KerGM: Kernelized Graph Matching

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Outline

- Introduction to Graph Matching
- Our Work
- Experiments

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Introduction to Graph Matching

Graph matching problem aims at finding the optimal correspondence between nodes.

Graph matching has many applications

- Image registration
- Pattern recognition
- Image segmentation
- Shape matching
- Object tracking
- Protein-protein interaction network alignment

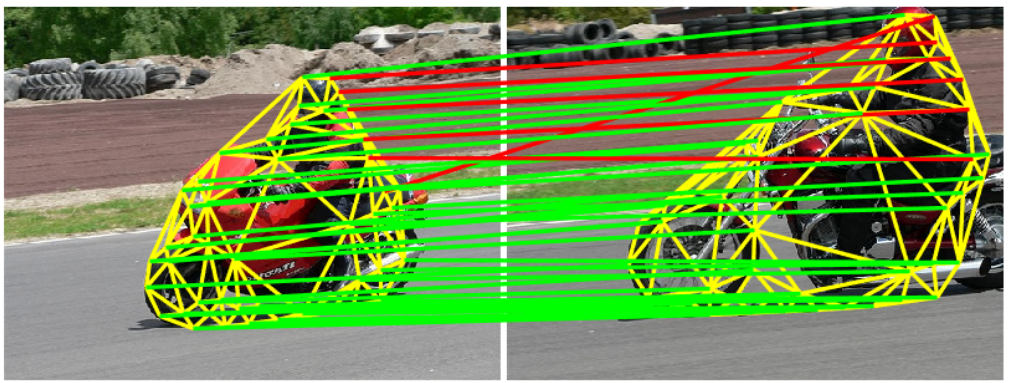

Figure 1: Landmarks matching in computer vision

Introduction to Graph Matching (Cont.)

Two quadratic assignment problems (QAPs) for graph matching

- The Koopmans-Beckmann's QAP

$$\max_{\boldsymbol{X}} \langle \boldsymbol{K}^N, \boldsymbol{X} \rangle_{\mathrm{F}} + \langle \boldsymbol{A}_1 \boldsymbol{X}, \boldsymbol{X} \boldsymbol{A}_2 \rangle_{\mathrm{F}}$$
$$\text{s.t. } \boldsymbol{X} \in \mathcal{P} = \{ \boldsymbol{X} \in \{0,1\}^{n \times n} | \boldsymbol{X}\vec{\mathbf{1}} = \vec{\mathbf{1}}, \boldsymbol{X}^T \vec{\mathbf{1}} = \vec{\mathbf{1}} \}, \tag{1}$$

  where $\boldsymbol{K}^N \in \mathbb{R}^{n \times n}$ is the node affinity matrix, $\boldsymbol{A}_1$ and $\boldsymbol{A}_2$ are the adjacency matrices of two graphs, and $\langle \cdot, \cdot \rangle_{\mathrm{F}}$ is the Frobenius inner product.

- The Lawler's QAP

$$\max_{\boldsymbol{X}} \langle \boldsymbol{K}^N, \boldsymbol{X} \rangle_{\mathrm{F}} + \mathrm{vec}(\boldsymbol{X})^T \boldsymbol{K} \mathrm{vec}(\boldsymbol{X}) \quad \text{s.t. } \boldsymbol{X} \in \mathcal{P}, \tag{2}$$

  where $\boldsymbol{K}$ is an $n^2 \times n^2$ matrix storing the edge affinities, defined such that

$$\boldsymbol{K}_{ia,jb} = \begin{cases} k^E(\vec{\boldsymbol{q}}^1_{ij}, \vec{\boldsymbol{q}}^2_{ab}), & \text{if } i \neq j, a \neq b, e^1_{ij} \in \mathcal{E}_1, \text{and } e^2_{ab} \in \mathcal{E}_2 \\ 0 & \text{otherwise} \end{cases}. \tag{3}$$

Introduction to Graph Matching (Cont.)

Pros and cons of two QAPs

- The Koopmans-Beckmann's QAP
  - It has well-designed convex and concave relaxations and has relatively low space complexity $O(n^2)$.
  - However, it doesn't consider the attribute information.

- The Lawler's QAP
  - It well encodes both the node and edge attributes.
  - However, it is not natural to obtain convex and concave relaxations and has extremely high space complexity $O(n^4)$ because of the affinity matrix $\boldsymbol{K}$.

Limitations of the Lawler's QAP

If we want to solve the Lawler's graph matching problem with more than 1, 000 nodes, we need to pre-compute a huge matrix $\boldsymbol{K}$ *of the size* $1,000,000 \times 1,000,000$.

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Our contributions

- We provide a unifying view for Koopman-Beckmann's and Lawler's QAPs, based on a very mild assumption that edge affinities are characterized by kernels.
- We rewrite Lawler's QAP as the Koopmann-Beckmann's alignment between two arrays in a reproducing kernel Hilbert space (RKHS), which allows us to solve it without computing the huge affinity matrix.
- We develop new and natural convex and concave relaxations for Lawler's QAP.
- We derive the efficient entropy-regularized Frank-Wolfe optimization algorithm for solving QAP.
- We conduct extensive experiments to demonstrate the superior performance of our kernelized graph matching algorithm. Notably, in practice, we can solve the Lawler's graph matching problem with thousands of nodes in about ten minutes.

KerGM: Kernelized Graph Matching

We assume that the edge affinity function $k^E : \mathbb{R}^{d_E} \times \mathbb{R}^{d_E} \to \mathbb{R}$ is a kernel. That is, there exist both an RKHS, $\mathcal{H}$, and an (implicit) feature map, $\psi : \mathbb{R}^{d_E} \to \mathcal{H}$, such that

$$k^E(\vec{\boldsymbol{q}}^1, \vec{\boldsymbol{q}}^2) = \langle \psi(\vec{\boldsymbol{q}}^1), \psi(\vec{\boldsymbol{q}}^2) \rangle_{\mathcal{H}}, \forall \vec{\boldsymbol{q}}^1, \vec{\boldsymbol{q}}^2 \in \mathbb{R}^{d_E}. \tag{4}$$

The Hilbert array representation of an attributed graph

For any graph $\mathcal{G}$ with edge attributes $\boldsymbol{Q} = [\vec{\boldsymbol{q}}_{ij} | e_{ij} \in \mathcal{E}]$, we can construct an array, $\boldsymbol{\Psi} \in \mathcal{H}^{n \times n}$:

$$\boldsymbol{\Psi}_{ij} = \begin{cases} \psi(\vec{\boldsymbol{q}}_{ij}) \in \mathcal{H}, & \text{if } (v_i, v_j) \in \mathcal{E} \\ 0_{\mathcal{H}} \quad \in \mathcal{H}, & \text{otherwise} \end{cases}, \text{where } 0_{\mathcal{H}} \text{ is the zero vector in } \mathcal{H}. \tag{5}$$

KerGM: Kernelized Graph Matching (Cont.)

Multiplications between a Hilbert array, $\boldsymbol{\Psi}$, and a matrix, $\boldsymbol{X}$

- $\boldsymbol{\Psi} \odot \boldsymbol{X} \in \mathcal{H}^{n \times n}$, where

$$[\boldsymbol{\Psi} \odot \boldsymbol{X}]_{ij} \triangleq \sum_{k=1}^{n} \boldsymbol{X}_{kj} \boldsymbol{\Psi}_{ik} \in \mathcal{H}. \tag{6}$$

- $\boldsymbol{X} \odot \boldsymbol{\Psi} \in \mathcal{H}^{n \times n}$, where

$$[\boldsymbol{X} \odot \boldsymbol{\Psi}]_{ij} \triangleq \sum_{k=1}^{n} \boldsymbol{X}_{ik} \boldsymbol{\Psi}_{kj} \in \mathcal{H}. \tag{7}$$

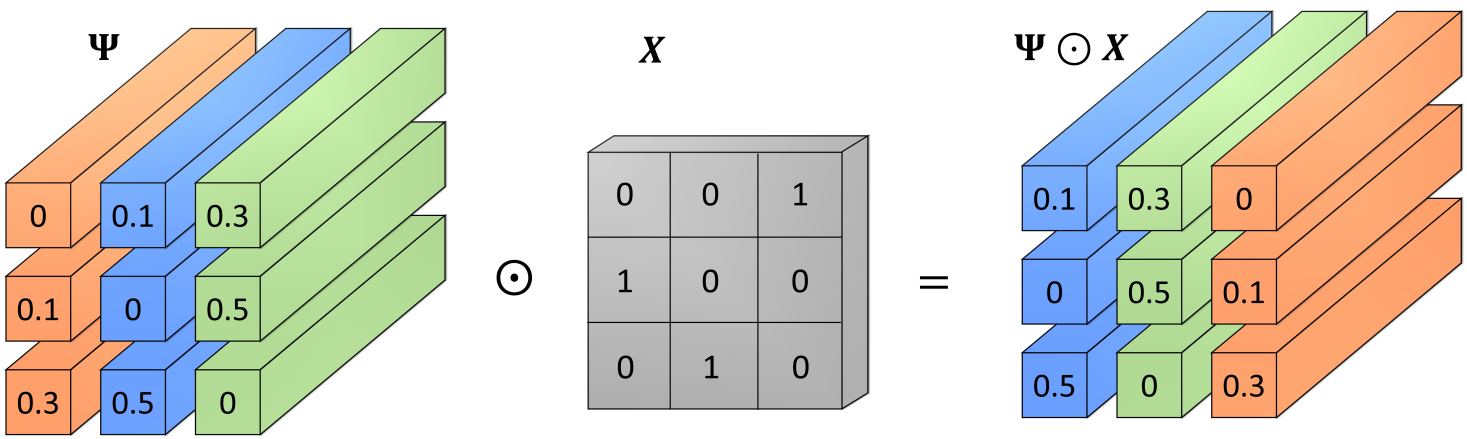

Figure 2: Visualization of the operation $\boldsymbol{\Psi} \odot \boldsymbol{X}$.

KerGM: Kernelized Graph Matching (Cont.)

Let $\boldsymbol{\Psi}^{(1)}$ and $\boldsymbol{\Psi}^{(2)}$ be the corresponding Hilbert arrays of graph $\mathcal{G}_1$ and graph $\mathcal{G}_2$, respectively. Then the Lawler's QAP can be written as

$$\begin{aligned} \max\ & J_{\mathrm{gm}}(\boldsymbol{X}) = \langle \boldsymbol{K}^N, \boldsymbol{X} \rangle_{\mathrm{F}} + \langle \boldsymbol{\Psi}^{(1)} \odot \boldsymbol{X}, \boldsymbol{X} \odot \boldsymbol{\Psi}^{(2)} \rangle_{\mathrm{F}_{\mathcal{H}}} \\ \text{s.t. } & \boldsymbol{X} \in \mathcal{P}. \end{aligned} \tag{8}$$

Remark 1. Recall the Koopmans-Beckmann's QAP is

$$\begin{aligned} \max_{\boldsymbol{X}}\ & \langle \boldsymbol{K}^N, \boldsymbol{X} \rangle_{\mathrm{F}} + \langle \boldsymbol{A}_1 \boldsymbol{X}, \boldsymbol{X} \boldsymbol{A}_2 \rangle_{\mathrm{F}} \\ \text{s.t. } & \boldsymbol{X} \in \mathcal{P}. \end{aligned} \tag{9}$$

Therefore the Lawler's QAP (8) can be rewritten as the form of the Koopmans-Beckmann's QAP.

Kernelized Graph Matching (Cont.)

Solving the Lawler's QAP

- The convex relaxation:

$$\min \ J_{\text{vex}}(\boldsymbol{X}) = -\langle \boldsymbol{K}^N, \boldsymbol{X} \rangle_{\text{F}} + \frac{1}{2} \| \boldsymbol{\Psi}^{(1)} \odot \boldsymbol{X} - \boldsymbol{X} \odot \boldsymbol{\Psi}^{(2)} \|^2_{\text{F}_{\mathcal{H}}} \quad \text{s.t. } \boldsymbol{X} \in \mathcal{D}. \tag{10}$$

- The concave relaxation:

$$\min \ J_{\text{cav}}(\boldsymbol{X}) = -\langle \boldsymbol{K}^N, \boldsymbol{X} \rangle_{\text{F}} - \frac{1}{2} \| \boldsymbol{\Psi}^{(1)} \odot \boldsymbol{X} + \boldsymbol{X} \odot \boldsymbol{\Psi}^{(2)} \|^2_{\text{F}_{\mathcal{H}}} \quad \text{s.t. } \boldsymbol{X} \in \mathcal{D}. \tag{11}$$

- The path-following strategy:

$$\min J_\alpha(\boldsymbol{X}) = (1-\alpha) J_{\text{vex}}(\boldsymbol{X}) + \alpha J_{\text{cav}}(\boldsymbol{X}) \quad \text{s.t. } \boldsymbol{X} \in \mathcal{D}. \tag{12}$$

- The entropy-regularized Frank-Wolfe optimization:

$$\min J_\alpha(\boldsymbol{X}) + \lambda \sum_{i,j=1}^{n} \boldsymbol{X}_{ij} \log \boldsymbol{X}_{ij} \quad \text{s.t. } \boldsymbol{X} \in \mathcal{D}. \tag{13}$$

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Experimental results on synthetic graphs

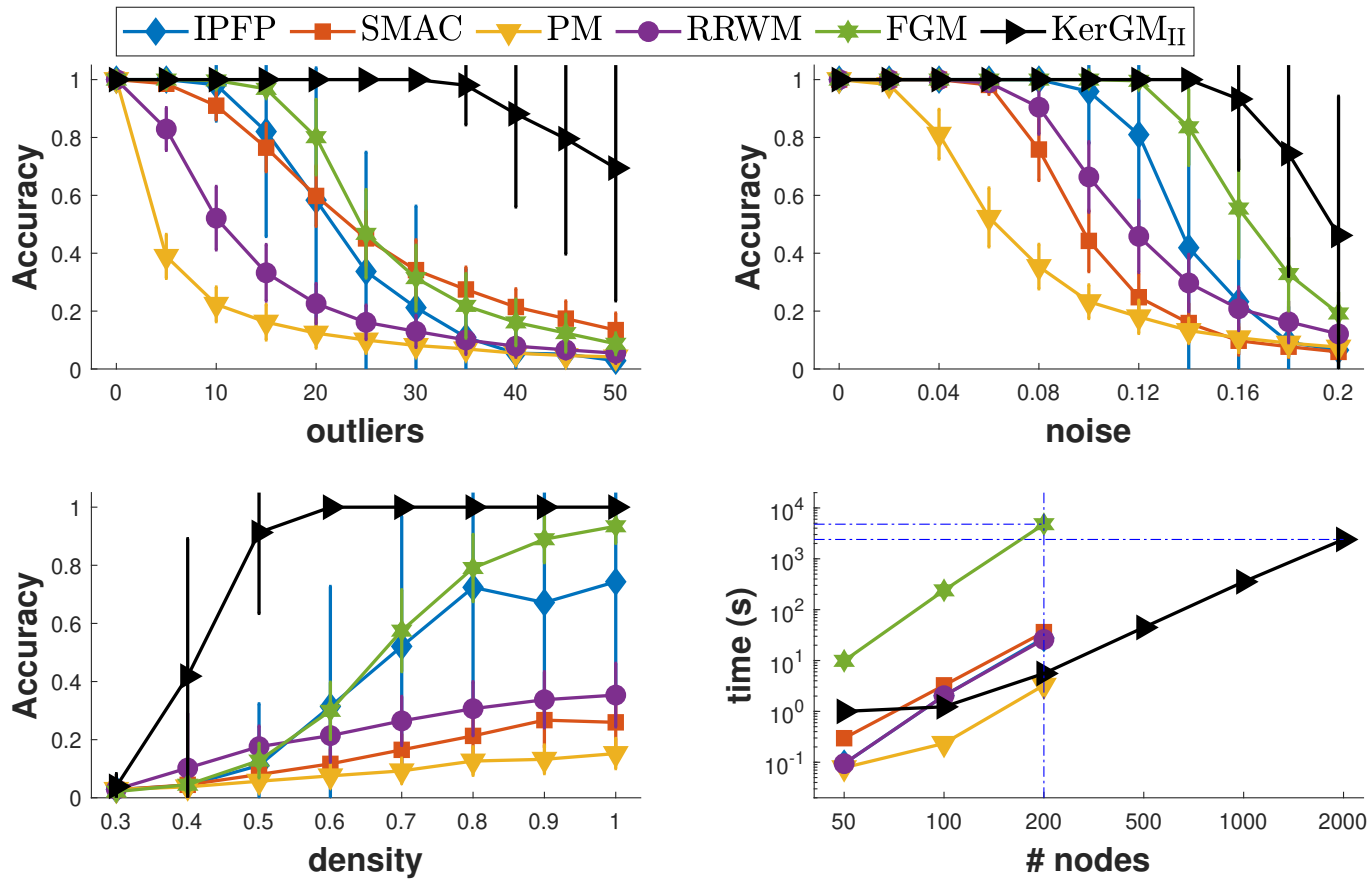

Figure 3: Compare the matching results of different agorithms on synthetic graph dataset.

Experimental results on protein-protein interaction networks

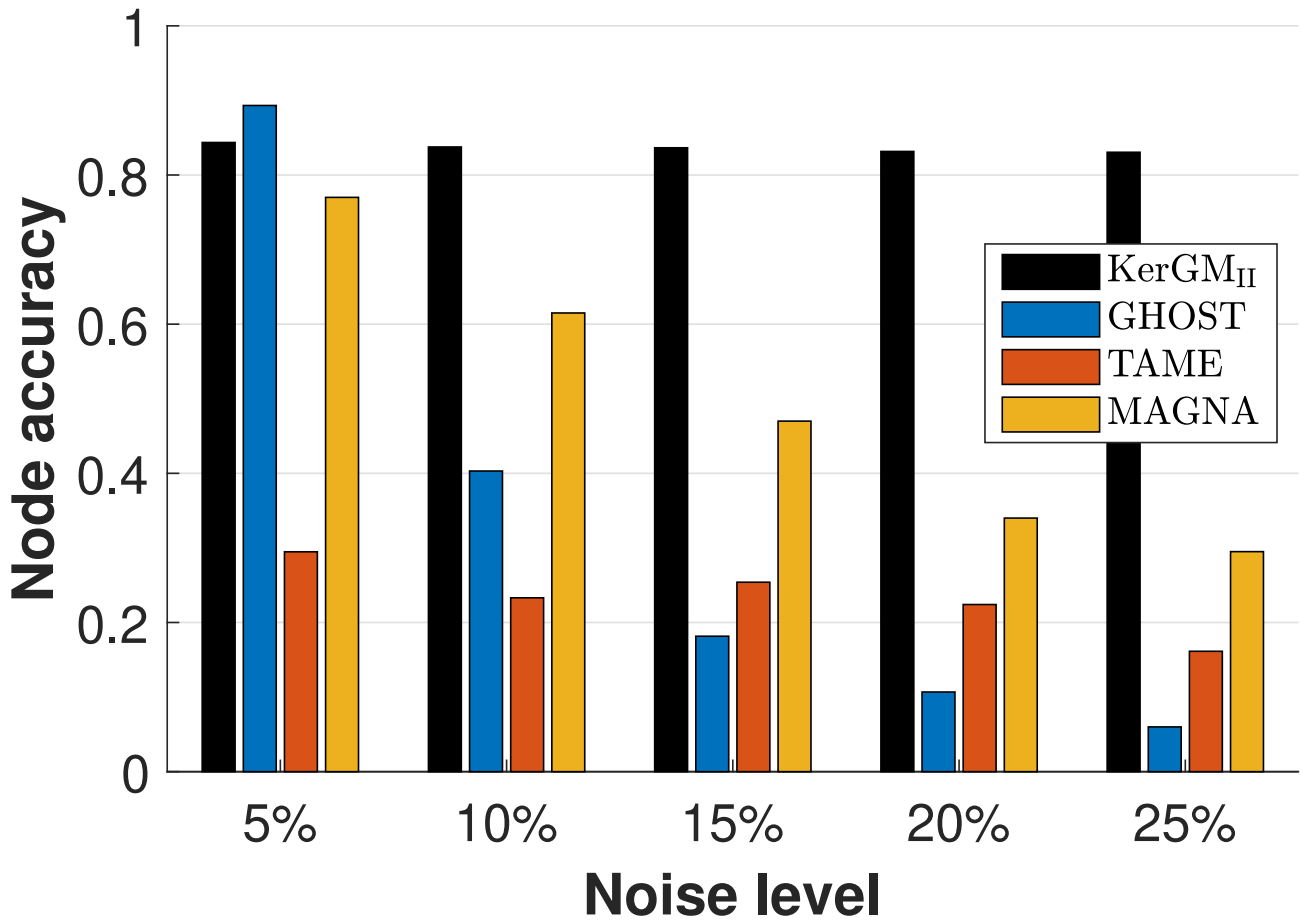

Figure 4: Results on PPI networks.