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Research Foundation Flanders ening new horizons



European Research Council

<u>OUTLINE</u>

Formalizing pattern mining

Case studies – Graph patterns – Subgroups – Visualizations

Open challenges

Summary



2

<u>A FORMALISATION OF</u> <u>PATTERN MINING</u>





4

Itemset: co-occurring attributes in binary data



Itemset: co-occurring attributes in binary data Association rule: locally 'predict' values of other attributes



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Clustering? Regression? Probabilistic model?



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Clustering? Regression? Probabilistic model?



. . .

Patterns specify some aspect of the data

Data \hat{X}



Lijffijt et al. 2010, De Bie 2011

Data \hat{X}

Data space Ω

- -Every $X \in \Omega$ is a value combination what could be \hat{X}
- $\, \hat{X}$ is constant, but we do not know the values



Lijffijt et al. 2010, De Bie 2011

what could be \hat{X} ne values

Data \hat{X}

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- -Every $X \in \Omega$ is a value combination what could be X
- -X is constant, but we do not know the values
- Pattern P is a set $P \subseteq \Omega$ s.t. $\hat{X} \in P$
- —That is, it may limit the possibilities for \hat{X}



Lijffijt et al. 2010, De Bie 2011



UNIFIED VIEW OF PATTERNS Data \hat{X} G = (V, E)

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UNIFIED VIEW OF PATTERNS Data \hat{X} G = (V, E)

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5

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In case V is known



UNIFIED VIEW OF PATTERNS Data \hat{X} G = (V, E) -Every $X \in \Omega$ is a value combination what could be X

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Certain edges that do or do not exist

Lijffijt et al. 2010, De Bie 2011

In case V is known



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6

UNIFIED VIEW OF PATTERNS Data \hat{X} – Data matrix

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6

UNIFIED VIEW OF PATTERNS Data \hat{X} – Data matrix

Data space Ω – All possible value combinations

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UNIFIED VIEW OF PATTERNS Data \hat{X} \checkmark Data matrix

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Range, moment, correlation, clustering, ...

Lijffijt et al. 2010, De Bie 2011

INTERESTINGNESS OF PATTERNS



Suppose: aim is to inform the user about the data



Suppose: aim is to **inform** the user about the data

Form of communication -Computer \xrightarrow{P} user



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Form of communication -Computer \xrightarrow{P} user



Central premise of pattern mining: Patterns can provide *information* in a compressed form

Suppose: aim is to **inform** the user about the data

Form of communication -Computer \xrightarrow{P} user

How to optimize this communication? \approx Maximal structure in minimal time



Central premise of pattern mining: Patterns can provide information in a compressed form

INFORMATION THEORETIC APPROACH

Pattern contains information

– What we really learn about data

Pattern has a descriptional complexity – How time consuming is it to internalize





De Bie 2011, 2013

9

INFORMATION THEORETIC APPROACH

Learning is being surprised –What we learn depends on what we know/expect

In particular, need to define Pr(P)

– Typically from mass or density function over Ω

Used a lot in data mining, but often implicitly – Models for random graphs, sequences, matrices, ...





De Bie 2011, 2013

BACKGROUND MODEL

Pr(P) is called the background model (or distribution)

- Many options
- Maximum Entropy model Tatti 2008, De Bie 2011
- Randomization Gionis et al. 2006, Lijffijt et al. 2014
- Other probabilistic models





BACKGROUND MODEL

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- Maximum Entropy model Tatti 2008, De Bie 2011
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- Other probabilistic models



Many options

Explicitly neutral model given certain expectations

BACKGROUND MODEL: EXAMPLE

Pr(P) is called the background model (or distribution)

Given a graph G = (V, E), and Ω all possible E –Without knowledge: MaxEnt dist. is Uniform over Ω -Given degree for every vertex: find MaxEnt dist. through optimization





BACKGROUND MODEL: EXAMPLE

Pr(P) is called the background model (or distribution)

Given a graph G = (V, E), and Ω all possible E –Without knowledge: MaxEnt dist. is Uniform over Ω -Given degree for every vertex: find MaxEnt dist. through optimization

Cannot do arbitrary constraints, but many types of expectations lead to tractable parameter inference



THE FORMALIZATION

Recall: pattern P is a set $\hat{X} \in P \subset \Omega$

Information Content (IC) of P is -log(Pr(P))

Description Length (DL) of P depends on syntax

Subjective Interestingness (SI) of *P* is $\frac{IC(P)}{DL(P)}$





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De Bie 2011, 2013

Derived from information gain

13

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Rate at which we gain information



De Bie 2011, 2013

Derived from information gain
THE FORSIED PROCESS

- 1. Background model
- 2. Pattern syntax
 - -IC & DL of patterns
- 3. Mining
- 4. Update background model
- 5. Iterative mining



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CONNECTIONS IN RELATIONAL DATA





RELATIONAL DATA

Example: Amazon ratings





Subject

RELATIONAL DATA

Example: Amazon ratings



Patterns like "Many customers rate all seven volumes of Harry Potter highly, which all belong to Fantasy and Fiction"



Subject

Fully connected set of entities







INFORMATION CONTENT

'Compression' due to fully connectedness -Only have to communicate vertices: $P \subseteq V$

If background model factorizes over edges:

$$IC(P) = \sum_{(v,w)\in P\times P} Pr((v))$$



(v, w))

DESCRIPTION LENGTH

Proportional to number of vertices:

$\mathrm{DL}(P) = \gamma |P| + \eta$

NB. Absolute values for SI are irrelevant, only ranking matters. Hence either parameter can be constant





RMiner: exhaustive candidate enumeration Spyropoulou et al. 2014 Constraint programming version: branch and bound

CP works well, but scalability remains an issue No heuristic algorithms developed yet



Guns et al. 2016

<u>CONNECTING TREES IN</u> <u>GRAPHS</u>



<u>EXAMPLE</u>







Given a query Q, integer k

- Pattern: arborescence of height $\leq k$ that connects Q
- -All leafs must be query nodes
- -May not exist



Given a query Q, integer k

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- All leafs must be query nodes
- -May not exist







QUANTIFICATION

Idea: tree is informative if

- -(links to) vertices are unexpected
- -vertices share parents







Non-informative

Non-minimal

Minimal and informative



QUANTIFICATION

Information Content like before

$$IC(P) = \sum_{(v,w)\in P\times P} Pr((v$$

Communicate (new) vertices + parent for each vertex

$$DL(T) = (|V_T| - |Q| + 1) \log(|V| - |Q| + 1) + |$$



(, w))

$|V_T| \log(|V_T| + 1)$



Heuristic construction of trees

-Not so straightforward to greedily construct a tree

Background distribution for growing graph: – Vertices can only have links to older vertices Parameter inference through intelligent grouping



EXAMPLE RESULT: KDD BEST PAPERS





The Nested Chinese Restaurant process and...

Reducing the sampling complexity of topic models

Topic models with power-law...

Reducing the sampling complexity of topic models

SUBGROUP DISCOVERY IN NUMERIC DATA





EXAMPLE



 $\widehat{\blacksquare}$ GHENT UNIVERSITY Lijffijt et al. under review

Condition $Z \rightarrow$ means are $f(\hat{X}_Z)$

Condition $Z \rightarrow$ variance in direction w is $g(\hat{X}_Z, w)$



Lijffijt et al. under review

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Condition $Z \rightarrow$ means are $f(\hat{X}_Z)$ Condition $Z \rightarrow$ variance in direction w is $g(X_Z, w)$



Condition: areas with few children

Lijffijt et al. under review

UANTIFICATION

Surprisal of the location

Surprisal of the spread

$$\operatorname{IC}(f(\hat{X}_Z)) = \log\left((2\pi)^d |\Sigma_Z|\right) / 2 + \left(f_Z^{d} |\Sigma_Z|\right) / 2 + \left(f_Z^{d}$$

 $\operatorname{IC}(g(\hat{X}_Z, w)) \approx \log\left(2^{\frac{m}{2}}\Gamma(m/2)\right)$

Description length

 $DL(\cdot) = \gamma |Cond|(+\gamma) + \eta$



$$f(\hat{X}_Z - \mu_Z)^T \Sigma_Z^{-1} \left(f(\hat{X}_Z - \mu_Z) \right) / 2$$

 $+\alpha - (m/2 - 1) \log \left(\left(g(\hat{X}_Z, w - \beta) / \alpha \right) + \left(g(\hat{X}_Z, w - \beta) / (2\alpha) \right) \right)$

ANTIFICATION

Surprisal of the location

Surprisal of the spread

 $\operatorname{IC}(g(\hat{X}_Z, w)) \approx \log\left(2^{\frac{m}{2}}\Gamma(m/2)\right)$

Description length

 $DL(\cdot) = \gamma |Cond|(+\gamma) + \eta$



 $IC(f(\hat{X}_{Z})) = \int D_{Z} \int$ $+\alpha - (m/2 - 1) \log \left(\left(g(\hat{X}_Z, w - \beta) / \alpha \right) + \left(g(\hat{X}_Z, w - \beta) / (2\alpha) \right) \right)$

ANTIFICATION

Surprisal of the location

Surprisal of the spread

$$IC(g(\hat{X}_Z, w)) \approx \log\left(2^{\frac{m}{2}}\Gamma(r) + \alpha - (m/2 - 1)\log\left(\left(g(\hat{X}_Z, w)\right)\right)\right)$$

Description length

 $DL(\cdot) = \gamma |Cond|(+ \gamma)|Cond|(+ \gamma$

Weigth times number of conditions + constant (+spread has one term more than location)



 $IC(f(\hat{X}_{Z})) = \int D_{Z} \int$ m/2)) $\hat{X}_Z, w - \beta \left(/ \alpha \right) + \left(g(\hat{X}_Z, w - \beta) / (2\alpha) \right)$

$$\gamma) + \eta$$



Finding subgroups:

Beam-search through off-the-shelf toolbox (Cortana)

Finding weight vector for spread pattern: Manifold learning toolbox (ManOpt)



Lijffijt et al. under review

VISUALIZATIONS AS PATTERNS





Synthetic Data Case Study









	3	4	5	6	7	8	9	10
H-	2.80+-	4.00e- 7	-7.5Ce- 7	-1.680- C	-1.13e- 6	-1.88e- G	1.45e- G	7.218-

Weight vector and (approximate) projection



GHENT UNIVERSITY De Bie et al. 2016 Kang et al. 2016 Puolamäki et al. 2016





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Weight vector and (approximate) projection



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De Bie et al. 2016 Kang et al. 2016 Puolamäki et al. 2016

Weight vector and (approximate) projection

15

10

-5

-10

-15

-20

-25







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Weight vector and (approximate) projection



Weight vector and (approximate) projection





Background model inference with gradient descent

Mining patterns is a manifold learning problem — Optimize through toolbox (ManOpt)







THE FORSIED PROCESS

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BACKGROUND MODEL

- How to provide specification as end-user
- -Objective
- -Subjective

Parameter inference (of MaxEnt model)



PATTERN SYNTAX

Should correspond to the task

- Probably constructed by researchers
- –Users need to be able to select appropriate syntax

- Not yet investigated: syntaxes with mixed relevance
- -E.g., for graphs with various vertex types



IC & DL OF PATTERNS

Requires extensive knowledge of maths

Not related to cognition yet in any way



MINE GOOD/BEST PATTERNS

All the usual algorithmic challenges

- -Typically NP-hard
 - Depends on b.g. model and pattern syntax
- Search strategies: greedy, beam search, branch & bound, SGD, black-box optimization
 - Consider bounds / approximability



n syntax rch, branch &

UPDATE BACKGROUND MODEL

Insert what the user has learned

How about forgetting?

What kind of inference capabilities do humans have? -Track remaining degree of vertices in graph, degrees of freedom for projections?



ITERATIVE MINING

May be possible to re-use state of previous mining step

- -E.g., in branch-and-bound
- -Non-overlapping patterns are generally unaffected

Iterative scheme has an 1-1/e bound for greedy -For the budget used so far







A generic approach to define patterns

Information Theory perspective on interestingness

Examples of mining interesting/surprising

- Dense and connecting vertex sets in graphs
- Subgroups in numeric data
- Projections for visualization

Many open challenges remaining



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