Spectral Graph Matching and Quadratic Relaxations

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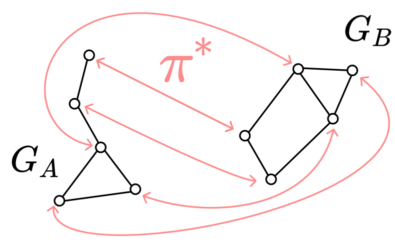
1 The Graph Matching Problem

1.1 General problem definition and initial remarks



Problem 1.1. *Given two edge-weighted graphs G_A, G_B, s.t. $|V(G_A)| = |V(G_B)|$ and $|E(G_a)| = |E(G_b)|$, let A and B denote their respective weighted adjacency matrices.* ***Graph Matching*** *(or network alignment) refers to finding a bijection π^* (which we can think of as a permutation $\pi \in \mathcal{S}_n$ on the n labels of the vertices in the set $V(G_B)$) between the vertex sets V_A, V_B of so that their edge sets E_A, E_B are maximally aligned (with respect to their weights). The optimal solution π^* of the graph matching problem satisfies:*

$$\max_{\pi^* \in \mathcal{S}_n} \sum_{i,j=1}^{n} A_{ij} B_{\pi(i)\pi(j)}. \tag{1}$$

Remark 1.1. ***Properties of the weighted adjacency matrix****, recall that given a graph $G = (V, E)$ and and edge-weighting function $w : E \to \mathbb{R}^+$ the adjacency matrix A associated with G, w is constructed as:*

$$(A_{ij} = w(e[i, j])).$$

Since the graph is undirected A is symmetric and positive semidefinite (i.e. $z^T A z \geq 0 \ \forall z \in \mathbb{R}^n$ is trivially true as $w(e) \geq 0 \ \forall e \in E(G)$). $\Rightarrow$ A has n real (not necessarily distinct positive) eigenvalues $\lambda_i \geq 0$.

Definition 1.1. *Given the adjacency matrix A of the graph G we write it's spectral decomposition as:*

$$(A_i j) = \left(\sum_{ij}^{n} \lambda_i u_i u_i^T \right),$$
$$A = Q \Lambda Q^T.$$

1.2 Gaussian Wigner Model description

Titou presents that, use the plots

2 A spectral algorithm for the graph matching problem

In the following section we use the following notation for the spectral decomposition of the adjacency matrices A and B of graphs G_A and G_B as:

$$A = \sum_{i=1}^{n} \lambda_i u_i u_i^T, \qquad B = \sum_{j=1}^{n} \mu_j v_j v_j^T,$$

where the eigenvalues are sorted such that:

$$\lambda_1 \geq ... \geq \lambda_n, \qquad \mu_1 \geq ... \geq \mu_n.$$

Algorithm 1: Graph Matching by Pairwise eigen-Alignment (GRAMPA)

Input: Weighted adjacency matrices $A, B \in \mathbb{R}^{n \times n}$ and tuning parameter $\eta \in \mathbb{R}$

Output: A permutation $\hat{\pi} \in \mathcal{S}_n$

Construct the similarity matrix:

$$\hat{X} = \sum_{i,j}^{n} w(\lambda j, \mu_j) u_i^T u_i \boldsymbol{J} v_j v_j^T \in \mathbb{R}^{n \times n}, \tag{2}$$

where $\boldsymbol{J}$ denotes the all ones $\mathbb{R}^{n \times n}$ matrix and w is the Cauchy kernel of bandwidth η.

$$w(x, y) = \frac{1}{(x-y)^2 + \eta^2}. \tag{3}$$

Output the permutation estimate $\hat{\pi}$ by rounding $\hat{X}$ to a permutation by solving the following linear assignment problem:

$$\hat{\pi} = \underset{\pi \in \mathbb{S}_n}{argmax} \sum_{i=1}^{n} \hat{X}_{i,\pi(i)}. \tag{4}$$

Property 2.1. *(**equivariance**) let $\hat{\pi}(A, B)$ denote the output of Algorithm 1, for any given permutation π on B (which gives the permuted matrix B^π constructed as $B^\pi_{ij} = B_{\pi i, \pi j}$) we have the following property:*

$$\pi \circ \hat{\pi}(A, B^\pi) = ... \tag{5}$$

2.1 Theorem 2.1 Outline

Noora writes out the outline, focus on the argmax bound

2.2 An optimization perspective on the problem

The problem as stated in (1) is an instance of the quadratic assignment problem a (QAP) which is NP-hard. Which can also be written in matrix notation as follows as a combinatorial optimization problem on permutation matrices $\Pi \in \mathcal{G}_n$:

$$\max_{\Pi \in \mathcal{G}_n} \langle A, \Pi B \Pi^T \rangle \iff \min_{\Pi \in \mathcal{G}_n} \|A - \Pi B \Pi^T\|_F^2 \iff \min_{\Pi \in \mathcal{G}_n} \|A\Pi - \Pi B\|_F^2$$

Which can in turn be relaxed from the set of permutations to it's convex hull (*the Birkhoff polytope*) into the following a quadratic program which is convex with respect to the relaxed permutation matrix X:

$$\min_{X \in \mathcal{B}_n} \|AX - XB\|_F^2 \tag{6}$$

Where the Birkhoff polytope is given by:

$$\mathcal{B}_n := \{X \in \mathbb{R}^{n \times n} : X\mathbf{1} = \mathbf{1}, X^T\mathbf{1} = \mathbf{1}, X_{ij} \geq 0 \ \forall i, j\},$$

with $\mathbf{1}$ denoting the all ones $1 \times n$ vector.

We will show that the spectral method we discuss in the next section outputs a matrix $\hat{X}$ which is a minimizer of the following quadratic problem:

$$\min_{X \in \mathcal{B}_n} \|AX - XB\|_F^2 + \frac{\eta^2}{2}\|X\|_F^2 - \mathbf{1}^T X \mathbf{1}. \tag{7}$$

Observe that for well chosen η (7) has the same solution as (6).

Titou writes out the convergence proof

3 Results

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