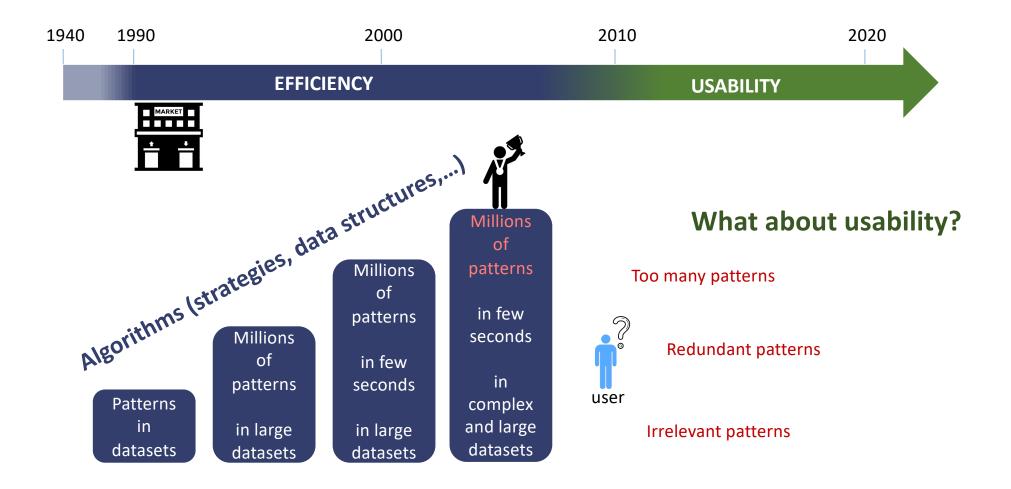
# Pattern Sets (DMV Lecture, M2 SIF)

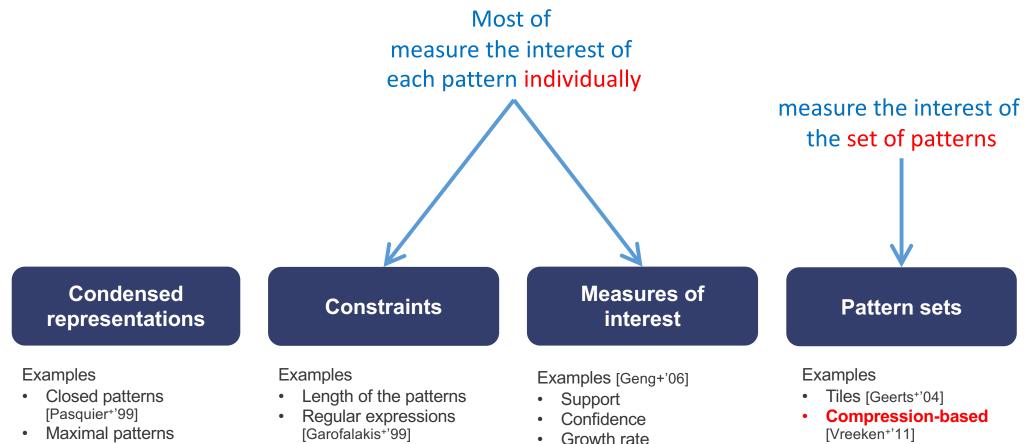
Peggy Cellier peggy.cellier@irisa.fr

Last revision: October 2023

# Pattern Mining: Efficiency, Efficiency, Efficiency



## How to manage the amount of Patterns?



• Swap randomization [Lijffijt+'12]

3

## **References and course material**

- [1] Krimp: mining itemsets that compress, Jilles Vreeken, Matthijs van Leeuwen, Arno Siebes, DMKD 2011
- [2] Slim: Directly Mining Descriptive Patterns, Koen Smets and Jilles Vreeken, SDM 2012
- [3] The Long and the Short of It: Summarising Event Sequences with Serial Episodes, Nikolaj Tatti and Jilles Vreeken, KDD 2012
- [4] <u>The Minimum Description Length Principle</u>, Peter Grünwald, MIT Press, 2007
- Some (lot of) slides come from the talk of Jilles Vreeken
  - <u>https://people.mmci.uni-saarland.de/~jilles/</u>
- Slides from the HDR of Peggy Cellier

# Outline

### 1. Introduction

#### 2. Compression based approaches

- 1. Motivations
- 2. Information theory and the MDL principle
  - Information theory
  - The MDL principle for pattern mining
- 3. Algorithms
  - Itemsets: Krimp (and SLIM)
  - Sequences: SQS
  - Graphs: Graph-MDL
- Conclusion

## Question

# How can we find useful patterns?

# **Standard pattern mining**

#### For a database db

- a pattern language L
- and a set of constraints C

#### the goal is to find the set of patterns $P \subseteq L$ such that

- each  $p \in P$  satisfies each  $c \in C$  on db
- and P is maximal

That is, find all patterns that satisfy the constraints

# **Problems in pattern paradise**

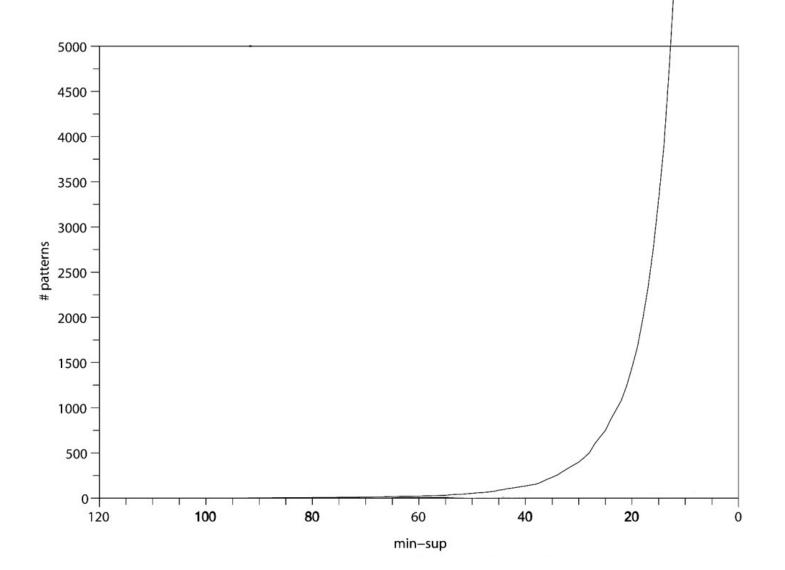
#### The pattern explosion problem

- I high thresholds
   I few, but well-known patterns
- Iow thresholds
   a gazillion patterns

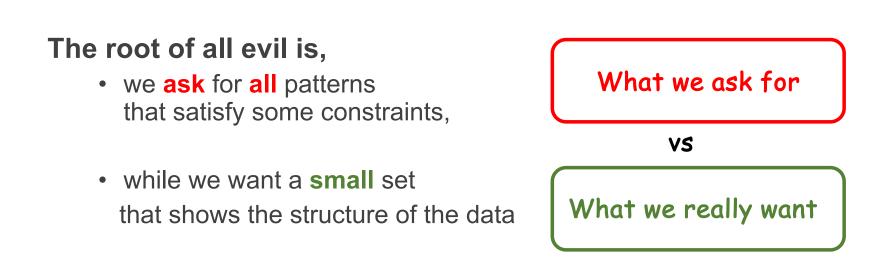
Many patterns are redundant



• The Wine dataset has 178 rows, 14 columns



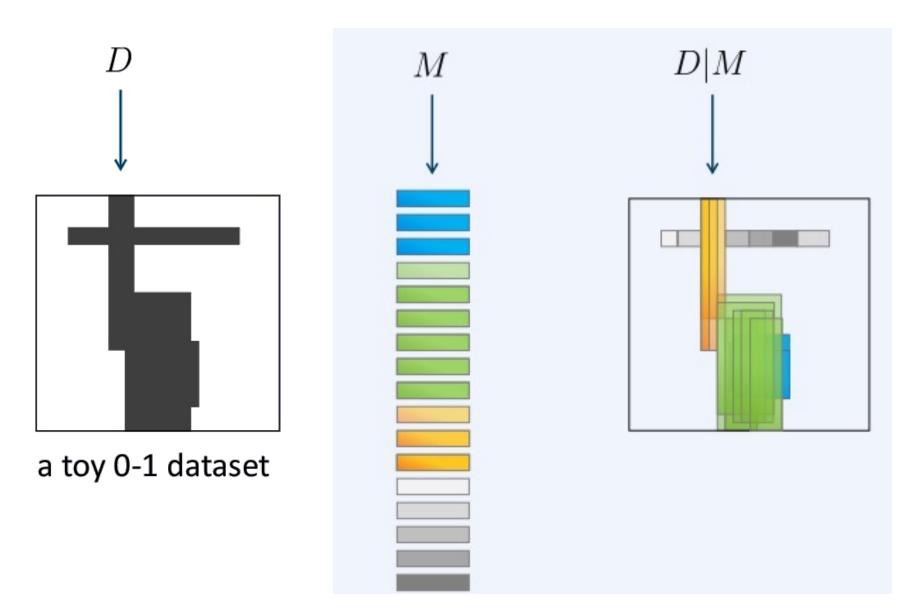
# Be careful what you wish for



In other words, we should ask for a set of patterns such that

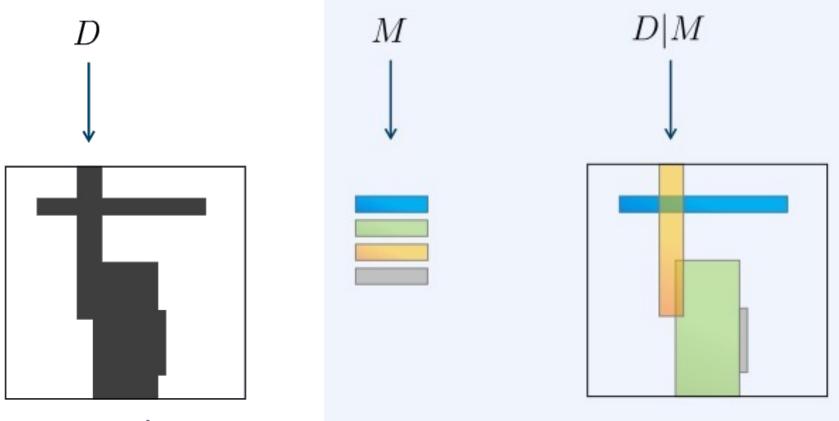
- all members of the set **satisfy** the constraints
- the set is **optimal** with regard to some criterion

# What we ask for



A pattern identifies local properties of the data (e.g., itemsets)

# What we really want



a toy 0-1 dataset

# How to do that?

How to find

- a subset of patterns
- describing data in a concise way

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[Risanen'78, Grünwald'00]

#### Models describe the data

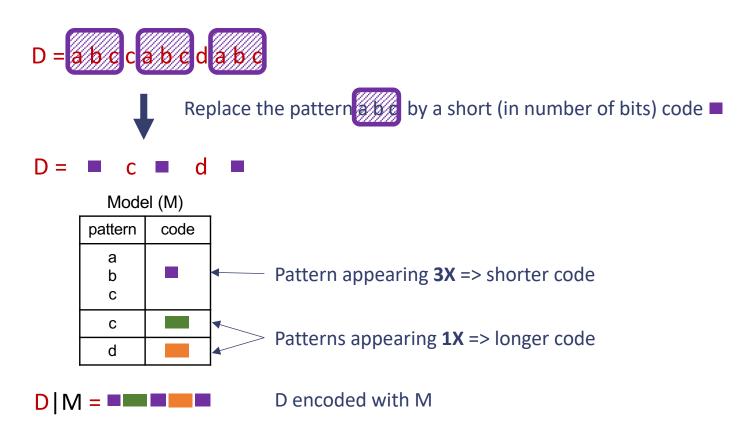
- that is, they capture regularities
- hence, in an abstract way, they compress it

The MDL principle makes this observation concrete:

``The model that best describes the data is the one that best compresses the data."

[Risanen'78, Grünwald'00]

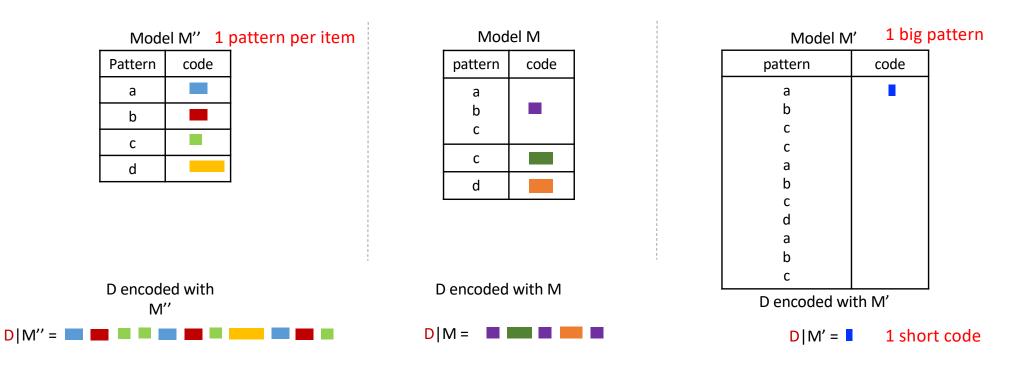
How to compress data? ⇒ take advantage of repetitions (patterns)



30

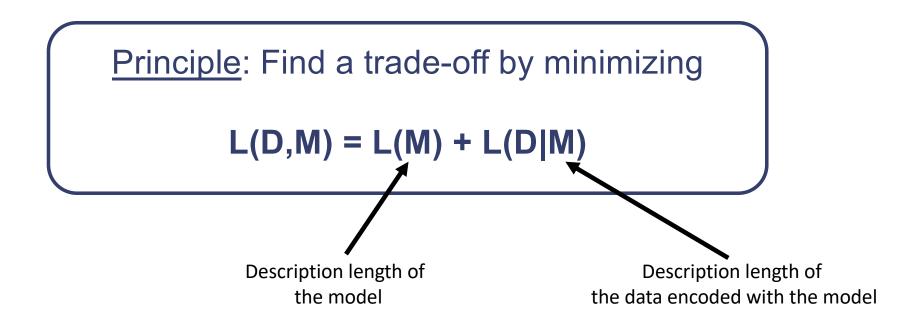
[Risanen'78, Grünwald'00]

# How to find the BEST compression? $\Rightarrow$ trade-off



[Risanen'78, Grünwald'00]

How to find the BEST compression?  $\Rightarrow$  trade-off



# Information theory and compression

#### The MDL principle is related to Kolmogorov Complexity

## Kolmogorov Complexity [Kolmogorov 1963]

the complexity of a string is the length of the smallest program that generates the string, and then halts

#### Kolmogorov Complexity is the ultimate compression

- recognizes and exploits **any** structure
- Uncomputable however...

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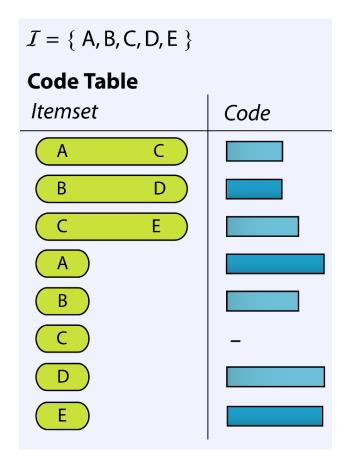
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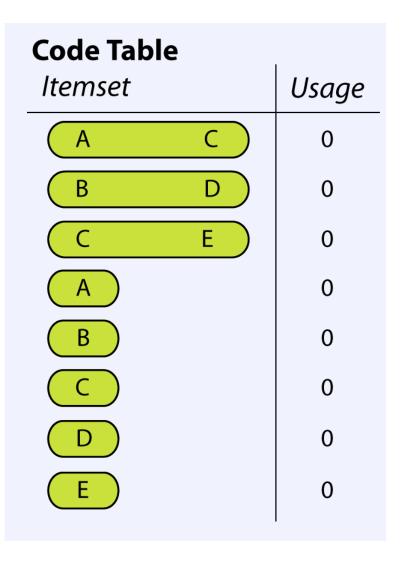
# The MDL principle for pattern mining

- Goal: reduce the number of extracted patterns
- Existing approaches for several pattern languages [Galbrun'22]
  - Examples
    - Itemsets: KRIMP [Vreeken+'11], SLIM [Smets+'12]
    - Sequences: SQS [Tatti+'12]
    - Graphs: GraphMDL [Bariatti+'20], GraphMDL+ [Bariatti+'21]

## Model = Code Table

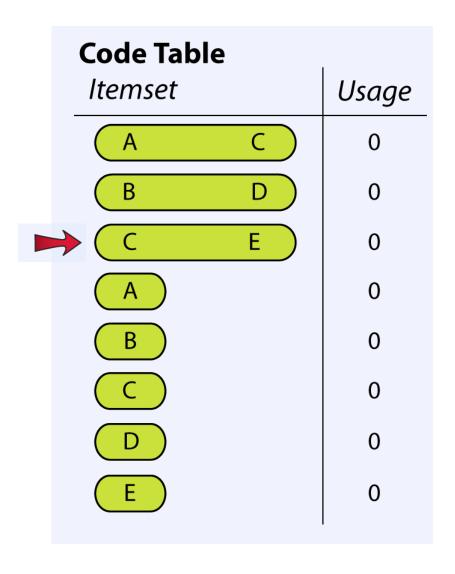
- Code Table (CT)
  - Set of itemsets + encoding





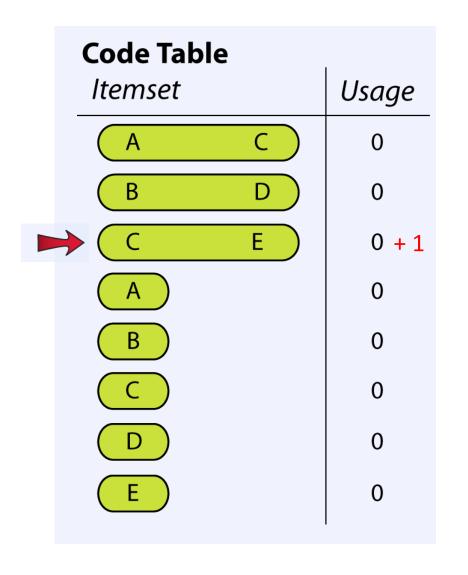


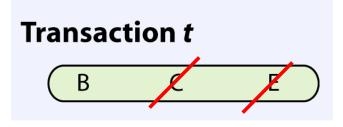
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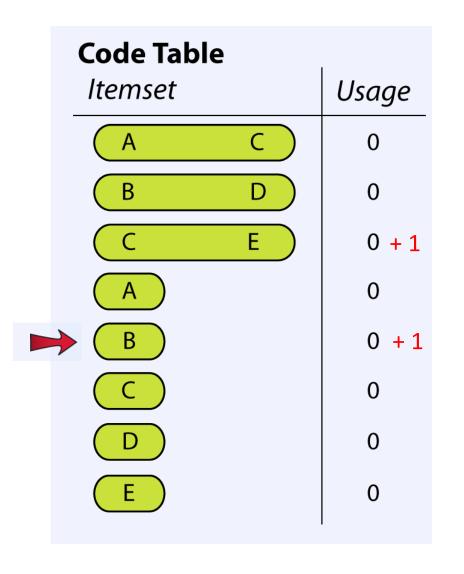


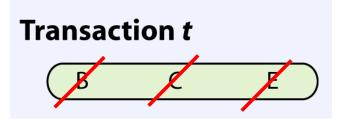
	В	С	E
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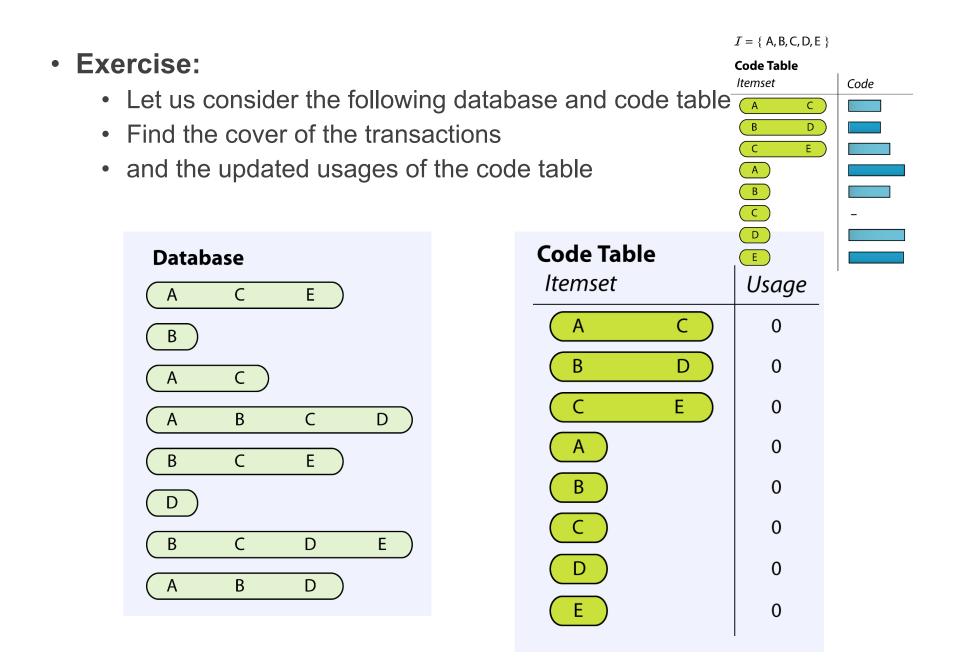






Cover of t		
С	E	В

## **Encoding a database: exercise**



# Solution

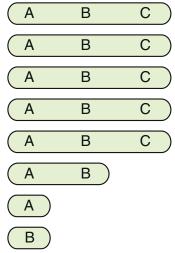
## **Standard Code Table**

#### ST: Standard Code table

• = only and all singleton itemsets

#### • Example

#### Database



Standard code table ST		
ltemset	Code	Usage
A		7
В		7
C		5

Cover with ST	Encoded with ST
A B C	
A B C	
A B C	
A B C	
A B C	
AB	
A	
В	

**Optimal codes** [Shannon 1948, Thomas & Cover 1991]

- What is the actual length of the codes? (in bits)
- For *c*∈*CT* we define

Α

• 
$$P(c|CT) = \frac{usage(c)}{\sum_{i \in CT} usage(i)}$$

where  $usage(j) = |\{t \in D \mid j \text{ in } cover(t, CT)\}|$ 

**Code Table** 

<u>Example</u>:  $P({A,C}) = 3/13$ •

> Length of the code

Itemset Usage Code The optimal code for the coding Α C 3 distribution *P* assigns a code to  $c \in CT$ В D 3 with length: [Shannon 1948] C E 2 Α 1  $L(c|CT) = -\log P(c|CT)$ B C 2 0 D 1 <u>Example</u>: L({A,C}) = -log(3/13) ≈ 2.12 **Database** Cover Database Ε 1 F Λ

## **Encoding a code table**

#### The size of a code table depends on

- the left column
  - length of itemsets as encoded with independence model
  - ST depends only from the data  $\rightarrow$  used to measure CT size
- the right column
  - the optimal code length based on usage of code table elements

#### Thus, the size of a code table is

$$L(CT | D) = \sum_{c \in CT: usage(c) \neq 0} L(c|ST) + L(c|CT)$$
Database
Database
Database
Dotabase

### **Encoding a database**

For  $t \in D$  we have

$$L(t|CT) = \sum_{c \in cover(t,CT)} L(c|CT)$$

Description length (DL) for one transaction of D

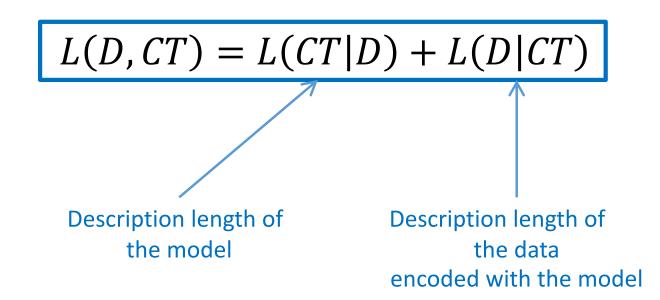
Hence we have

$$L(D|CT) = \sum_{t \in D} L(t|CT)$$

Sum of the DL of all transactions of D

**The Total Size** 

The total size of data and code table is



This is the MDL measure that we want to minimize

## And now, the optimal code table...

#### Easier said than done

- The number of possible code tables is huge
- No useful structure to exploit

• Hence, we resort to heuristics

# Outline

### 1. Introduction

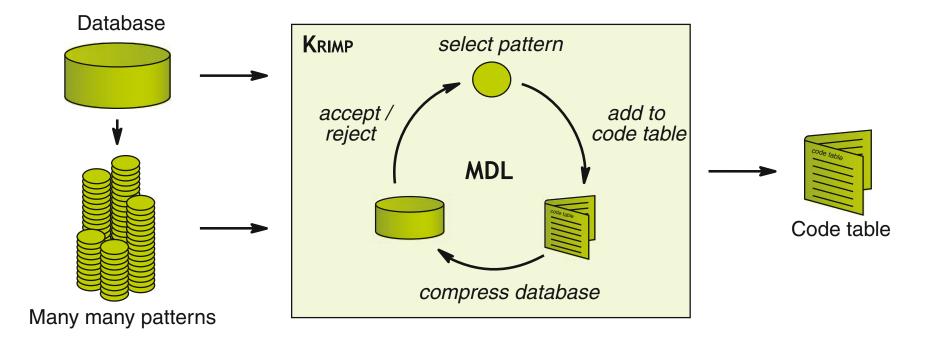
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## KRIMP

#### • KRIMP

- Based on MDL
- And heuristics



# **KRIMP** algorithm

#### Algorithm 3 The KRIMP Algorithm

**Input:** A transaction database  $\mathcal{D}$  and a candidate set  $\mathcal{F}$ , both over a set of items  $\mathcal{I}$ **Output:** A heuristic solution to the Minimal Coding Set Problem, code table CT 1:  $CT \leftarrow \text{Standard Code Table}(\mathcal{D})$  $supp_D(X) \downarrow |X| \downarrow$  Lexicographically  $\uparrow$ 2:  $\mathcal{F}_o \leftarrow \mathcal{F}$  in Standard Candidate Order 3: for all  $F \in \mathcal{F}_o \setminus \mathcal{I}$  do Add the candidate one by one  $CT_{\mathcal{C}} \leftarrow (CT \cup F)$  in **Standard Cover Order**  $|X| \downarrow supp_{\mathcal{D}}(X) \downarrow$  Lexicographically 4: if  $L(\mathcal{D}, CT_c) < L(\mathcal{D}, CT)$  then 5:  $CT \leftarrow CT_c$ 6: end if 7: 8: end for 9: return CT

## **Improvement by Pruning**

#### • Example

• Let us consider 3 code tables

 $CT_{1} = \{\{X_{1}, X_{2}\}, \{X_{1}\}, \{X_{2}\}, \{X_{3}\}\}\$   $CT_{2} = \{\{X_{1}, X_{2}, X_{3}\}, \{X_{1}, X_{2}\}, \{X_{1}\}, \{X_{2}\}, \{X_{3}\}\}\$   $CT_{3} = \{\{X_{1}, X_{2}, X_{3}\}, \{X_{1}\}, \{X_{2}\}, \{X_{3}\}\}\$ 

- And assume that  $sup(\{X_1, X_2, X_3\}) = sup(\{X_1, X_2\}) 1$
- KRIMP will never consider  $CT_3$
- But it is possible that  $L(D, CT_3) < L(D, CT_2)$ 
  - => Problem:  $CT_3$  will not be considered
- Solution: pruning in the code table that KRIMP is considering

## **Improvement by Pruning**

#### • When pruning?

- When an itemset *F* is added to the code table
- At line 6 of KRIMP Algorithm

#### Which itemsets have to be tested?

- Only ones for which the usage has decreased
- Because their code length has increased

#### Algorithm 4 Code Table Post-Acceptance Pruning

**Input:** Code tables  $CT_c$  and CT, for a transaction database  $\mathcal{D}$  over a set of items  $\mathcal{I}$ , where  $\{X \in CT\} \subset \{Y \in CT_c\}$  and  $L(\mathcal{D}, CT_c) < L(\mathcal{D}, CT)$ .

**Output:** Pruned code table  $CT_p$ , such that  $L(\mathcal{D}, CT_p) \leq L(\mathcal{D}, CT_c)$  and  $CT_p \subseteq CT_c$ .

1:  $PruneSet \leftarrow \{X \in CT \mid usage_{CT_c}(X) < usage_{CT}(X)\}$  Only itemsets with decreased usage

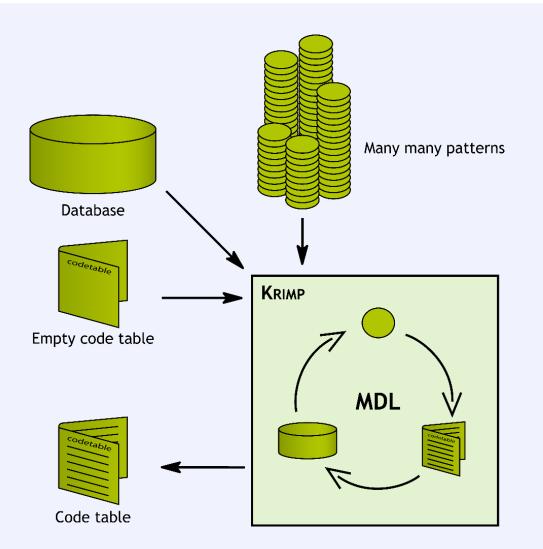
2: while *PruneSet* 
$$\neq \emptyset$$
 do

- 3: PruneCand  $\leftarrow X \in PruneSet$  with lowest  $usage_{CT_c}(X)$   $usage \downarrow = code length \uparrow$
- 4:  $PruneSet \leftarrow PruneSet \setminus PruneCand$
- 5:  $CT_p \leftarrow CT_c \setminus PruneCand$
- 6: if  $\dot{L}(\mathcal{D}, CT_p) < L(\mathcal{D}, CT_c)$  then Compare the length of D without the itemset
- 7:  $PruneSet \leftarrow PruneSet \cup \{X \in CT_p \mid usage_{CT_p}(X) < usage_{CT_c}(X)\}$
- 8:  $CT_c \leftarrow CT_p$
- 9: **end if**

#### 10: end while

11: **return** *CT*<sub>*c*</sub>

# KRIMP



- mine candidates from D
- iterate over candidates
   Standard Candidate Order
- covers data greedily
  - no overlap
  - Standard Code Table Order
- select by MDL
  - better compression? candidates may stay, reconsider old elements

#### So, are KRIMP code tables good?

#### At first glance, yes

- the code tables are characteristic in the MDL-sense
  - they compress well
- the code tables are small
  - they consist of few patterns
- the code tables are specific
  - they contain relatively long itemsets

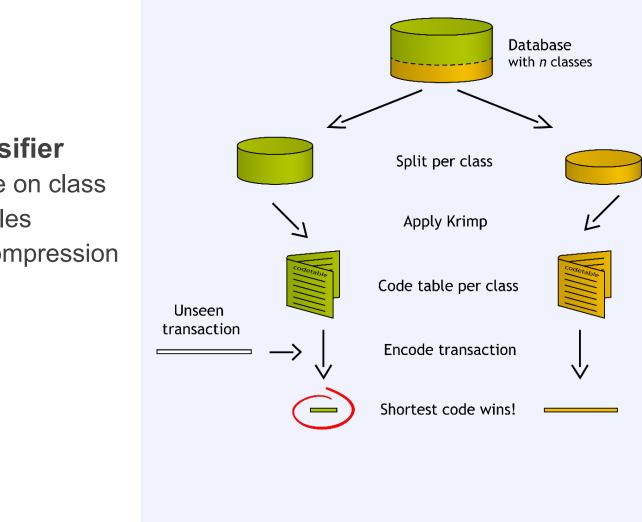
#### But, are these patterns useful?

## The proof of the pudding

#### The quality of the KRIMP code tables was tested by

- classification (ECML PKDD'06)
- measuring dissimilarity (KDD'07, ECML PKDD'15)
- generating data (ICDM'07)
- concept-drift detection (ECML PKDD'08)
- estimating missing values (ICDM'08)
- clustering (ECML PKDD'09)
- sub-space clustering (CIKM'09)
- anomaly detection (SDM'11, CIKM'12, SDM'17)
- characterising uncertain 0-1 data (SDM'11)
- tag-recommendation (IDA'12)
- Web semantic (Semantic Web'20)

## Example: How to use KRIMP for Classification



- The Krimp classifier
  - Split database on class
  - Find code tables
  - Classify by compression

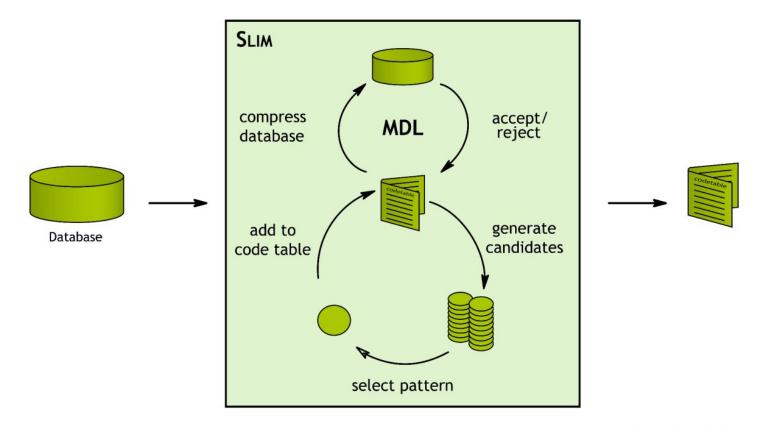
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- Any-time version of KRIMP
- Generate-and-select instead of generate-then-select



(Smets & Vreeken, 2012

# **SLIM** algorithm

### Algorithm 2 The SLIM Algorithm

**Input:** A transaction database  $\mathcal{D}$  over a set of items  $\mathcal{I}$ 

- **Output:** A heuristic solution to the Minimal Coding Set Problem, code table CT
  - 1.  $CT \leftarrow \mathbf{Standard} \ \mathbf{Code} \ \mathbf{Table}(\mathcal{D})$
  - 2. for  $F \in \{X \cup Y : X, Y \in CT\}$  in Gain Order do usage
  - 3.  $CT_c \leftarrow (CT \oplus F)$  in Standard Cover Order
  - 4. if  $L(\mathcal{D}, CT_c) < L(\mathcal{D}, CT)$  then  $|X| \downarrow supp_D(X) \downarrow$  Lexicographically  $\uparrow$
  - 5.  $CT \leftarrow post-prune(CT_c)$
  - 6. **end if**
  - 7. end for

8. return CT

Note: At line 2 a list of the top-k candidates is kept in case the selected candidate fails the test at line 4

## SLIM: example (with simplifications)

<ul> <li>Let us assume</li> </ul>	transactions	description
<ul> <li>A set of items I={A, B, C, D}</li> </ul>	T1	ABC
<ul> <li>And a database D</li> </ul>	T2	BCD
	Т3	AB
	Τ4	ВC

T5

#### Apply 2 steps of the loop of SLIM on D

- For a sake of simplicity
  - No postpruning

Memo: Length(t) =  $-\log 2(\frac{usage(t)}{\Sigma_{y \in CT} usage(y)})$ 

Memo
-log2(5/12) = 1.26
-log2(3/12) = 2
-log2(2/12) = 2.58
-log2(3/9)=1.58
-log2(2/9) = 2.16
-log2(1/9) = 3.16

В

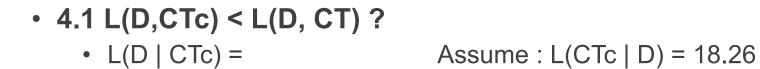
D

• 1. Computation of the standard code table

	pattern	support	usage	usage list	length	code
CT = ST =						

 2.1 Selection of a candidate F as the union of 2 elements of CT

• 3.1 Computation of the new CTc



• L(D | CT) = Assume : L(CT | D) = 15.16

 2.2 Selection of a candidate F as the union of 2 elements of CT

• 3.1 Computation of the new CTc

- 4.1 L(D,CTc) < L(D, CT) ?
  - L(D | CTc) =

assume L(CTc | D) = 25.74

## SLIM

#### Characteristics

- Any-time algorithm
- It considers at each step the refinement of the CT that provides most gain
  - Thanks to heuristics
- Parameter-free (no minsup)

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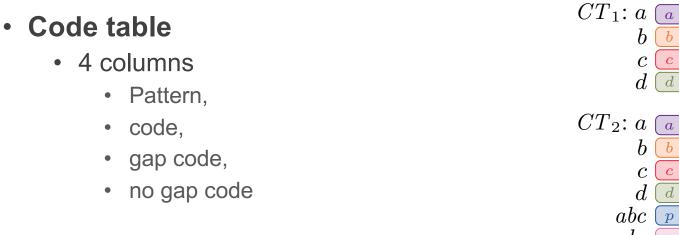
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- SQS read « squeeze »
- MDL for sequences

# Data $D: \underline{a, b, d, c, a, d, b, a, a, b, c}$

## **MDL** for event sequences

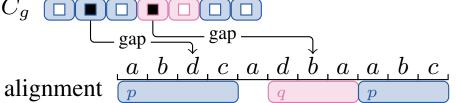


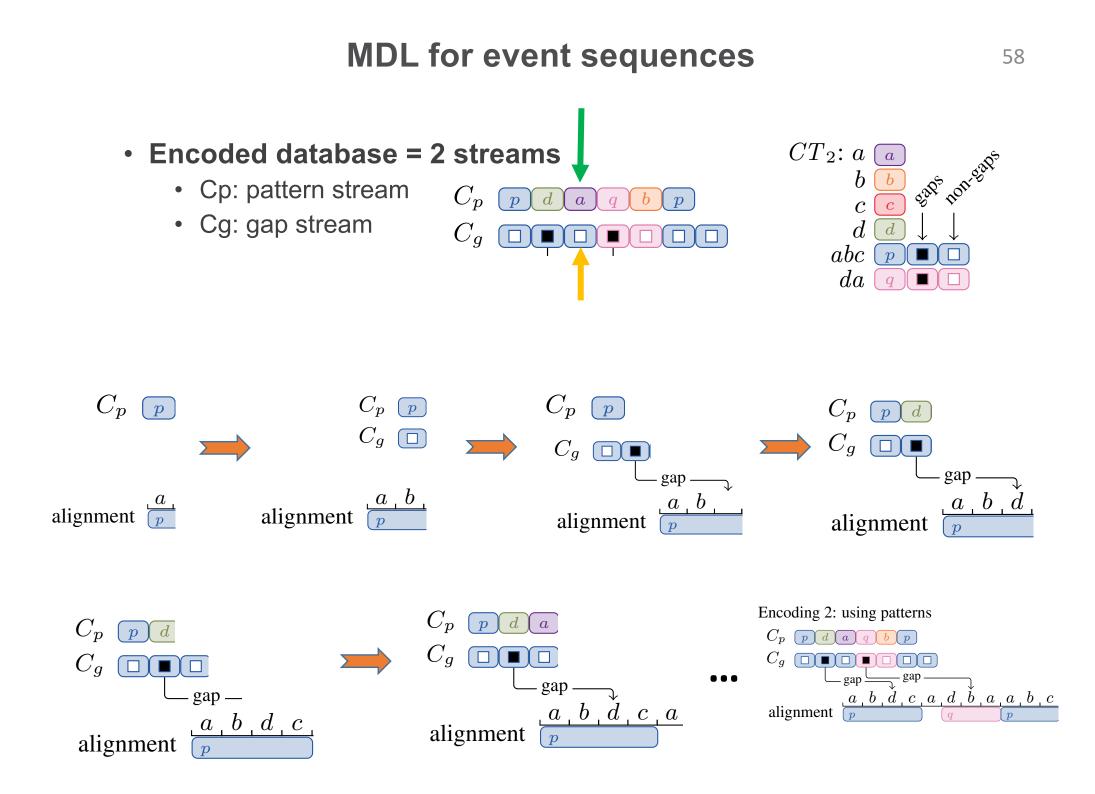
- Encoded database = 2 streams
  - Cp: pattern stream
  - Cg: gap stream

Encoding 1: using only singletons

 $C_p$  abd c ad b a a b c

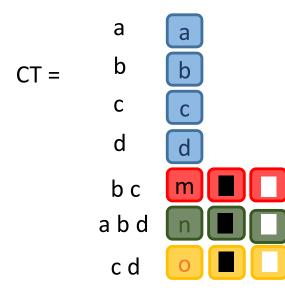
# Encoding 2: using patterns $C_p \quad p \quad d \quad a \quad q \quad b \quad p$ $C_g \quad \Box \quad \Box \quad \Box \quad \Box \quad \Box$

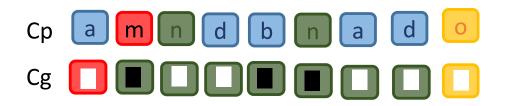




#### Exercise

- Let us consider the following code table and the following streams
- Give the decoded sequence





## SQS

#### **Encoding length**

• Patterns

$$L(code_p(X) \mid CT) = -\log\left(\frac{usage(X)}{\sum_{Y \in CT} usage(Y)}\right)$$

- Let
  - gaps(X) = number of gaps in the usage of pattern X
  - *fills*(*X*) = number of non-gaps in the usage of pattern X

• Note: 
$$fills(X) = usage(X)(|X| - 1)$$

• Gaps

$$L(code_g(X) \mid CT) = -\log\left(\frac{gaps(X)}{gaps(X) + fills(X)}\right)$$

• Non-gaps

$$L(code_n(X) \mid CT) = -\log\left(\frac{fills(X)}{gaps(X) + fills(X)}\right)$$

#### **Encoding length**

• Pattern stream

$$L(C_p \mid CT) = \sum_{X \in CT} usage(X)L(code_p(X))$$

• Gap stream

$$L(C_g \mid CT) = \sum_{\substack{X \in CT \\ |X| > 1}} \left( gaps(X)L(code_g(X)) + fills(X)L(code_n(X)) \right)$$

• Database D with a code table CT

$$L(D \mid CT) = L_{\mathbb{N}}(|D|) + \sum_{S \in D} L_{\mathbb{N}}(|S|) + L(C_p \mid CT) + L(C_g \mid CT)$$

$$464$$

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## SQS (optional)

#### Just for information but not to learn: encoding of the code table

• Length of a pattern X

$$L(X, CT) = L_{\mathbb{N}}(|X|) + L_{\mathbb{N}}(gaps(X) + 1) + \sum_{x \in X} L(code_p(x \mid ST))$$

#### Length of the code table

 $L(CT \mid C) = L_{\mathbb{N}}(|\Omega|) + L_U(||D||, |\Omega|) +$ 

$$L_{\mathbb{N}}(|\mathcal{P}|+1) + L_{\mathbb{N}}(usage(\mathcal{P})+1) +$$

$$L_U(usage(\mathcal{P}), |\mathcal{P}|) + \sum_{X \in \mathcal{P}} L(X, CT)$$

## **SQS-CANDIDATES**

#### Same idea as KRIMP

- Input:
  - a set of candidate patterns extracted by an other pattern mining algorithm
- Method
  - Try to add one by one each candidate and see if the compression is better

```
Algorithm 3: SQS-CANDIDATES(\mathcal{F}, D)input : candidate patterns \mathcal{F}<br/>output : set of non-singleton patterns \mathcal{P} that heuristically<br/>minimise the Minimal Code Table ProblemSort patterns1 order patterns X \in \mathcal{F} based on L(D, \{X\});<br/>2 \ \mathcal{P} \leftarrow \emptyset;<br/>3 foreach X \in \mathcal{F} in order doWith pattern, gain?4if L(D, \mathcal{P} \cup X) < L(D, \mathcal{P}) then<br/>5\mathcal{P} \leftarrow \mathsf{PRUNE}(\mathcal{P} \cup X, D, \mathsf{false}); Pruning step6 \ \mathcal{P} \leftarrow \mathsf{PRUNE}(\mathcal{P}, D, \mathsf{true});<br/>7 \text{ order patterns } X \in G by L(D, \mathcal{P}) - L(D, \mathcal{P} \setminus X);<br/>8 return \mathcal{P};
```

#### **SQS-SEARCH**

#### • Same idea as SLIM

- Any-time algorithm
- Free-parameter

A	Algorithm 6: SQS-SEARCH(D)
	<b>input</b> : database $D$
	<b>output</b> : significant patterns $\mathcal{P}$
1	$\mathcal{P} \leftarrow \emptyset; A \leftarrow \mathrm{Sqs}(D, \emptyset);$
2	while changes do
3	$  \mathcal{F} \leftarrow \emptyset;$
4	foreach $P \in CT$ do add ESTIMATE $(P, A, D)$ to $\mathcal{F}$ ;
5	foreach $X \in \mathcal{F}$ ordered by the estimate do
6	<b>if</b> $L(D, \mathcal{P} \cup X) < L(D, \mathcal{P})$ then
7	$ \qquad \qquad$
8	<b>if</b> X is added <b>then</b> test recursively X augmented with
	events occurring in the gaps;
9	$\mathcal{P} \leftarrow PRUNE(\mathcal{P}, D, true);$
	order patterns $X \in G$ by $L(D, \mathcal{P}) - L(D, \mathcal{P} \setminus X)$ ;
11	
11	return $\mathcal{P}$ ;

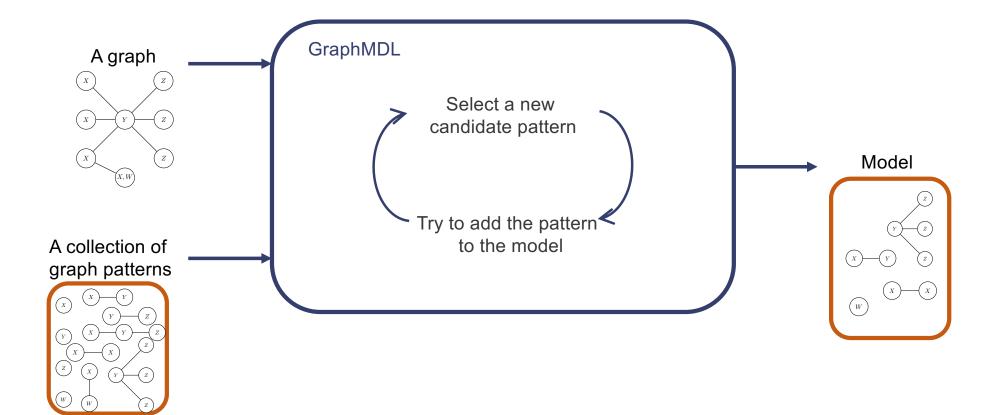
# Outline

#### 1. Introduction

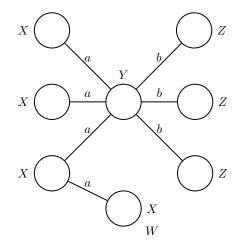
#### 2. Compression based approaches

- 1. Motivations
- 2. Information theory and the MDL principle
  - Information theory
  - The MDL principle for pattern mining
- 3. Algorithms
  - Itemsets: Krimp (and SLIM)
  - Sequences: SQS
  - Graphs: GraphMDL
- Conclusion

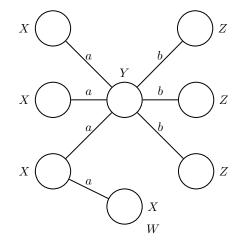
## GraphMDL [IDA'20]

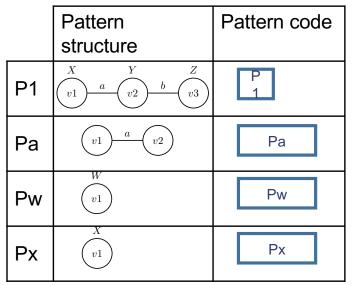


• Graph

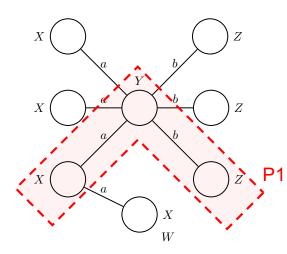


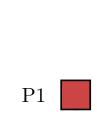
• Graph

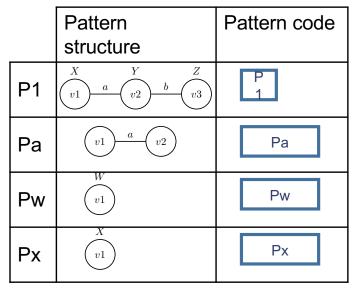




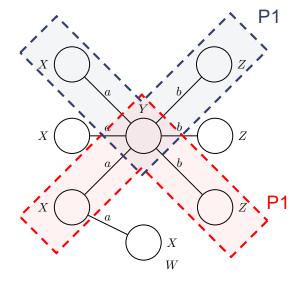
• Graph

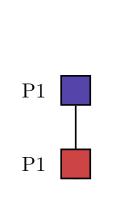


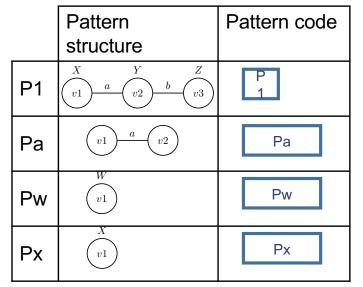




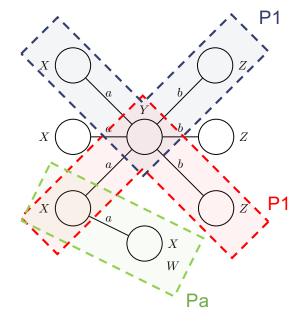
• Graph

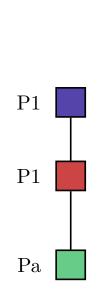


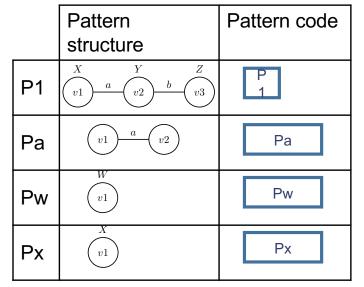




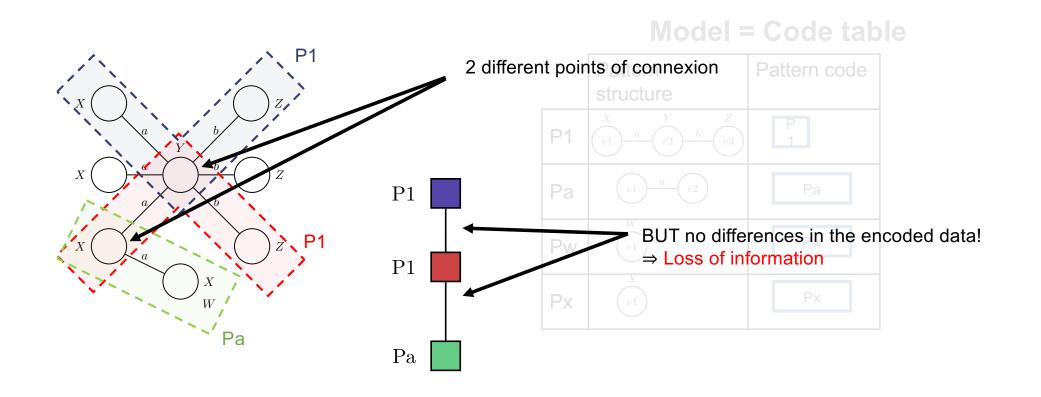
• Graph





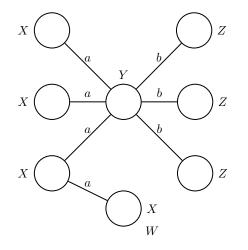


• Graph



## **GraphMDL: Ports**

• Graph



#### Model = Code table

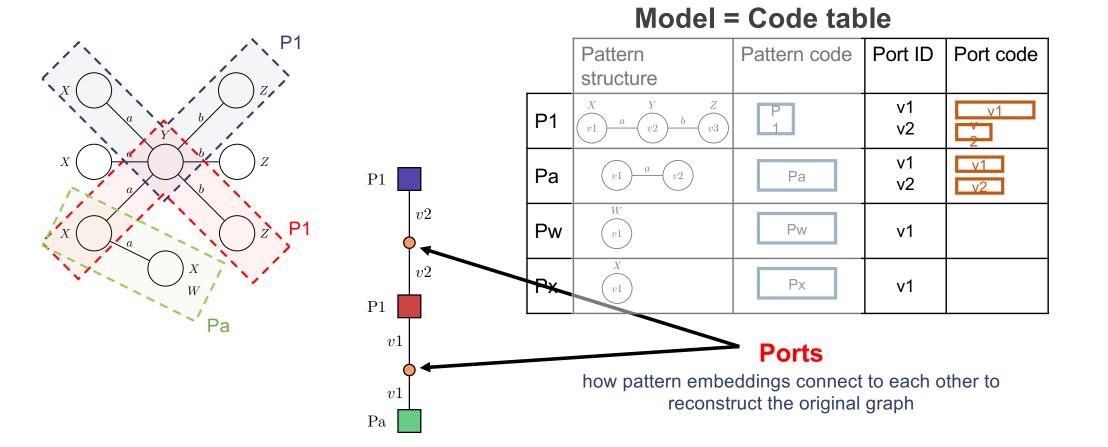
	Pattern	Pattern code	Port ID	Port code
	structure			
P1	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	P 1	v1 v2	v1 Ž
Ра		Pa	v1 v2	v1 v2
Pw		Pw	v1	
Px	X v1	Px	v1	

#### **Ports**

how pattern embeddings connect to each other to reconstruct the original graph

## **GraphMDL: Ports**

• Graph



# **GraphMDL: Experiments**

#### • 3 datasets

- AIDS-CA, AIDS-CM: about molecules (few labels, many cycles)
  - National Cancer Institute AIDS antiviral sceen data
- UD-PUD-En: about dependency trees of english sentences (many labels, no cycles)
  - Universal dependencies project

Quantitative resul	Dataset <b>tS</b>	gSpan minsup	# Candidate patterns input	# Selected patterns output
	AIDS-CA	20%	2194	115
	AIDS-CA	15%	7867	123
	AIDS-CA	10%	20596	148
	AIDS-CM	20%	433	111
	AIDS-CM	15%	779	131
	AIDS-CM	10%	2054	163
	AIDS-CM	5%	9943	225
	UD-PUD-En	10%	164	162
	UD-PUD-En	5%	458	249
	UD-PUD-En	1%	6021	523
	UD-PUD-En	0%	233434	773

Drastic reduction

• Relatively stable in the number of selected patterns

# GraphMDL+

#### • GraphMDL+ as SLIM and SQS-Search

- Generate-and-select algorithm
- Any-time algorithm
- Free-parameter

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# If we have time Mining Periodic Patterns with a MDL Criterion

Esther Galbrun, Peggy Cellier, Alexandre Termier, Bruno Crémilleux

## Conclusions

- MDL is great for picking important and useful patterns
- KRIMP, SQS, GRAPHMDL approximate the MDL ideal very well
  - vast reduction of the number of itemsets
  - works for other pattern types equally well: itemsets, sequences, streams
- Local patterns and information theory
  - naturally induce good classifiers, clusterers, distance measures
  - with instant characterisation and explanation,
  - and, without (explicit) parameters

## Conclusions

#### When using MDL for pattern mining

- Question 1: what kind of model to use?
  - Data modelisation
- Question 2: how to encode the database? the model?
  - Information theory
- Question 3: how to find the « best » (or at least one good) model?
  - Algorithmic

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