Spectral Graph Matching and Quadratic Relaxations

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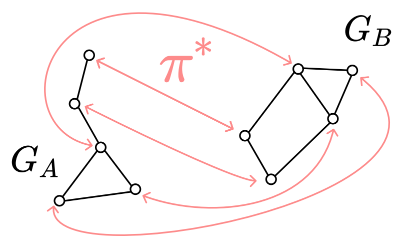
May 8, 2022

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 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:

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

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:

$$\min_{X \in \mathcal{B}_n} \|AX - XB\|_F^2 + \frac{\eta^2}{2}\|X\|_F^2 - \mathbf{1}^T X \mathbf{1}. \tag{3}$$

Observe that for well chosen η (3) has the same solution as (2).

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:

$$\hat{X} = \sum_{i,j}^{n} w(\lambda j, \mu_j) u_i^T u_i \boldsymbol{J} v_j v_j^T \in \mathbb{R}^{n\times n}, \tag{4}$$

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

$$w(x, y) = \frac{1}{(x-y)^2 + \eta^2}. \tag{5}$$

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

$$\hat{\pi} = \underset{\pi\in\mathbb{S}_n}{argmax} \sum_{i=1}^{n} \hat{X}_{i,\pi(i)}. \tag{6}$$

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:*

$$\pi \circ \hat{\pi}(A, B^\pi) = \tag{7}$$