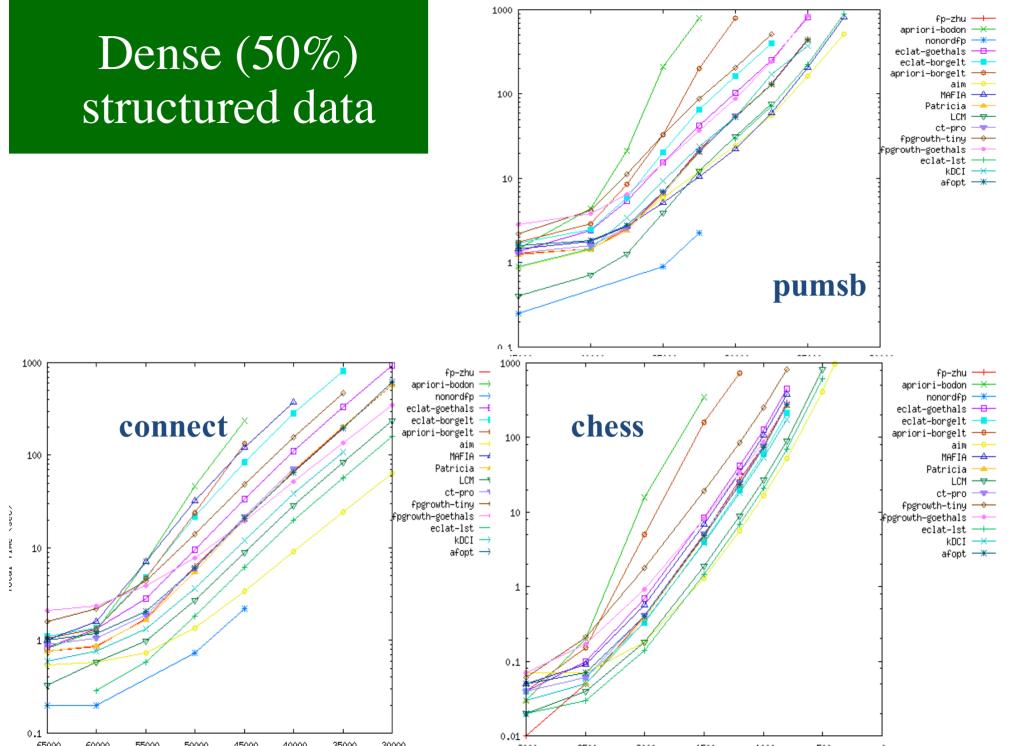
# Real-world data(sparse) memory usage

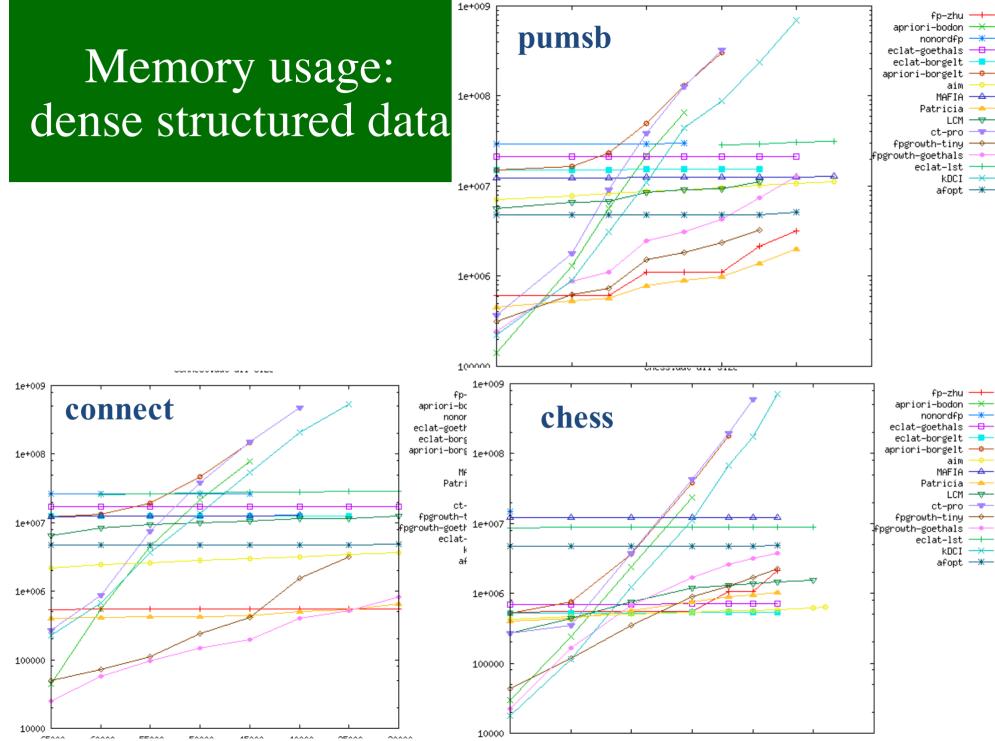
1e+009

1e+008

1e+007







# Dense real-world/ Large scale/ data

accidents

1e+009

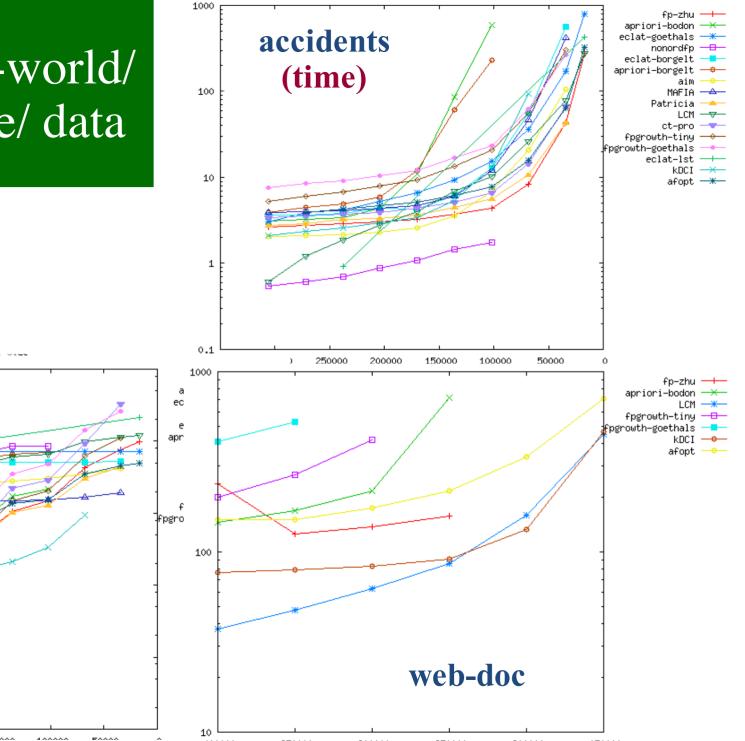
1e+008

1e+007

1e+006

100000

10000



## **Other Frequent Patterns**

• Bottom-wideness, delivery and database reduction are available for many kinds of other frequent pattern mining

- + string, sequence, time series data
- + matrix
- + geometric data, figure, vector
- + graph, tree, path, cycles...



# 3-3 Closed Itemset Enumeration

# Disadvantage of Frequent Itemset

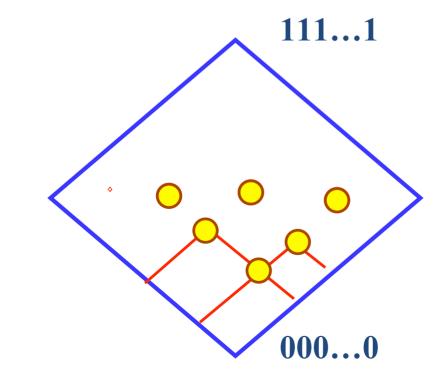
- To find interesting(deep) frequent itemsets, we need to set σ small numerous solutions will appear
- Without loss of information, we want to shift the problem (model)

### 1. maximal frequent itemsets

included in no other frequent itemsets

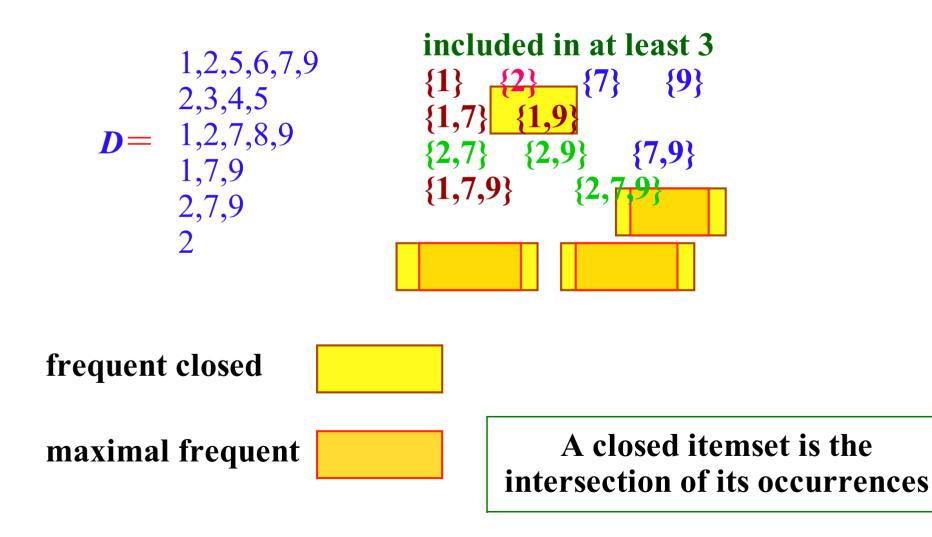
### 2. closed itemsets

maximal among those having the same occurrence set



## Ex) Maximal Frequent / Closed Itemsets

• Classify frequent itemsets by their occurrence sets



## Advantage and Disadvantage

#### maximal

- existence of output polynomial time algorithm is open
- fast computation is available by pruning like maximal cliques
- few solutions but sensitive against the change of o

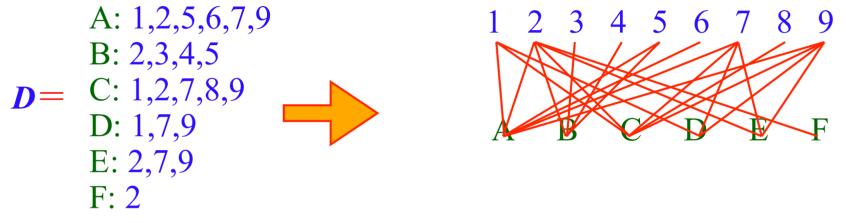
#### closed

- polynomial time enumeratable by reverse search
- discrete algorithms and bottom-wideness fasten computation
- no loss w.r.t occurrence sets
- no advantage for noisy data (no decrease of solution)

#### Both can be enumerated O(1) time on average, 10k-100k / sec.

# **Bipartite Graph Representation**

• Items and transactions are vertices, and the inclusion relations are the edges



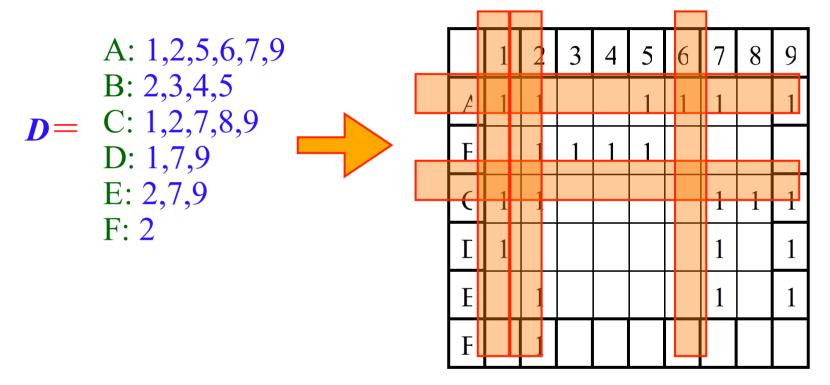
- itemset and transactions including it bipartite clique of the graph
- itemset and its occurrence set

bipartite clique maximal on the transaction side

• closed itemset and its occurrence set maximal bipartite clique

## From Adjacency Matrix

• See the adjacency matrix of the bipartite graph



• itemset and transactions including it a submatrix all whose cells are 1

# Methods for Closed Itemset Enumeration

#### Based on frequent itemset enumeration

- enumerate frequent itemsets, and output only closed ones
- can not get advantage of fewness of closed itemsets

### • Storage + pruning

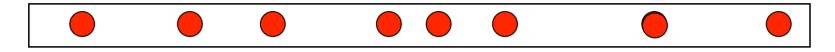
- store all solutions found, and use them for pruning
- pretty fast
- memory usage is a bottle neck

### • Reverse search + database reduction (LCM)

- computation is efficient
- no memory for previously found solutions

# Neighbor Relation of Closed Itemsets

• Remove items from a closed itemset, in decreasing ordering

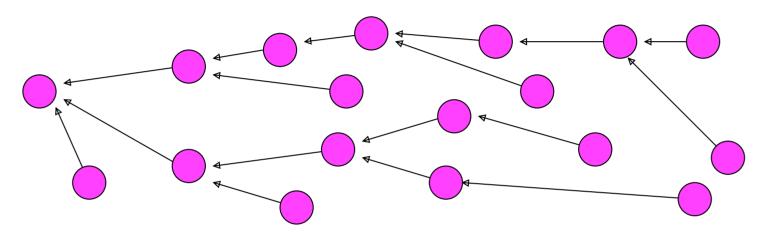


- At some point, occurrence set expands
- Compute the closed itemset of the expanded occurrence set
- The obtained closed itemset is the **parent** (uniquely defined)
- Frequency of the parent is always larger than the child, thus the parent-child relation is surely acyclic

The parent-child relation induces a directed spanning tree

### Reverse Search

Parent-child relation induces a directed spanning tree



#### **DFS search on the tree can find all solutions**

- Enumeration method for all children of a parent is enough to search
- If children are found polynomial time on average, output polynomial

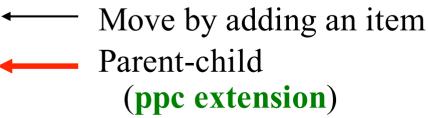
(child is obtained by adding an item to the parent)

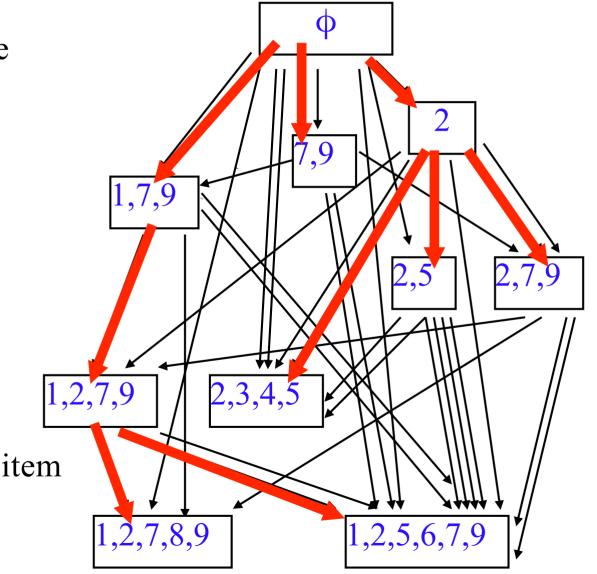
Acyclic relation and polytime children enumeration are sufficient to polytime enumeration of any kind of objects

## Ex) Parent-child Relation

• All closed itemsets of the following database, and the parent-child relation

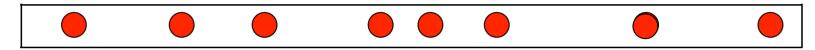
 $D = \begin{array}{c} 1,2,5,6,7,9\\ 2,3,4,5\\ 1,2,7,8,9\\ 1,7,9\\ 2,7,9\\ 2\end{array}$ 





# Computing the Children

Let e be the item removed most recently to obtain the parent
 By adding e to the parent, its occurrence set will be the occurrence set of the child



A child is obtained by adding an item and computing the closed itemset

However, itemsets obtained in this way are not always children

Necessary and sufficient condition to be a child is "no item appears preceding to e" by closure operation

## Database Reduction

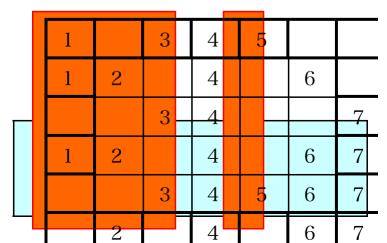
We want to reduce the database as frequent itemset enumeration
However, can not remove smaller items (than last added item e) computation of ppc extension needs them

• However,

+ if larger items are identical, included in Occ at the same time
+ so, only the intersection of the smaller parts is needed
store the intersection of transactions having the same large items

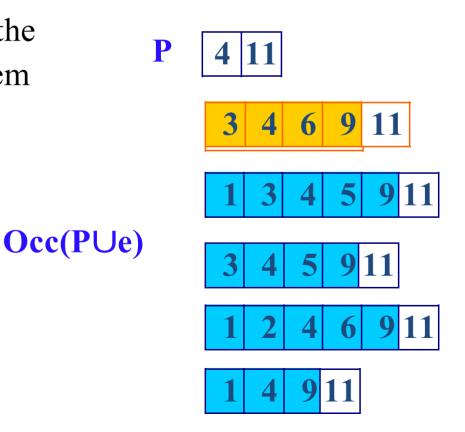
• The intersection of many transactions has a small size

#### no much loss compared with large **o**



# Cost for Comparison

- We can simply compute the intersection of Occ(PUe), but would be redundant. We do just "checking the equality of the intersection Occ(PUe) and P", thus no need to scan all We can stop when we confirmed that they are different
- Trace each occurrence of **PUe** in the increasing order, and check each item appears all occurrences or not
- If an item appears in all, check whether it is included in **P** or not
- Proceed the operations from the last operated item



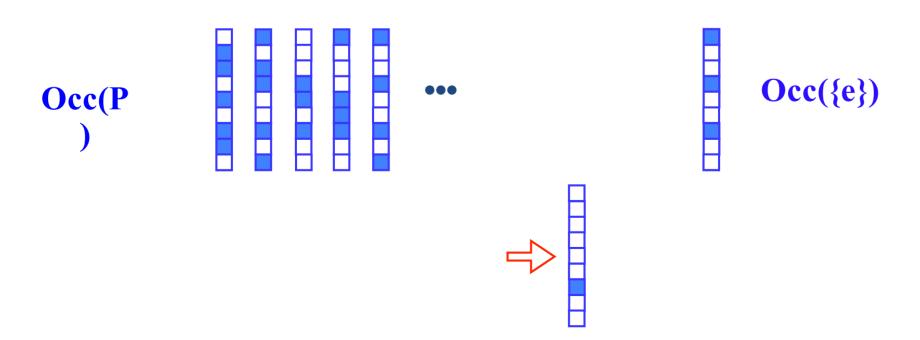
# Using Bit Matrix

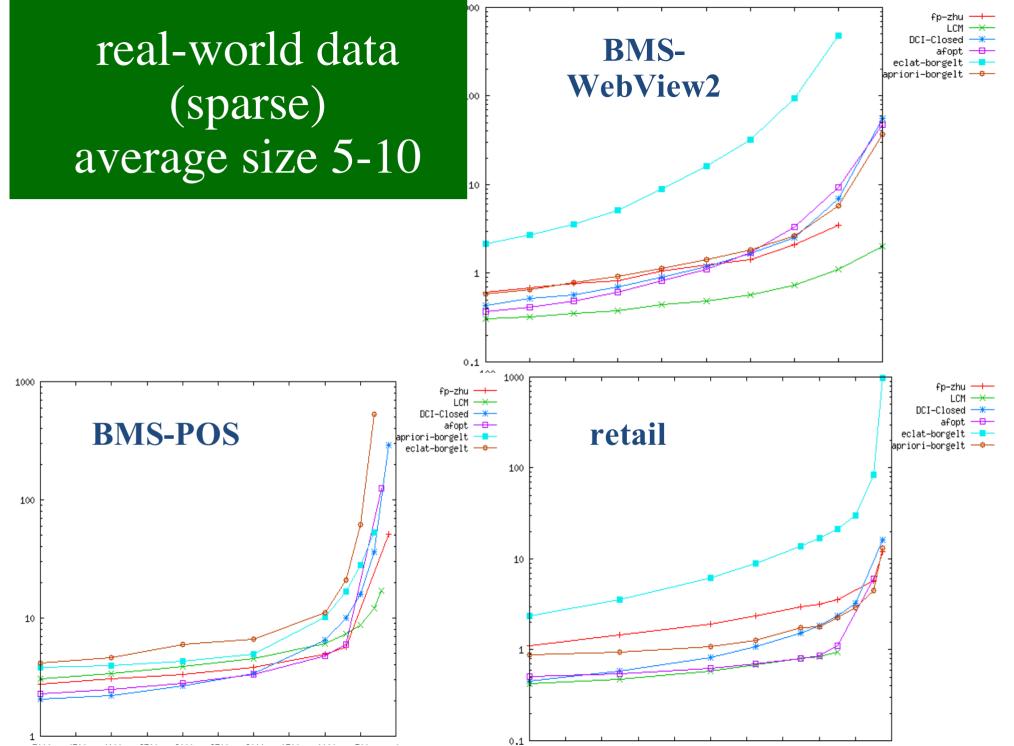
- Sweep pointer is a technique for sparse style data. We can do better if we have adjacency matrix
- But, adjacency matrix is so huge (even for construction)
- Use adjacency matrix when the occurrence set becomes sufficiently small

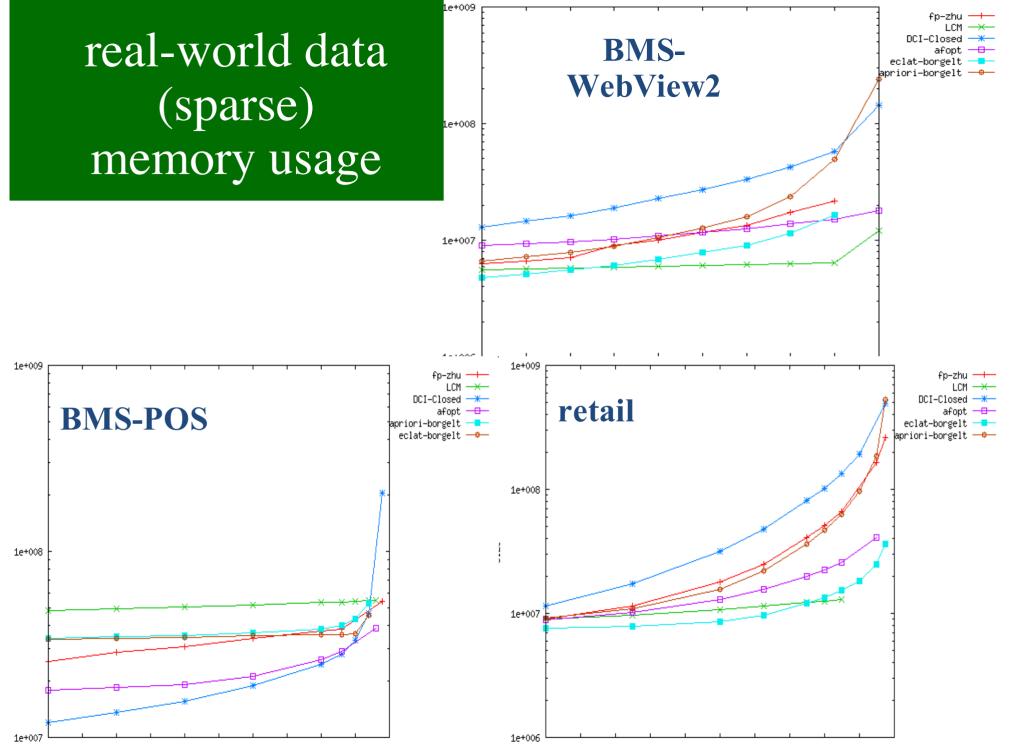
By representing the matrix by bitmap, each column (corresponding to an item) fits one variable!

# O(1) Time Computation of Bit Matrix

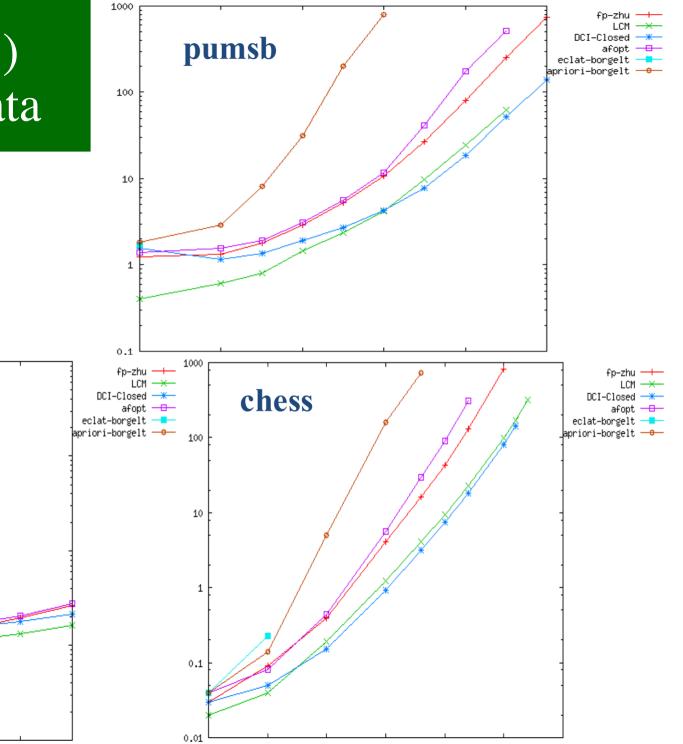
- By storing the occurrences including each item by a variable, we can check whether all occurrence of PUe includes an item or not in O(1) time
- Take the intersection of bit patterns of Occ({i}) and Occ(P Ue)
- If i is included in all occurrences of PUe, their intersection is equal to Occ({i})







# dense (50%) structured data



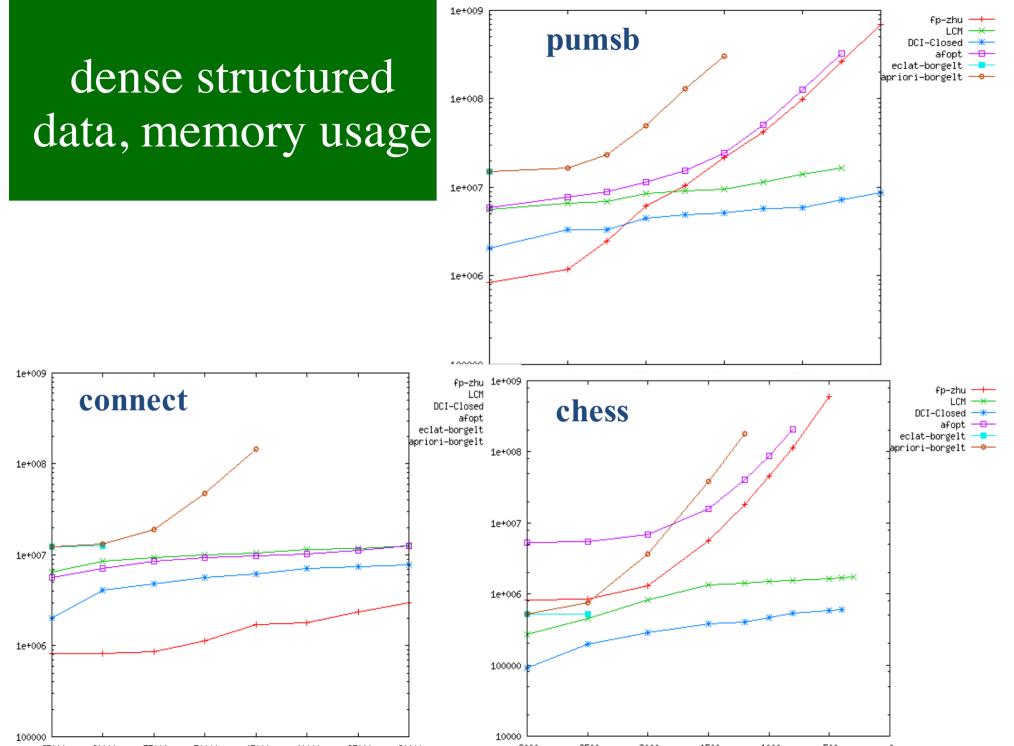
0.1

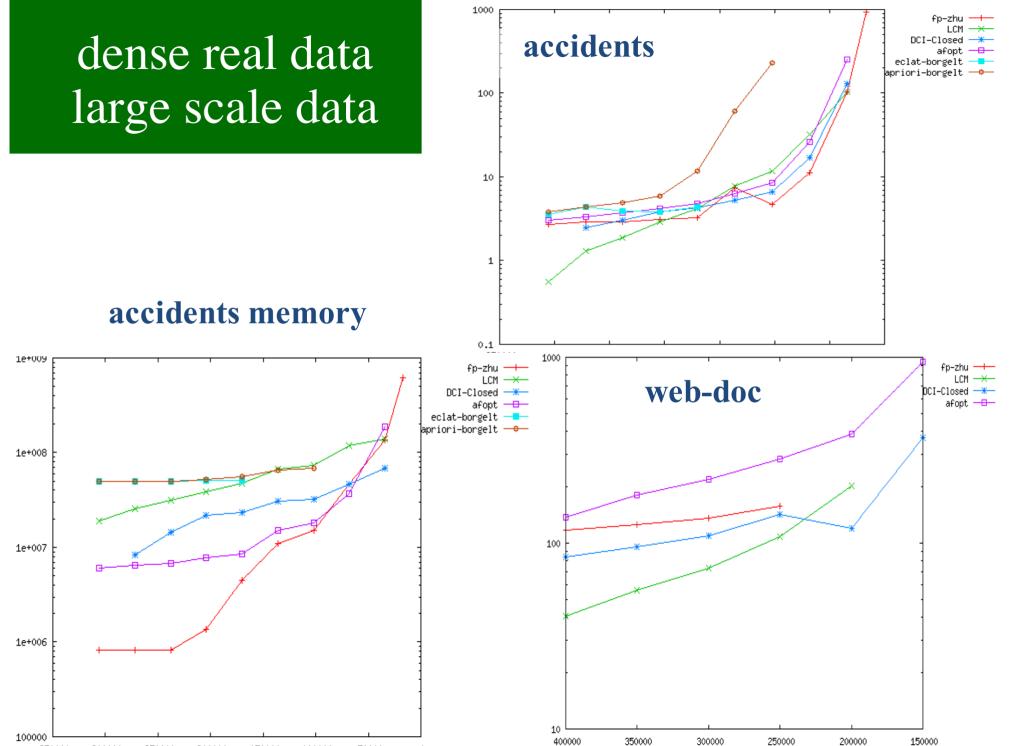
1000

100

10

connect

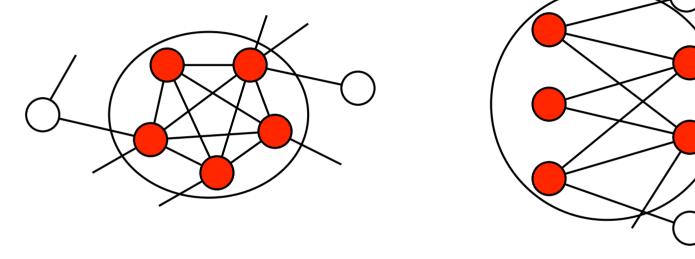




# 3-4 Maximal Clique Enumeration

## **Clique Enumeration**

**Clique:** a subgraph that is a complete graph (any two vertices are connected



- Finding a maximum size is NP-complete
- Bipartite clique enumeration is converted to clique enumeration
- Finding a maximal clique is easy ( O(|E|) time )
- Many researches and many applications, with many models

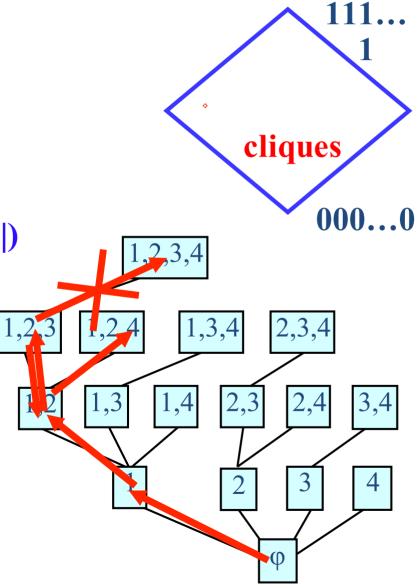
### Monotone

• Set of cliques is monotone, since any subset of a clique is also a clique

Backtracking works

• The check being a clique takes O(|E|) time, and at most |V| recursive calls

O(|V| |E|) per clique

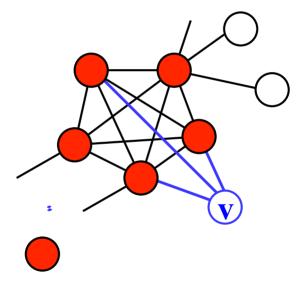


# Like Refine Search

We want to find vertices can be added to a clique
 Addible adjacent to all vertices of clique
 keep the set of addible vertices (CAND) in advance

• When add a vertex v to clique, addible vertex is still addible adjacent to v

The update involved by adding v intersection of CAND and N(v) (N(v) is the neighbors of v)



 $O(\delta(v))$  time per iteration, where  $\delta(v)$  is the degree of v

# Adjacency on Maximal Cliques

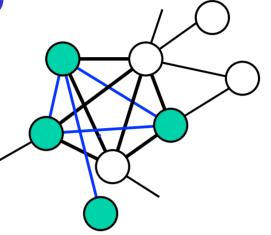
- C(K) := lexicographically smallest maximal clique including K (greedily add vertices from smallest index)
- For maximal clique **K**, remove vertices iteratively, from largest index
- At the beginning C(K) = K, but at some point  $C(K) \neq$  original  $K_{C}$
- Define the parent **P(K)** of **K** by the maximal clique (uniquely defined).
- The lexicographically smallest maximal clique (= root) has no parent
- **P(K)** is always lexicographically smaller than **K** the parent-child relation is acyclic, thereby induces tree

# Finding Children

K[v]: The maximal clique obtained by adding vertex v to K, remove vertices not adjacent to v, and take C()
 K[v] := C(K ∩ N(v)∪{v})

• K' is a child of K K' = K[v] for some v

**K**[**v**] for all **v** are sufficient to check



• For each **K**[**v**], we compute **P**(**K**[**v**]) If it is equal to **K** to, **K**[**v**] is a child of **K** 

All children of K can be found by at most |V| checks, thus an iteration takes O(|V| |E|) time O(|V| |E|) per maximal clique

• Note that C(K) and P(K) can be computed in O(|E|) time

## Pseudo Code for Maximal Clique

```
EnumMaxcliq (K)

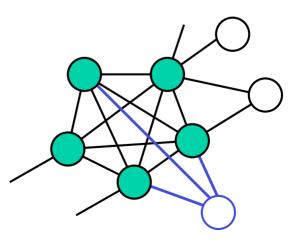
1. output K

2. for each vertex v not in K

3. K' := K[v] \quad (= C(K \cap N(v) \cup v))

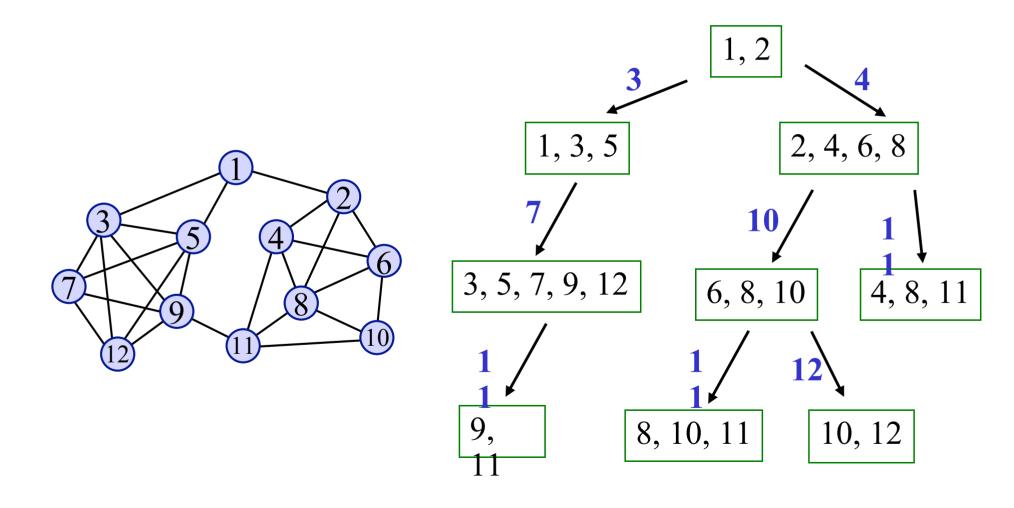
4. if P(K') = K then call EnumMaxcliq (K)

5. end for
```



## Example

### • The parent-child relation on the left graph



# Example

- The parent-child relation on the left graph
- The red-lines are moves by **K**[**v**] 1, 2 1, 3, 5 2, 4, 6, 8 10 6 3, 5, 7, 9, 12 4, 8, 11 6, 8, 10 8 9, 8, 10, 11 10, 12

# Finding Children Quickly

• K[v]: The maximal clique obtained by adding vertex v to K, remove vertices not adjacent to v, and take C()  $K[v] := C(K \cap N(v) \cup \{v\})$ 

• K' is a child of K K' = K[v] for some v

• v is adjacent no vertex in K  $K[v] = C(\{v\})$  P(K[v]) is root

if  $\mathbf{K} \neq \text{root}$ , v is adjacent none of  $\mathbf{K}$   $\mathbf{K}[v]$  is not a child

We have to check only the vertices adjacent to some of K, that are at most  $(\Delta + 1)2$ 

# Computing C(K)

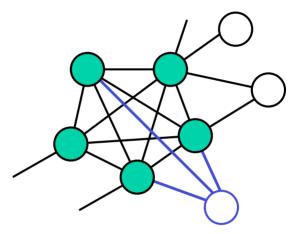
- CAND(K) : the set of vertices adjacent all vertices in K
- To compute C(K), we add to K the minimum index among CAND(K), until CAND(K) = ♦
- CAND(KUv) = CAND(K)  $\cap$  N(v) thus computable in O( $\Delta$ ) time ( $\Delta$ : maximum degree)
- Repetitions (=maximum clique size) is at most Δ, the total time is O(Δ2)

**C(K)** can be computed in **O(\Delta 2)** time

# Computing P(K)

Let r(v) be #vertices in K adjacent to v
 r(v) = |K| ⇒ addible to K

 Delete vertices in K from maximum index, and update r(v) for all necessary v (deletion of u needs O(δ(u)) time for update)

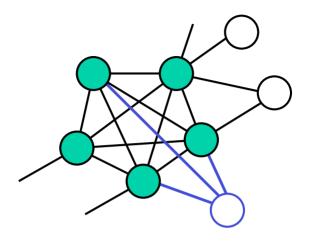


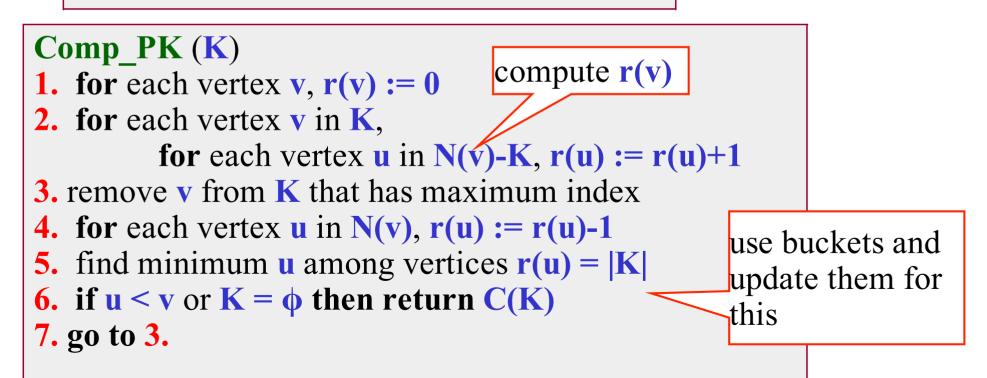
- If a vertex v satisfies r(v) = |K| after deleting u, compare v and u
- If v < u, C(K-{,...,v}) never include u, thus it is the parent

#### **P(K)** can be computed in **O(\Delta 2)** time

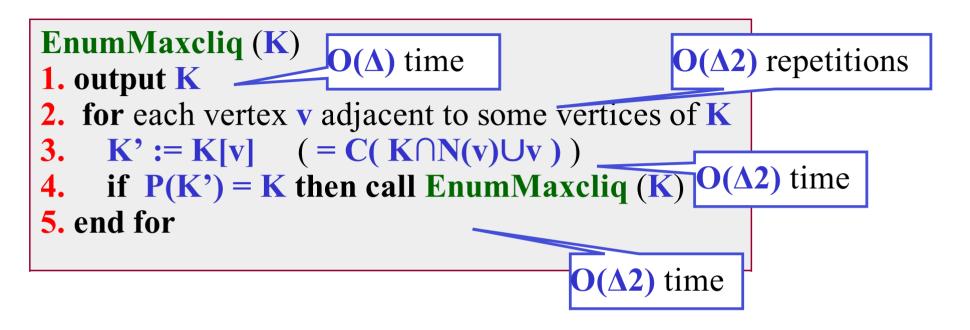
# **Two Routines**

Comp\_CK (K={v1,...,vk}) 1. K' := K, CAND := N(v1)  $\cap ... \cap N(vk)$ 2. if CAND =  $\phi$  return K' 3. v := minimum vertex in CAND 4. K' := K'Uv, CAND := CAND  $\cap N(v)$ 5. go to 2.

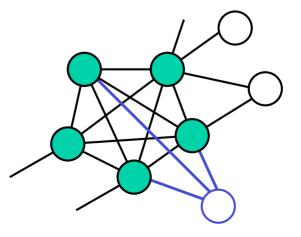




# **Complexity Analysis**



• Taken together, each iteration takes  $O(\Delta 4)$  time



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#### **Frequent Itemsets**

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### Clique

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# Exercise 3

# Speed up

**3-1.** We want to design an algorithm for enumerating four cycles (cycles of length four) in a huge sparse graph. When the algorithm recursively adds an edge, how can we speed up iterations by removing unnecessary parts from input graphs recursively.

**3-2.** For given **m** permutations of  $1, \dots, n$ , we want to enumerate all subsequences appearing at least **k** of them. How can we reduce the database to reduce the computation time?

(subsequence is a sequence of numbers such that the numbers appear in the sequence without changing the order. For example, (1,2,3) is a subsequence of (1,4,2,5,6,3).

**3-3.** We want to enumerate independent sets (no two vertices are connected). What data structure can we use to speed up iterations?

# Speed up

**3-4.** We can construct an algorithm for enumerating all paths connecting given vertices **s** and **t**, by adding an edges one by one recursively. For large scale graphs, what should we do for modeling, and speeding up?

**3-5.** What kind of techniques should we use to speed up the algorithm for enumerating pseudo cliques in a large scale graph?

**3-6.** A leaf-elimination ordering of a tree **T** is a vertex ordering obtained by removing leaves of **T** iteratively. Design an algorithm for enumerating all leaf-elimination ordering, and way to speed up. Discuss about the complexity.

# Speed up

3-7. A decreasing sequence of numbers a1,...,an is a subsequence b1,...,bm s.t. bi > bi+1 holds for any i (subsequence is a sequence of numbers that appears in a1,...,an without changing the order). Design an algorithm to enumerate all "maximal" decreasing ordering (we assume that no two numbers are the same).

**3-8.** For a Markov chain defined on state set V, design an algorithm to enumerate all state sequences starting from  $S \in V$ , with moving 10 times. Discuss about speeding up.

## Bottom-wideness

**3-9.** We first find a triangle **X** from a graph and iteratively add vertices to **X** which is adjacent to at least 3 vertices of **X**, to make a cluster (we do this to enumerate clusters). We want to enumerate all such structures, so how can we make the algorithm efficient?

**3-10.** For given a set of axis-parallel rectangles in a plane, we want to enumerate all rectangles obtained by intersecting of some rectangles in the set. Discuss available enumeration techniques, and #solutions.

**3-11.** For given a set of data strings, we want enumerate all strings s.t. there are at least **o** substrings of some data strings have Hamming distance at most k to the string. Consider how to construct efficient algorithm with bottom-wideness.

3-12. Design an algorithm for enumerating all vertex sets U of a graph G=(V,E) s.t. the maximum degree in G[U] is at most k. Discuss about speeding up, and existence of polynomial time algorithm for enumerate only maximal ones.

**3-13.** For given a database whose records are graphs having a common vertex set, design an algorithm for enumerating pairs of graphs s.t., the symmetric difference between them is composed of at most k edges.