A Least Square Approach to Semi-supervised Local Cluster Extraction

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Abstract

A least square semi-supervised local clustering algorithm based on the idea of compressed sensing are proposed to extract clusters from a graph with known adjacency matrix. The algorithm is based on a two stage approaches similar to the one in [26]. However, under a weaker assumption and with less computational complexity than the one in [26], the algorithm is shown to be able to find a desired cluster with high probability. Several numerical experiments including the synthetic data and real data such as MNIST, AT&T and YaleB human faces data sets are conducted to demonstrate the performance of our algorithm.

1 Introduction

Informally speaking, graph clustering is a problem of dividing the set of vertices of a graph into subsets in a way which makes more edges within each subset, and fewer edges between different subsets. When analyzing a graph, one of people’s primary interest is to find the underlying clustered structure of the graph, as the vertices in the same cluster can reasonably be assumed to have some latent similarity. Even though for data set which are not presented as graphs, it can be done by first creating a suitable auxiliary graph based on the data, for example, the $K$-nearest-neighbors ($K$-NN) graph, and then apply graph clustering techniques on this auxiliary graph.

Graph clustering problem has become prevalent recently in areas of social network study [16], [20] and [24], image classification [6], [7] and [40], natural language processing [11] and [31]. For example, suppose a social network graph has vertices which represents users of a social network (e.g. Facebook, LinkedIn), then the edges could represent users which are connected to each other. The sets of nodes with high inter-connectivity, which we call them communities or clusters, could represent friendship groups or co-workers. By identifying those communities we can suggest new connections to users. Note that some networks are directed (e.g. Twitter, Citation Networks), which could make community detection more subtle. For the scope of this paper, we will only be focusing on weighted undirected graphs.

The classical graph based clustering problem is a global clustering problem which assigns every vertex a unique cluster, assuming there are no multi-class vertices. It is usually considered as an unsupervised learning problem which can be done by using method such as spectral clustering [29], [34], [48] or ways of finding an optimal cut of the graph [12], [13], these approaches are generally computational expensive and hard to implement for large data sets. It can also be done semi-supervisely, such as [25], [21] and [47]. However, sometimes it is only of people’s interests in finding one certain

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cluster which contains the target vertices, given some prior knowledge of a small portion of labels for the entire true cluster, which is usually attainable for real data. This type of problem is called local clustering, or local cluster extraction, which loosely speaking, is defined to be the problem which takes a set of vertices \( \Gamma \) with known labels, called seed vertices, as input, and returns a cluster \( C^\# \) such that \( \Gamma \subset C^\# \). In this paper, we proposed a new approach using the ideas of compressed sensing and method of least square together to solve it effectively.

The local clustering problem hasn’t been studied exhaustively, and many aspects of the local clustering problem still remain open. Some recent related work are [18], [45], [46], [42], and [26]. Especially the work in [26], which is one of the recent works with the same setting as ours. However, as we will see in the numerical experiments section, our approach outperforms them in terms of both the accuracy and efficiency.

The main contribution of this paper is that it proposes the local cluster extraction algorithms \texttt{LeastSquareClustering} and \texttt{IterLeastSquareClustering} which improves the results in [26]. The subsequent sections in this paper are structured as follows. In Section 2 we give brief introductions to the concept of in spectral clustering such as graph Laplacian and Theorem 2.1, we also make the assumptions for the graph model which we will use later for theoretical analysis. In Section 3 we introduce the main algorithms for solving the local cluster extraction problem in two stages show the correctness of our algorithms asymptotically. In Section 4 we analyze the asymptotic complexity for our algorithms. In Section 5 several synthetic and real data sets are used to evaluate the performance of the algorithms and we also compared the performance with the state-of-the-art results.

2 Preliminaries and Models

2.1 Notations and Definitions

We use standard notation \( G = (V,E) \) to denote the graph \( G \) with the set of vertices \( V \) and set of edges \( E \). For the case \( |V| = n \), we identify \( V \) with the set of integers \( [n] := \{1,2,\cdots,n\} \). We use \( A \) to denote the adjacency matrix (possibly weighted but weights are non-negative) of \( G \), so in the undirected case, \( A \) is a symmetric matrix. Let \( D \) be the diagonal matrix \( D = \text{diag}(d_1,d_2,\cdots,d_n) \), where each \( d_i \) is the degree of vertex \( i \). We have the following definition.

**Definition 2.1.** The unnormalized Graph Laplacian is defined as \( L = D-A \). There are also two other graph Laplacians which are symmetric graph Laplacian \( L_{\text{sym}} := I - D^{-1/2}AD^{-1/2} \), and the random walk graph Laplacian \( L_{\text{rw}} := I - D^{-1}A \).

The following theorem serves as the fundamental theorem for solving graph clustering in our approach, we omit the proof here by directly referring to [8] and [29].

**Theorem 2.1.** Let \( G \) be an undirected graph with non-negative weights. Then the multiplicity \( k \) of the eigenvalue \( 0 \) of \( L \) (\( L_{\text{rw}} \)) equals to the number of connected components \( C_1,C_2,\cdots,C_k \) in \( G \), and the indicator vectors \( \mathbf{1}_{C_1},\cdots,\mathbf{1}_{C_k} \) on these components span the kernel of \( L \) (\( L_{\text{rw}} \)).

Let us further introduce some notations which we will use later. Suppose for the moment we have information about structure of the underlying clusters for each vertex, then it is useful to write \( G \) as a union of two edge-disjoint subgraphs \( G = G^{\text{in}} \cup G^{\text{out}} \) where \( G^{\text{in}} = (V,E^{\text{in}}) \) consists of only intra-connection edges, and \( G^{\text{out}} = (V,E^{\text{out}}) \) consists of only inter-connection edges. We will use \( d_i^{\text{in}} \) to denote the degree of vertex \( i \) in the subgraph \( G^{\text{in}} \), and \( d_i^{\text{out}} \) to denote the degree of vertex \( i \) in the subgraph \( G^{\text{out}} \). We will also use \( A^{\text{in}} \) and \( L^{\text{in}} \) to denote the adjacency matrix and graph Laplacian associated with \( G^{\text{in}} \), and \( A^{\text{out}} \) and \( L^{\text{out}} \) to denote the adjacency matrix and graph Laplacian associated
with \( G_{\text{out}} \). Note that these notations are just for convenience for the analysis in the next section, in reality we will have no assurance about which cluster each individual vertex belongs to, so we will have no access to \( A_{\text{in}} \) and \( L_{\text{in}} \). It is also worthwhile to point out that \( A = A_{\text{in}} + A_{\text{out}} \) but \( L \neq L_{\text{in}} + L_{\text{out}} \) in general. In addition, we will use \(|L|\) to denote the same matrix \( L \) with the entries in absolute value instead of the original entries in \( L \).

### 2.2 Graph Model Assumption

We make the following assumption for our analysis of graph model in the asymptotic perspective.

**Assumption 1.** Suppose \( G = (V, E) \) can be partitioned into \( k = O(1) \) connected components such that \( V = C_1 \cup \cdots \cup C_k \), where each \( C_i \) is the underlying vertex set for each connected component of \( G \).

(I): The degree of each vertex is asymptotically the same for vertices belong to the same cluster \( C_i \).

(II): The degree \( d_{\text{out}}^i \) is small relative to degree \( d_{\text{in}}^i \) asymptotically for each vertex \( i \in V \).

The random graphs which satisfies assumption (I) is not uncommon, for example, the Erdős-Rényi (ER) model \( G(n, p) \) with \( p \sim \frac{\omega(n) \log(n)}{n} \) for any \( \omega(n) \to \infty \), see [15] and [9]. A natural generalization of the ER model is the stochastic block model (SBM) [19], which is a generative model for random graphs with certain edge densities within and between underlying clusters, such that the edges within clusters are more dense than the edges between clusters. In the case of each cluster has the same size and the intra- and inter-connection probability are the same among all the vertices, we have the symmetric stochastic block model (SSBM). It is worthwhile to note that the information theoretical bound for exact cluster recovery in SBM are given in [11] and [2]. It was also shown in [26] that a general SBM with certain choice of parameters can be clustered by using a compressed sensing approach. Our model requires a weaker assumption than the one in [26], indeed, we remove the assumption on the eigenvalues of graph Laplacian \( L \) in [26]. Therefore, our model will be applicable to a broader range of random graphs.

### 3 Cluster Extraction Algorithms

For simplicity, we will use \( L \) and \( L_{\text{in}} \) to denote \( L_{\text{rw}} \) and \( L_{\text{in}}^{\text{rw}} \) respectively. Our analysis is based on the following key observation. Suppose for the moment graph \( G \) has \( k \) connected components \( C_1, \cdots, C_k \), i.e., \( L = L_{\text{in}} \). Suppose further that we have access to the information about the structure of \( L_{\text{in}} \), then we can write the graph Laplacian \( L_{\text{in}} \) into a block diagonal form. Therefore to find all the clusters, it is equivalent to find the first \( k \) eigenvectors of \( L_{\text{in}} \).

\[
L = L_{\text{in}} = \begin{pmatrix}
L_{1_{\text{in}}} & * & * \\
* & L_{2_{\text{in}}} & * \\
* & * & \ddots \\
* & * & * & L_{k_{\text{in}}}
\end{pmatrix}
\]

Suppose now we are interested in finding the cluster with the smallest number of vertices, say \( C_1 \), which corresponds to \( L_{1_{\text{in}}} \). By Theorem 2.1, \( \{1_{C_1}, \cdots, 1_{C_k}\} \) forms a basis of the kernel \( W_0 \) of \( L \). Note that all the \( 1_{C_i} \) have disjoint supports, so for \( w \in W_0 \) and \( w \neq 0 \), we can write

\[
w = \sum_{i=1}^{k} \alpha_i 1_{C_i}
\]
with some $\alpha_i \neq 0$. Therefore, if $1_{C_1}$ has the fewest non-zero entries among all elements of $W_0 \setminus \{0\}$, then we can find it by solving the following minimization problem:

$$
\min \|w\|_0 \quad \text{subject to} \quad L^{in}w = 0 \quad \text{and} \quad w \neq 0.
$$

(1)

This problem can be solved using methods such as greedy algorithms in compressed sensing as explained in [26]. However, we will propose a different approach to tackle it in this paper and demonstrate that the new approach is more effective numerically and require a fewer number of assumptions.

### 3.1 Least Square Cluster Pursuit

We will use $L_C$ and $L_C^{in}$ to denote the submatrices of $L$ and $L^{in}$ with column indices subset $C \subset V = [n]$ respectively. Now consider problem (1) again, instead of finding $C$ directly, let us try to find what are not in $C_1$. Suppose there is a superset $\Omega \subset V$ such that $C_1 \subset \Omega$, and $C_i \not\subset \Omega$ for all $i = 2, \cdots, n$. Then we know

$$
L^{in}1_\Omega = L^{in}(1_{\Omega \setminus C_1} + 1_{C_1}) = L^{in}1_{\Omega \setminus C_1} + L^{in}1_{C_1} = L^{in}1_{\Omega \setminus C_1}.
$$

Letting $y := L^{in}1_\Omega$, we see that solving Problem (1) will be equivalent to solve the following problem (2), but with some condition imposed.

$$
\arg \min_{w \in \mathbb{R}^n} \|L^{in}x - y\|_2
$$

(2)

Note that solving Problem (2) directly will give $x^* = 1_\Omega \in \mathbb{R}^n$ and $x^* = 1_{\Omega \setminus C_1} \in \mathbb{R}^n$ both as solutions. By setting the columns $L^{in}_{V \setminus \Omega} = 0$, solving Problem (2) is equivalent to solving

$$
\arg \min_{x \in \mathbb{R}^{|\Omega|}} \|L^{in}_{\Omega}x - y\|_2.
$$

(3)

Directly solving Problem (3) gives at least two solutions $x^* = 1 \in \mathbb{R}^{|\Omega|}$ and $x^* = 1_{C_1^c} \in \mathbb{R}^{|\Omega|}$, where the latter one is much more informative for us to extract $C_1$ from $\Omega$ than the former. So we need to find a way to avoid the non-informative solution $x^* = 1$ but keep the informative one $x^* = 1_{C_1^c}$.

We can achieve this by removing a proportion of column indices set $T$ from $\Omega$. Let us consider

$$
\arg \min_{x \in \mathbb{R}^{|\Omega \setminus T|}} \|L^{in}_{\Omega \setminus T}x - y\|_2,
$$

(4)

where now $1 \in \mathbb{R}^{|\Omega \setminus T|}$ is not a solution to (4) any more. However, if we can assure a suitable subset $T$ such that $T \subset C_1$, then $1_{C_1^c} \in \mathbb{R}^{|\Omega \setminus T|}$ is still a solution to it, since $L^{in}_{\Omega \setminus T}1_{C_1^c} = L^{in}1_{\Omega \setminus C_1} = 0$. Note that problem (4) has a unique solution because it is a least square problem with matrix $L^{in}_{\Omega \setminus T}$ of full column rank. This idea leads to Algorithm 1.

**Remark 3.1.** Note that there are certainly some other heuristic ways to choose the indices set $T$, based on different measures on $L_\Omega$ and $y$. For example, we can choose a set of seeds for $T$ if we are given some seeds of the concerned cluster. But the way we choose $T$ in this paper is based on the following observation. Suppose $L = L^{in}$, $\Omega \supset C_1$ and $\Omega \not\supset C_i$ for $i = 2, \cdots, k$. Then $|L_a| \cdot |y| = 0$ for all $a \in C_1$, and $|L_a| \cdot |y| > 0$ for all $a \in \Omega \setminus C_1$. We impose the absolute value rather than direct dot product in order to have fewer cancellation between vector components when summing over the entrywised products. In practice, the size of $\gamma$ will not matter too much as long as it is not being pushed too extreme.
Lemma 3.1. Let $L = I - D^{-1} A$ and $y = L \Omega$. Let $T$ be the set of column indices of $\gamma \cdot |\Omega|$ smallest components of the vector $|L\Omega|^T \cdot |y|$ (Here the absolute value operation is entrywise).

Let $x^\#$ be the solution to
\[
\arg\min_{x \in \mathbb{R}^{|\Omega| - |T|}} \|L_{\Omega \setminus T} x - y\|_2
\] obtained by using an iterative least square solver.

Let $W^\# = \{ i : x_i^\# > R \}$. 

Ensure: $C_i^\# = \Omega \setminus W^\#$.

Algorithm 1 LeastSquareClusterPursuit

Require: Adjacency matrix $A$, vertex subset $\Omega \subset V$, least square threshold parameter $\gamma \in (0,1)$, and rejection parameter $R \in [0,1]$.

• Compute $L = I - D^{-1} A$ and $y = L \Omega$.
• Let $T$ be the set of column indices of $\gamma \cdot |\Omega|$ smallest components of the vector $|L\Omega|^T \cdot |y|$ (Here the absolute value operation is entrywise).
• Let $x^\#$ be the solution to
\[
\arg\min_{x \in \mathbb{R}^{|\Omega| - |T|}} \|L_{\Omega \setminus T} x - y\|_2
\]

Remark 3.2. As indicated in [26], we can reformulate problem (1) as solving
\[
\arg\min_{x \in \mathbb{R}^n} \{ \|Lx - y\|_2 : \|x\|_0 \leq s \}
\]

by applying the greedy algorithms such as subspace pursuit [10] and compressed sensing matching pursuit (CoSaMP) [33]. Or alternatively, we can consider the LASSO [39] [41] form of the problem
\[
\arg\min_{x \in \mathbb{R}^n} \{ \|Lx - y\|_2^2 + \lambda \|x\|_1 \} = \arg\min_{x \in \mathbb{R}^n} \{ \|Lx - y\|_2^2 + \lambda \|x\|_0 \}.
\]
The reason that Lasso is a good way to interpret this problem is that the solution $x^*$ we are trying to solve for is the sparse indicator vector which satisfies $\|x^*\|_1 = \|x^*\|_0$. We will implement these two ideas in the numerical results section for the comparison.

However, in reality we have no access to $L^m$, what we know only is $L$ and in general $L \neq L^m$. But we hope the solution to the above problem associated with $L$ will not be perturbed too much from the solution $1_C^\#$ associated with $L^m$ if the difference between $L$ and $L^m$ is relative small and the subset $T \subset \Omega$ is chosen to be appropriate. Let us make this precise by first quoting the following standard result in numerical analysis.

Lemma 3.1. Let $\| \cdot \|$ be an operator norm, $A \in \mathbb{R}^{n \times n}$ be a non-singular square matrix, $x \in \mathbb{R}^n$, $y \in \mathbb{R}^n$. Let $\hat{A}$, $\hat{x}$, $\hat{y}$ be perturbed measurements of $A$, $x$, $y$ respectively. Suppose $Ax = y$, $\hat{A}x = \hat{y}$, and suppose further $\operatorname{cond}(A) < \|A\| \|A^{-1}\|^{-1}$, then
\[
\frac{\|\hat{x} - x\|}{\|x\|} \leq \frac{\operatorname{cond}(A)}{1 - \operatorname{cond}(A) \|A^{-1}\|} \left( \frac{\|\hat{A} - A\|}{\|A\|} + \frac{\|\hat{y} - y\|}{\|y\|} \right).
\]
The above lemma tells us that the size of $\operatorname{cond}(A)$ is significant in determining the stability of the solution $x$ is with respect to small perturbations on $A$ and $y$. For the discussion from now on, we will use $\| \cdot \|$ to denote the standard vector or matrix induced two-norm $\| \cdot \|_2$ unless state otherwise. The next lemma asserts the invertibility of $(L_{\Omega \setminus T}^m)^T L_{\Omega \setminus T}^m$ and gives an estimation bound of its condition number.

Lemma 3.2. Let $V = \bigcup_{i=1}^k C_i$ be the disjoint union of $k = O(1)$ underlying clusters with size $n_i$, and assume (I). Let $d_j$ be the degree for vertex $j \in V = [n]$, $n_1 = \min_{i \in [k]} n_i$, and suppose $\Omega \subset V$ be such that $\Omega \supset C_1$ and $\Omega \not\supset C_i$ for $i = 2, \ldots, k$. Then
(i). If $T \subset C_1$, then $(L_{\Omega \setminus T}^n)^	op L_{\Omega \setminus T}^n$ is invertible.

(ii). Suppose further $[3n^2] \leq |T| < n_1$ and $|\Omega| \leq [\frac{5n^3}{2}]$. Then $\text{cond}((L_{\Omega \setminus T}^n)^	op L_{\Omega \setminus T}^n) \leq 4$ almost surely as $n_1 \to \infty$, e.g. when $n \to \infty$.

Proof. The invertibility is straightforward since $L_{\Omega \setminus T}^n$ is of full column rank, therefore $(L_{\Omega \setminus T}^n)^	op L_{\Omega \setminus T}^n$ is invertible. Without loss of generality, let us assume that the column indices of $L_{\Omega \setminus T}^n$ are already permuted such that the indices number is in the same order relative to their underlying clusters. Now since $(L_{\Omega \setminus T}^n)^	op L_{\Omega \setminus T}^n$ is in a block form, to estimate the condition number, we only need to estimate the largest and smallest eigenvalues for each block. Writing $L_{\Omega \setminus T}^n = [l_{ij}]$ and $(L_{\Omega \setminus T}^n)^	op L_{\Omega \setminus T}^n = [s_{ij}]$, for each $i \in C_1 \setminus T$, $s_{ii} = \sum_{k=1}^n l_{ki}l_{ki} = \sum_{k=1}^n l_{ki}^2 = 1 + \frac{1}{n_1}$, and for $i, j \in C_1 \setminus T$ with $i \neq j$, $s_{ij} = \sum_{k=1}^n l_{ki}l_{kj} = \sum_{k=1}^n l_{ki}l_{kj}$. Note that the probability of having an edge between $i$ and $j$ given degree sequences $d_1, \ldots, d_n$, equals to $\frac{d_id_j}{\sum_i d_i}$, assuming that the existence of an edge between two vertices is proportional to their degrees. So $s_{ij}$ equals to $-\frac{1}{d_i}$ with probability $\frac{d_id_j}{\sum_i d_i}$, which implies $\mathbb{E}(s_{ij}) = -\frac{d_id_j}{\sum_i d_i}$; $l_{ij}$ equals to $-\frac{1}{d_i}$ with probability $\frac{d_id_j}{\sum_i d_i}$, which implies $\mathbb{E}(l_{ij}) = -\frac{d_i}{\sum_i d_i}$.

Hence the expectation

\[
\mathbb{E}(s_{ij}) = \mathbb{E}\left(\sum_{k=1}^n l_{ki}l_{kj}\right) = \sum_{k=1}^n \mathbb{E}(l_{ki})\mathbb{E}(l_{kj}) = \sum_{k=1}^n \mathbb{E}(l_{ki})\mathbb{E}(l_{kj}) = \frac{d_id_j}{\sum_i d_i} \cdot \left(\frac{1}{d_i} - \frac{1}{d_j}\right) + \frac{d_id_j}{\sum_i d_i} \cdot \left(\frac{1}{d_i} - \frac{1}{d_j}\right) + \frac{d_id_j}{\sum_i d_i} \cdot \left(\frac{1}{d_i} - \frac{1}{d_j}\right) = \frac{d_id_j}{\sum_i d_i} \cdot \frac{1}{n_1}.
\]

By the law of large numbers, $s_{ij} \to -\frac{2}{n_1} + \frac{1}{n_1}$ almost surely as $n_1 \to \infty$. Therefore for $i \in C_1 \setminus T$, we have

\[
\sum_{j \in C_1 \setminus T, j \neq i} |s_{ij}| \to |C_1 \setminus T| \cdot \left(\frac{2}{n_1} - \frac{1}{n_1}\right) = \frac{n_1}{4} \cdot \left(\frac{2}{n_1} - \frac{1}{n_1}\right) \leq \frac{1}{2}
\]

almost surely as $n_1 \to \infty$. Similarly, for each $i \in C_k \cap (\Omega \setminus C_1), k \geq 2$, we have $s_{ii} = 1 + \frac{1}{d_i}$, and $\sum_{j \in C_k \cap (\Omega \setminus C_1), j \neq i} |s_{ij}| \to \frac{n_1}{4} \cdot \left(\frac{2}{n_1} - \frac{1}{n_1}\right) \leq \frac{1}{2}$ almost surely as $n_1 \to \infty$.

Now we apply Gershgorin’s circle theorem to bound the spectrum of $(L_{\Omega \setminus T}^n)^	op L_{\Omega \setminus T}^n$. For all $i \in \Omega \setminus T$, the circles are centered at $1 + \frac{1}{d_i}$, with radius less than or equal to $\frac{1}{2}$ almost surely, hence $\sigma_{\text{min}}((L_{\Omega \setminus T}^n)^	op L_{\Omega \setminus T}^n) \geq \frac{1}{2}$ and $\sigma_{\text{max}}((L_{\Omega \setminus T}^n)^	op L_{\Omega \setminus T}^n) \leq \frac{3}{4} + \frac{1}{d_i} \leq 2$, almost surely. Therefore we have

\[
\text{cond}((L_{\Omega \setminus T}^n)^	op L_{\Omega \setminus T}^n) = \frac{\sigma_{\text{max}}((L_{\Omega \setminus T}^n)^	op L_{\Omega \setminus T}^n)}{\sigma_{\text{min}}((L_{\Omega \setminus T}^n)^	op L_{\Omega \setminus T}^n)} \leq 4
\]

almost surely, as desired. \(\square\)

Remark 3.3. Note that there is a minor difficulty in estimating the expectation of inner product between two different columns of $L_{\Omega \setminus T}^n$. The computation assumes the independence of degree distribution of each individual vertex within each cluster, but this may not be true in general for arbitrary graph. However, the independence will occur if the asymptotic uniformity of the degree distribution within each cluster is assumed, that is why our model needs this assumption.
Now the perturbed problem \( (5) \) is equivalent to solving \((L_{Ω,T}^{\top}L_{Ω,T})x^\# = L_{Ω,T}^{\top}y = L_{Ω,T}^{\top}(L_{Ω,T}1_{Ω})\),
while the unperturbed problem \( (1) \) is to solve \((L_{Ω,T}^{\top})^nL_{Ω,T}^{\top}x^* = (L_{Ω,T}^{\top})^ny = (L_{Ω,T}^{\top})^n(L_{Ω,T}^{\top}1_{Ω})\). Let \( M := L - L^i \), \( M_{Ω} := L_{Ω} - L_{Ω}^i \), and \( M_{Ω,T} := L_{Ω,T} - L_{Ω,T}^i \). Now let us give an estimate for \( M \).

**Lemma 3.3.** Let \( L \) be the graph Laplacian of \( G \) and \( M := L - L^i \). Let \( \epsilon_i := \frac{d_{out}}{d_i} \) for all \( i \) and \( \epsilon_{max} := \max_{i \in [n]} \epsilon_i \). Then \( \|M\| \leq 2\epsilon_{max} \).

**Proof.** Let \( \delta_{ij} \) denote the Kronecker delta symbol, observe that

\[
L_{ij} := \delta_{ij} - \frac{1}{d_i}A_{ij} = \delta_{ij} - \frac{1}{d_i} + \frac{\epsilon_i}{d_i} (A_{ij}^{in} + A_{ij}^{out}).
\]

Since \( \epsilon_i := \frac{d_{out}}{d_i} \), we have \( \frac{1}{d_i} = \frac{1}{d_i^{in} + d_i^{out}} = \frac{1}{d_i^{in}} - \frac{\epsilon_i}{d_i^{in}} \). So we have

\[
L_{ij} = \delta_{ij} - \left( \frac{1}{d_i^{in}} - \frac{\epsilon_i}{d_i^{in}} \right) (A_{ij}^{in} + A_{ij}^{out})
\]

\[
= \left( \delta_{ij} - \frac{1}{d_i^{in}} A_{ij}^{in} \right) - \frac{1}{d_i^{in}} A_{ij}^{out} + \epsilon_i \frac{1}{d_i^{in}} (A_{ij}^{in} + A_{ij}^{out})
\]

\[
= L_{ij} - \frac{1 - \epsilon_i}{d_i^{in}} A_{ij}^{out} + \epsilon_i \frac{1}{d_i^{in}} A_{ij}^{in}.
\]

Therefore \( M_{ij} = -\frac{1 - \epsilon_i}{d_i^{in}} A_{ij}^{out} + \epsilon_i \frac{1}{d_i^{in}} A_{ij}^{in} \). To bound the spectral norm we apply Gershgorin’s circle theorem, noting that \( M_{ii} = 0 \) for all \( i \), hence

\[
\|M\|_2 = \max\{|\lambda_i| : \lambda_i \text{ eigenvalue of } M\} \leq \max_i \sum_j |M_{ij}|
\]

\[
= \max_i \left\{ \frac{1 - \epsilon_i}{d_i^{in}} \sum_j A_{ij}^{out} + \frac{\epsilon_i}{d_i^{in}} \sum_j A_{ij}^{in} \right\}
\]

\[
= \max_i \left\{ \frac{1 - \epsilon_i}{d_i^{in}} d_i^{out} + \frac{\epsilon_i}{d_i^{in}} d_i^{in} \right\} = 2 \max_i \epsilon_i = 2\epsilon_{max}.
\]

This completes the proof. \( \square \)

Next we will have the following result.

**Lemma 3.4.** \( \|L_{Ω,T}^{in}(L_{Ω,T}^{in})^\top 1_{Ω}\| \geq \frac{\sqrt{|Ω \cap C_1|}}{2} = \frac{\sqrt{n}}{4} \) almost surely.

**Proof.** Note that \( \|L_{Ω,T}^{in}(L_{Ω,T}^{in})^\top 1_{Ω}\| = \|(L_{Ω,T}^{in})^\top L_{Ω,T}^{in} 1_{Ω}\| \). Let us estimate \( \|(L_{Ω,T}^{in})^\top L_{Ω,T}^{in} 1_{Ω}\| \). Similar to the computation we did in Lemma 3.2, for each \( i \in C_1 \setminus T \), we have \( s_{ii} = 1 + \frac{1}{d_i^{in}} \), \( \sum_{j \in C_1} s_{ij} = 0 \), and \( \sum_{j \in Ω \setminus C_1} s_{ij} = 0 \). For each \( i \in C_k \cap (Ω \setminus C_1) \), \( k \geq 2 \), we have \( s_{ii} = 1 + \frac{1}{d_i^{in}} \), \( \sum_{j \in C_1} s_{ij} = 0 \), and \( \sum_{j \in Ω \cap (Ω \setminus C_1)} s_{ij} \rightarrow \frac{n_k}{2} \cdot \left( -\frac{n}{n_k} + \frac{1}{n_k} \right) \geq -\frac{1}{2} \) almost surely. Therefore, the row sum of \( (L_{Ω,T}^{in})^\top L_{Ω,T}^{in} \) for row \( i \in C_1 \setminus T \) equals to zero, and the row sum \( (L_{Ω,T}^{in})^\top L_{Ω,T}^{in} \) for row \( i \in Ω \setminus C_1 \) larger than \( \frac{1}{2} \) almost surely. Hence \( \|(L_{Ω,T}^{in})^\top L_{Ω,T}^{in} 1_{Ω}\| \geq \frac{\sqrt{|Ω \cap C_1|}}{2} = \frac{\sqrt{n}}{4} \) almost surely. \( \square \)

Now let us use previous lemmas to establish that the difference between perturbed solution and unperturbed solution is small in the order of \( \epsilon_{max} \).
Theorem 3.1. Under the same assumptions as Lemma 3.2, let $\mathbf{x}^{\#}$ be the solution to the perturbed problem (7), and $\mathbf{x}^* = \mathbf{1}_{C_1} \in \mathbb{R}^{[\Omega]-[T]}$ which is the solution to the unperturbed problem (4). Then
\[
\frac{||\mathbf{x}^{\#} - \mathbf{x}^*||}{||\mathbf{x}^*||} = O(\epsilon_{\max}).
\]
almost surely for large $n_1$.

Proof. By Lemma 3.3 we have $||M|| \leq 2\epsilon_{\max}$. Therefore
\[
||\tilde{A} - A|| = ||(L_{\Omega,T})^T L_{\Omega,T} - (L_{\Omega,T}^m)^T L_{\Omega,T}^m|| = \|(L_{\Omega,T}^m)^T M_{\Omega,T} + M_{\Omega,T}^T L_{\Omega,T}^m + M_{\Omega,T}^T M_{\Omega,T}||
\leq \|(L_{\Omega,T}^m)^T M_{\Omega,T}|| + \|M_{\Omega,T}^T L_{\Omega,T}^m|| + \|M_{\Omega,T}^T M_{\Omega,T}||
\leq (2||L_{\Omega,T}^m|| + ||M_{\Omega,T}||) \cdot ||M_{\Omega,T}||
\leq (2||L_{\Omega,T}^m|| + ||M||) \cdot ||M|| \leq 4\epsilon_{\max} \cdot (||L_{\Omega,T}^m|| + \epsilon_{\max}).
\]

For each $i \in \Omega \setminus T$, we have $||L_i|| \geq 1$, and $\sigma_{\max}((L_{\Omega,T}^m)^T L_{\Omega,T}^m) = ||(L_{\Omega,T}^m)^T L_{\Omega,T}^m|| = \sigma_{\max}(L_{\Omega,T}^m) = ||L_{\Omega,T}^m||^2 \geq \max_{i \in \Omega \setminus T} ||L_i||^2 \geq 1$. Hence
\[
\frac{\|(L_{\Omega,T}^m)^T L_{\Omega,T} - (L_{\Omega,T}^m)^T L_{\Omega,T}^m||}{\|(L_{\Omega,T}^m)^T L_{\Omega,T}^m||} \leq \frac{(2||L_{\Omega,T}^m|| + ||M||) \cdot ||M||}{\|(L_{\Omega,T}^m)^T L_{\Omega,T}^m||^2}
\leq \frac{4\epsilon_{\max}}{||L_{\Omega,T}^m||^2} + \frac{4\epsilon_{\max}^2}{||L_{\Omega,T}^m||^2} \leq 4(\epsilon_{\max} + \epsilon_{\max}^2). \tag{8}
\]

We also have
\[
||\tilde{y} - y|| = \|(L_{\Omega,T})^T (L_1 \Omega) - (L_{\Omega,T}^m)^T (L_1 \Omega)|| = \|(L_{\Omega,T}^m)^T M_{\Omega,T}^T (L_1 \Omega) - (L_{\Omega,T}^m)^T (L_1 \Omega)||
\leq \sqrt{\Omega} \cdot \|(L_{\Omega,T}^m)^T M_{\Omega,T}^T L_{\Omega,T}^m + M_{\Omega,T}^T M_{\Omega,T} M_\Omega \cdot 1_\Omega||
\leq \sqrt{\Omega} \cdot \|2||L_{\Omega,T}^m|| + ||M_{\Omega,T}|| \cdot ||M||
\leq \sqrt{\Omega} \cdot (2||L_{\Omega,T}^m|| + 2\epsilon_{\max}) \cdot 2\epsilon_{\max} = 2\sqrt{5\epsilon_{\max}} \cdot (||L_{\Omega,T}^m|| + \epsilon_{\max}) \cdot \epsilon_{\max}.
\]

Next by Lemma 3.4 $||L_{\Omega,T}^m|| \geq \sqrt{(1 + \epsilon_{\max})/2} = \frac{\sqrt{m}}{4}$ almost surely, therefore we have
\[
\frac{\|(L_{\Omega,T})^T L_1 \Omega - (L_{\Omega,T}^m)^T L_1 \Omega||}{\|(L_{\Omega,T}^m)^T L_1 \Omega||} \leq \frac{2\sqrt{5\epsilon_{\max}} \cdot (||L_{\Omega,T}^m|| + \epsilon_{\max}) \cdot \epsilon_{\max}}{\sqrt{m}/4} = 8\sqrt{5\epsilon_{\max}} \cdot (||L_{\Omega,T}^m|| + \epsilon_{\max})
\leq 8\sqrt{5\epsilon_{\max}} \cdot (\sqrt{2} + \epsilon_{\max}) = 8\sqrt{10\epsilon_{\max}} + 8\sqrt{5\epsilon_{\max}^2}.
\]
The second inequality holds because $\sigma_{\max}((L_{\Omega,T}^m)^T L_{\Omega,T}^m) \leq 2$ for the similar reasoning in Lemma 3.2 by using Gershgorin’s circle theorem, so $||L_{\Omega,T}^m|| \leq \sqrt{2}$. Now applying Lemma 3.2 and Lemma 3.1 with $A = (L_{\Omega,T}^m)^T L_{\Omega,T}, \tilde{A} = (L_{\Omega,T})^T L_{\Omega,T}, \mathbf{y} = L_{\Omega,T}^m \mathbf{1}_\Omega, \tilde{\mathbf{y}} = L_{\Omega,T} \mathbf{1}_\Omega$, we have
\[
\frac{||\mathbf{x}^{\#} - \mathbf{x}^*||}{||\mathbf{x}^*||} \leq \frac{\text{cond}((L_{\Omega,T}^m)^T L_{\Omega,T}^m) \cdot (4\epsilon_{\max} + 4\epsilon_{\max}^2 + 8\sqrt{10\epsilon_{\max}} + 8\sqrt{5\epsilon_{\max}}^2)}{1 - \text{cond}((L_{\Omega,T}^m)^T L_{\Omega,T}^m) \cdot (4\epsilon_{\max} + 4\epsilon_{\max}^2)}
\leq \frac{16(1 + 2\sqrt{10}\epsilon_{\max}) + (1 + 2\sqrt{5})\epsilon_{\max}^2}{1 - 16\epsilon_{\max} + 1 + \epsilon_{\max}} = O(\epsilon_{\max}).
\]
Next we can estimate the size of the symmetric difference between output $C_1^\#$ and the true cluster $C_1$ relative to the size of $C_1$, the symmetric difference is defined as $C_1^\# \triangle C_1 := (C_1^\# \setminus C_1) \cup (C_1 \setminus C_1^\#)$. Let us state another lemma before we establish the result.

**Lemma 3.5.** Let $T \subset [n]$, $v \in \mathbb{R}^n$, and $W^\# = \{ i : v_i > R \}$. Suppose $\|1_T - v\| \leq D$, then $|T \triangle W^\#| \leq \frac{D^2}{R^2}$.

**Proof.** Let $U^\# = [n] \setminus W^\#$ and write $v = v_{U^\#} + v_{W^\#}$, where $v_{U^\#}$ and $v_{W^\#}$ are the parts of $v$ supported on $U^\#$ and $W^\#$. Then we can write

$$\|1_T - v\|^2 = \|1_{T \cap W^\#} - (v_{W^\#})_{T \cap W^\#}\|^2 + \|(v_{W^\#})_{W^\# \setminus T}\|^2 + \|1_{T \setminus W^\#} - v_{U^\#}\|^2.$$ 

Since $\|(v_{W^\#})_{W^\# \setminus T}\|^2 \geq R^2 \cdot |W^\# \setminus T|$ and $\|1_{T \setminus W^\#} - v_{U^\#}\|^2 \geq R^2 \cdot |T \setminus W^\#|$, we have

$$R^2 \cdot |T \triangle W^\#| = R^2 \cdot (|T \setminus W^\#| + |W^\# \setminus T|) \leq \|(v_{W^\#})_{W^\# \setminus T}\|^2 + \|1_{T \setminus W^\#} - v_{U^\#}\|^2 \leq \|1_T - v\|^2.$$

Hence $|T \triangle W^\#| \leq \frac{\|1_T - v\|^2}{R^2} \leq \frac{D^2}{R^2}$. \hfill \qed

**Theorem 3.2.** Suppose $0.1 \leq R \leq 0.9$. Under the same assumptions as Theorem 3.1, we have

$$\frac{|C_1^\# \triangle C_1|}{|C_1|} \leq O(\epsilon_{\text{max}}^2).$$

In other words, the error rate of successfully recovering $C_1$ is at most a constant multiple of $\epsilon_{\text{max}}^2$.

**Proof.** From Theorem 3.1 we have $\|x^\# - x^\ast\| = \|x^\# - 1_{\Omega \setminus C_1}\| \leq O(\epsilon_{\text{max}}) \cdot \|x^\ast\| \leq O(\epsilon_{\text{max}} \sqrt{n_1})$. Then by Lemma 3.5 we get $|W^\# \triangle (\Omega \setminus C_1)| \leq O(\epsilon_{\text{max}}^2 n_1)$. Since $C_1^\# = \Omega \setminus W^\#$, it then follows $|C_1^\# \triangle C_1| \leq O(\epsilon_{\text{max}}^2 n_1)$, hence $\frac{|C_1^\# \triangle C_1|}{|C_1|} = O(\epsilon_{\text{max}}^2)$ as desired. \hfill \qed

### 3.2 Random Walk Threshold

In order to apply Algorithm 1, we have to have a "good" superset which contains $C_1$. The task for this subsection is to find such a superset $\Omega$ from the given seed vertices $\Gamma$. We will apply a simple diffusion based random walk algorithm on $G$ to find such $\Omega$. Note that there are also other sophisticated algorithms such as [3] [23] [43] to achieve this goal, but we do not analyze them here as our purpose is just to implement a fast way of obtaining a set $\Omega \supset C_1$. This leads to Algorithm 2, note that this algorithm is also described in [26], but the difference is that in implementation, we will allow a larger $\epsilon$ to decrease the chances of missing any vertices in $C_1$ based on the natural differences of our approaches.

**Algorithm 2 RandomWalkThreshold**

**Require:** Adjacency matrix $A$, a random walk threshold parameter $\epsilon \in (0, 1)$, a set of seed vertices $\Gamma \subset C_1$, estimated size $\hat{n}_1 \approx |C_1|$, and depth of random walk $t \in \mathbb{Z}^+$. 

- Compute $P = AD^{-1}$ and $v^0 = D1_\Gamma$.
- Compute $v^{(t)} = P^t v^{(0)}$.
- Define $\Omega = \mathcal{L}(1+\epsilon)\hat{n}_1(v^{(t)})$.

**Ensure:** $\Omega = \Omega \cup \Gamma$. 

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Let us first consider the case $\Gamma$ random walk with seed vertices $\Omega$. Given seed vertices $\Gamma$, our goal is to enter the target cluster $C_1$. Similar to Theorem 7.1, we get that the limiting probability of finally being at each vertex will be the same, but now there is a trade-off between the size of $\Gamma$ and the depth of the random walk. In order to fully explore the target cluster, we can apply the above argument to each individual vertex in $\Gamma$. Then we have $\mathbb{P}\left( \sum_{j \in C_1} v_j^{(t)} = \|v(t)\|_1 \right) \geq (1 - \epsilon_{\max})^t \geq 1 - t\epsilon_{\max} = 1 - O(\epsilon_{\max})$.

Suppose now $|\Gamma| > 1$, we can apply the above argument to each individual vertex in $\Gamma$, where the random walk starting from each vertex can be considered independently, therefore we have $\mathbb{P}\left( \sum_{j \in C_1} v_j^{(t)} = \|v(t)\|_1 \right) \geq (1 - \epsilon_{\max})^{|\Gamma|} \geq 1 - t\epsilon_{\max}|\Gamma| = 1 - O(\epsilon_{\max})$.

**Remark 3.4.** It is worthwhile to note that we do not want $t$ to be too large, one reason is that Theorem 3.3 tells us that the probability of staying within the target cluster $C_1$ decreases as $t$ increases. An alternative interpretation is that we can treat our graph $G$, suppose connected, as a time homogeneous finite state Markov chain with evenly distributed transition probability determined by the vertex degree between adjacent vertices. Since $G$ is connected, then $G$ is certainly irreducible and aperiodic. By Theorem 7.1, we get that the limiting probability of finally being at each vertex will be the same, regardless of what the seed set $\Gamma$ is. We provide further details about finite state Markov chains in the Appendix. Meanwhile, we do not want $t$ to be too small as well, otherwise the random walk will not be able to explore all the reachable vertices. There is a trade-off between the size of $\Gamma$ and the random walk depth $t$, where a smaller size of $\Gamma$ usually induces a larger $t$ in order to fully explore the target cluster.

### 3.3 Local Cluster Extraction

Let us now combine the previous two subroutines into our local clustering algorithm **LeastSqureClustering**. In practice, we may want to vary the number of iterations $\text{MaxIter}$ based on the number of examples in the data set in order to achieve a better performance. For the purpose theoretical analysis, let us fix $\text{MaxIter} = 1$.

**Remark 3.5.** The hyperparameter $\text{MaxIter}$ in the algorithm is usually chosen based on the size of initial seed vertices $\Gamma$ relative to $n$, we do not have a formal way of choosing the best $\text{MaxIter}$ rather than choose it heuristically. In practice, we believe $\text{MaxIter} \leq 3$ will do a very good job mostly.
Algorithm 3 LeastSqureClustering

Require: Adjacency matrix $A$, a random walk threshold parameter $\epsilon \in (0, 1)$, a set of seed vertices $\Gamma \subset C_1$, estimated size $\hat{n}_1 \approx |C_1|$, depth of random walk $t \in \mathbb{Z}^+$, least square parameter $\gamma \in (0, 0.8)$, and rejection parameter $R \in [0, 1)$.

• for $i = 1, \ldots, \text{MaxIter}$
  • $\Omega \leftarrow$ RandomWalkThreshold$(A, \Gamma, \hat{n}_1, \epsilon, t)$.
  • $\Gamma \leftarrow$ LeastSquareClusterPursuit$(A, \Omega, R, \gamma)$.
• end

Let $C_1^\# = \Gamma$.

Ensure: $C_1^\#$.

The analysis in previous two subsections give that the difference between true cluster $C_1$ and the estimated $C_1^\#$ is relative small compared to the size of $C_1$, this can be written more formally using the asymptotic notation.

**Theorem 3.4.** Suppose $\epsilon_{\text{max}} = o(1)$ and $\text{MaxIter} = 1$, then under the assumptions of Theorem 3.2 and 3.3, we have $P(\frac{|C_1^\# \triangle C_1|}{|C_1|} \leq o(1)) = 1 - o(1)$.

**Proof.** By Theorem 3.3, we have that the probability of $\Omega \supset C_1$ after RandomWalkThreshold is $1 - O(\epsilon_{\text{max}}) = 1 - o(1)$. Then by Theorem 3.2, the error rate is at most a constant multiple of $\epsilon_{\text{max}}^2$ after LeastSquareClusterPursuit. Putting them together, we have $P(\frac{|C_1^\# \triangle C_1|}{|C_1|} \leq o(1)) = 1 - o(1)$. \[\square\]

### 3.4 From Local to Global

We can make one step further by applying LeastSquareClustering iteratively on the entire graph to extract all the underlying clusters. That is, we remove $C_i^\#$ each time after the algorithm finds it, and updates the graph $G$ by removing the subgraph spanned by vertices $C_i^\#$ successively. We summarize the algorithm as IterLeastSqureClustering. However, we will not analyze further the theoretical guarantees of the iterative version the algorithm, but rather provide with numerical examples in the later section to show its effectiveness and efficiency.

Algorithm 4 IterativeLeastSqureClustering

Require: Adjacency matrix $A$, random walk threshold parameter $\epsilon \in (0, 1)$, least square parameter $\gamma \in (0, 0.8)$, rejection parameter $R \in [0, 1)$, depth of random walk $t \in \mathbb{Z}^+$. Seed vertices for each cluster $\Gamma_i \subset C_i$, estimated size $\hat{n}_i \approx |C_i|$ for $i = 1, \ldots, k$.

• for $i = 1, \ldots, k$
  • Let $C_i^\#$ be the output of LeastSquareClustering.
  • Let $G^{(i)}$ be the subgraph spanned by $C_i^\#$.
  • Updates $G \leftarrow G \setminus G^{(i)}$.
• end

Ensure: $C_1^\#, \ldots, C_k^\#$. 

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4 Computational Complexity

First, note that if $A, D, P$ are stored as sparse matrices, then for each $t$ in the second step of RandomWalkThreshold, the computation will have a complexity $O(nd_{\text{max}})$, where $d_{\text{max}}$ is the maximal degrees among all the vertices. Then the algorithm RandomWalkThreshold has a time complexity $O(nd_{\text{max}}t + n\log(n))$, where the $O(n\log(n))$ part comes from the third step of sorting. If we take $t$ to be a $O(1)$ with respect to $n$, then we have the time complexity $O(nd_{\text{max}} + n\log(n))$.

For algorithm LeastSquareClusterPursuit, the first step takes time $O(nd_{\text{max}})$, second step takes time $O(nd_{\text{max}} + n\log(n))$, where the $O(nd_{\text{max}})$ part comes from matrix vector multiplication, and $O(n\log(n))$ part comes from sorting.

Note that the standard way of solving the least square problem in the third step by finding the matrix inverse could cost a lot in computation. However, if an iterative method such as conjugate gradient descent is used (during our implementation, we used the lsqr function in Matlab) instead, given that the matrices are associated with well behaved condition numbers, then as pointed out by [33], it requires only a constant number of iterations to get a well approximated least square solution. In the implementation, we apply ten iterations for lsqr. Since the cost for each iteration in conjugate gradient descent equals to a few operations of matrix vector multiplication, which is $O(nd_{\text{max}})$, the total cost for LeastSquareClusterPursuit is $O(nd_{\text{max}} + n\log(n))$.

As a consequence, the total run time for LeastSquareClustering is $O(nd_{\text{max}} + n\log(n))$, and the total run time for IterLeastSquareClustering is $O(knd_{\text{max}} + kn\log(n))$. In the case of $k = O(1)$, the total run time are $O(nd_{\text{max}} + n\log(n))$, whereas the run time in [26] is $O(nd_{\text{max}}\log(n))$. For the regime $d_{\text{max}} = O(\omega(n)\log n)$ where $\omega(n) \to \infty$, our algorithm is slightly favored in terms of efficiency, which can also be seen from the numerical examples given in the next section.

5 Numerical Experiments

In this section, we evaluate the performance of our algorithm on synthetic SSBM model, network data on political blogs, MNIST data, AT&T human faces data and YaleB human faces data. We use CP+RWT and ICP+RWT [26] as baseline method to compare their performance. We also apply Lasso method as a subroutine to replace the least square step in LSC for comparison purpose. The standard spectral clustering (SC) algorithm is also being considered as another baseline method. For the implementation of LSC and ILSC, we use Matlab lsqr function as our iterative least square solver to solve equation (5). For the implementation of CP+RWT and ICP+RWT, we replace (5) in Step 3 of Algorithm 1 by solving (6) the same way as [26]. For the implementation of Lasso method, we solve (7) using the standard Matlab Lasso solver as a subroutine. We tune the rejection parameters $R$ for all algorithms and regularized parameter $\lambda$ in Lasso appropriately to make the output $C^\#_i$ of each algorithm approximately the same size for comparison purpose. Some more implementation details are summarized in the Appendix.

5.1 Synthetic Data

We first test our algorithms on the symmetric stochastic block model $SSBM(n, k, p, q)$ with different choices of parameters. The parameter $n$ indicates the total number of vertices, $k$ indicates the number of clusters, $p$ is the probability of having an edge between any two vertices within each cluster, and $q$ is the probability of having an edge between any two vertices from different clusters. Figure 1 gives an illustration of such a synthetic random graph model with three underlying clusters. By tuning the parameters, we achieve the experimental results shown in Table 1. We also run the experiments on stochastic block model for non-symmetric case and obtained similar gaps in accuracy and run time.
as in Table 1. For the implementation of symmetric stochastic block model, we use three vertices
with given label as our seed vertices under 500 repetitions, and we focus on only recovering the target
cluster.

Figure 1: A Symmetric Stochastic Block Random Graph with Three Underlying Clusters.

Table 1: Performance of finding $C_1$ using LSC, CP+RWT and LASSO with $k = 3$.

| $n$  | $p$ | $q$  | LSC  | Time  | CP+RWT | Time  | LASSO | Time  |
|------|-----|------|------|-------|--------|-------|-------|-------|
| 300  | 0.1 | 0.005| 99.8%| 4.7 ms| 99.6%  | 17.7 ms| 99.2% | 13.7 ms|
| 300  | 0.1 | 0.01 | 97.7%| 4.6 ms| 95.1%  | 13.5 ms| 96.6% | 14.7 ms|
| 1200 | 0.1 | 0.01 | 100% | 35.9 ms| 99.9% | 52.4 ms| 99.9% | 117.2 ms|
| 1200 | 0.1 | 0.02 | 99.6%| 37.6 ms| 97.4% | 42.9 ms| 99.6% | 126.8 ms|
| 4800 | 0.1 | 0.01 | 100% | 0.37 s | 100%  | 0.43 s | 100%  | 1.65 s |
| 4800 | 0.1 | 0.03 | 99.9%| 0.39 s | 99.4% | 0.50 s | 99.9% | 1.69 s |
| 4800 | 0.1 | 0.035| 98.6%| 0.39 s | 92.7% | 0.44 s | 98.6% | 1.70 s |
| 19200| 0.1 | 0.01 | 100% | 4.30 s | 100%  | 9.12 s | 100%  | 28.2 s |
| 19200| 0.1 | 0.04 | 99.9%| 6.70 s | 99.3% | 11.35 s| 99.9% | 30.6 s |
| 19200| 0.1 | 0.045| 99.0%| 7.71 s | 93.8% | 12.40 s| 99.0% | 33.6 s |

5.2 Network Data

We test our algorithms on the data from "The political blogosphere and the 2004 US Election" [3],
which contains a list of political blogs that were classified as liberal or conservative, and links between
the blogs. See Figure 2 as an illustration for the community structure (Figure source [3]). As explained
by Abbe and Sandon in [2], their simplified algorithm gave a reasonably good classification 37 times
out of 40 trials. Each of these trials classified all but 56 to 67 of the 1222 vertices in the graph main
component correctly. According to [2], the state-of-the-art described in [49] before the work in [2]
gives a lowest value at 58, with the best algorithms around 60 while algorithms regularized spectral
methods such as the one in [36] obtain about 80 errors. In our experiments, given eight labeled seeds,
the algorithm LSC succeeds 25 trials among a total of 30 trials, and among those 25 trials, the average
number of misclassified node is 78. which is comparable to the state-of-the-art result.
5.3 Human Faces Data

Two human faces datasets are also considered for evaluating the performance of our algorithms.

5.3.1 AT&T Faces Data

The AT&T Database of Faces [38] contains gray scale images for 40 different people of pixel size $56 \times 46$. Images of each person are taken under 10 different conditions, by varying the three perspectives of faces, lighting conditions, and facial expressions.

![AT&T Faces Data](image)

We use part of this data set by randomly selecting 10 people such that each individual has 10 images. We randomly permute the images as shown on the left of Figure 3, and compute its adjacency matrix $A$. 

![AT&T Faces Data](image)
based on the preprocessing method discussed in Appendix 7.2.2. Then we iteratively apply Algorithm 3 and try to recover all the 10 images belong to the same individual. The desired permutation of these individual images after iteratively performing Algorithm 3 are shown on the right of Figure 3. Some more details of the implementation regarding to the hyperparameters tuning are summarized in Appendix 7.2.1. The performances of our algorithm compared with other methods are summarized in Table 2 under 500 repetitions. Note that the spectral clustering method is unsupervised, hence its accuracy does not affected by the percentage of labeled data.

Table 2: Average F1 Scores of Recovering All Clusters for AT&T Data.

| Labeled Data % | 10  | 20  | 30  |
|----------------|-----|-----|-----|
| LSC            | 96.5% | 97.5% | 98.2% |
| CP+RWT         | 92.2% | 95.7% | 97.1% |
| LASSO          | 88.2% | 91.1% | 92.4% |
| SC             | 95.8% | 95.8% | 95.8% |

5.3.2 Yale Faces Data

The "Extended Yale Face Database B (YaleB)" [17] dataset contains 16128 gray scale images of 28 human subjects under 9 poses and 64 illumination conditions. We use part of this data set by randomly selecting 20 images from each person after some preprocessing, see Appendix 7.2.2. The images are randomly permuted and we aim to recover all the clusters by iteratively performing Algorithm 3. Figure 4 shows the randomly permuted images on the left side and the desired result on the right side. The performances of our algorithm compared with others are summarized in Table 3 under 500 repetitions.

Table 3: Average F1 Scores of Recovering All Clusters for YaleB Data.

| Labeled Data % | 5  | 10  | 20  |
|----------------|----|-----|-----|
| LSC            | 92.1% | 96.0% | 96.1% |
| CP+RWT         | 89.2% | 93.7% | 93.9% |
| LASSO          | 90.3% | 93.8% | 93.8% |
| SC             | 93.8% | 93.8% | 93.8% |

5.4 MNIST Data

We also test our algorithm on the MNIST data, which is a famous machine learning benchmark dataset in classification that consists of 70000 grayscale images of the handwritten digits 0-9 of size 28 × 28 with approximately 7000 images of each digit. We used a certain percentage of vertices with given label within each of the ten clusters as our seed vertices, the performance ILSC and ICP+RWT are summarized in Tables 4 under 100 repetitions.

We also compare ILSC with several other state-of-the-art semi-supervised methods on MNIST. As we can see in Table 5, ILSC outperforms the other algorithms except for the Ladder Networks which uses more information of labels and involved in a deep neural network architecture that requires training on GPUs for hours.
Figure 4: YaleB Faces Data (random permutation on the left, perfect recovering on the right)

Table 4: Average Accuracy of Recovering All Clusters for MNIST Data.

| Labeled Data % | ILSC  | Run Time | ICP+RWT | Run Time |
|----------------|-------|----------|---------|----------|
| 0.5            | 97.30%| 15.5 s   | 96.41%  | 18.1 s   |
| 1              | 97.73%| 15.3 s   | 97.32%  | 19.1 s   |
| 1.5            | 98.03%| 15.4 s   | 97.44%  | 19.8 s   |
| 2              | 98.17%| 15.5 s   | 97.52%  | 21.4 s   |
| 2.5            | 98.27%| 15.4 s   | 97.50%  | 22.1 s   |

Table 5: Comparing ILSC to other State-of-the-Art Semi-supervised Algorithms on MNIST.

| Methods                                   | Labeled Data | Accuracy |
|-------------------------------------------|--------------|----------|
| LapRF [47]                                | 600          | 95.6%    |
| TVRF [47]                                 | 600          | 96.8%    |
| ICP+RWT [26]                              | 700          | 97.3%    |
| Multi-Class MBO with Auction Dynamics [21] | 700          | 97.4%    |
| ILSC (this paper)                         | 700          | 97.7%    |
| AtlasRBF [35]                             | 1000         | 96.4%    |
| Pseudo-label [27]                         | 1000         | 96.6%    |
| DGN [22]                                  | 1000         | 97.6%    |
| ILSC (this paper)                         | 1000         | 98.0%    |
| Ladder Networks [37]                      | 1000         | 99.2%    |
6 Conclusions

In this paper, we proposed a semi-supervised local clustering algorithm LeastSquareClustering (LSC) and IterLeastSquareClustering (ILSC). The LSC is obtained through a two stages approach. In the first stage, we found a superset of the target cluster which will almost certain to contain the seed vertices set by running RandomWalkThreshold on the seed vertices. In the second stage, we developed a least square based approach LeastSquareClusterPuruist as our pursuit step to find the complement of target cluster within the superset. The ILSC is obtained by iteratively applying LSC with the updates of the underlying graph. We validate our algorithms by evaluating it on Stochastic Block Model, political blog data, MNIST data, AT&T human faces and YaleB human faces data. Our algorithms LSC and ILSC achieve a better performance than their counterparts CP+RWT and ICP+RWT [26] both in accuracy and efficiency. It also achieves very competitive results compared with other state-of-the-art semi-supervised clustering algorithms.

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7 Appendix

7.1 Finite State Markov Chains

For completeness, we briefly introduce the concept of Markov chains and state the fundamental theorem of Markov chains in this subsection.

For a finite state space $\Omega$, we say a sequence of random variables $X_t$ on $\Omega$ is a Markov chain if for all $t$ and all $x_0, \ldots, x_t, y \in \Omega$, we have

$$P(X_{t+1} = y|X_0 = x_0, \ldots, X_t = x_t) = P(X_{t+1} = y|X_t = x_t).$$

In other words, the probability of being at the current state is only determined by the immediate previous state. We consider time homogeneous one step transition matrix as

$$P(x, y) = P(X_{t+1} = y|X_t = x).$$

The $t$-step transition matrix is naturally defined as

$$P^t(x, y) = \begin{cases} P(x, y) & t = 1, \\ \sum_{z \in \Omega} P(x, z)P^{t-1}(z, y) & t > 1. \end{cases}$$

We say a distribution $\pi$ over $\Omega$ is a stationary distribution if it is invariant with respect to the transition matrix, i.e.,

$$\pi(y) = \sum_{x \in \Omega} \pi(x)P(x, y), \text{ for all } y \in \Omega.$$

**Definition 7.1.** A Markov chain is called irreducible if for all $x, y \in \Omega$, there exists $t$ such that $P^t(x, y) > 0$.

**Definition 7.2.** A Markov chain is called aperiodic if for all $x \in \Omega$, $\gcd\{t : P^t(x, x) > 0\} = 1$. (Here $\gcd$ stands for the greatest common divisor.)

The following theorem, originally proved in [14], details the essential property of irreducible and aperiodic Markov chains.

**Theorem 7.1.** (Fundamental Theorem of Markov Chains) For a finite irreducible and aperiodic Markov Chain, there exists a unique stationary distribution $\pi$ such that

$$\lim_{t \to \infty} P^t(x, y) = \pi(y) \text{ for all } x, y \in \Omega.$$

**Proof.** We omit the proof here by referring to [14], [4] and [28] for interested readers.

7.2 Further Details on Numerical Experiments

We provide with some more specific details in this subsection for implementing the numerical experiments in the previous sections.
7.2.1 Parameters Tuning

For each cluster to be recovered, we sampled the seed vertices $\Gamma_i$ uniformly from $C_i$ during all implementations. We fix the random walk depth with $t = 3$ and use random walk threshold parameter $\epsilon = 0.6$ for all of our experiments. We vary the rejection parameters $R \in (0, 1)$ for each specific experiments based on the estimated sizes of clusters. In the case of no knowledge of estimated sizes of clusters nor the number of clusters are given, we may have to refer to the spectra of graph Laplacian and use the large gap between two consecutive spectrum to estimate the number of clusters, and then use the average size to estimate the size of each cluster.

We fix the least square threshold parameter with $\gamma = |\hat{n}_1|/5$, which is totally heuristic. However, the performance of algorithms will not perturbed too much by varying $\gamma \in (0, 0.5)$, as long as we do not push $\gamma$ too extremely. The hyperparameter MaxIter is choosen according to the size of initial seed vertices relative to the total number of vertices in the cluster. For purely comparison purpose, we keep MaxIter = 1 for MNIST data. By experimenting on different choices of MaxIter, we find that the best performance for AT&T data occurs at MaxIter = 2 for 10% seeds and MaxIter = 1 for 20% and 30% seeds. For YaleB data, the best performance occurs at MaxIter = 2 for 5%, 10%, and 20% seeds. Therefore we choose to use these MaxIters in our implementation.

7.2.2 Image Data Preprocessing

We performed some data preprocessing techniques on YaleB data to avoid the poor quality images. Specifically, we abandoned the pictures which are too dark, and we cropped each image into size of $54 \times 46$ to reduce the effect of background noise. For the remaining qualified pictures, we randomly selected 20 images for each person.

All the image data in MNIST, AT&T, YaleB needs to be firstly constructed into an auxiliary graph before the implementation. Let $x_i \in \mathbb{R}^n$ be the vectorization of each image image from the original data set, we define the following affinity matrix of the $K$-NN auxiliary graph \cite{21} \cite{48} based on Gaussian kernel.

$$A_{ij} = \begin{cases} 
  e^{-\|x_i - x_j\|^2/\sigma_i \sigma_j} & \text{if } x_j \in NN(x_i, K) \\
  0 & \text{otherwise}
\end{cases}$$

The notation $NN(x_i, K)$ is the set of $K$-nearest neighbours of $x_i$, and $\sigma_i = \|x_i - x_i^{(r)}\|$ where $x_i^{(r)}$ is the $r$-th closest point of $x_i$. Note that the above $A_{ij}$ is not necessary symmetric, so we consider $\tilde{A}_{ij} = A^T A$ for symmetrization. Alternatively, one may also want to consider $\tilde{A} = \max\{A_{ij}, A_{ji}\}$ or $\tilde{A} = (A_{ij} + A_{ji})/2$. We then use $\tilde{A}$ as the input adjacency matrix for our algorithms.

We fix the local scaling parameters $K = 15$, $r = 10$ for the MNIST data, $K = 8$, $r = 5$ for the YaleB data, and $K = 5$, $r = 3$ for the AT&T data during implementation.