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WHERE WITH A DECEMBER

Graph Exploration: From the User to Large Graphs

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Who we are



Davide Mottin

- graph mining, novel query paradigms, interactive methods
- <u>https://hpi.de/en/mueller/team/davide-mottin.html</u>



Emmanuel Müller

- graph mining, stream mining, clustering and outlier mining on graphs, streams, and traditional databases
- http://hpi.de/en/mueller/prof-dr-emmanuel-mueller.html

Big data and novice users







Data exploration



Efficiently extracting knowledge from data even if we do not know exactly what we are looking for

Idreos et al., Overview of Data Exploration Methods, SIGMOD 2015

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The importance of graphs



Lost in the graph?



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Current: Visualization tools







Several visualization tools:

- General: Gephi, GraphViz, ...
- Biological: Cytoscape, Network Workbench
- Social: EgoNet, NodeXL, ...
- Relational: Tulip

but

- No Scalability to large networks!
- **No** for novice users
- Limited expressivity

Current: Query languages

SELECT ?name ?email WHERE

?person a foaf:Person .
?person foaf:name ?name .
?person foaf:mbox ?email .

SPARQL

Query languages **ARE**:

- Expressive
- Powerful
- Scalable
- Compact

g.V().hasLabel('movie').as('a','b').
where(inE('rated').count().is(gt(10))).
select('a','b').
by('name').
hu(inE('rated').unlues('stern').mean())

```
by(inE('rated').values('stars').mean()).
```

order().

by(select('b'),decr). limit(10

GREMLIN

MATCH (node1:Label1)-->(node2:Label2) WHERE node1.propertyA = {value} RETURN node2.propertyA, node2.propertyB

CYPHER

but

- Not user friendly
- No guided search
- Not interactive
- Not scalable

This tutorial is about ...

- Algorithms for helping the user finding the wanted information
- Approximate search on graphs to assist the user in finding the information
- Interactive methods on graphs based on user feedback
- Automatically discovery of portions of graphs using examples

NOT about

- Visualization methods for graphs
- Query languages and semantics
- Efficient indexing methods
- Pure machine learning on graphs

Our graph exploration taxonomy



Graph exploration taxonomy



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Graph exploration taxonomy



- 2. Space restriction methods
- 3. Graph Reweighting

Graph exploration taxonomy



The graph exploration ... graph



Tutorial outline

Background (5 min)

Graph models, subgraph isomorphism, subgraph mining, graph clustering



Challenges and discussion

We are here

Background (5 min)

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Graphs





- Undirected Graphs
 - Co-authorship, Roads, Biological
- Directed graphs
 - Follows, ...
- Labeled Graphs
 - Knowledge graphs, ...
- Probabilistic graphs
 - Causal graphs

Graph databases (set of graphs)



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Graph Isomorphism



Given two graphs, $G_1: \langle V_1, E_1, l_1 \rangle$, $G_2: \langle V_2, E_2, l_2 \rangle$ G_1 is isomorphic G_2 iff exists a **bijective** function $f: V_1 \rightarrow V_2$ s.t.: 1. For each $v_1 \in V_1$, $l(v_1) = l(f(v_1))$ 2. $(v_1, u_1) \in E_1$ iff $(f(v_1), f(u_1)) \in E_2$

Subgraph Isomorphism



A graph , $Q: \langle V_Q, E_Q, l_Q \rangle$ is subgraph isomorphic to a graph $G: \langle V, E, l \rangle$ if exists a subgraph $G' \sqsubseteq G$, isomorphic to Q

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Graph Clustering and Community Detection



Given: graph with nodes, edges, labels



Discover: a partitioning of communities

$$C = \{C_1, C_2, C_3, ..., C_k\}$$

- Optimize a given quality criterion Q(C), e.g. *Modularity* or other measures
- Is an **NP-hard problem** to find the optimal partitioning

We are here

Background (5 min)

Graph models, subgraph isomorphism, subgraph mining, graph clustering

Exploratory Graph Analysis (20 min)

Focused Graph Mining (20 min)

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Refinement of Query Results (20 min)



Challenges and discussion

Exploratory Search

Approximate Graph Search

- Given an imprecise query find the closest answers to that query
- User perspective: no need to know about the entire details of the data

Searching by Example

- Given an example from the results, find the other results of an unspecified query
- User perspective: it is not necessary to know how to describe the results

Approximate Graph Search



- Structural mapping: Strong-simulation (Ma et al.)
- Node similarity approaches: P-homomorphism (Fan et al.), Nema (Khan et al.)
- Probabilistic approaches: SLQ (Yang et al.)

Subgraph isomorphism issues



Fan, W., Li, J., Ma, S., Wang, H. and Wu, Y.. Graph homomorphism revisited for graph matching. PVLDB, 2010

Strong simulation

Revise subgraph isomorphism: Instead of bijection, compute a binary relation between nodes



Ma, S., Cao, Y., Fan, W., Huai, J. and Wo, T. Strong simulation: Capturing topology in graph pattern matching. TODS, 2014

Strong simulation

	Given $Q: \langle V_q, E_q, l_q \rangle$ and data graph $G: \langle V, E, l \rangle$, a	Graph Simulation
	binary relation $S \subseteq V_q \times V$ is said to be a dual	[Milner 1989]
	simulation if	
	• for each $(u, v) \in S$, $l(u) = l(v)$	
	• for each $v \in V_Q$ exists a node $u \in V s.t.(v,u) \in S$	
ality	- for each edge $(v, v') \in E_q$, there exists an edge $(u, u') \in E$ such that $(v', u') \in S$	Parent-child relationship
na	- for each edge $(v'', v) \in E_q$, there exists an edge $(u'', u) \in E$ such that $(v'', u'') \in S$	Child-parent relationship

- The matching subgraph is:
- connected graph
- the diameter is not larger than twice the diameter of the query

Ma, S., Cao, Y., Fan, W., Huai, J. and Wo, T. Strong simulation: Capturing topology in graph pattern matching. TODS, 2014

Locality

Properties of Strong Simulation

If Q matches G, via subgraph isomorphism, then Q matches G, via strong simulation

If Q matches G, via strong simulation, then Q matches G, via dual simulation

If Q matches G, via dual simulation, then Q matches G, via graph simulation



Ma, S., Cao, Y., Fan, W., Huai, J. and Wo, T. Strong simulation: Capturing topology in graph pattern matching. TODS, 2014

NeMa

Relax **p-homomorphism**:

- Structure and some labels are unknown
- Node closed in the query must be closed in the graph



Khan, A., Wu, Y., Aggarwal, C.C. and Yan, X. Nema: Fast graph search with label similarity. PVLDB, 2013

NeMa: compute node vectors



Khan, A., Wu, Y., Aggarwal, C.C. and Yan, X. Nema: Fast graph search with label similarity. PVLDB, 2013



Given Q and G, find the mapping ϕ with the minimum cost $C(\phi)$

Khan, A., Wu, Y., Aggarwal, C.C. and Yan, X. Nema: Fast graph search with label similarity. PVLDB, 2013

SLQ

Similar to **NEMA** Assume that a match is obtained by a sequence of transformations of the query nodes into the graph



Yang, S., Wu, Y., Sun, H. and Yan, X. Schemaless and structureless graph querying. PVLDB, 2014.



Problem

- How to learn the parameters α_i , β_i ?
- How to find the matching with the highest score?

Yang, S., Wu, Y., Sun, H. and Yan, X. Schemaless and structureless graph querying. PVLDB, 2014.

Querying by Example



Exemplar Queries (Mottin et al.), GQBE (Jayaram et al.)

NOT approximate queries:

a result to an approximate query is the closest possible to the query itself

Exemplar Queries

Input: Q_e , an example element of interest **Output**: set of elements in the desired result set

Exemplar Query Evaluation

- evaluate Q_e in a database D, finding a sample s
- find the set of elements *a* similar to *s* given a *similarity relation*

Mottin, D., Lissandrini, M., Velegrakis, Y. and Palpanas, T. Exemplar queries: Give me an example of what you need. PVLDB 2014

Exemplar Queries


Computing exemplar queries

NP-complete (subgraph isomorphism) $O(|V|^4)$ (simulation)



Pruning technique:

 Compute the neighbor labels of each node

 $W_{n,a,i} = \{n_1 | l(n_1, n_2) = a \lor \in N_{i-1}(n)\}$

- Prune nodes not matching query nodes neighborhood labels
- Apply the technique iteratively on the query nodes



Mottin, D., Lissandrini, M., Velegrakis, Y. and Palpanas, T. Exemplar queries: Give me an example of what you need. PVLDB 2014

Graph query by example (GQBE)

In GQBE Input is a set of (disconnected) entity mention tuples



Jayaram, N., Khan, A., Li, C., Yan, X. and Elmasri, R. Querying knowledge graphs by example entity tuples. TKDE, 2015

GQBE

NP-hard



1. Find the maximum query graph

- Neighborhood Graph with m edges having the maximum weight
- 2. Find all the answers subgraph isomorphic to the query graph
- Rank the answers and return the top-k tuples

Answer score:

- Sum of query graph weights
- Similarity match between edges in the answer and the query

$$\mathsf{match}(e, e') = \begin{cases} \frac{\mathsf{w}(e)}{|E(u)|} & \text{if } u = f(u) \\ \frac{\mathsf{w}(e)}{|E(v)|} & \text{if } v = f(v) \\ \frac{\mathsf{w}(e)}{\min(|E(u)|, |E(v)|)} & \text{if } u = f(u), v = f(v) \\ 0 & \text{otherwise} \end{cases}$$

Jayaram, N., Khan, A., Li, C., Yan, X. and Elmasri, R. Querying knowledge graphs by example entity tuples. TKDE, 2015

We are here

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Challenges and discussion

Graph Mining – a very broad topic

Link Prediction

Community Detection

Anomaly Detection

Frequent Subgraph Mining

Graph Partitioning

... many more ...

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Graph Mining Focused on User Interest

We consider "user interest" at a major tool for adaptive graph mining

- In contrast to raw analysis of graphs
 (i.e. with no or very little user interaction)
- Example (modularity based clustering):

Given a graph discover best partitioning of the nodes

Optimize a given quality criterion Q(C), e.g. *Modularity* or other measures

- Where is the user interest in such definitions?
- How to include the user into the loop?
- How do we need to change the algorithmic search?



Focus: Given a Set of Query Nodes

Given Q nodes (by the user)

How can we **find the center-piece node** that has direct or indirect connections to all or most of these nodes?

- Neither a clustering of nodes
- Nor the shortest path between pairs of nodes
- Nor any other graph mining method (with lack of user input)

H. Tong & C. Faloutsos: Center-Piece Subgraphs: Problem Definition and Fast Solutions. (KDD 2006)

Focused Communities: Given a Set of Seed Nodes

Traditional detection of **communities** as **internally dense subgraphs** (e.g. measured by modularity or conductance)

Given seed nodes (by the user)

Perform selective search for communities local community detection seed set expansion

- Global search is not appropriate for such local/selective models
- Communities may overlap or coincide

C. Staudt, Y. Marrakchi, H. Meyerhenke: Detecting Communities Around Seed Nodes in Complex Networks (BigData 2014)

Egoistic Focus on Yourself: Ego-Nets

For a given node consider their neighbors and the connections among these neighbors

Compute ego-nets for each given node that is of interest.

Useful for link prediction, community detection, anomaly detection, and many more, as pre-processing (feature extraction).



Epasto et al. Ego-Net Community Mining Applied to Fried Suggestion. (VLDB 2015)

Mining Attributed Graphs

Different graph mining techniques

- Clustering / graph partitioning / ...
- Community detection and anomaly detection

Used assumption: **Homophily** has to be fulfilled for **all** the attributes

Problem: disassortative mixing [Newman 2003] hinders the detection of communities (i.e. similarity assessment of nodes)

Solution: Selection of relevant views ensuring homophily

Newman. Mixing patterns in networks. Physical Review, 2003

0

age

Multiple Views in Attributed Graphs

Different structures depending on the subset of attributes



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Multiple Views in Attributed Graphs

Different structures depending on the subset of attributes



Specialized Approaches

Frequent subgraph mining, subspace clustering ...

- Local selection of the attributes
- Individual subgraphs





First Idea: Local Context Selection

Local Context:

- Subset of relevant attributes
- Selection w.r.t. a subgraph

How to **define a local context** for each node?

How to **efficiently** select only the **relevant attributes**?



Model dependent solution for community outlier mining

- Statistical test of attribute value distribution for each local context
- Measure deviation of each node w.r.t. its local context only

Iglesias et al. Local Context Selection for Outlier Ranking in Graphs with Multiple Numeric Node Attributes (SSDBM 2014)

Selection of Congruent Subspaces (ConSub)

Definition: Congruent subspaces

- Mutual similarity between attribute values in subspace S
- Significantly more edges than expected by a random distribution

Constraint Subgraph $G_{C,S}$

• Set of constraints formed by all the pairs $(I_j = [low_j, high_j], A_j \in S)$



Iglesias et al. Statistical Selection of Congruent Subspaces for Mining Attributed Graphs (ICDM 2013)

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S ={age,income} nodes with 45 ≤ age ≤ 60 and 1900 ≤ income ≤ 4500





Iglesias et al. Statistical Selection of Congruent Subspaces for Mining Attributed Graphs (ICDM 2013)

Focus on User Preference

Examples for user preference:

- attribute weighting
- examples of similar nodes
- some notion of similarity



examples of similar nodes



attribute weighting

Focused Selection of Subsaces (FocusCO)

Decoupled mining for given user preference

- 1. Infer similarity measure
- 2. Re-weighting of graph edges
- 3. Community detection & community outlier mining



Perozzi et al. Focused Clustering and Outlier Detection in Large Attributed Graphs (KDD 2014)

Knowledge Discovery by Focused Graph Mining

Example Sociology:

hypothesis testing vs. hypothesis generation



We are here

Background (5 min)

Graph models, subgraph isomorphism, subgraph mining, graph clustering

Exploratory Graph Analysis (20 min)

Focused Graph Mining (20 min)



Refinement of Query Results (20 min)



Challenges and discussion

Refinement of Graph Query Results

Reformulation and Refinement

- Generate reformulations (explanations) for query with too-many too few results
- Explain results by providing summaries
- User perspective: even if the query is imprecise the system provides assistance

Top-k results

- Use user feedback to find the k results with the highest score
- User perspective: the results are potentially the most preferred items

Skyline queries

- Optimize one single
- User perspective: sh

Not in this tutorial 😕 le when finding results of a query

Those nodes/graphs that are no worse than others

Reformulation and Refinement



- Query Reformulation approaches: in Graph Databases (Mottin et al.), in connected networks (Vasilyeva et al.)
- Result summarization approaches: top-k representative (Ranu et al.), keyword induced result summarization (Wu et al.)

Graph Query Reformulation



Mottin, D., Bonchi, F. and Gullo, F. Graph Query Reformulation with Diversity. KDD, 2015

Graph Query Reformulation



Mottin, D., Bonchi, F. and Gullo, F. Graph Query Reformulation with Diversity. KDD, 2015

Why empty, Why so-many answers in graphs



Vasilyeva, E., Thiele, M., Bornhövd, C. and Lehner, W.. Answering "Why Empty?" and "Why So Many?" queries in graph databases. JCSS, 2016

Why empty, Why so-many answers in graphs



Vasilyeva, E., Thiele, M., Bornhövd, C. and Lehner, W.. Answering "Why Empty?" and "Why So Many?" queries in graph databases. JCSS, 2016

Top-k representative queries

Graphs are points in a metric space with d as a distance function



Select k=2 relevant objects

Top-2 answer: g_1, g_2



- Object is relevant
- O Object is non-relevant

Two objects are close if they are similar

Ranu, S., Hoang, M. and Singh, A. Answering top-k representative queries on graph databases. SIGMOD, 2014

Top-k representative queries

Result of a query



Vector graph \vec{g}_i : vectorial representation of G_i

Example: Binding compatibility with m proteins, frequent subgraphs, belonged communities

Query: function from \vec{g} to [-1,1], $q: \vec{g} \rightarrow [-1,1]$

Example: Molecules with some properties, graphs with some structure, some community

Top-k Representative queries: $A = \arg \max_{S} \{\pi_{\theta}(S) | S \subseteq R(q), |S| = k\}$ where R(q) = results of q, $\pi_{\theta}(S)$ =**representative power** of S, given threshold θ

Ranu, S., Hoang, M. and Singh, A. Answering top-k representative queries on graph databases. SIGMOD, 2014

Representative power

R(q) = answers to the query

• q : query

θ -neighborhood

- $N_{\theta}(G) = \{G' \in R(q) | d(G, G') \le \theta\}$
- θ : distance threshold
- d(G, G'): graph edit distance



Given a set of graphs S

• Representative power of S

•
$$\pi_{\theta}(S) = \frac{|\bigcup_{G \in S} N_{\theta}(G)|}{R(q)}$$
 Represent the coverage of a graph neighborhood

$$\pi(\{G_1, G_3\}) = \frac{7}{8}$$
$$\pi(\{G_1, G_2\}) = \frac{4}{8}$$

Ranu, S., Hoang, M. and Singh, A. Answering top-k representative queries on graph databases. SIGMOD, 2014

Summarizing graph results

Query: keyword query on graph

e.g., Jaguar, America, History



Wu, Y., Yang, S., Srivatsa, M., Iyengar, A. and Yan, X. Summarizing answer graphs induced by keyword queries. PVLDB, 2013

Summarizing graph results



Two problems

- 1. Minimum α -summarization: find the **minimum size** summary which covers at least α
- 2. K-summarization: find K 1-summaries with minimum total size that form a K-partition on the answer graph sets (no repeated answers)

Wu, Y., Yang, S., Srivatsa, M., Iyengar, A. and Yan, X. Summarizing answer graphs induced by keyword queries. PVLDB, 2013

Summarizing graph results



Summarizing graph results algorithms

1-summarization

- 1. Based on dominance relation: a node n1 dominates n2 if they have the same label and each path from a keyword pair that contains n2 also contains n1
- 2. Discover dominance relation and remove dominated nodes until no change

α -summarization

- 1. Greedy heuristic: compute 1-summaries for all keyword paths
- 2. Merge summaries with the minimum merge cost (extra edges added)
- 3. Repeat until the desired α is reached

K-summarization

- 1. Select K answer graphs as centers
- 2. Refine the clusters merging answer graphs with minimum merge cost until convergence
- 3. Compute 1-summary graphs for each cluster

Wu, Y., Yang, S., Srivatsa, M., Iyengar, A. and Yan, X. Summarizing answer graphs induced by keyword queries. PVLDB, 2013

NP-complete

PTIME

NP-complete

Top-k Results



- Diversified top-k graph pattern matching (Fan et al.)
- Exploiting relevance feedback in knowledge graph search (Su et al.)
- Top-k interesting subgraph discovery in information networks (Gupta et al.)
- Querying web-scale information networks through bounding matching scores (Jin et al.)

Diversified top-k graph pattern matching

Query: Find good PM (project manager) candidates collaborated with PRG (programmer), DB (database developer) and ST (software tester).



Find matches using graph simulation, which computes a binary relation on the pattern nodes in Q and their matches in G

Fan, W., Wang, X. and Wu, Y. Diversified top-k graph pattern matching. VLDB, 2013

Diversified top-k graph pattern matching



Pattern Q

- Graph pattern matching revised
 - extend a pattern with a designated output node \boldsymbol{u}_0
 - matches Q(G): the matches of u₀
 - readily extends to multiple output nodes
- Problem:
 - Find (diversified) top-K matches for graph pattern matching with a designated output node.

Fan, W., Wang, X. and Wu, Y. Diversified top-k graph pattern matching. VLDB, 2013
Diversified top-k graph pattern matching



Fan, W., Wang, X. and Wu, Y. Diversified top-k graph pattern matching. VLDB, 2013

Finding Top-k Matches (acyclic)



We are here

Background (5 min)

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Summary of Exploratory Graph Analysis

Approximate Queries

- User query is imprecise
- By-Example methods
- User query is an example result



- Only need a partial knowledge on the data
- No need for complicate query languages (use examples, partial descriptions)
- The query adapts to user need
- Enable exploratory search by using small queries on the data

Challenges for Exploratory Graph Analysis



Summary of Focused Graph Mining

The focus on individual user interest ... as Query to the Graph Mining System ... as Seed Node(s) for Local Search ... as Attributes and Weights

- get or infer user interest
 → unexpected results
- interactive exploration
 → intuitive parametrization
- adaptive graph mining
 → individual local search



Challenges for Focused Graph Mining

User interactivity in the graph mining process

- unsupported in most of the current graph mining algorithms
- huge variety of user interactions possible
- feedback loop needs to be <u>unified</u> and become <u>exchangeable</u>



Revolution of formal models and search algorithms

- insufficient extensions of existing models and algorithms
- <u>adaptive steering</u> of algorithms vs. fixed parametrization
- evaluation of algorithms with <u>user studies</u>



Scalability of algorithms for real-time interaction

- NP-hard problems, heuristic algorithms, ..., still not scalable
- exploit the user interest for pruning the search space

Summary of Refinement of Query Results

Refinement

The user query is too restrictive or too generic

Top-k Results

 Queries typically have inexact matches

Skyline Queries

 Find small set of interesting items with many dimensions and incremental updates

- The user might have a very generic idea of how to describe the structure of interest
- The system guides the user towards the answer with simple steps
- The results are explained with reformulations
- The queries can be inexact



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Challenges for Refinement of Query Results



The missing tiles in graph exploration



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Slides: https://hpi.de//mueller/tutorials/graph-explorationsigmod.html

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