Iterative graph alignment via supermodular approximation

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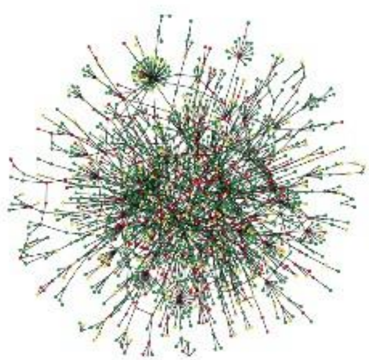
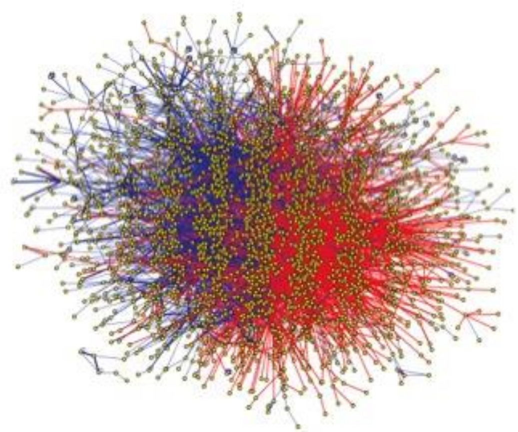
Graph Matching

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}$$





$$\mathbf{B} = \begin{bmatrix} 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \end{bmatrix}$$

$\mathbf{A} \in \mathbb{R}_+^{n_A \times n_A}$ $\quad$ $\mathbf{B} \in \mathbb{R}_+^{n_B \times n_B}$

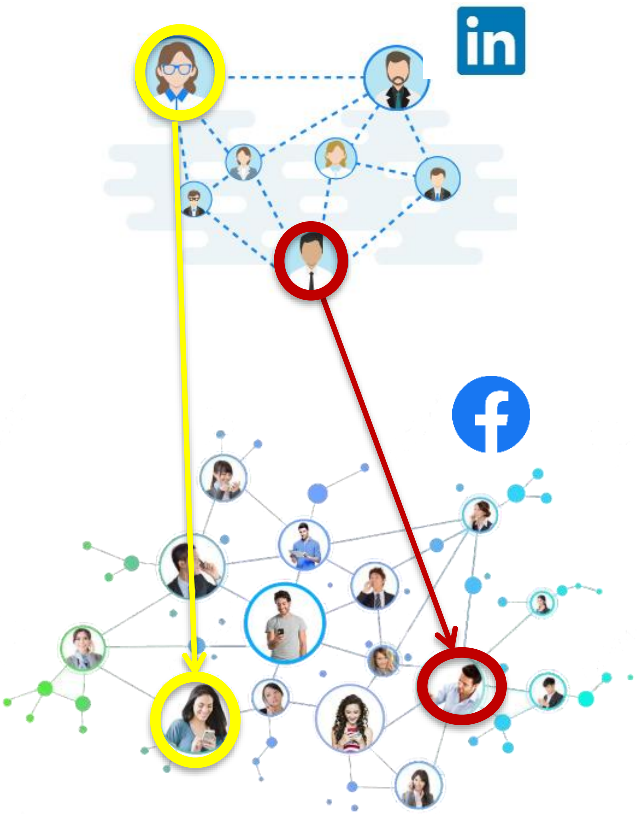
- Problem: Find correspondence mapping between vertex sets that best preserves adjacency relations

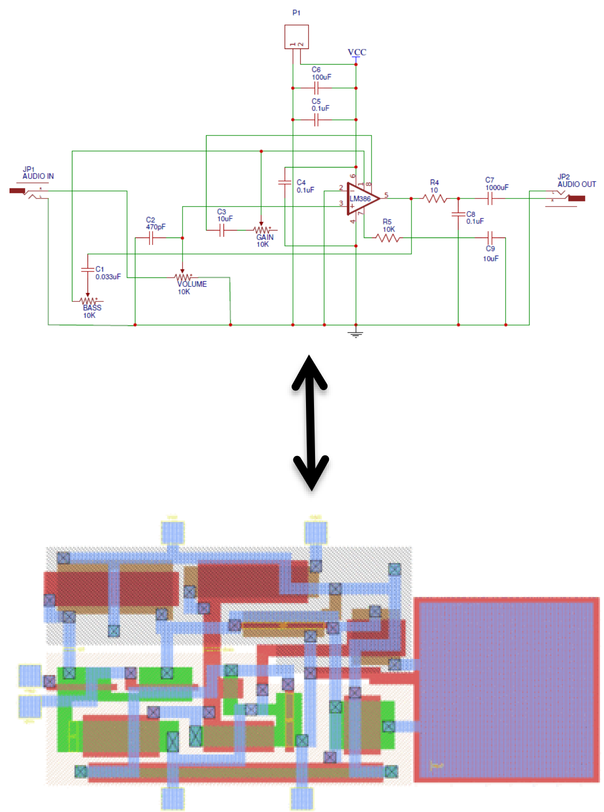
Minimize edge disagreements

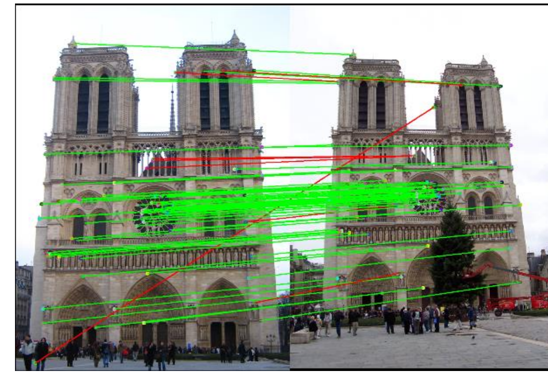
$$\begin{aligned} \min. \quad & \boxed{\|\mathbf{B} - \mathbf{P}\mathbf{A}\mathbf{P}^T\|_F^2} \\ \text{s.t.} \quad & \mathbf{P} \in \mathcal{P} := \{\mathbf{P} \in \{0,1\}^{n_B \times n_A} \mid \mathbf{P}^T\mathbf{P} = \mathbf{I}\} \end{aligned}$$

Correspondence mappings

Applications







Scene matching

Network de-anonymization

Electronic circuit design

Ontology alignment

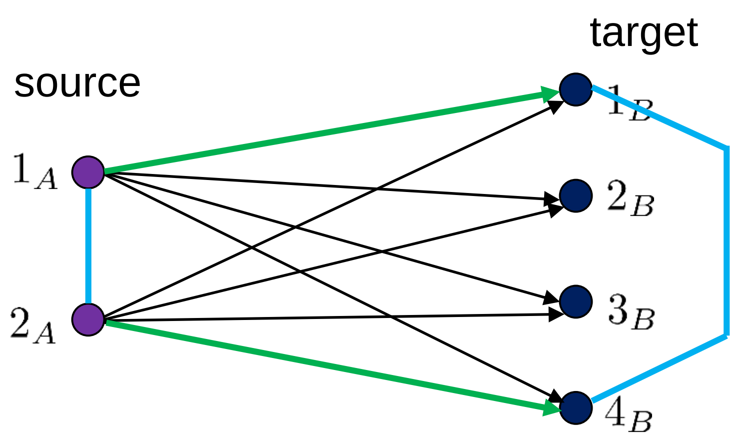
Graph Matching

- Vectorization: Define $\mathbf{x} = \mathrm{vec}(\mathbf{P}), n = n_A n_B$

$$\begin{aligned} \max. \quad & \boxed{\left\{ f(\mathbf{x}) := \mathbf{x}^T (\mathbf{A} \otimes \mathbf{B}) \mathbf{x} \right\}} \\ \text{s.t.} \quad & \mathbf{x} \in \mathcal{M} \end{aligned}$$

Maximize edge overlap

Set of maximum cardinality matchings in $\mathcal{G}_C$



$$\mathcal{G}_C = (\mathcal{V}_A \cup \mathcal{V}_B, \mathcal{E}_C)$$

Computational Challenges

- Graph Matching
  - Corresponds to a quadratic assignment problem [Koopmans-Beckmann 57]
- Theoretical: [Sahni-Gonzalez 76]
  - NP-hard (contains subgraph isomorphism as a special case)
  - NP-hard to approximate within constant-factor of optimum
- Practical:
  - Space and time complexity of computing + storing $\mathbf{A} \otimes \mathbf{B}$
  - Requires quadratic memory in the size of the graphs

Prior Art

Linear programming relaxation [Sherali-Adams 13]

Semidefinite programming relaxation [Sherali-Adams 13]

Spectral methods: [Umeyama 1988, Singh *et al.* 09, Feizi *et al.* 19]

Continuous domain

Branch and bound [Bazara 83]

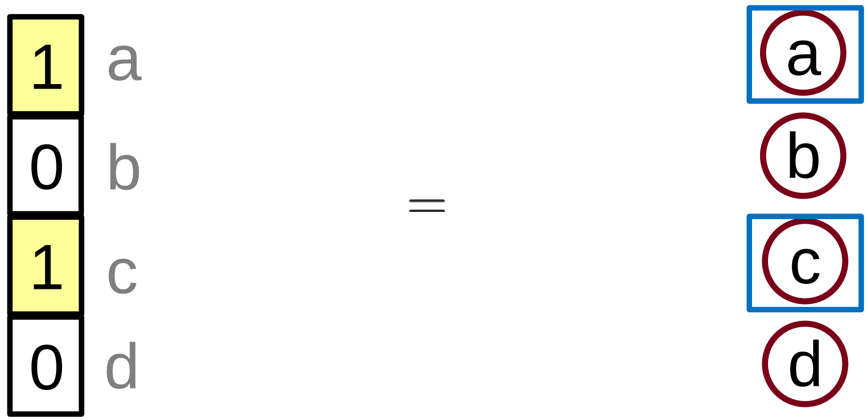
Message passing [Bayati *et al.* 10]

Discrete domain

Problem Reformulation

- Is there a more principled approach that works entirely in the combinatorial domain?
  - Represent discrete function as a set function

$\mathbf{x} \in \mathcal{M}$ $\qquad\qquad$ $\mathbf{x} = \mathbf{1}_{\mathcal{S}}$



$f : \{0,1\}^n \to \mathbb{R}$ $\qquad\qquad$ $F : 2^n \to \mathbb{R}$

  - Discrete problem = subset selection problem

Problem Reformulation

- Final formulation:

$$\boxed{\max_{\mathcal{S}\in\mathcal{I}_A\cap\mathcal{I}_B} \left\{ F(\mathcal{S}) := \mathbf{1}_{\mathcal{S}}^T(\mathbf{A}\otimes\mathbf{B})\mathbf{1}_{\mathcal{S}} \right\}}$$

where $\mathcal{I}_A = \{\mathcal{S}\subset\mathcal{E}_C, |\mathcal{S}\cap\delta(i)|\leq 1, \forall\, i\in\mathcal{V}_A\},$

$\mathcal{I}_B = \{\mathcal{S}\subset\mathcal{E}_C, |\mathcal{S}\cap\delta(j)|\leq 1, \forall\, j\in\mathcal{V}_B\}$

- Conventional wisdom:
  - Constraints are "harder" to handle compared to the objective

- Our perspective:
  - The opposite is true
  - Constraints: $\mathcal{S}\in\mathcal{I}_A\cap\mathcal{I}_B \Leftrightarrow$ matroid intersection

A closer look: objective function

- Key fact: $F(\mathcal{S})$ is a monotone, supermodular function [Konar-Sidiropoulos 19]

- Monotonicity: $\mathcal{A} \subseteq \mathcal{B} \implies F(\mathcal{A}) \leq F(\mathcal{B})$

- Supermodularity: For all $\mathcal{A} \subseteq \mathcal{B} \subseteq \mathcal{E}_C \setminus \{e\}$

$$F(\mathcal{A} \cup \{e\}) - F(\mathcal{A}) \leq F(\mathcal{B} \cup \{e\}) - F(\mathcal{B})$$

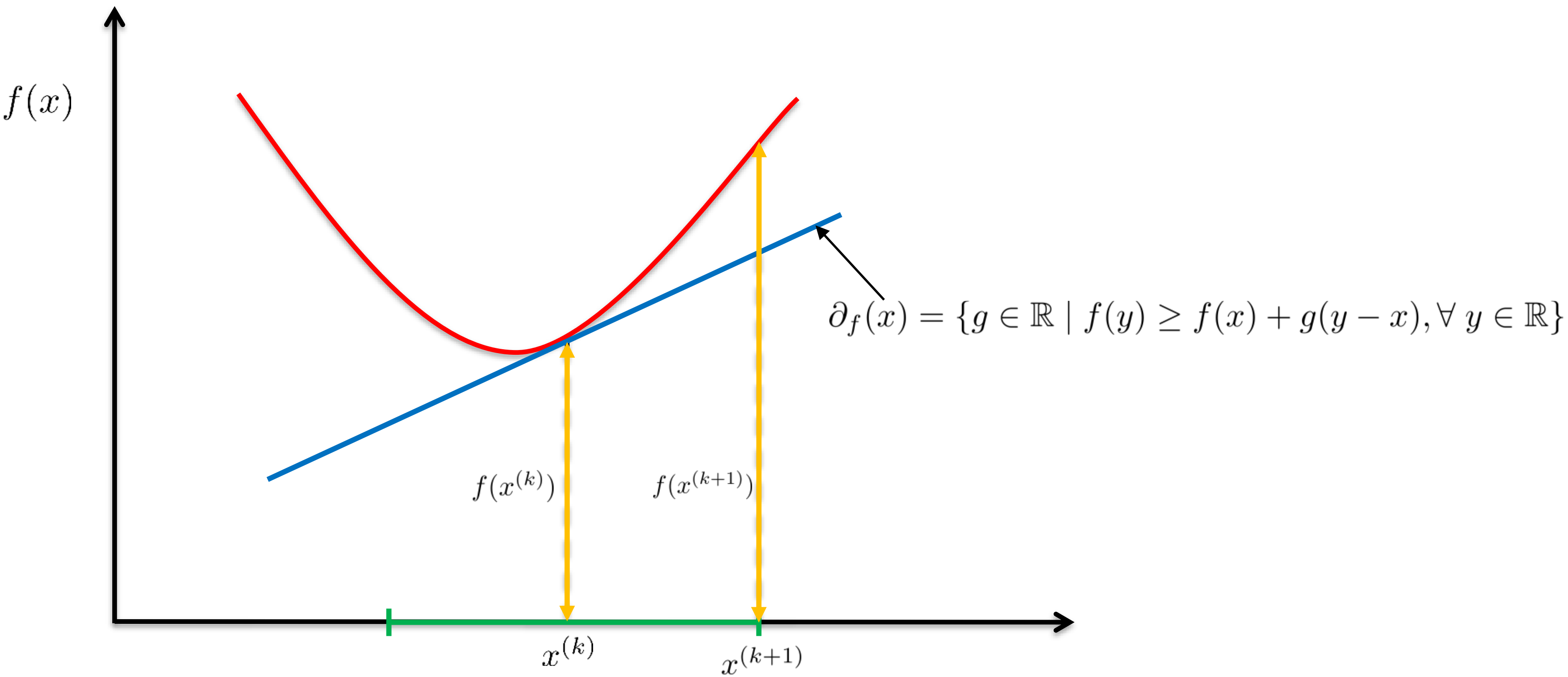
An improving returns property, reminiscent of convexity

Graph Matching

- Key Result:
  - Graph matching is a supermodular maximization problem subject to matroid intersection constraints!
- Take-away:
  - Constraints are manageable, but objective function is difficult to maximize
- Can we exploit supermodularity for approximate maximization?

Majorization Minimization

- Main Idea:
  - Iteratively maximize sequence of global lower bounds on reward



Does the idea carry over to the discrete domain?

Discrete Majorization Minimization

- **Key fact:** Supermodular functions possess (discrete) subgradients! [Jegelka-Bilmes 11]

$$\partial_F(\mathcal{X}) = \{\mathbf{g} \in \mathbb{R}^n \mid F(\mathcal{Y}) \geq F(\mathcal{X}) + G(\mathcal{Y}) - G(\mathcal{X}), \forall\, \mathcal{Y} \subseteq \mathcal{E}_C\}$$

where $G(\mathcal{Y}) = \mathbf{g}^T \mathbf{1}_\mathcal{Y} = \sum_{i \in \mathcal{Y}} g_i$

- **Construction of global lower bound:** [Bai-Bilmes 18]
  - Pick any $\mathbf{g} \in \partial_F(\mathcal{X})$, and define

$$m_\mathcal{X}(\mathcal{Y}) := F(\mathcal{X}) + G(\mathcal{Y}) - G(\mathcal{X})$$

  - Furthermore:

$m_\mathcal{X}(\mathcal{X}) := F(\mathcal{X})$ and $m_\mathcal{X}(\mathcal{Y}) \leq F(\mathcal{Y}), \forall\, \mathcal{Y} \subseteq \mathcal{E}_C$

A global lower bound on the reward function!

Discrete Majorization Minimization

- **Simplification:** For any given $\mathcal{S} \subseteq \mathcal{M}$

Option I: $$g_1(j) = \begin{cases} 2\mathrm{deg}_B(\pi(i))\mathrm{deg}_A(i), & \forall\, j \in \mathcal{S} \\ 2\mathbf{b}_{\bar{\pi}(i)}^T \mathbf{P}\mathbf{a}_i, & \forall\, j \notin \mathcal{S} \end{cases}$$

OR

Option II: $$g_2(j) = \begin{cases} 2\mathbf{b}_{\pi(i)}^T \mathbf{P}\mathbf{a}_i, & \forall\, j \in \mathcal{S} \\ 0, & \forall\, j \notin \mathcal{S} \end{cases}$$

- No Kronecker products required!
- In practice, use Option II (linear memory in size of input graph)

Discrete Majorization Minimization

- The algorithm:
  - Initialization: $\mathcal{S}^{(0)} \in \mathcal{M}$
  - Iterate: $k = \{0, 1, 2 \cdots\}$
    - Obtain subgradient $\mathbf{g}^{(k)} \in \partial_F(\mathcal{S}^{(k)})$
    - Compute update

$$\mathcal{S}^{(k+1)} \in \arg \max_{\mathcal{S} \in \mathcal{I}_A \cap \mathcal{I}_B}. \left\{ m_{\mathcal{S}^{(k)}}(\mathcal{S}) := F(\mathcal{S}^{(k)}) + \boxed{G_k(\mathcal{S})} - G_k(\mathcal{S}^{(k)}) \right\}$$

$$\updownarrow$$

$$\boxed{\mathcal{S}^{(k+1)} \in \arg \max_{\mathcal{S} \in \mathcal{I}_A \cap \mathcal{I}_B}. \left\{ G_k(\mathcal{S}) = (\mathbf{g}^{(k)})^T \mathbf{1}_{\mathcal{S}} \right\}}$$

Linear assignment / maximum weight bipartite matching problem

    - Repeat

Discrete Majorization Minimization

- Features:
  - Purely combinatorial - solves a few weighted bipartite matching problems
  - Guaranteed to improve the reward function:

$$F(\mathcal{S}^{(0)}) \leq F(\mathcal{S}^{(1)}) \leq F(\mathcal{S}^{(2)}) \leq F(\mathcal{S}^{(3)}) \leq \cdots$$

  - Guaranteed to maintain feasibility:

$$\mathcal{S}^{(k)} \in \mathcal{M}, \forall\, k \ \in \{0, 1, 2, \cdots\}$$

  - Complexity: Dominated by cost of solving weighted bipartite matching problem
    - (For $n_A = n_B$) Hungarian algorithm [Kuhn-Munkres 58] / Jonker-Volgenant algorithm [Jonker-Volgenant, 87]
    - (For $n_A < n_B$) Network-Simplex algorithm [Orlin 97]
    - Greedy matching
    - Sinkhorn Matrix Balancing [Cuturi 13, Sinkhorn 67]

Exact

Inexact

Experiments

❑ Setup:

- Given real world graph $\mathbf{A}$, generate noisy graph $\mathbf{B}$

$$\mathbf{B} = \underbrace{\mathbf{P}}_{\text{Ground-truth correspondence}}(\mathbf{A} + \underbrace{\boxed{(\mathbf{1} - \mathbf{A}) * \mathbf{Q}}}_{\text{Add extra edges}})\mathbf{P}^T$$

  - where $\mathbf{Q}$ is a random Erdos-Renyi noise graph

❑ Benchmarks:

  - Umeyama's Method: full EVD of each adjacency [Umeyama 1988]
  - Eigen-Align (EA): top eigen-vector of each adjancency [Feizi *et. al* 2016]
  - IsoRank: Random-walk based [Singh *et. al* 2008]
  - Feature Engineering (FE): local + egonet features [Berlingerio *et. al* 2012]
- Apply greedy matching on output of each algorithm to obtain final correspondence mapping

Experiments

- Implementation:
  - Initialization: Use output of FE
  - Regularization: Use node-level similarity matrix of FE
  - Inner-solver:
    - Exact: Jonker-Volgenant algorithm
    - Inexact: 5 iterations of Sinkhorn Matrix balancing + Greedy

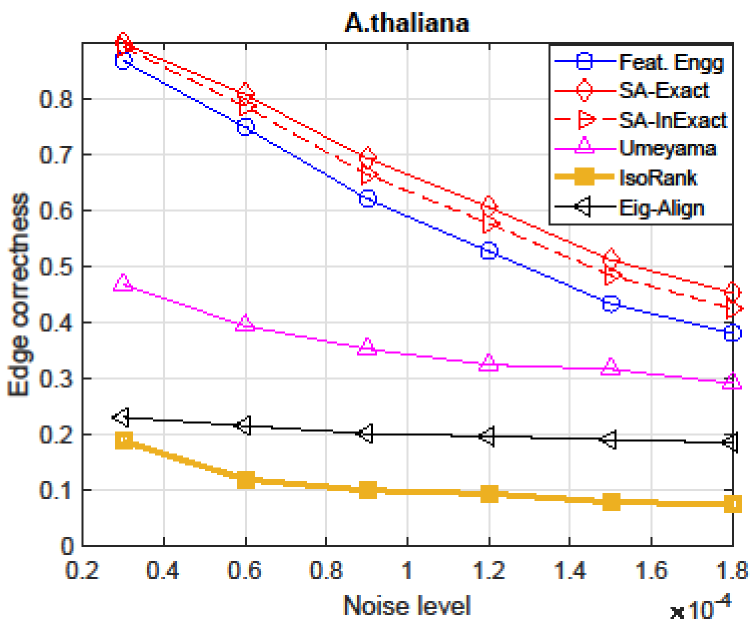
- Evaluation Metrics:
  - Edge correctness
  - Relative degree difference (by degree)

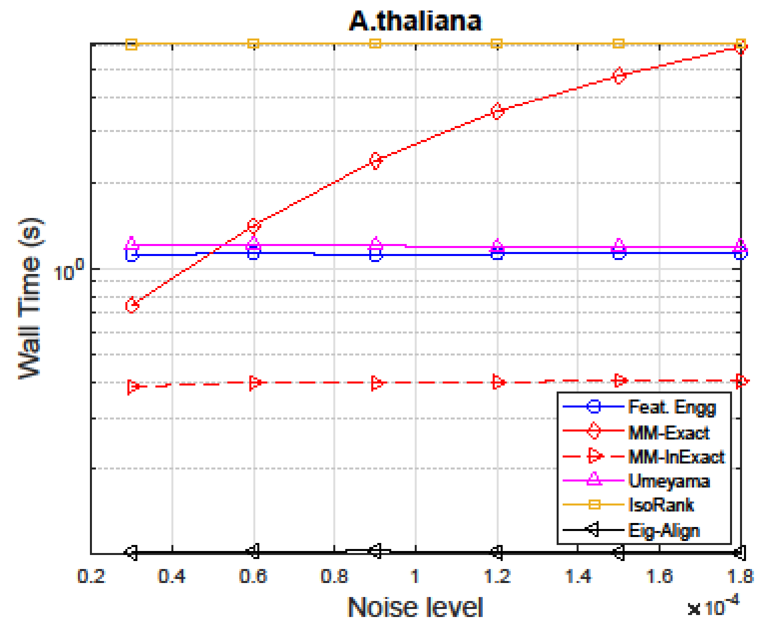
$$\mathrm{rdd}(i, \pi(i)) = \left(1 + \frac{|\deg(i) - \deg(\pi(i))|}{(\deg(i) + \deg(\pi(i)))/2}\right)^{-1}$$

  - Runtime

Results

A. Thaliana (PPI): n = 2,082, m = 4,145





15 % accuracy improvement over FE, MM-Inexact best performance overall

Results

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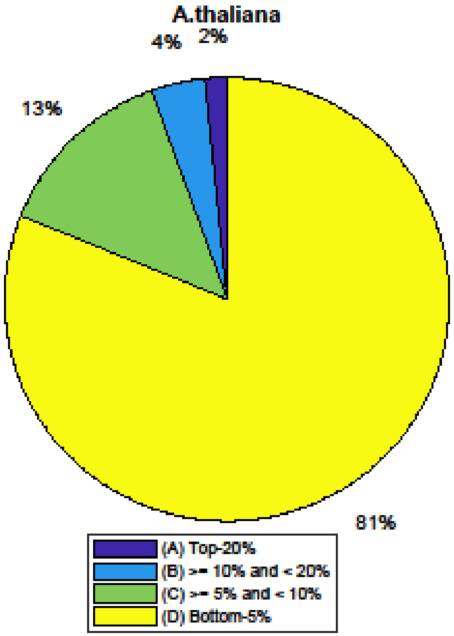
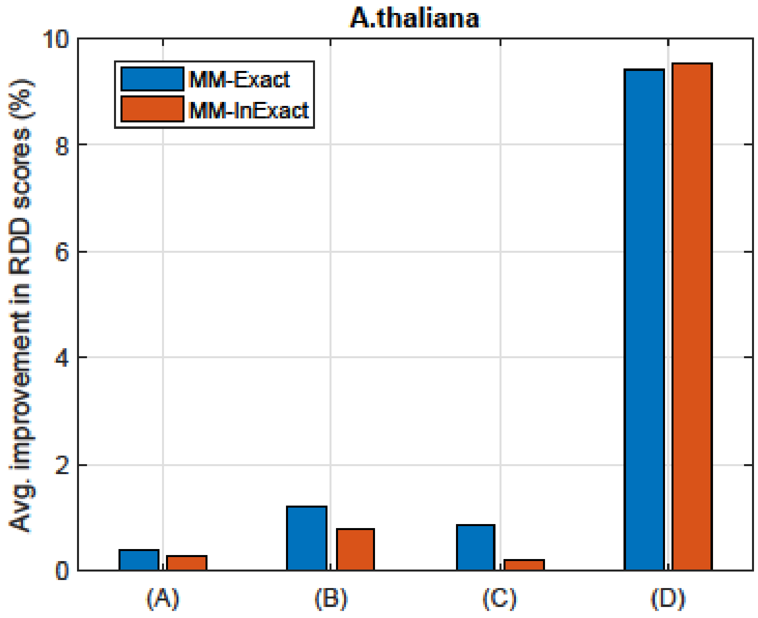




Significant improvement in RDD alignment scores for bottom 5% nodes

Conclusions

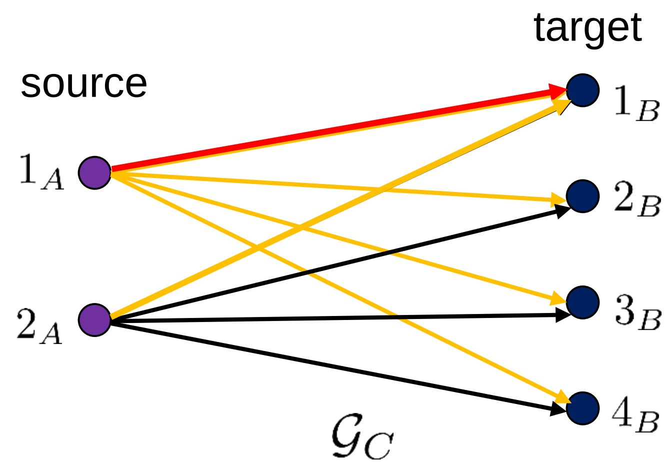
- Graph Matching through the lens of supermodularity:
  - Maximizing a supermodular function subject to matroid intersection constraints
  - Combinatorial local search based on discrete MM
    - Solve a sequence of bipartite matching problems
    - Does not require computing expensive Kronecker products
    - FE + Inexact version yields state-of-the-art performance on real-world data

- Future Work:
  - Instance specific approximation guarantees
  - Joint embedding + matching

Thank you!

A closer look: the constraints

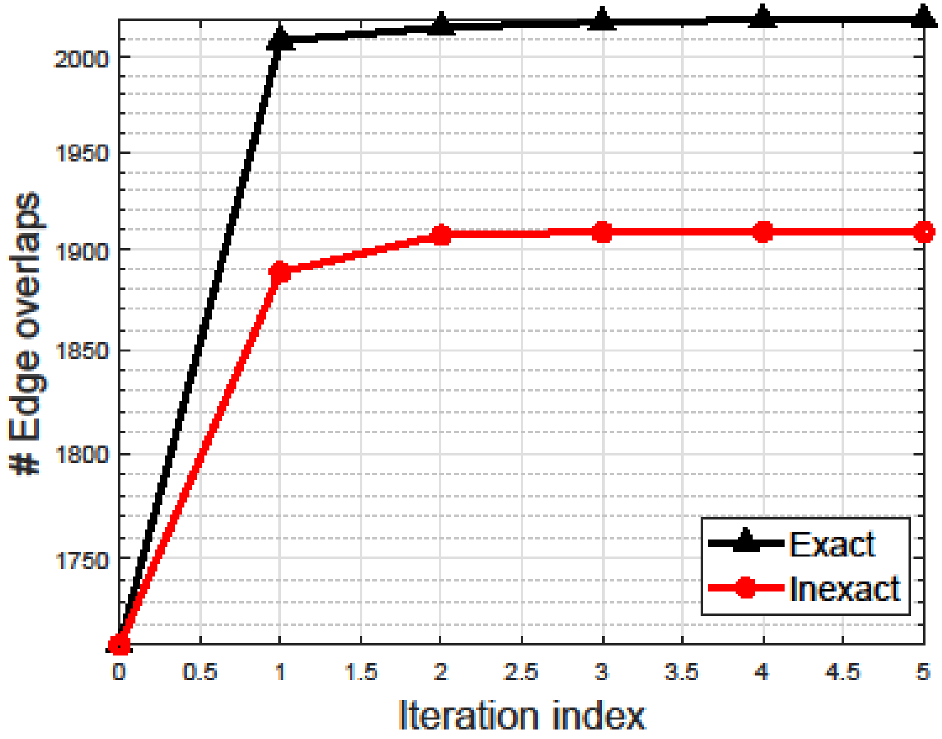
- Interpretation: $\mathcal{S} \in \mathcal{I}_A \cap \mathcal{I}_B$



- Set $\mathcal{I}_A$:
  - For every source vertex, only one outgoing edge can be selected
  - A partition matroid on the edges of $\mathcal{G}_C$
- Set $\mathcal{I}_B$:
  - For every target vertex, only one incoming edge can be selected
  - Also a partition matroid on the edges of $\mathcal{G}_C$
- Matching sets equivalent to intersection of partition matroids

Exact or Inexact?

A. Thaliana (PPI): n = 2082, m = 4145



Inexact: 5 % performance loss, 10x speedup, approx. convergence in 1 iteration

Setup

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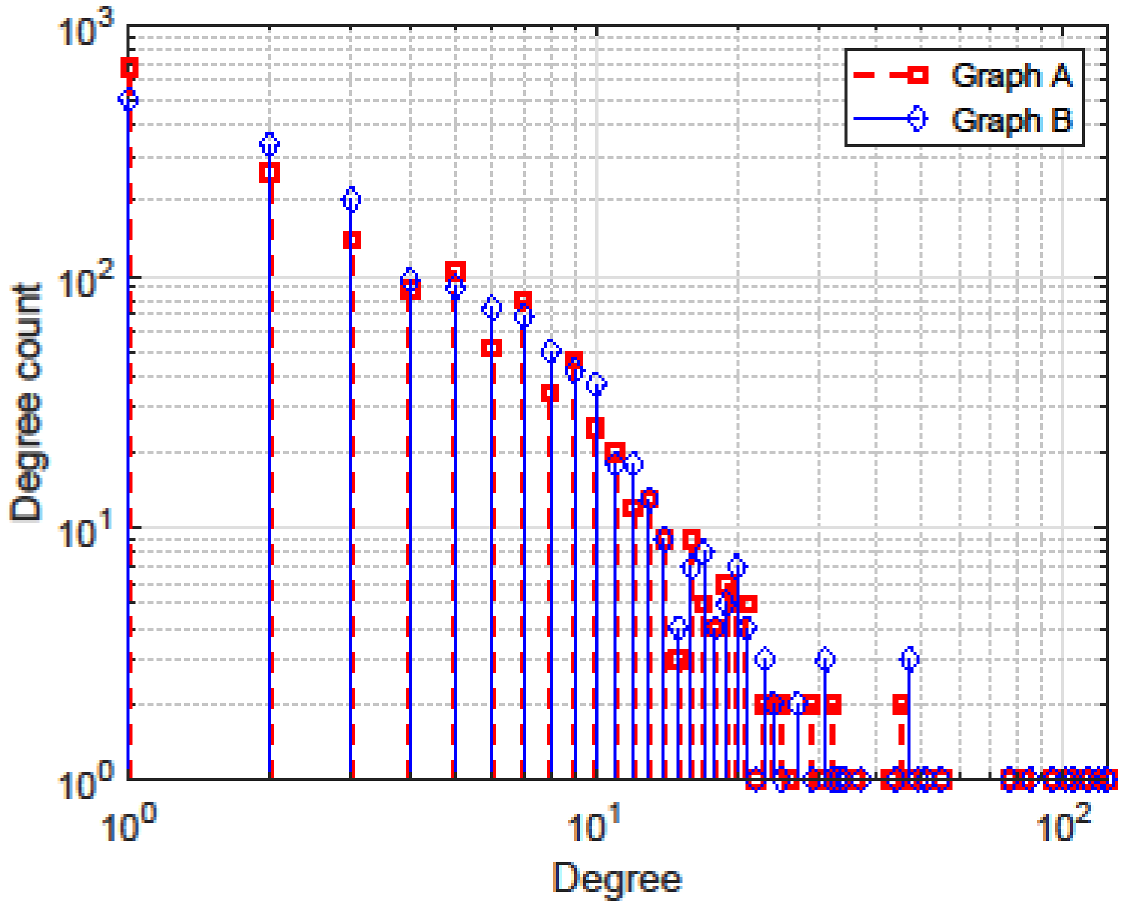
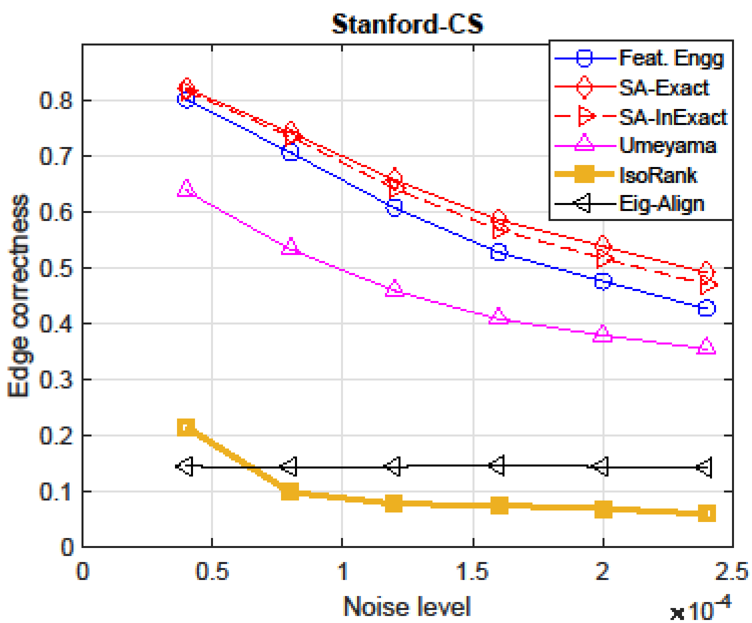
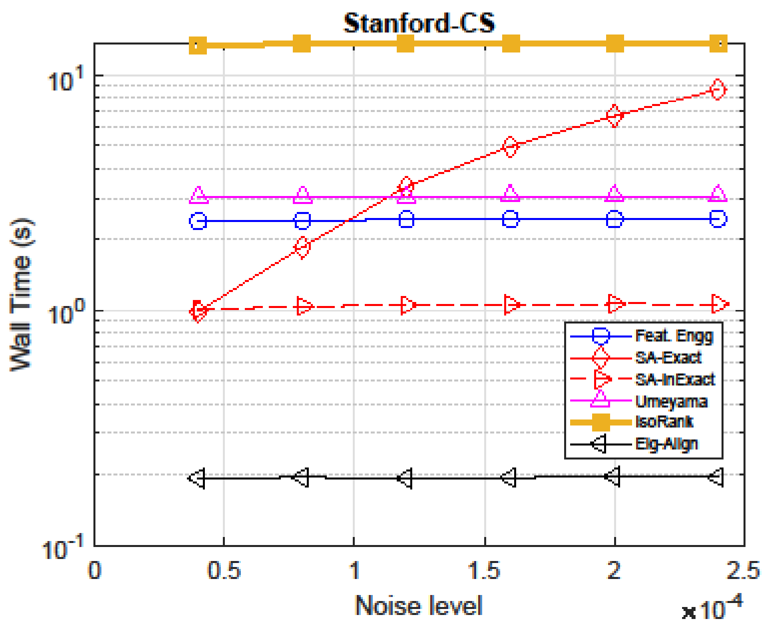


Results

Stanford-CS (web): n = 2,759, m = 10,270





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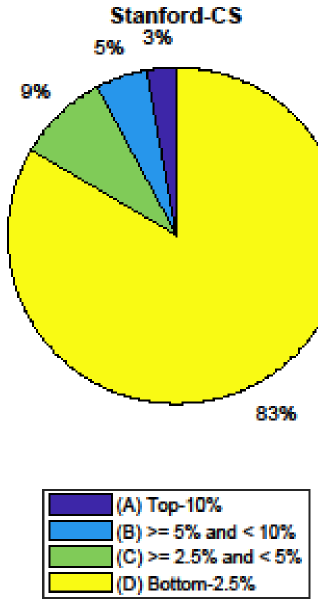
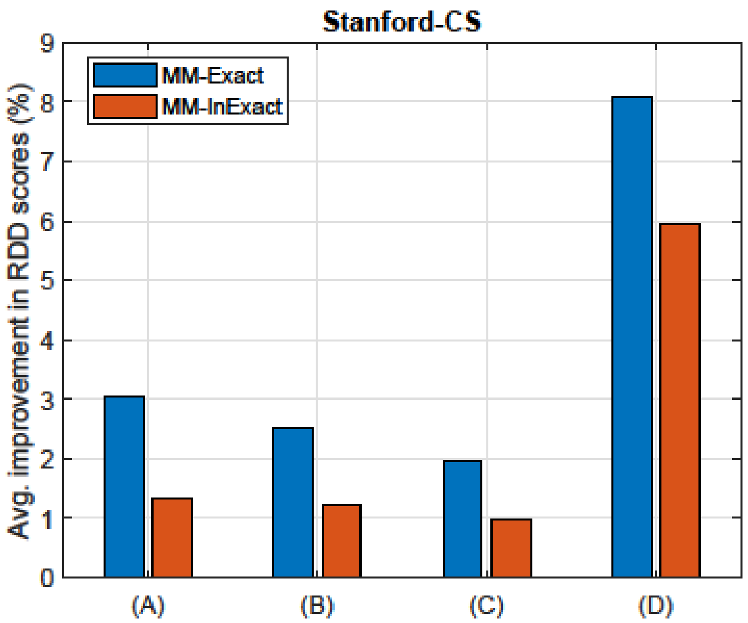
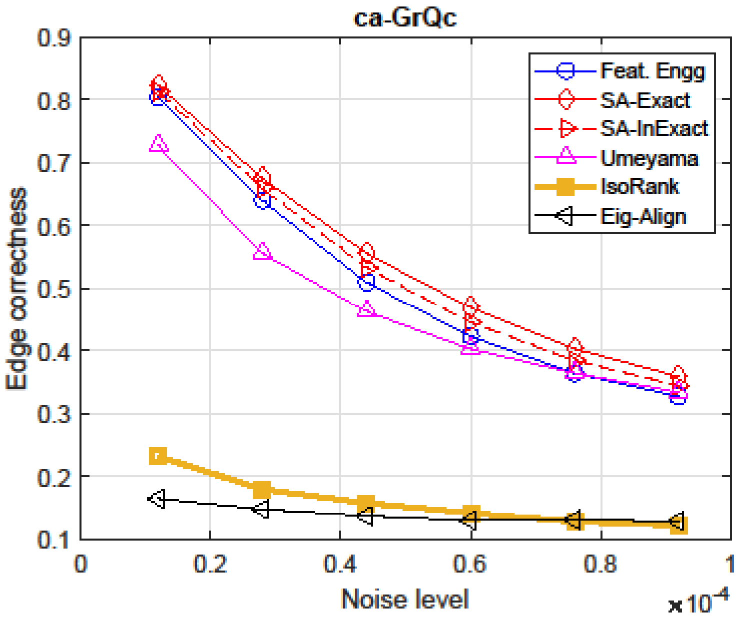


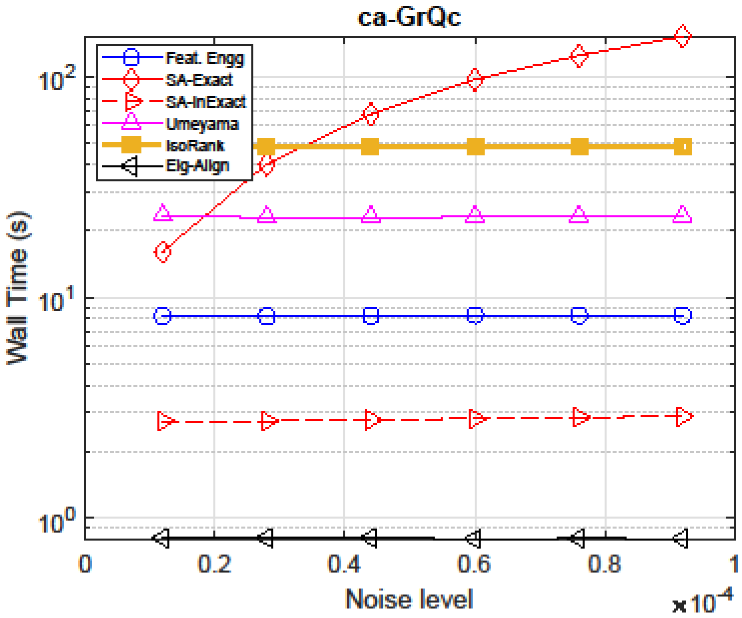


Significant improvement in RDD alignment scores of bottom 5% nodes

Results

Ca-GrQc (co-authorship): n = 5,242, m = 14,490





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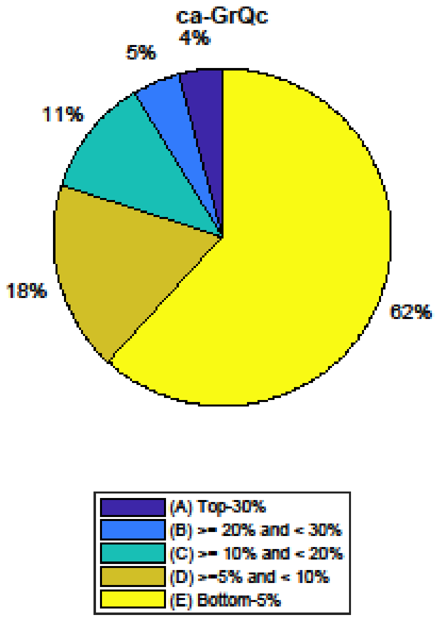

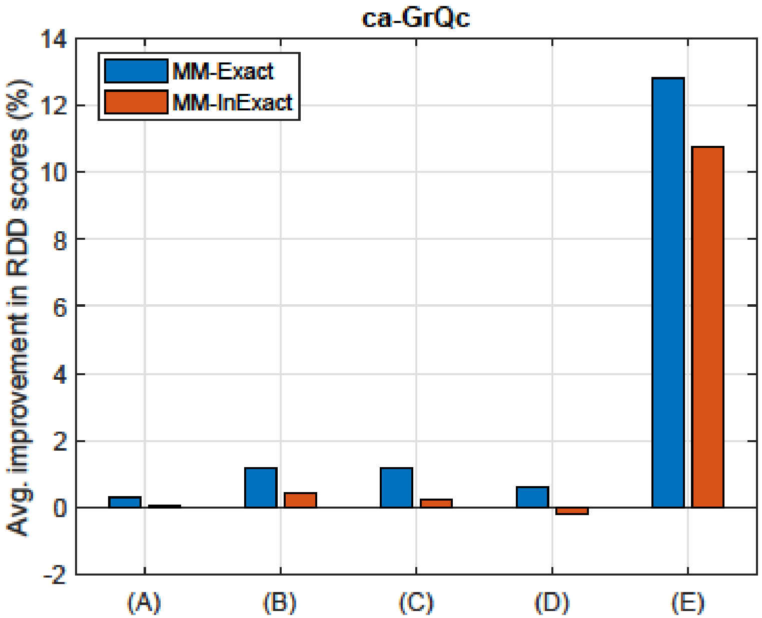

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