Projected power iteration for network alignment

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ABSTRACT

The network alignment problem asks for the best correspondence between two given graphs, so that the largest possible number of edges are matched. This problem appears in many scientific problems (like the study of protein-protein interactions) and it is very closely related to the quadratic assignment problem which has graph isomorphism, traveling salesman and minimum bisection problems as particular cases. The graph matching problem is NP-hard in general. However, under some restrictive models for the graphs, algorithms can approximate the alignment efficiently. In that spirit the recent work by Feizi and collaborators introduce EigenAlign, a fast spectral method with convergence guarantees for Erdős-Rényi graphs. In this work we propose the algorithm Projected Power Alignment, which is a projected power iteration version of EigenAlign. We numerically show it improves the recovery rates of EigenAlign and we describe the theory that may be used to provide performance guarantees for Projected Power Alignment.

Keywords: Quadratic assignment, graph matching, projected power iteration

1. INTRODUCTION

Data science aims to extract information from data, usually by first proposing a model for the sought information, and then solving an optimization problem of the form

\begin{equation}
\text{minimize } f_D(x) \quad \text{subject to } x \in S.
\end{equation}

In (1), $D$ is the data for the problem, that can be thought to belong to a large set $\mathcal{D}$ of all possible problems; and $S$ is the set of all feasible solutions for (1).

For instance, the network alignment or graph matching problem consists in, given two graphs $G_1$ and $G_2$ with $n$ vertices, to find the best permutation to align $G_1$ with $G_2$. If $G_1$ and $G_2$ are isomorphic, then a solution is an isomorphism between them. If they are not, the solution is the permutation that matches the largest amount of edges possible between $G_1$ and $G_2$. The network alignment problem has an optimization formulation of the form (1) that we describe in Section 1.1 where $S$ is the (discrete) set of $n \times n$ permutation matrices. Network alignment is a relevant problem for many scientific applications, including computational biology\textsuperscript{4}, computer vision\textsuperscript{2} and linguistics.\textsuperscript{3} In computational biology, network alignment is a useful tool for studying protein-protein interactions.\textsuperscript{4} Network alignment is closely related with the more general quadratic assignment problem that has the traveling salesman problem and the minimum bisection as particular cases. We give a broad description of network alignment and quadratic assignment in Section 1.1 but for now we still consider the setting of the generic optimization problem (1).

The optimization problem (1) arising from data science is quite often NP-hard and therefore there is no hope to find an efficient algorithm that would find the exact solution for every $D$. However, being NP-hard is a statement about the hardest instance of the problem, and quite often, efficient algorithms can be used to solve or find an approximate solution for (1) for a large subset of $\mathcal{D}$. Examples of such phenomenon include but are not restricted to convex relaxations. The approach may have started with the seminal work of Goemans and Williams\textsuperscript{5} and became very popular after compressed sensing.

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Efficient algorithms may give satisfactory solutions to the problem (1) for \( D \in \mathcal{D} \) where \( \mathcal{D} \) is a proper subset of all possible data instances \( \mathcal{D} \). Therefore it is natural (and a common practice within the applied mathematics, theoretical computer science and statistics communities) to study such algorithms under certain generative models. In those cases, the data is assumed to be generated by a specific probabilistic model which many times can be interpreted as

\[
D = \text{signal} + \lambda \text{noise},
\]

where the signal is structured (usually sparse or low rank) and the noise obeys a simple probabilistic model and it is somehow incoherent with the signal structure. The classic mixtures of Gaussians and the currently popular stochastic block model\(^6\) can be seen as examples of generative models of form (2). When designing a generative model for a problem of the form (1), a natural structure for the signal is one that makes the solution of (1) obvious. For instance, the stochastic ball model\(^6\) was introduced by Nellore and Ward in order to study the performance of a clustering algorithm, and it consists of points drawn from disjoint unit balls, making the solution to the clustering problem apparent.

In the case of the network alignment, we may let \( D_\lambda = (G_1, G_2 := P^T G_1 P + E_\lambda) \) where \( P \) is an \( n \times n \) permutation matrix and \( G_1 \) may itself obey a generative model such as Erdős-Rényi. (Here we are abusing the notation and using \( G_1 \) and \( G_2 \) the adjacency matrix of said graphs.) The matrix \( E_\lambda \) is the noise, for instance switching randomly a \( \lambda \) fraction of the edges (from 0 to 1 or from 1 to 0). For \( \lambda = 0 \) (\( E_\lambda = 0 \)) a solution of the network alignment problem is the permutation \( P \), however the solution is not necessarily unique. In this context the permutation \( P \) is considered to be the planted solution or ground truth for the alignment problem. If the noise level \( \lambda \) is small and \( G_1 \) is well-conditioned (namely \( G_1 \) is a sufficiently large asymmetric graph) one expects that \( P \) continues to be a solution of (1) for \( D_\lambda \) until some threshold \( \lambda^*(G_1) \) where \( P \) stops being the solution of (1) but maybe the solution \( P^* \) is correlated with \( P \). When \( \lambda \) is too large then we expect \( P^* \) not to contain meaningful information about \( P \), and it makes no sense to think of \( P \) as the planted solution anymore. These statistical thresholds for recovery and weak recovery are classic statistical questions and had been studied for the stochastic block model\(^6\). For the graph matching problem there exists partial results\(^8\) but the problem is still open.

A completely different question is whether one can find the solution of (1) in polynomial-time. An active research area in Theoretical Computer Science and Statistics is to understand the interplay between statistical and computational detection thresholds for community detection problem.\(^6\) See\(^9,10\) for other examples of statistical inference tradeoffs under computational constraints. Algorithms studied in this context include spectral methods, projected power iteration and approximate message passing. In some restrictive cases, these algorithms are proven to achieve recovery all the way to the threshold where recovery is possible. There is a very nice explanation of this phenomenon and how different algorithms relate to each other by Perry and collaborators\(^11\). Another line of algorithms that has been explored towards these problems are automatically learned algorithms using data-driven techniques like neural networks\(^12,13\). One issue to stress is that algorithms designed to address problem (1) under a certain model of the form (2) may be over fitting the statistical model and may not work under small modifications as it has recently been observed using semi-random models\(^14\).

Returning to the network alignment problem and the model \( D_\lambda \) we defined, at \( \lambda = 0 \) the question is equivalent to the graph isomorphism problem for which Babai recently has announced a quasi-polynomial algorithm\(^15\). However, depending on the generative model, the problem can be much simpler like for friendly graphs.\(^16\) Efficient heuristic algorithms of graph matching for special applications are available without theoretical guarantees and the reader is referred to comprehensive surveys.\(^17,18\) In this paper we define Projected Power Alignment, a projected power iteration algorithm based on EigenAlign. EigenAlign is a spectral method recently introduced by Feizi and collaborators\(^19\) based on an relaxation of the quadratic assignment problem.

**Our contribution**

In this paper we propose an algorithm, Projected Power Alignment, which is a projected power iteration version for the spectral algorithm EigenAlign.\(^19\) We numerically compare its performance with EigenAlign for the Erdős-Rényi with noise generative model.
Future work includes the study of the evolution equation for Projected Power Alignment, study of the statistical thresholds for recovery for the Erdős-Rényí model and an approximate message passing version of our algorithm.

Organization of this paper
In Section 1.1 we review the quadratic assignment problem, and in Section 1.2 we explain the algorithm EigenAlign which we use as a baseline for our projected power iteration alignment algorithm. In Section 1.3 we describe projected power iteration algorithms. In Section 2 we introduce our projected power iteration for alignment. In Section 3 we present numerical simulations.

1.1 Graph matching and Quadratic assignment
Graph matching is a classic problem in theoretical computer science. Given two graphs with $n \times n$ adjacency matrices $G_1, G_2$, the graph matching problem asks for the best permutation matrix to align them. Mathematically it can be expressed as

$$\min_{X \in \Pi} \|G_1 X - X G_2\|_F^2,$$

where $\Pi$ is the set of all permutation matrices of size $n \times n$. Graph matching is closely related with the quadratic assignment problem, that has the graph isomorphism, traveling salesman problem, Gromov-Hausdorff distance and the minimum bisection as particular cases.

The quadratic assignment problem (QAP) and graph isomorphism were deeply investigated in computer science literature from a worst-case point of view. QAPs in general are known to be NP-hard to solve exactly and even to approximate, no polynomial time algorithm can be guaranteed to approximate the solution up to a small constant factor. Graph isomorphism problem is a very special case of QAP, that in our case asks the existence of such $X \in \Pi$ that vanishes (3). It is not known whether the graph isomorphism problem is in P or not, despite the recent advancement that proposed a quasi-polynomial time algorithm.

The data science approach has shifted the focus from worst-case performance to average-case complexity. Namely finding a polynomial time algorithm that works for most cases. For instance, community detection, although classically studied as NP-hard min-bisection problem, recently revealed interesting information-theoretic analysis and efficient algorithms with high probability guarantees under stochastic block model.

Our problem in the random case can be described as follows. Assume we have two unlabeled graphs $G_1$ and $G_2$, that are noisy observations from an underlying graph. Noise here refers to edge addition or deletion. Since $G_1$ and $G_2$ are observations of the same graph they induce a planted bijection across the node sets of the two graphs and our goal is to recover it. Equivalently it can be stated as having observed two adjacency graphs $G_1$ and $G_2$ where $G_2 = PG_1P^T + W$ for some $P \in \Pi$ and noise matrix $W$, can we recover $P$? Note that the maximum a posteriori estimate of $P$ is the solution of graph matching problem provided independent small noise.

Let us consider $G_1$ to be an from Erdős-Rényi graph on $n$ nodes and edges independently drawn with probability $p$. In the noiseless case (the isomorphism problem on random graphs from ER($n$, $p$) distribution) the problem can be efficiently solved with high probability by canonical labeling provided $p \in [\Theta\left(\frac{\ln n}{n}\right), 1 - \Theta\left(\frac{\ln n}{n}\right)]$. This range of $p$ covers the region of almost sure asymmetry for ER($n$, $p$) by a constant factor. Therefore there are efficient algorithms that are order optimal. Despite the success with high probability of polynomial-time algorithms in graph isomorphism, there is no known efficient algorithm for the general case ($W \neq 0$) that is of satisfying success with respect to information theoretic bounds. In fact, the information theoretic bounds have been only recently studied.

1.2 The spectral method EigenAlign
Given two unweighted undirected graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ with $n$ vertices each, the EigenAlign algorithm first defines the alignment matrix $A(G_1, G_2)$. The alignment matrix that is a $n^2 \times n^2$ that encodes
pairwise information of edges of $G_1$ and $G_2$ giving a score to whether edges match or not. Namely,

$$A[(i,j'),(r,s')] = \begin{cases} 
  s_1 & \text{if } (i,r) \in E_1 \text{ and } (j',s') \in E_2 \\
  s_2 & \text{if } (i,r) \notin E_1 \text{ and } (j',s') \notin E_2 \\
  s_3 & \text{otherwise} 
\end{cases} \quad (\text{edge mismatch}).$$

This definition can be extended for weighted or undirected graphs. The network alignment on the matrix $A$ is

$$\text{minimize}_y \ y^T A y \quad (5)$$

subject to

$$\sum_i y_{i,j'} = 1 \quad \text{for all } j' \in V_2$$

$$\sum_{j'} y_{i,j'} = 1 \quad \text{for all } i \in V_1$$

$$y_{i,j'} \in \{0,1\} \quad \text{for all } (i,j') \in V_1 \times V_2.$$

Note that the constraints in (5) are equivalent to asking $y$ to be the vectorization of a permutation matrix. Using properties of the Kronecker product we have $\text{Trace}(G_1 X G_2 X^\top) = \text{vec}(X)^\top G_1 \otimes G_2 \text{vec}(X)$ and one can check that

$$y^T A y = \text{Trace}(G'_1 X G'_2 X^\top) + \text{constant}$$

where $\text{vec}(X) = y$ and

$$G'_1 = G_1 + \frac{s_3 - s_2}{s_1 + s_2 - 2s_3}$$

$$G'_2 = (s_1 + s_2 - 2s_3)G_2 + (s_2 - s_3) \quad (6)$$

The EigenAlign algorithm reads as follows:

0. Compute $A$ as in (4).

1. Compute $v$ the top eigenvector of $A$.

2. Solve the maximum weight bipartite graph matching by solving the following optimization:

$$\text{maximize}_y \ v^\top y, \quad (8)$$

subject to

$$\sum_i y_{i,j'} = 1 \quad \text{for all } j' \in V_2$$

$$\sum_{j'} y_{i,j'} = 1 \quad \text{for all } i \in V_1$$

$$0 \leq y_{i,j'} \leq 1 \quad \text{for all } (i,j') \in V_1 \times V_2$$

Note the solution of (8) is always integral (i.e. $y_{i,j'} \in \{0,1\}$ for all $(i,j') \in V_1 \times V_2$) because (8) is a totally unimodular linear program. The parameters suggested for EigenAlign are $s_1 = \alpha + \epsilon$, $s_2 = 1 + \epsilon$, $s_3 = \epsilon$, for $\epsilon = 0.001$ and

$$\alpha = 1 + \frac{\#\text{matches}}{\#\text{mismatches}}.$$  

This choice of parameters is motivated by keeping the weights of matches and mismatches balanced in the objective function and observed to lead to better performance as reported in Feizi’s paper.
1.3 Projected power iteration

Projected power iteration method was proposed by Journé et.al. for sparse PCA problem\(^{[19]}\) and at each iteration \(t\), it can simply be expressed as

\[
v_{t+1} = \mathcal{F}(Av_t) \tag{9}
\]

where \(A\) is the matrix whose leading eigenvector is to be computed and \(\mathcal{F}\) is a non-linear projection. The starting point \(v_0\) can be chosen arbitrarily.

At the same time as projected power method was introduced another branch of algorithms with a very similar idea, called iterative thresholding, was popular in compressed sensing applications\(^{[31]}\). Although much more efficient than convex \(\ell_1\) relaxation algorithms, iterative thresholding was not as accurate. The improvement on iterative thresholding that equalized their accuracy to convex relaxation without sacrificing efficiency is achieved by adding a correction term to each iterate, called onsgar term in statistical physics. The motivation for the onsgar term is due to belief propagation algorithms\(^{[32]}\) and hence the algorithm with corrected iterates is called approximate message passing (AMP). Projected power method or AMP have been successfully applied to eigenproblems in different contexts, each of them taking advantage of the specific structure of the set in which the problem is defined in the projection step of the algorithm. These include constrained PCA\(^{[33][34]}\), phase synchronization\(^{[11][35]}\) and community detection\(^{[36][37]}\). For some generative random models AMP is shown to achieve statistical upper bounds on accuracy by inspection of state evolution equations\(^{[34]}\).

2. PROJECTED POWER ALIGNMENT

The algorithm we propose, Projected Power Alignment, constructs the alignment matrix \(A\) in the same fashion as EigenAlign\(^{[4]}\), and likewise EigenAlign computes the top eigenvector of \(A\) as an initialization step. Instead of rounding the top eigenvector to a permutation matrix with a linear program, Projected Power Alignment does a projection step by rounding the vector into a permutation in a greedy fashion (for efficiency purposes) and then iteratively alternates between multiplying by \(A\) and rounding.

\[
\begin{align*}
0. \text{Compute } A \text{ as in } [4]. \\
1. \text{Let } v^0 \text{ the top eigenvector of } A. \\
2. \text{For } t = 1, \ldots \text{ until convergence or time out} \\
   (a) \text{ Let } u^{t+1} = Av^t. \\
   (b) \text{Greedily round } u^{t+1} \text{ into a permutation matrix by rounding the largest entry of } u_{i,j}^{t+1} \text{ to 1 } \\
   \text{and setting the remaining elements of its row and column to 0 iteratively until we obtain } \\
   \text{the permutation matrix } v^{t+1} = \mathcal{F}(u^{t+1}).
\end{align*}
\]

State evolution analysis, as mentioned before, is the key to characterize the performance of power iteration method or AMP. Its hypothesis is that at each iteration \(t\) the iterand can be approximated as the optimal solution and an added independent gaussian noise with diminishing variance if SNR of the original problem is large enough. This remarkable observation was rigorously proven in\(^{[38][39]}\) in the case the matrix \(A\) is assumed to be drawn from a distribution \(A\) satisfying certain conditions. Although our problem has important differences than PCA or sparse recovery context, which these proofs are built in, a recent paper shows statistical equivalence of community detection and PCA with gaussian noise, namely guessing the leading eigenvector of \(A\) where

\[
A = \sqrt{\frac{\lambda}{n}}xx^T + Z
\]

where \(x\) is the vector of community assignments (-1 or 1), \(Z\) is gaussian symmetric matrix independent of \(x\) and \(\lambda\) is a function of the difference between intra and inter-community edge probabilities. We suspect such equivalence holds for our problem too so we could use state evolution analysis for AMP of PCA. However we defer this to future work.
3. NUMERICAL SIMULATIONS

In Figure 1 we report on numerical experiments where we compare the recovery rates of Projected Power Alignment with EigenAlign under the Erdős-Renyi model. We draw $G_1$ to be an Erdős-Renyi graph with edge probability $p$ and and $G_2 = P^T \tilde{G}_1 (\odot E_\lambda) P$ where $\tilde{G}_1$ is a noisy version of $G_1$ according to the noise model used in the EigenAlign paper. Namely

$$\tilde{G}_1 = G_1 \odot (1 - Q) + (1 - G_1) \odot Q$$

where $\odot$ denotes the Hadamard product, and $Q$ is a symmetric binary random matrix whose edges are drawn i.i.d. from a Bernoulli distribution with $\mathbb{P}[Q(i,j) = 1] = \lambda$. We say $\lambda$ is the noise level.

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Figure 1. Recovery rates for EigenAlign (left) and Projected Power Alignment (right) for the Erdős-Renyí with noise model described in Section 3. We take $p = 0.2$ (top line) and a logarithm scale for enhancing visualization. We take the same plot of $p = 0.2$ with a linear scale (middle line). We take $p = 0.5$ and a linear scale (bottom line). Darker color correspond to higher recovery rate. The recovery rate is computed as the average performance among 20 independent experiments. Note that both algorithms obtain perfect recovery rate in the noiseless case. Note that, consistently with the theory by Feizi and collaborators, the recovery rate seems to (modestly) increase with $n$ for $p = 0.2$ but decrease with $n$ for $p = 0.5$. 
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