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Knowledge discovery from multi-relational data







Knowledge discovery from multi-relational data



Biological knowledge discovery





Automatically discover *surprising* multi-relational "3C" (coalitions, connections, & chains) patterns.



STRUCTURED AND UNSTRUCTURED DATA

We consider **two** types of input data, or 'pattern spaces'

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 $by \ using \ a \ trick$

PATTERNS

Bicluster: connected entity set

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Redescription: bicluster pair identifying (roughly) the same entities for shared domain

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Bicluster: connected entity sets

Redescription: bicluster pair identifying (roughly) the same entities for shared domain

Bicluster Chain: A **chain** of redescriptions

BICLUSTER CHAINS

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SURPRISING PATTERNS

'Just mine biclusters!' - nope.

'Just mine redescriptions!' - better, but still nope.

We are after *chains* of biclusters, such that plots in the data are revealed

and, we want *only* those chains *that stand out* from what we already know

Related

Maximal Completely Connected Subgraphs

• Spyropoulou & De Bie (2011)

CONNECTING TO MCCS

We mine chains of *redescriptions*

transform

probabilistic model of the data

entity-entity graph or document-entity db

Chain of **redescriptions** surprising wrt margins **and** all mined chains

mine

Automatically discover *surprising* multi-relational "3C" (coalitions, connections, & chains) patterns.

ITERATIVE MINING

Knowledge *changes* during data analysis

• **interestingness** of chains changes depending on what results we study/reject

Static ranking of results is overly simplistic • leads to redundancy – hides interesting results

How can we score results based on (accumulated) background knowledge?

What prior should we use?

MAXIMUM ENTROPY MODELLING

'the best distribution p^* satisfies the background knowledge, but makes **no further** assumptions'

> very useful for data mining: **unbiased** measurement of subjective interestingness

> > (Jaynes 1957; De Bie 2009)

MAXENT FOR BINARY DATA

Tiles

- A tuple of row IDs and column IDs from the given binary data matrix *D*.
- Frequency of a Tile

$$\gamma_T = fr(T; D) = \frac{1}{|\sigma(T)|} \sum_{(i,j) \in \sigma(T)} D(i,j)$$

where D(i, j) represents the (i, j) entry in D, and $\sigma(T)$ represents the set of all the entries in tile T.

MAXENT FOR BINARY DATA

Needed: MaxEnt model for tiles

• we use the model by Tatti & Vreeken (2011), De Bie (2011)

$$p_{\mathcal{T}}^* = \arg \max_{p \in \mathcal{P}} H(p)$$

where

$$\mathcal{P} = \{ p \mid fr(T; p) = \gamma_T, \forall T \in \mathcal{T} \}$$
$$H(p) = -\sum_{D \in \mathcal{D}} p(D) \log p(D)$$
$$fr(T; p) = \frac{1}{|\sigma(T)|} \sum_{(i,j) \in \sigma(T)} p((i,j) = 1)$$

BACKGROUND KNOWLEDGE

Background information in terms of Tiles

- \mathcal{T}_{col} : a set of column margin tiles
- \mathcal{T}_{row} : a set of row margin tiles *per entity domain*
- \mathcal{T}_{dom} : a set of entity domain tiles

$$\mathcal{T}_{back} = \mathcal{T}_{row} \cup \mathcal{T}_{col} \cup \mathcal{T}_{dom}$$

MEASURING SURPRISINGNESS

Evaluating a bicluster chain

- 1) Convert the chain into a set of tiles (depends on data model, see paper)
- 2) Infer the MaxEnt model
- 3) Calculate surprisingness through divergence

 $s_{global}(B) = KL(P_B||P_{back})$

$$s_{local}(B) = -\sum_{T \in \mathcal{T}_B} \sum_{(i,j) \in \sigma(T)} \log p^*((i,j) = D(i,j))$$

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.86	.98	.92	.85	.77	.40	.67	.55
.75	.96	.85	.73	.62	.24	.50	.37
.86	.98	.92	.85	.77	.40	.67	.55
.44	.85	.60	.42	.30	.08	.21	.13
.20	.63	.31	.61	.48	.15	.36	.25
.30	.76	.45	.74	.63	.25	.50	.37
.30	.76	.45	.74	.63	.25	.50	.37
.11	.47	.19	.45	.32	.09	.22	.15
.20	.63	.31	.61	.48	.15	.36	.25

SEARCHING GOOD CHAINS Super Naïve Strategy:

- 1) Mine all the biclusters!
- 2) Construct all the chains!
- 3) Evaluate all subsets of *k* chains!
- 4) Choose the most surprising set.

SEARCHING GOOD CHAINS Slightly Less Naïve Strategy:

- 1) Mine all the biclusters!
- 2) Construct all the chains!
- 3) While not yet chosen k chains: evaluate each chain C against P_{back} greedily choose most surprising C back \leftarrow back + C, and infer P_{back}

SEARCHING GOOD CHAINS Our strategy:

1) Mine all the biclusters!

2) while not yet mined k chains: find most surprising bicluster B_0 , while there is a redescription B_i of B_{i-1} add most surprising B_i to chain $back \leftarrow back + C$, and re-infer P_{back}

Datasets Statistics

	Number of	Number of	Doc–Entity	Entity-Entity	
Dataset	Documents	Entities	%1s	min $\%1s$	max $\%1s$
Synthetic 1k	1000	1000	0.01 - 0.05	0.01	0.05
Synthetic 2k	2000	2000	0.01 - 0.05	0.01	0.05
Synthetic 3k	3000	3000	0.01 - 0.05	0.01	0.05
Synthetic 5k	5000	5000	0.01 - 0.05	0.01	0.05
Synthetic 10k	10000	10000	0.01 - 0.05	0.01	0.05
Atlantic Storm	111	716	0.0179	0.0261	0.0608
Crescent	41	284	0.0425	0.0357	0.136
Manpad	47	143	0.0299	0.0385	0.0714

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First things first: Synthetic Data

• can we uncover the plot?

Second things second: Synthetic Data

can we tell when to stop? 0

Runtime Performance

Real Data

Aalto University VirginiaTech XPERIMENT RESULTS

Iterative Knowledge Discovery

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$C_3: \ldots$

 C_1 :

Arnold C. Ryder

Wr.

Nashville

- Ralph T., who is a member of Aryan Militia, bought weapons and sells them to George W. (Muhammad J.) who is a member of Al-Denver Queda.
- Ralph T. meets Kamel J. Colorado in Atlanta in Atlanta, Georgia, and Kamel J. drives a truck from Atlanta to St. Paul, Minnesota. He probably transports weapons.

• Arnold C. (Abu H.)., who was a suspect of the 9/11attack and spent time in Afghanistan, rents a U-Hual truck and drives it from Boulder, Colorado to Los Angeles. He probably transports the weapons.

state University

 C_2 :

 C_2

 C_3

Army rmy Clon Brotherhiner Color

Denver

of Colorado

of Colorado

User

Feedback

 C'_1 :

ammed H.

"FBI Arvan Militia

• Homer W., who is a member Army CID Brotherhood of Aryan Brotherhood of *Colorado*, sells the weapons to John H., who is a member of Al-Queda, in Colorado.

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CONCLUSION

• Applicable to analyze multi-relational unstructured or discrete data

• Discover surprising entity coalitions with new data modeling primitives and algorithms

• Experiments on both synthetic and real datasets show that elaborate 'plots' can be detected

• Support human-in-loop iterative knowledge discovery

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