Notes for graph-matching theory

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1 Problem Setup

Given two weighted graphs G_1, G_2 with $|G_1| = |G_2| = N$ and weight matrices W_1, W_2, our goal is to find a graph isomorphism $\rho : G_1 \to G_2$ that preserves the edge weights as much as possible. An isomorphism of graphs can be thought of as a permutation of indices $1, 2, \ldots, N$. Let P be the matrix corresponding to this permutation. Then, in detail, our goal is to find

$$\operatorname{argmin}_{P \text{ a permutation}} \left\| W_1 - P W_2 P^T \right\|_F^2 . \tag{1}$$

This problem is NP-hard, so instead we solved the relaxed problem

$$\operatorname{argmin}_{Q \text{ orthogonal}} \left\| W_1 - Q W_2 Q^T \right\|_F^2 . \tag{2}$$

This problem has a closed-form solution using eigendecompositions of the weight matrices. The background theory is presented below.

2 Graph Matching Theorem

The proof structure below was adapted from [1, 2]

Theorem 2.1. Let $A, B \in \mathbb{R}^{n \times n}$ symmetric, positive definite, with eigendecompositions $A = U A_0 U^T, B = V B_0 V^T$. Then

$$\operatorname{argmin}_{Q \text{ orthogonal}} \left\| A - Q B Q^T \right\|_F^2 = U V^T, \tag{3}$$

3 Background

Theorem 3.1. Let $A, B \in \mathbb{R}^{n \times n}$ symmetric matrices with eigenvalues $\alpha_1 \geq \alpha_2 \geq \cdots \geq \alpha_n$ and $\beta_1 \geq \beta_2 \geq \cdots \geq \beta_n$, respectively. Then

$$\|A - B\|_F^2 \geq \sum_{i=1}^{n} |\alpha_i - \beta_i|^2 . \tag{4}$$

Lemma 3.2. Let $A_0, B_0 \in \mathbb{R}^{n\times n}$ be diagonal matrices, and let

$$Q = \text{argmin}_{VV^T=I} \left\| A_0 - VB_0V^T \right\|_f^2 . \tag{5}$$

Then Q is a permutation matrix.

Proof. First, we convert the problem into a trace minimization, as

$$\begin{aligned} \left\| A_0 - VB_0V^T \right\|_F^2 &= \text{tr}\left((A_0 - VB_0V^T)(A_0^T - VB_0^TV^T) \right) . &(6)\\ &= \text{tr}\left(A_0A_0^T + B_0B_0^T - A_0VB_0^TV^T - VB_0V^TA_0^T \right) . &(7)\\ &= \text{tr}\left(A_0A_0^T + B_0B_0^T \right) + \text{tr}\left(-A_0VB_0^TV^T - VB_0V^TA_0^T \right) . &(8)\end{aligned}$$

Define

$$\begin{aligned} r(V) &= \text{tr}\left(-A_0VB_0^TV^T - VB_0V^TA_0^T \right) . &(9)\\ &= \sum_{i,j} -2\alpha_i\beta_jV_{ij}^2 &(10)\end{aligned}$$

Then we have that

$$Q = \text{argmin}_{VV^T=I} r(V). \tag{11}$$

Here is where the problem becomes more complicated. Let W be the entry-wise square of V

$$W_{ij} = V_{ij}^2. \tag{12}$$

Then W is a *doubly-stochastic matrix*. That is,

$$\sum_{i=1}^n W_{ij} = 1 \qquad \sum_{j=1}^n W_{ij} = 1 \qquad W_{ij} \geq 0 \tag{13}$$

for all i, j. Let $\mathcal{X}$ be the set of doubly-stochastic matrices, and

$$\mathcal{W} = \{W \in \mathbb{R}^{n\times n} \ : \ W \text{ is the elementwise square of a unitary } V\}. \tag{14}$$

Then we have that $\mathcal{W} \subseteq \mathcal{X}$. The Birkhoff-von Neumann theorem [3] states that $\mathcal{X}$ is a closed convex polyhedron in $\mathbb{R}^{n^2}$, where the vertices are exactly the permutation matrices. If we reimagine $r(V)$ as a function of W, then it is a linear form. Furthermore, the set of minimizers of a linear form over closed bounded convex set always includes a vertex. Therefore there is a permutation matrix Q such that

$$Q = \text{argmin}_{W\in\mathcal{X}} r(W). \tag{15}$$

Since each permutation matrix is also in $\mathcal{W}$, and $\mathcal{W} \subseteq \mathcal{X}$ we have that

$$Q = \text{argmin}_{VV^T=I} r(V). \tag{16}$$

This is exactly what we were trying to prove. $\square$

With the lemma proved, the theorem then becomes relatively simple. Here is the proof:

Proof. Let A_0, B_0 be the diagonal matrices of eigenvalues corresponding to A, B, with

$$A = UA_0U^T \tag{17}$$

$$B = UVB_0V^TU^T. \tag{18}$$

Then we have that $\|A - B\|_F^2 = \left\|A_0 - VB_0V^T\right\|_F^2$. Let

$$P = \text{argmin}_{VV^T=I} \left\|A_0 - VB_0V^T\right\|_F^2. \tag{19}$$

Then the above lemma gives that P is a permutation matrix. Therefore we have that

$$\|A - B\| \geq \left\|A_0 - PB_0P^T\right\|_F^2 = \sum_{i=1}^{n} \left(\alpha_i - \beta_{p(i)}\right)^2, \tag{20}$$

where p is the permutation on indices corresponding to the matrix P.

To finish the proof, we show that P can be chosen to be the identity permutation. Recall that we initially ordered $\alpha_1 \geq \alpha_2 \geq \cdots \geq \alpha_n$, $\beta_1 \geq \beta_2 \geq \cdots \geq \beta_n$. Suppose that $p(i) \neq i$ for some i. For ease of notation we will say $p(1) = 2$, and $p(3) = 1$. Define the updated permutation $\tilde{p}$ by $\tilde{p}(1) = 1$ and $\tilde{p}(3) = 2$ (and $p(j) = \tilde{p}(j)$ for all other j). We will show that

$$\sum_{i=1}^{n} \left(\alpha_i - \beta_{p(i)}\right)^2 \geq \sum_{i=1}^{n} \left(\alpha_i - \beta_{\tilde{p}(i)}\right)^2. \tag{21}$$

Most terms in the above inequality cancel. We need only show

$$(\alpha_1 - \beta_2)^2 + (\alpha_3 - \beta_1)^2 \geq (\alpha_1 - \beta_1)^2 + (\alpha_3 - \beta_2)^2. \tag{22}$$

This last inequality comes from simple algebra. We know that

$$(\alpha_1 - \alpha_3)(\beta_1 - \beta_2) \geq 0, \tag{23}$$

and this came be rearranged to get the desired result. This means that if the original P is not the identity permutation, we can iteratively update it by applying transpositions to get the identity. So we have proved that

$$\|A - B\| \geq \sum_{i=1}^{n} \left(\alpha_i - \beta_i\right)^2. \tag{24}$$

$\square$

4 Proof of Graph Matching Theorem

Proof. To put this in the context of the previous work, note that

$$\left\|A - QBQ^T\right\|_F^2 = \left\|A_0 - U^TQVB_0V^TQ^TU\right\|. \tag{25}$$

In the proof of theorem 3.1, it was shown that this equation is minimized by choosing $Q = UV^T$. $\square$

References

[1] S. Umeyama. An eigendecomposition approach to weighted graph matching problems. *IEEE Trans. Pattern Anal. Mach. Intell.*, 10(5):695–703, September 1988. 2

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[3] G. Birkhoff. Three observations on linear algebra. *Univ. Nac. Tacuman Rev. Ser.*, A(5):147–151, 1946. 3