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Matching graphs with equal number of nodes

Given weighted graphs G_1, G_2 with $n = |G_1| = |G_2|$, and corresponding weight matrices W_1, W_2 , we wish to find a graph homomorphism $\phi: G_1 \to G_2$ that preserves the weights as best as possible. This is easiest to express if we think of ϕ as a permutation on the ordering of nodes $1, \ldots, n$. We are trying to find

$$\operatorname{argmin}_{P \text{ a permutation matrix}} \left\| W_1 - PW_2 P^T \right\|.$$

First we do dimension reduction using eigenvectors of the Graph Laplacian. Have L_1, L_2 be the Graph Laplacians for G_1, G_2 , respectively. Let U_1, U_2 be the matrices formed by picking the k eigenvectors with the smallest eigenvalues (so each U is $n \times k$). The rows of U_i represent the images of each graph node after the dimension reduction. Matching rows of U_1 to rows of U_2 would find the desired permutation, but there is a problem with the sign-ambiguity of the eigenvectors. For now, we handle this by assuming we have already matched one point in G_1 with one point in G_2 . We can then compare the corresponding rows of U_1, U_2 and fix the signs as we go.

To perform the rest of the matching, define

$$U = U_2 U_1^T.$$

The ij-th entry of U represents the quality of the match between the i-th row of U_2 and the j-th row of U_2 . Use the Hungarian algorithm on the matrix U to find a matching that maximizes the sum of the individual match qualities.

Example Calculation

Say we have n = 4 and k = 2, and we calculate

$$U_1 = \begin{pmatrix} 0.4970 & -0.0018 \\ 0.5030 & -0.0058 \\ -0.5054 & -0.7033 \\ -0.4946 & 0.7109 \end{pmatrix}$$

$$U_2 = \begin{pmatrix} 0.5016 & -0.0006 \\ 0.4984 & -0.0000 \\ -0.4995 & 0.7074 \\ -0.5005 & -0.7068 \end{pmatrix}$$

Then

$$U = U_2 U_1^T = \begin{pmatrix} 0.2493 & 0.2523 & -0.2530 & -0.2485 \\ 0.2477 & 0.2507 & -0.2519 & -0.2465 \\ -0.2495 & -0.2554 & -0.2451 & 0.7500 \\ -0.2474 & -0.2476 & 0.7500 & -0.2549 \end{pmatrix}$$

Let's label the nodes of G_1 as x_1, \ldots, x_4 , and the nodes of G_2 as y_1, \ldots, y_4 . Then from U we see that x_4 matches to y_3 , x_3 matches to y_4 . x_1, x_2 and y_1, y_2 should match to each other somehow, but there is no strong reason to choose one matching or the other.

Example Picture

See figure 1. Here we have two different 2-dimensional datasets, X_1, X_2 . X_1 is shown in the plane z = 0, with blue dots. X_2 is shown in the plane z = 1, with orange dots. Both datasets consist of a point cluster of 50 points, as well as a line segment of 100 points.

For each dataset, we form a weight matrix by considering the L^2 distance between points. These matrices are then input into the algorithm above to form a matching. In the figure, matching points are joined by a line. We use k=4 eigenvectors (chosen mostly arbitrarily).

Next thing to do

Obviously, there is a lot left to do. First, I want to update the algorithm to be able to handle a partial matching. The benefit of this algorithm is that the matrix U gives a numerical value to the quality of matches between different points. We should be able to use this to decide what constitutes a "good" match, and which matches are "bad". In the final algorithm, we expect our input graphs to be sufficiently different, and we don't want to create any "bad" matches. Rather, we leave those points unmatched.

Second, we should be able to handle the case when $|G_1| \neq |G_2|$. Right now, the algorithm will run in this scenario, but the output doesn't seem optimal. See figure 2. In this example the set X_1 (blue) has 150 points, and X_2 (orange) has 90 points. When matching the line segments, it seems to prioritize points at the corners. I'm not sure why yet. I think those points are the most different from the points closer to the center of the line segments, which is why they are matched.

Third, maybe we should think about making this algorithm semisupervised. It's easy to enforce certain node-matchings by editing the matrix U to give a high value to those matchings, but I don't think that fully uses the assumption that two nodes match. Somehow this should suggest more matchings with nearby nodes, but I'm not sure how to do that yet.

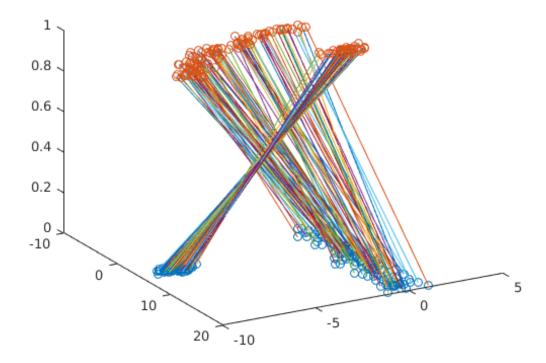


Figure 1: Example Graph matching. 150 nodes in both sets.

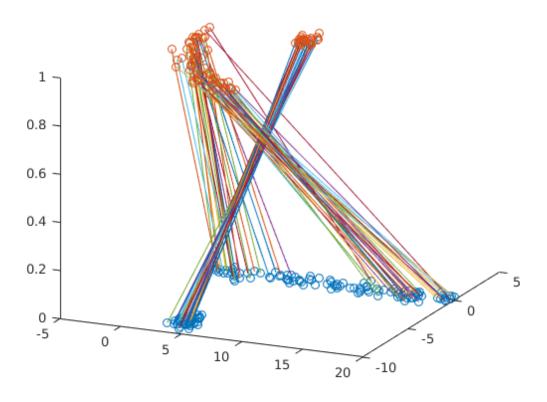


Figure 2: 150 nodes in blue set. 90 nodes in orange set.