## Making Sense of (Multi-)Relational Data

Part II: Exploration through targeted patterns
Jefrey Lijffijt
Eirini Spyropoulou

## Tijl De Bie

## Approaches

- Safarii / "Multi-Relational Data Mining"
- RDB-Krimp
- Inductive Logic Programming


## Safarii / "Multi-Relational Data Mining"

## Data

- Relational database / E-R model


| Atom |  |  |
| :---: | :---: | :---: |
| id | mol_id | element |
| 1 | 1 | C |
| 2 | 1 | O |
| 3 | 1 | O |
| 4 | 2 | H |
| 5 | 2 | H |
| 6 | 2 | O |
|  |  |  |

Knobbe (2004)
Bond

| id | atom1 | atom2 | type |
| :---: | :---: | :---: | :---: |
| 1 | 1 | 2 | double |
| 2 | 1 | 3 | double |
| 3 | 4 | 6 | single |
| 4 | 5 | 6 | single |
|  |  |  |  |

Figure 3.2 Relational representation of $\mathrm{CO}_{2}$ and $\mathrm{H}_{2} \mathrm{O}$.

## Data

- Relational database / E-R model



## Example pattern

- Pattern =
all molecules with
at least one bond and a $C$ atom


Knobbe (2004)

Pattern syntax

- Individuals are records in the target table, along with its associations and associated parts
- The units which we want to predict/describe
- A subgroup is a set of individuals


## Pattern syntax

- Pattern = subgroup = selection graphs


Pattern syntax

- Pattern = subgroup = selection graphs
- Mining is then refinement of selection graphs
- Conditioning: choose subset of values ( $=, \geq, \leq$ )
- Association: add an association


## Pattern syntax

- Simple case: condition \& association refinement


Pattern syntax

Molecule

| id | name |
| :---: | :---: |
| 1 | $\mathrm{CO}_{2}$ |
| 2 | $\mathrm{H}_{2} \mathrm{O}$ |
|  |  |

Knobbe (2004)

| Atom |  |  |
| :---: | :---: | :---: |
| id | mol id | element |
| 1 | 1 | C |
| 2 | 1 | O |
| 3 | 1 | O |
| 4 | 2 | H |
| 5 | 2 | H |
| 6 | 2 | O |
|  |  |  |

Bond

| id | atom1 | atom2 | type |
| :---: | :---: | :---: | :---: |
| 1 | 1 | 2 | double |
| 2 | 1 | 3 | double |
| 3 | 4 | 6 | single |
| 4 | 5 | 6 | single |
|  |  |  |  |

Figure 3.2 Relational representation of $\mathrm{CO}_{2}$ and $\mathrm{H}_{2} \mathrm{O}$.

## Implementation of MRDM: Safarii

- Relational association rule discovery
- Find refinements using aggregation
- Categorical: select an attribute-value
- Numerical: exists $\leq, \geq$, $\min \leq, \max \geq$
- These are SQL primaries, there are many more possibilities

Algorithmic approach

- Restrict \# associations, \# refinements
- Generate SQL queries, push workload to DB
- Aggregation is greedy
- Choose only optimal split at runtime
- Essentially a form of local discretisation


## Algorithmic approach

## Knobbe (2004)

- Patterns are also SQL queries


```
SELECT DISTINCT TO.id
FROM molecule T0, bond T1, atom T2
WHERE TO.id = T1.molecule_id and TO.id = T2.molecule_id
AND T2.element = 'C'
```


## Interestingness

- Several objective interestingness measures
- support $(S \rightarrow T)=P(S T)$
- coverage $(S \rightarrow T)=P(S)$
- accuracy $(S \rightarrow T)=P(T \mid S)$
- $\operatorname{specificity~}(S \rightarrow T)=P(\neg S \mid \neg T)$
- sensitivity $(S \rightarrow T)=P(S \mid T)$
- novelty $(S \rightarrow T)=P(S T)-P(S) \cdot P(T)$


## Interestingness

- Several objective interestingness measures
- Steer aggregation
- Rank rules


## Predicting bad loans

Knobbe (2004)

## RDB-Krimp

## Data

- Relational database / E-R model
- Table defined as: key, foreign keys, attributes
- Categorical attributes only


## Koopman \& Siebes (2009)

| $\mathbf{T}^{\mathbf{i}}$ |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{K}^{\mathbf{i}}$ | $\mathrm{F}_{\mathrm{j}}$ | $\mathrm{A}^{\mathrm{i}}{ }_{1}$ | $\mathrm{~A}^{\mathrm{i}}{ }_{2}$ |  |  |
| k | k | $\mathrm{k}_{\mathrm{j}}$ | $\mathrm{V}_{1}$ |  |  |


| $\mathbf{T}^{\mathbf{2}}=$ LOAN |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| loan ID | account | Date | Amount | Duration | Payment |  |
| 30 | 10 | I $06 / 2008$ | 10245 | 12 | A |  |
| 31 | 10 | $09 / 2008$ | 13722 | 24 | B |  |
| 32 | 11 | $08 / 2006$ | 27313 | 36 | B |  |
| 33 | 12 | $09 / 2006$ | 27147 | 12 | B |  |
| 34 | 12 | $05 / 2008$ | 27194 | 36 | D |  |
| 35 | 13 | $09 / 2008$ | 30289 | 12 | B |  |
| 36 | 13 | $06 / 2008$ | 18203 | 12 | C |  |


| $\mathrm{T}^{3}=\mathbf{O R D E R}$ |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ordern ${ }_{\text {ID }}$, account ${ }_{\text {ID }}$, Bank-To, Amount-To, Amount , Type |  |  |  |  |  |  |  |  |  |  |
| 20 | 1 | 10 | 1 | ST | I | 141 |  | 1000 |  | UVER |
| 21 | 1 | 10 | 1 | QR | I | 359 |  | 2000 |  | SIPO |
| 22 | 1 | 11 | 1 | YZ | 1 | 850 |  | 1000 |  | SIPO |
| 23 | I | 13 | 1 | ST | 1 | 283 |  | 1000 |  | NULL |
| 24 | 1 | 13 |  | OP |  | 850 |  | 2000 |  | SIPO |


| $\mathbf{T}^{4}=$ DISPOSITION |  |  |  |
| :---: | :---: | :---: | :---: |
| dispID | account ID | Type |  |
| 40 | 1 | 10 | OWNER |
| 41 | 11 | DISPONENT |  |
| 42 | 11 | OWNER |  |
| 43 | 12 | DISPONENT |  |
| 44 | 12 | OWNER |  |

## Pattern syntax

- Given a target table $T$ with key $K$
- Pattern =
selection of attribute values (conj + disj) of $T$
\& selection of attribute values (conj + disj) for tables with $K$ as foreign key


## $P_{1}$ : ACCOUNT(\{ Frequency $\left.=2\right\}$ )

[ [ ORDER(\{ Bank-To=ST, Amount=1000 \}), ORDER(\{ Amount=2000, Type=SIPO \}) ],
[ [ LOAN(\{ Date='06/2008', Duration=12 \}), LOAN(\{ Date='09/2008', Payment=B \}) ] ]
$P_{2}$ : ACCOUNT $(\{$ Frequency $=3\})$
[ [ DISPOSITION(\{ Type = Disponent \}), DISPOSITION(\{ Type = Owner \}) ] ]
frequency $\left(P_{1}\right)=2, \operatorname{count}\left(P_{1}\right)=10, \operatorname{size}\left(P_{1}\right)=9$
frequency $\left(P_{2}\right)=2, \operatorname{count}\left(P_{2}\right)=6, \operatorname{size}\left(P_{2}\right)=3$
Partially Covered Database

| $\mathbf{T}^{\mathbf{1}}=$ ACCOUNT |  |  |
| :---: | :---: | :---: |
| account $_{\text {ID }}$ | Frequency | Date |
| 10 | 2 | $06 / 2007$ |
| 11 | 3 | $03 / 2006$ |
| 12 | 3 | $08 / 2006$ |
| 13 | 2 | $03 / 2006$ |
| 14 | 1 | $05 / 2008$ |
| 15 | 3 | $03 / 2006$ |
| 16 | 2 | $06 / 2007$ |


| $\mathbf{T}^{\mathbf{2}}=$ LOAN |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| loan $_{\text {ID }}$ | account $_{\text {ID }}$ | Date | Amount | Duration | Payment |  |
| 30 | 10 | $06 / 2008$ | 10245 | 12 | A |  |
| 31 | 10 | $09 / 2008$ | 13722 | 24 | B |  |
| 32 | 11 | $08 / 2006$ | 27313 | 36 | B |  |
| 33 | 12 | $09 / 2006$ | 27147 | 12 | B |  |
| 34 | 12 | $05 / 2008$ | 27194 | 36 | D |  |
| 36 | 13 | $06 / 2008$ | 18203 | 12 | C |  |
| 35 | 13 | $09 / 2008$ | 30289 | 12 | B |  |


| T ${ }^{3}=$ ORDER |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  | Amount-To | Amount | Type |
| 20 | 1 | 10 | $1 / \mathrm{ST} / 1$ | 141 | 11000 / | UVER |
| 21 | 1 | 10 | QR | 359 | 1/2000/ | SÍPO $/$ |
| 22 | 1 | 11 | 1 YZ | 850 | , 1000 | SIPO |
| 23 | 1 | 13 | YST/ | 283 | $1 / 1000 / 1$ | NULL |
| 24 | 1 | 13 | 1 OP | 850 | 12000 | SIPO/ |


| $\mathbf{T}^{4}=$ DISPOSITION |  |  |  |
| :---: | :---: | :---: | :---: |
| dispID | account ID | Type |  |
| 40 | 10 | OWNER |  |
| 41 | 11 | DISPONENT |  |
| 42 | 11 | OWNER |  |
| 43 | 1 | 12 |  |$:$ DISPONENT

Algorithmic (enumeration) approach

- Run FARMER for every table in DB as target
- FARMER (Nijssen \& Kok, 2003) is an ILP algorithm for enumeration of frequent 'queries'
- Exhaustive search with minsup threshold


## Interestingness

- Main contribution of RDB-Krimp
- Find concise set of local patterns that together describe the DB well
$\rightarrow$ Minimum Description Length principle
- Two part code L(H) + L(D|H)


## Interestingness

- Greedy approximation algorithm:

1. Initialise pattern set as all singletons
2. Try insert patterns one by one

- Keep if total description length decreases
- No guarantees on optimality

Candidate Set Growth


Code Table Growth


## Inductive Logic Programming

## (Probabilistic) Inductive Logic Programming

- Field of research
- Also related to / equivalent with probabilistic logic learning, statistical relational learning, logical and relational learning
- Ultra brief review
- We are not experts
- Too much to cover


## Data

- Logical representation
- Also an E-R model ?

Pattern syntax

- Generalises all pattern mining syntaxes discussed here
- Can derive predicates (rules)
- Can have no antecedent $\rightarrow$ association but not 'rule'
- Terms can be variables rather than constants
daughter(C, P) :- female(C), mother(P, C)
[De Raedt \& Kersting, 2008]

Algorithmic approach

- Very different terminology
- Logic, but
- Various frameworks (entailment, interpretations, proofs)
- Also based on 'generality' (= monotonicity)
- Search can easily become very costly


## Interestingness

- Objective interestingness measures have been employed
- Frequency
- Confidence
- ...


## De Raedt (2008)

## Case I:Structure Activity Relationship Prediction

Actıve

nitrofurazone


4-nitropenta[cd]pyrene
[Srinivasan et al.AlJ 96]

Structural alert:

Inactive


6-nitro-7,8,9,10-tetrahydrobenzo[a]pyrene


4-nitroindole

Data $=$ Set of Small Graphs

## Dehaspe's Warmr ~ Apriori

## PARTICIPANT Table

| NAME | JOB | COMPANY | PARTY | R_NUMBER |
| :---: | :---: | :---: | :---: | :---: | :---: |
| adams | researcher | scuf | no | 23 |
| blake | president | jvt | yes | 5 |
| king | manager | ucro | no | 78 |
| miller | manager | jvt | yes | 14 |
| scott | researcher | scuf | yes | 94 |
| turner | researcher | ucro | no | 81 |


| COMPANY Table |  |
| :---: | :---: |
| COMPANY | TYPE |
| jvt | commercial |
| scuf | university |
| ucro | university |

COURSE Table

| COURSE | LENGTH | TYPE |
| :---: | :---: | :---: |
| cso | 2 | introductory |
| erm | 3 | introductory |
| so2 | 4 | introductory |
| srw | 3 | advanced |


| SUBSCRIPTION Table |  |
| :---: | :---: |
| NAME | COURSE |
| adams | erm |
| adams | so2 |
| adams | srw |
| blake | cso |
| blake | erm |
| king | cso |
| king | erm |
| king | so2 |
| king | srw |
| miller | so2 |
| scott | erm |
| scott | srw |
| turner | so2 |
| turner | srw |

- Knobbe, Arno (2004). Multi-Relational Data Mining. PhD Thesis, Utrecht University.
- Koopman, Arne \& Siebes, Arno (2009). "Characteristic Relational Patterns". In Proc. of KDD 2009, pp 437-446, ACM, New York.
- De Raedt, Luc \& Kersting, Kristian (2008). Probabilistic Inductive Logic Programming, Springer.
- De Raedt, Luc (2007). "Logic, Probability and Learning". Tutorial at ACAI.
- De Raedt, Luc (2008). "Logical and Relational Learning Revisited". Tutorial at ICML.

