



UNIVERSITY
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Department of Information
Engineering and Computer Science

dbTrento

YAHOO!
LABS

Graph Query Reformulation with Diversity

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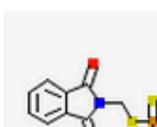
Pattern search

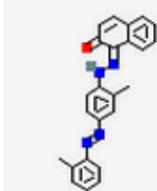
Query OS(=O)=O

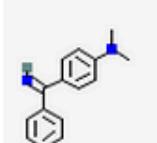
PubChem Compound Save search Limits Advanced

Display Settings: Summary, 20 per page, Sorted by Default order Send to:

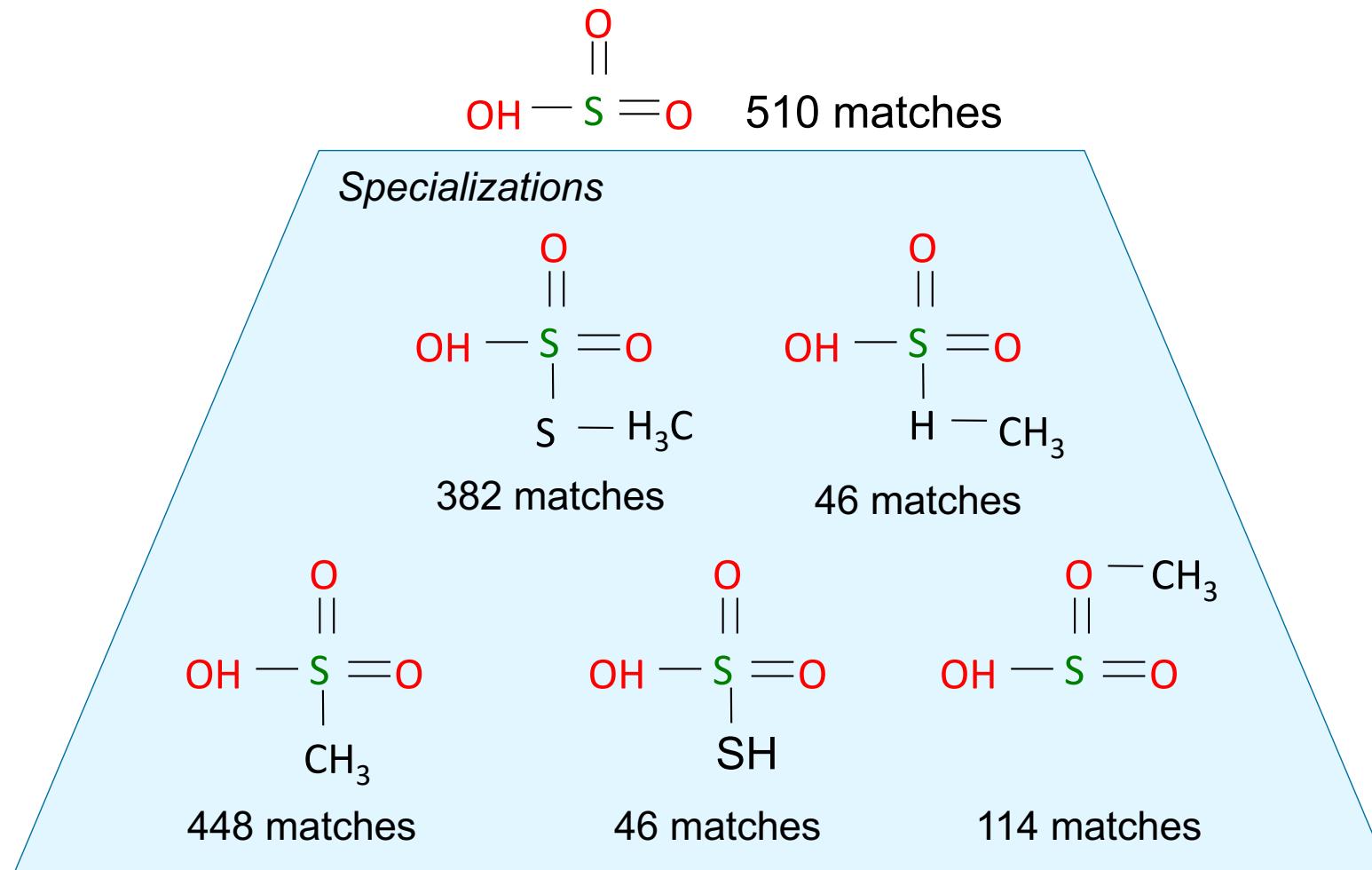
Results: 1 to 20 of 510 << First < Prev Page of 49 Next > Last >>

1.  • Too many matches
• Results are not grouped

2. 
IUPAC name: (1Z)-1-[[2-methyl-4-[(2-methoxyphenyl)diazenyl]phenyl]hydrazinyl]...
Create Date: 2005-09-09
CID: 5876571
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [PubMed \(MeSH Keyword\)](#) [Active in 7 of 209 BioAssays](#)

3. 
Basic Yellow 2; Auramine O; Auramin ...
MW: 303.829680 g/mol MF: C₁₇H₂₂ClN₃
IUPAC name: 4-[4-(dimethylamino)benzenecarboximidoyl]-N,N-dimethylanilin...
Create Date: 2005-08-08

Finding specializations



Applications

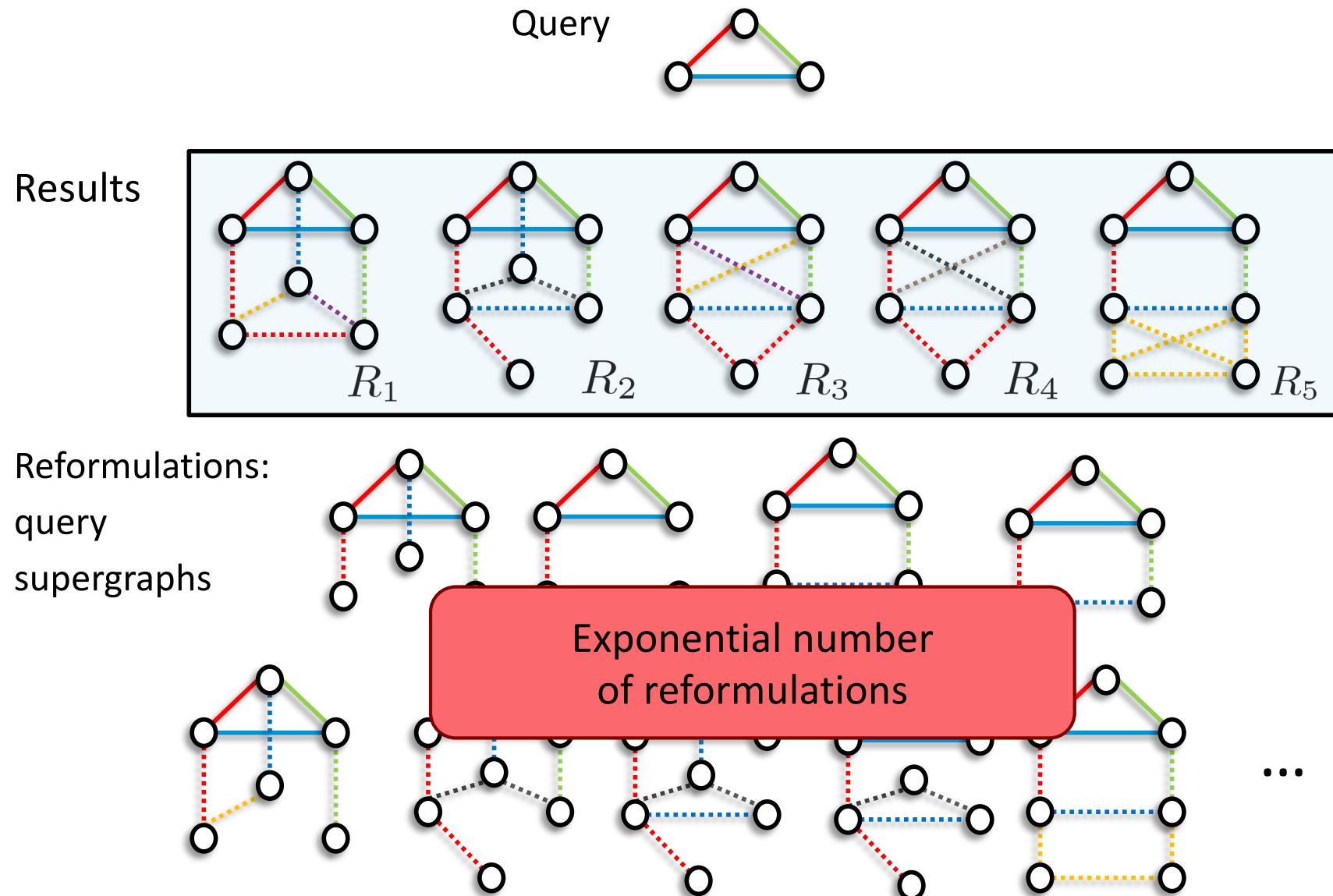
- Finding groups of molecules having a particular reagent
- Analyze a set of proteins to find diseases
- Workflow optimization
- Anomalies detection in a network
- Finding similar 3D shape search

Dealing with specializations in web and relational data

- Faceted Search
 - present aspects of the results [Roy08]
- **Query reformulation**
 - Modify some of the query conditions
 - In structured databases [Mishra09]
 - In web search [Dang10]

Frist Study of Problem on GRAPHS

Graph Query Reformulation



Challenges

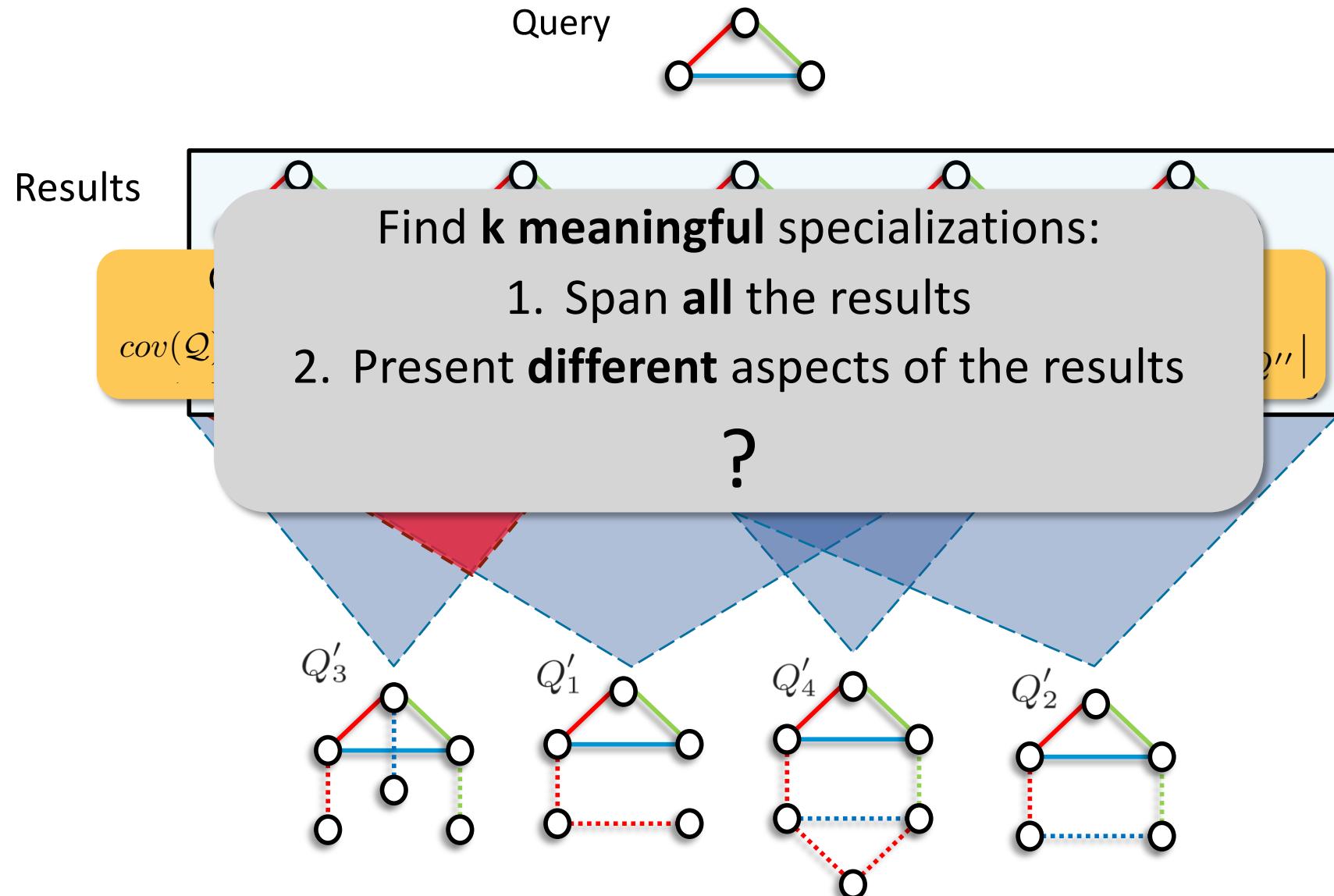
- The number of reformulation is exponential
- Quantify the interestingness of a reformulation
- Finding query reformulations is **NP**-complete

Our Approach

Graph Query Reformulation with Diversity

- Finds k *meaningful* specializations efficiently

Finding Meaningful Specializations



Graph Query Reformulation with Diversity

Problem

Find a set \mathcal{Q}^* of k specializations of Q that maximize a combination of **coverage** and **diversity**

$$f(\mathcal{Q}) = cov(\mathcal{Q}) + \lambda \sum_{Q', Q'' \in \mathcal{Q}} div(Q', Q'')$$

$$\mathcal{Q}^* = \arg \max_{\mathcal{Q} \subseteq \mathbb{S}_Q} f(\mathcal{Q})$$

$$\text{subject to} \quad |\mathcal{Q}| = k.$$

Theorem (NP-hardness)

The problem reduces to **MAX-SUM Diversification** Problem, so it is NP-hard

Solution: Greedy Algorithm

Greedy

While k-specializations are not found

1. Find the specialization leading to the maximum increment of the objective function (marginal gain)
2. Add the specialization to the results

Theorem

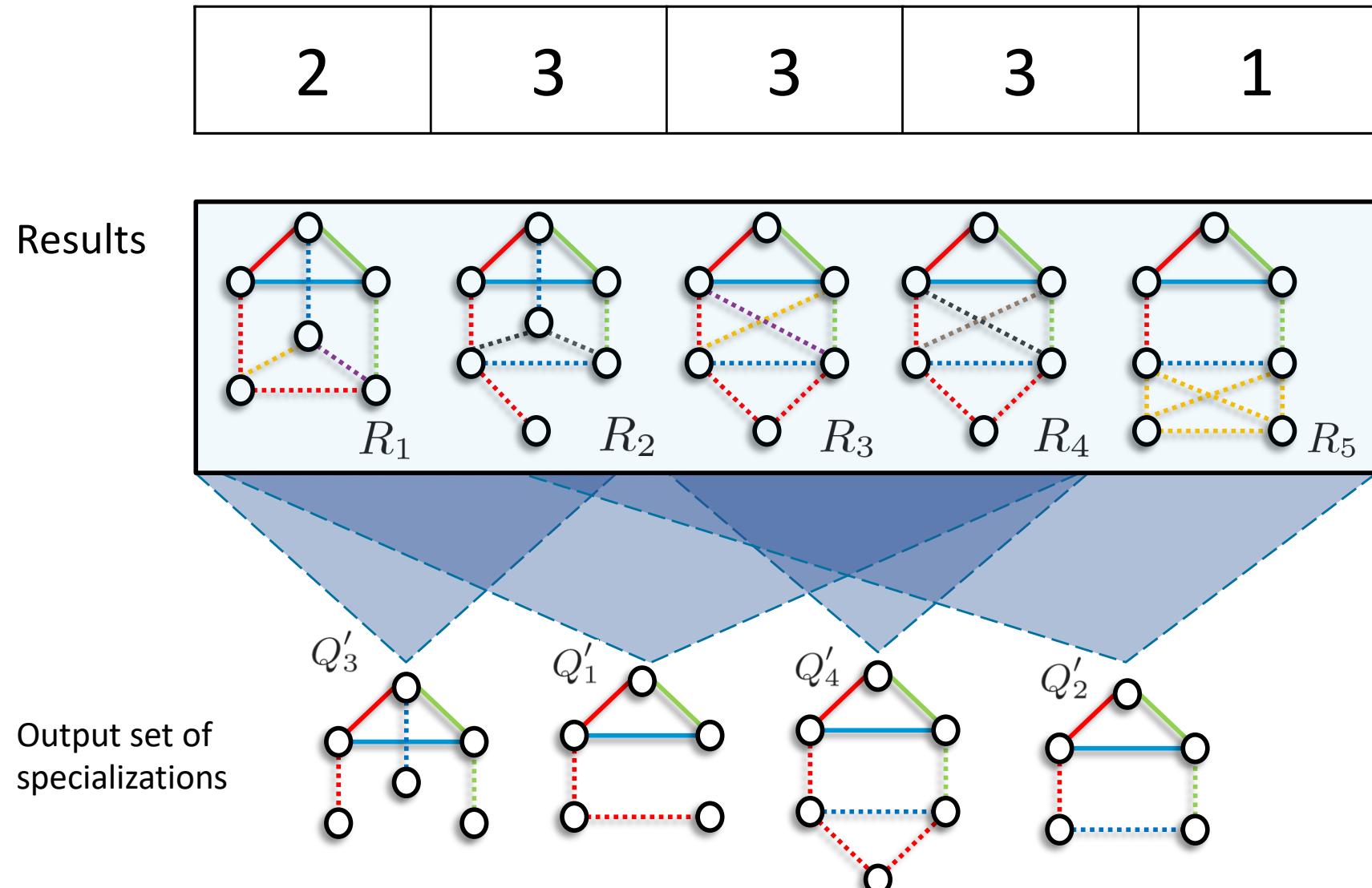
The algorithm is a $\frac{1}{2}$ -approximation

Finding the maximum gain is
#P-complete [Valiant79]

Solution

Fast_MMPG: Branch and bound algorithm with quality guarantees

The multiplicity vector



Upper bound on the Marginal gain

Lemma

The marginal gain increases if the multiplicity of the considered item is where $\leq \frac{|\mathcal{Q}|}{2}$ is the number of reformulations in the reformulated set constructed so far.

Upper bound : is the value of the objective function considering only results with multiplicity $\leq \frac{|\mathcal{Q}|}{2}$

Theorem

For a reformulation $Q' \in \mathbb{S} \setminus \mathcal{Q}$ it holds that

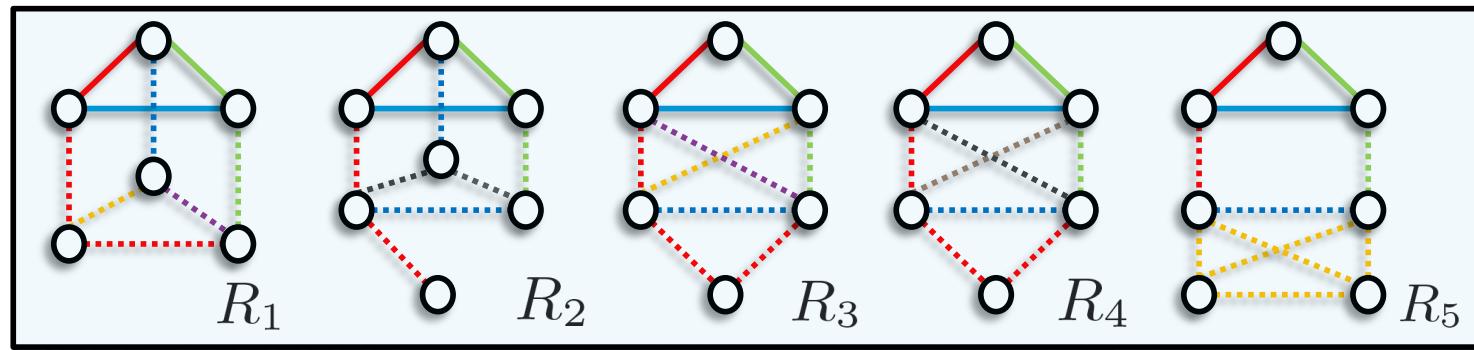
$$\begin{aligned} \max_{Q'' \in \mathcal{T}_{Q'}} \Delta_f(\mathcal{Q}, Q'') &\leq \overline{\Delta_f}(\mathcal{Q}, Q') = \\ &= \frac{1}{2} \vec{u}_{\mathcal{Q}} \cdot \vec{x}_{Q^*} + \lambda (\|\vec{m}_{\mathcal{Q}}\| + |\mathcal{Q}| \times \|\vec{x}_{Q^*}\| - 2 \vec{m}_{\mathcal{Q}} \cdot \vec{x}_{Q^*}). \end{aligned}$$

Upper bound

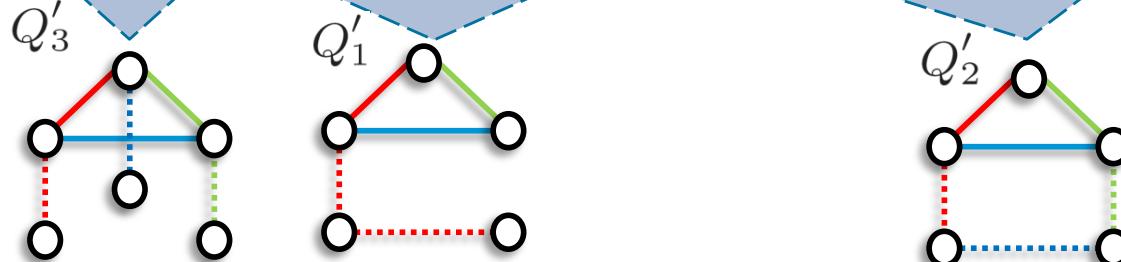
$$\leq \frac{|Q|}{2}$$



Results



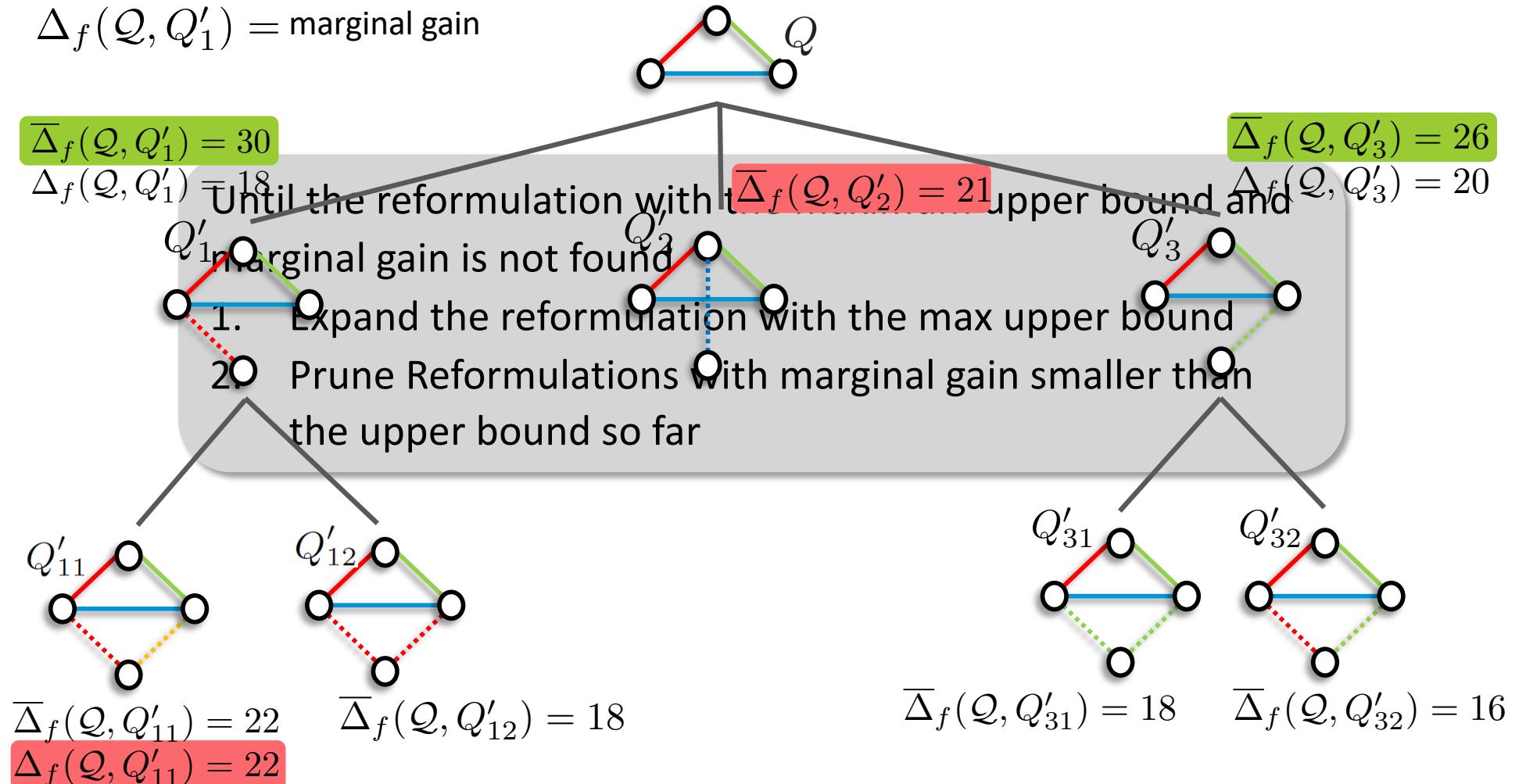
Output set of reformulations



The Fast_MMMPG Algorithm

$\overline{\Delta}_f(Q, Q'_1) = \text{upper bound}$

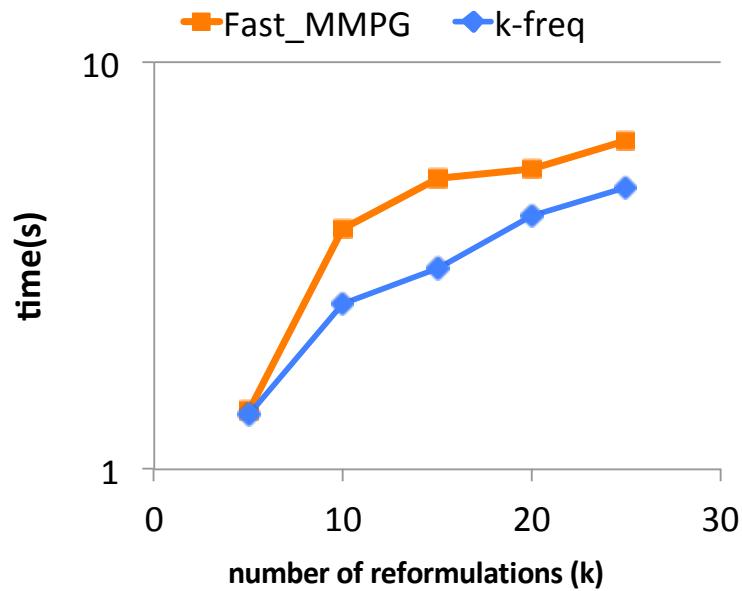
$\Delta_f(Q, Q'_1) = \text{marginal gain}$



Experimental Setup

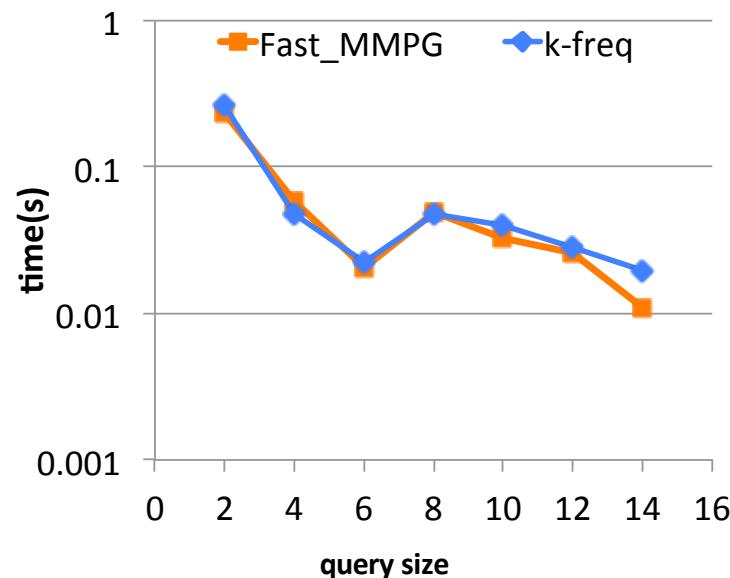
- **Datasets:**
 - AIDS: 10k chemical compounds
 - Financial: 17k transaction workflows
 - Web: 13k interactions with a recommender system
- **Baseline algorithms:**
 - k-freq: returns top-k frequent supergraphs of a query
 - LIndex: informative patterns index
- **Experiments:**
 - Time and objective function value varying k , query size, λ
 - Anecdotal
 - Scalability

Time Comparison



Number of reformulations

1. k-freq runs only slightly faster
2. Time increases linearly in k
3. Fast_MMPG has real-time performance



Query size

1. Fast_MMPG comparable to k-freq
2. Time decreases with query size (less reformulations)

Objective function gain

	λ				
	0	0.01	0.05	0.1	0.5
Fast_MMPG	433	613	1 345	2 260	9 566
k-freq	409	540	1 063	1718	6 954
gain (%)	6	12	21	24	27

Analysis

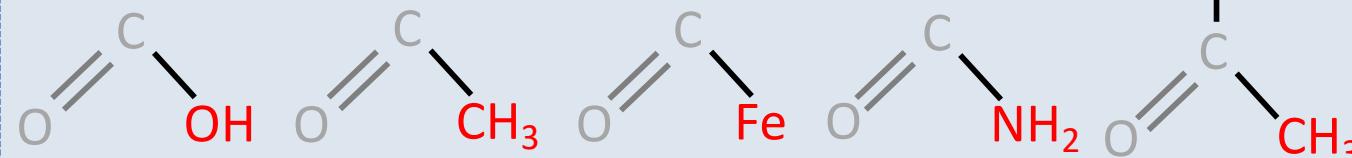
1. Lambda correctly moves the objective function towards diversity
2. k-freq only captures coverage

$$f(\mathcal{Q}) = cov(\mathcal{Q}) + \lambda \sum_{Q', Q'' \in \mathcal{Q}} div(Q', Q'')$$

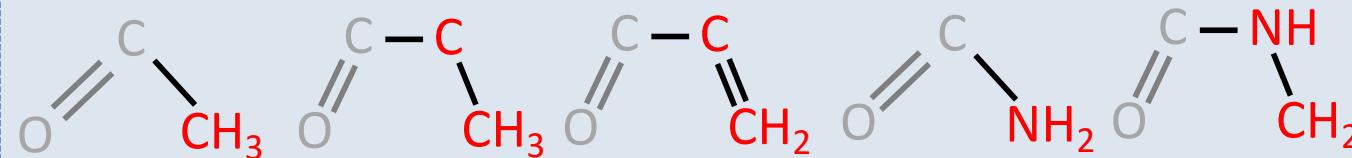
Qualitative evaluation

Query $\text{C} = \text{O}$

Fast_MMPG



k-freq

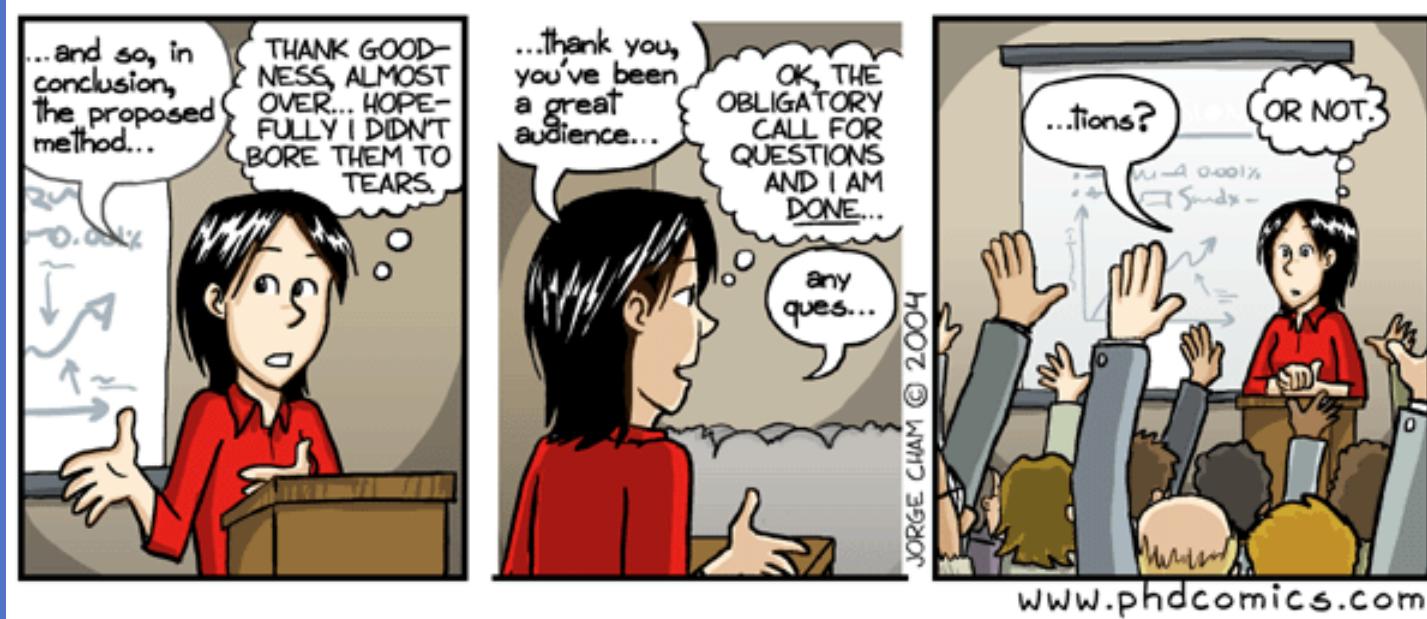


Analysis

- k-freq finds reformulation of the same superquery
- Fast_MMPG returns reformulations with more diversified structures

Conclusions

- First study of the problem in **graph databases**
- **Principled** objective function optimizing
coverage and **diversity**
- Algorithmic solutions **with quality guarantees**
and **real time responses**



Thank you!

Questions?