Chapter 1

Spectral Community Detection

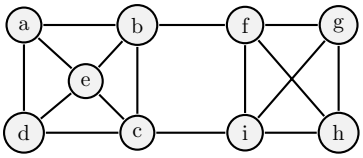
Contributed by Satyaki Sikdar

1.1 Introduction

Humans are highly selective when choosing whom they interact with. This is visible when people choose whom they want to be friends with from a group of people, or when researchers choose their collaborators. Social scientists call this process link formation. As expected, the process of link formation in complex networks is deliberate and non-random. As a result, not every node gets the same share of edges to connect to. A small number of nodes, called hubs, become part of the majority of the links, whereas the other nodes share a modest number of links among them [3]. In the world wide web and social networks, hubs hold a position of authority and influence. For example, Facebook, Google, and Amazon dominate their respective domains despite the presence of hundreds of competitors [20]. This is partly attributed to their being hubs in the complex network of the World Wide Web.

Sociologists first studied the theory of link formation in social networks, looking at the interaction between groups of people. The findings identified *homophily* [34], or the tendency of individuals to bond with other individuals they share a collective identity — gender, race, class, political views, and social roles, as the main driving force [10, 1, 35]. This not only results in the formation of links but also determines their strength. More frequent, stronger ties form between more similar users, and weaker ties which keep the network together form sporadically [17]. This leads to the formation of communities or clusters in the network, with nodes in each community having more links to other nodes in the same community than to the nodes in the rest of the network. This effect is not restricted to just social networks. In specific networks, communities make intuitive sense. For example, in social and telecommunication networks, clusters represent social circles; in collaboration networks, the clusters represent researchers working on similar areas of research, and so on. Moreover, communities are often nested, with smaller communities combining to form larger communities [26]. In the collaboration network of researchers across multiple disciplines, each discipline could be separable into large individual clusters, and inside each of them, there could be smaller clusters representing sub-disciplines. Extracting this higher-order interaction between the nodes is very useful in tasks like graph mining and graph compression. Community detection techniques therefore are used widely in many graph compression [22] and summarization algorithms [23].

While the presence of community structure in complex networks is ubiquitous, the degree of expression varies. In networks like the collaboration network among researchers [37], the clusters are highly separable. Researchers are more much more likely to collaborate with people who



(a) An undirected graph G with 9 nodes and 16 edges.

$$\mathcal{L} = \begin{array}{c} \\ \text{a} \\ \text{b} \\ \text{c} \\ \text{d} \\ \text{e} \\ \text{f} \\ \text{g} \\ \text{h} \\ \text{i} \end{array} \begin{array}{c} \begin{array}{ccccccccc} \text{a} & \text{b} & \text{c} & \text{d} & \text{e} & \text{f} & \text{g} & \text{h} & \text{i} \end{array} \\ \begin{pmatrix} 3 & -1 & & -1 & -1 & & & & \\ -1 & 4 & -1 & & -1 & -1 & & & \\ & -1 & 4 & -1 & -1 & & & & -1 \\ -1 & & -1 & 3 & -1 & & & & \\ -1 & -1 & -1 & -1 & 4 & & & & \\ & -1 & & & & 4 & -1 & -1 & -1 \\ & & & & & -1 & 3 & -1 & -1 \\ & & & & & -1 & -1 & 3 & -1 \\ & & -1 & & & -1 & -1 & -1 & 4 \end{pmatrix} \end{array}$$

(b) The Laplacian matrix $\mathcal{L}$ of G. The 0 entries are omitted for clarity.

$$\begin{array}{c} \\ \text{a} \\ \text{b} \\ \text{c} \\ \text{d} \\ \text{e} \\ \text{f} \\ \text{g} \\ \text{h} \\ \text{i} \end{array} \begin{array}{c} \\ \begin{pmatrix} -0.378 \\ -0.178 \\ -0.378 \\ -0.332 \\ -0.178 \\ +0.291 \\ +0.291 \\ +0.431 \\ +0.431 \end{pmatrix} \end{array}$$

(c) The Fiedler vector $\mathcal{F}$ of G

Figure 1.1: A graph and its Laplacian matrix and Fiedler vector

work in similar areas as them. The small group of researchers who do inter-disciplinary research keep the entire network connected. However, in some cases, as in friendship networks, the clusters represent social circles, which by nature are overlapping and messy [30]. Most community detection algorithms usually are more effective in graphs where the clusters are well defined. This chapter describes a particular class of spectral algorithms which are designed to find disjoint communities in undirected networks.

1.2 The Problem as a Graph

In a graph $G = (V, E)$ where V is the set of nodes and E is the set of edges, a community detection algorithm generates a cover $\mathbb{C} = \{C_1, C_2, \cdots, C_k\}$ of k communities where nodes lying in the same community are placed in the same set, and $\bigcup_i C_i = V$, that is, every node in the network is assigned to at least one community.

In disjoint community detection, each node is assigned to exactly one community. Formally, $\forall\ i, j,\ C_i \cap C_j = \emptyset$. In comparison, in overlapping community detection, each node can be a part of multiple communities, that is, $\exists\ i, j,\ C_i \cap C_j \neq \emptyset$.

The intuition behind community structures given in Section 1.1 can be formalized as follows. For a community C with n_C nodes, let $n_{int}(C)$ and $n_{ext}(C)$ denote the internal and external edge counts, signifying the number of edges having both endpoints and exactly one endpoint in C respectively. Both these counts are normalized to get the internal and external edge densities represented by $\delta_{int}(C)$ and $\delta_{ext}(C)$ respectively. The numerator of $\delta_{ext}(C)$ is also called the cut value of C ($\text{cut}(C)$). For a good clustering $\mathbb{C}$, the internal edge density for each cluster should be much greater than the external edge density. Mathematically,

$$\delta_{int}(C) = \frac{\sum_{\substack{i \in C \\ j \in C}} A_{ij}}{\binom{n_C}{2}} \qquad \delta_{ext}(C) = \frac{\sum_{\substack{i \in C \\ j \notin C}} A_{ij}}{n_C \cdot (n - n_C)} \qquad \text{cut}(C) = \sum_{\substack{i \in C \\ j \notin C}} A_{ij}$$

where A and n represent the adjacency matrix and the number of nodes in the graph G.

1.2.1 The Laplacian Matrix

The Laplacian matrix plays a central role in spectral graph theory. For a connected undirected graph $G = (V, E)$ with adjacency matrix $A_{n\times n}$, the Laplacian matrix $\mathcal{L}_{n\times n}$ is defined as $\mathcal{L} = D - A$, where $D_{n\times n}$ is a diagonal matrix where D_{ii} is the degree of node i. See Figure 1.1b to see the Laplacian matrix of a toy undirected graph described in Figure 1.1a.

By construction, the Laplacian has some beneficial mathematical properties, some of which are discussed now. $\mathcal{L}$ is symmetric and consists of only real-valued elements. Therefore, it has real eigenvalues, and the eigenvectors are orthogonal and have real entries. In addition to this, $\mathcal{L}$ is positive semidefinite (since $\vec{x}^T M \vec{x} \geq 0$ for all real-valued $\vec{x}$), so, the eigenvalues of $\mathcal{L}$ are non-negative. For example, the sorted eigenvalues of the toy graph G are (0, 0.649, 3.198, 3.326, 4, 4.554, 4.641, 5.382, 6.246) respectively.

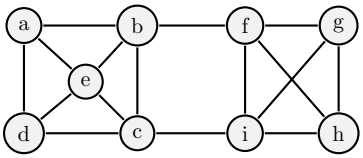
The smallest eigenvalue λ_1 of $\mathcal{L}$ is 0 with eigenvector $v_1 = (1, \ldots, 1)^T$, since the rows of $\mathcal{L}$ sum to zero. This eigen-pair (λ_1, v_1) is called trivial. The second smallest eigenvalue λ_2 and it's corresponding eigenvector v_2 encodes a lot of topological information about the graph G. This was first discovered by Fiedler [14] and are therefore named after him. The Fiedler vector v_2 of the toy graph is given in Figure 1.1c. For more properties of the Fiedler vector, see [11]. Section 1.4.1 discusses how the Fiedler vector can be used to find bipartitions.

1.3 Some Realistic Data Sets

Almost all complex networks are expected to have some amount of community structure when compared to a random graph of similar size. As described in Section 1.1, graphs with well defined clusters are expected to contain a large number of triangles [6] as they are indicative of the presence of local cliques.

Due to the universality of the phenomenon, it is observed in graphs of all scales. In the case of Facebook, the famous social network, their user graph as of 2014 had 1.39 billion active users and 400 billion edges [9]. Co-authorship networks are another class of networks that are of great interest to researchers. In Computer Science, for example, DBLP stores the information of 4.3 million publications made by 2.1 million authors across over 5,000 conferences as of September 2018. This sheer scale dramatically magnifies the difficulty level of the problem. However, through the advances in research in distributed computing and using novel computing paradigms [41, 31, 46, 32], researchers can crunch these massive networks and run the necessary algorithms.

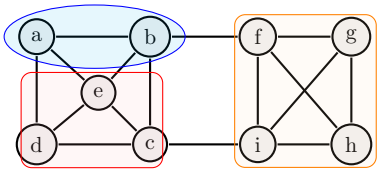
Several repositories of real-life networks exist on the internet [12, 29, 24]. There also exists several artificial graph generation algorithms which produce synthetic graphs having a defined community structure which are frequently used to validate the effectiveness of community detection algorithms. The *planted partition model* [13] for example, takes in the number of nodes n, the number of communities l, and the mixing parameter μ as an input. A node shares a fraction $1 - \mu$ of its links with the other nodes of its community and a fraction μ with the other nodes in the network. A lower μ signifies a more prominent community structure. The planted partition model generates a network having l groups of (nearly) equal size. Benchmarks like the *LFR benchmark graph generator* [27] is more flexible than the planted partition model. In addition to the parameters in the previous model, it allows the user more control over the degree distribution as well as the size distribution of the communities. This model has been extended to generate directed graphs with possibly overlapping community structures as well [25].



(a) The same undirected graph G from Figure 1.1a

	v_1	v_2	v_3
a	−0.378	0.521	−0.428
b	−0.178	0.418	0.463
c	−0.378	−0.521	−0.428
d	−0.332	0	0.104
e	−0.178	−0.418	0.463
f	0.291	0.232	0.172
g	0.291	−0.232	0.172
h	0.431	0	−0.26
i	0.431	0	−0.26

(b) Eigenvectors corresponding to 3 smallest positive eigenvalues of Laplacian $\mathcal{L}$ of G.



(c) 3 Clusters found by K-means with k=3 on the *normalized* matrix in (b)

Figure 1.2: A graph, its unnormalized eigenvectors corresponding to 3 smallest positive eigenvalues, and the resulting clustering

1.4 SCD - A Key Graph Kernel

Community detection is a widely studied area of research. Researchers have chosen multiple approaches to tackle this problem. A few popular ones involve using spectral techniques [36], graph sparsification [5, 44], traversals [40, 4], and greedy optimization of quality measures like modularity [7]. For a more comprehensive review of existing methods, see [15, 16].

For this report, two spectral clustering techniques are now described in detail.

The core premise of spectral clustering is that the eigenvectors of the matrices associated with a graph encode local information which can be used for clustering the nodes. The advantages of the spectral clustering methods come from their efficiency and mathematical elegance. Additionally, they usually have provable bounds of the quality of clusters produced [8]. For a survey on spectral graph clustering methods, see [36].

The nodes and edges in a graph are conventionally described in an abstract space where the conventional notion of distance between objects does not apply. This is unlike a metric space, where each object is embedded in d-dimensions. Conventional machine learning tasks like classification or clustering expect the input data to be in a metric space, so they cannot be directly used for data represented as graphs. Spectral clustering, however, generates a d-dimensional metric space embedding of the nodes, i.e., each node gets assigned a d-dimensional coordinate. In addition to that, it ensures that the nodes that share direct links, or that are part of the same cluster, are spatially closer too. This results in the transfer of the link and community information from the abstract space to the metric space. In the bipartition algorithm described in Section 1.4.1, each node is embedded in 1-dimensional (metric) space, while in the algorithm in Section 1.4.2, it is k-dimensional.

1.4.1 Spectral bipartition

Hagen et al. [18] proposed an algorithm whose pseudocode is given in Algorithm 1. Nodes are divided into two clusters p_1 and p_2 depending on whether the corresponding entry in the Fiedler vector is above or below the given threshold r. The choice of r therefore influences the quality of clusters. Popular choices for r include 0 and the median value of the Fiedler vector. For example,

for $r = 0$ for the Fiedler vector in Figure 1.1c for the graph in Figure 1.1a finds two clusters {a, b, c, d, e} and {f, g, h, i}.

The computation of the Fiedler vector dominates the computational complexity of the algorithm. The fastest known method, the Lanczos method [28] takes linear time i.e., $O(|V|+|E|)$. So, the overall time complexity of Algorithm 1 is also $O(|V| + |E|)$.

1.4.2 k-way spectral partition

Ng et. al [39] extends the idea of bipartition described above into k-way partitions as follows. Instead of using just the Fiedler vector, they use the eigenvectors corresponding to the k-smallest positive eigenvalues of the Laplacian as a matrix of order $|V| \times k$. By doing so, they generate a k-dimensional embedding for each of the nodes. Additionally, each row of this matrix is normalized by its L_2 norm since in practice, normalized data tends to produce better quality clusters. These embeddings are then clustered using any conventional spatial clustering algorithm like K-means [19] to find k clusters. The pseudocode of this algorithm is given in Algorithm 2.

The running time of the algorithm is dominated by the eigendecomposition and the time taken by K-means to converge. In practice, the method seems to work fast and scales linearly with the size of the graph.

1.4.3 Computing Eigen-decompositions

Central to spectral clustering is the computation of eigenvalues and eigenvectors. This report looks at three popular eigen-decomposition, viz., the Lanczos algorithm with Implicitly Restarted Arnoldi Methods [28], Locally Optimal Block Preconditioned Conjugate Gradient method (LOBPCG) [43], and Trace Minimization Algorithm for the Generalized Eigenvalue problem (TraceMIN) [42]. All these algorithms are conveniently implemented in the NetworkX and SciPy libraries which makes for easy comparison of these methods. The Lanczos and the LOBPCG methods use BLAS and ARPACK libraries [21, 28], and therefore are parallel in nature. This results in reduced running times compared to the serially implemented TraceMIN algorithm. Also, the Lanczos sacrifices numerical stability and accuracy for speed.

To test out the performance of each of the methods, Fiedler vectors $\mathcal{F}$ were computed 5 times for each of the graphs described in Table 1.1. The running time as well as the maximum Mean Absolute Error (MAE) was computed between all pairs of $\mathcal{F}$ for a given method, and were plotted for comparisons in Figure 1.3. The results are quite surprising as all the three methods have almost identical MAE values while the Lanczos algorithm is consistently the fastest among the three.

1.5 Prior and Related Work

Spectral clustering remains a popular choice for finding clusters for reasons mentioned in Section 1. While the core premise of using eigendecompositions to encode structural similarity is shared across all the methods, each algorithm has its own uniqueness built into it and sees applications in a variety of domains, like computer vision [45, 33] and VLSI design [2]. In each of these methods, some variant of the minimum-cut problem is solved. Additionally, there have been methods like [38] which maximizes the modularity of the partitions. For a more detailed overview of spectral clustering techniques, see [36].

Algorithm 1 Approximate minimum cut of a connected graph G for a given threshold r

```
1: procedure approx_min_cut(G(V, E), r)
2:     clusters ← ∅
3:     if G has fewer than 2 nodes then
4:         clusters ← V
5:     else
6:         fiedler ← Fiedler vector of G
7:         p1 ← ∅
8:         p2 ← ∅
9:         for u ∈ V do
10:            if fiedler[u] < r then
11:                p1 ← p1 ∪ {u}
12:            else
13:                p2 ← p2 ∪ {u}
14:        clusters ← clusters ∪ { p1}
15:        clusters ← clusters ∪ { p2}
16:    return clusters
```

Algorithm 2 k-way spectral partitioning of a connected graph G

```
1: procedure k_way_spectral(G(V, E), k)
2:     clusters ← ∅
3:     if G has fewer than k nodes then
4:         clusters ← V
5:     else
6:         L ← Laplacian matrix of G
7:         evecs ← matrix of eigenvectors corresponding to k-smallest positive eigenvalues of L
8:         Normalize each row of evecs by its L2 norm
9:         Run K-means clustering on evecs to find k clusters ℂ = {C1, ··· , Ck} using Euclidean
   distance
10:        clusters ← ℂ
11:    return clusters
```

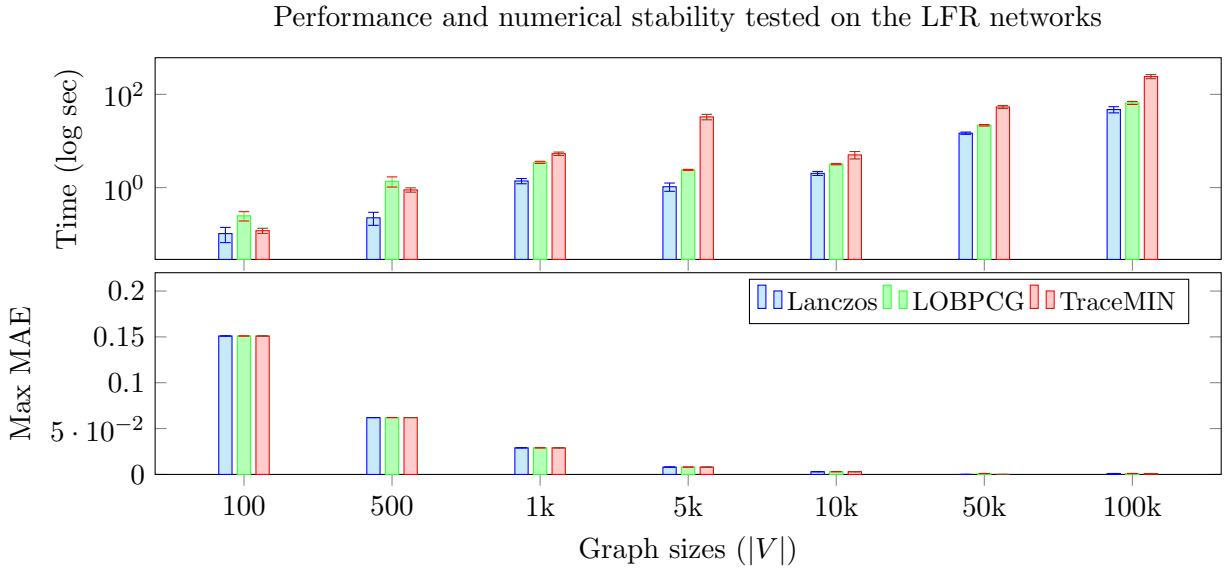


Figure 1.3: Running times and numerical stability of the eigen-decomposition algorithms on the LFR networks described in Table 1.1. Lower is better. The Lanczos method consistently performs better than the rest.

1.6 A Sequential Algorithm

For implementing Algorithms 1 and 2, we use Python with `NetworkX`[1], `numpy`[2], `scipy`[3], and `scikit-learn`[4] libraries. `NetworkX` provides easy to use containers for graphs as well as supporting functions like computing the Laplacian matrix and the Fiedler vector of a graph. `SciPy` facilitates easy computation of eigenvectors of arbitrary matrices and `scikit-learn` has a built-in implementation of the K-means algorithm.

1.7 A Reference Sequential Implementation

Python implementation of Algorithm 1

```
import networkx as nx

def approx_min_cut(G, r):
    assert nx.is_connected(G), "the graph must be connnected"

    clusters = []
    if G.order() < 2:
        clusters = list(G.nodes())
    else:
        # compute the Fiedler vector
        fiedler_vec = nx.fiedler_vector(G, method='lanczos')
```

[1] `https://networkx.github.io`
[2] `http://www.numpy.org`
[3] `https://www.scipy.org`
[4] `http://scikit-learn.org`

```
        # p1 and p2 stores the nodes in each partition
        p1, p2 = set(), set()

        for node_id, fiedler_val in zip(G.nodes(), fiedler_vec):
            if fiedler_val < r:
                p1.add(node_id)
            else:
                p2.add(node_id)

        clusters.append(p1)
        clusters.append(p2)
    return clusters
```

Python implementation of Algorithm 2

```
import networkx as nx
import numpy as np
import scipy.sparse.linalg
from sklearn.cluster import KMeans
import sklearn.preprocessing

def k_way_spectral(G, k):
    assert nx.is_connected(G), "the graph must be connnected"

    clusters = []
    if G.order() < k:
        clusters = list(G.nodes())
    else:
        L = nx.laplacian_matrix(G)

        # compute the first k + 1 eigenvectors
        _, eigenvecs = scipy.sparse.linalg.eigs(L.asfptype(), k=k+1, which='SM')

        # discard the first trivial eigenvector
        eigenvecs = eigenvecs[:, 1:]

        # normalize each row by its L2 norm
        eigenvecs = sklearn.preprocessing.normalize(eigenvecs)

        # run K-means
        kmeans = KMeans(n_clusters=k).fit(eigenvecs)
        cluster_labels = kmeans.labels_

        clusters = [[] for _ in range(max(cluster_labels) + 1)]

        for node_id, cluster_id in zip(G.nodes(), cluster_labels):
            clusters[cluster_id].append(node_id)
    return clusters
```

1.8 Sequential Scaling Results

The experiments were run on one node of the CRC cluster with 64 cores and 128 GB memory. The graphs were generated using the LFR benchmark, with more details given in Table 1.1. The top plot in Figure 1.3 shows the Python running times for Fiedler vector computations.

Table 1.1: Graph statistics for the LFR networks with $\langle k \rangle \approx 16,\ \gamma = -2,\ \beta = -1,\ \mu = 0.1$. $\langle k \rangle$, ρ, and $\#\Delta$s represent the average degree, graph density (%), and the number of triangles respectively.

Graph Name	$\lvert V \rvert$	$\lvert E \rvert$	$\langle k \rangle$	ρ	$\#\Delta$s
100	100	795	15.9	16%	2 834
500	500	3 825	15.3	3%	12 296
1k	1 000	7 692	15.384	1.5%	21 491
5k	5 000	38 247	15.298	0.3%	31 063
10k	10 000	76 325	15.265	0.15%	47 136
50k	50 000	383 778	15.351	0.03%	183 152
100k	100 000	765 073	15.30	0.01%	329 364

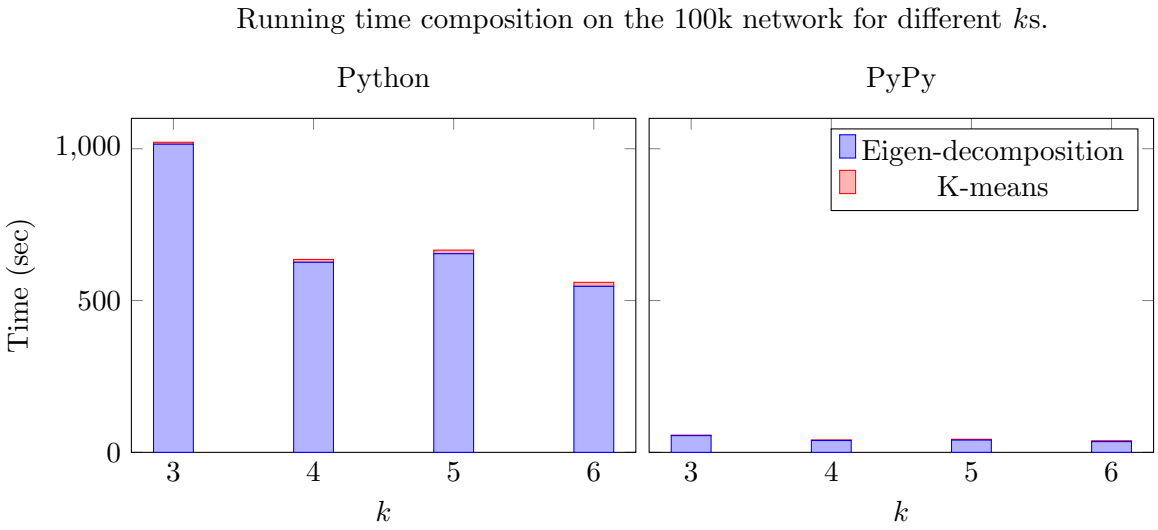


Figure 1.4: Running time plots for the k-way spectral clustering algorithm for both Python and PyPy implementations using the Lanczos algorithm. Lower is better. Most of the time is spent in the eigen-decomposition algorithm.

Similarly, Figure 1.4 shows the running time for the k-way spectral clustering for both Python and PyPy[5] implementations. Eigen-decomposition dominates the CPU time over the K-means clustering. PyPy definitely achieves a huge speedup compared to the regular Python interpreter.

1.9 A Parallel Algorithm

I feel the PyPy implementation does not qualify as a parallel implementation, mostly because PyPy runs the exact same code and does the optimizations behind the scenes.

I recently came across a parallel C++ spectral clustering implementation which uses MPI. I do plan on getting those data in the report over the winter break.

Hence, the sections 1.10 and 1.11 are empty.

[5] `https://www.pypy.org`

1.10 A Reference Parallel Implementation

1.11 Parallel Scaling Results

1.12 Conclusion

This report covers the Spectral Community Detection kernel. It starts by looking at the causality behind the formation of communities, and then formalizes the problem in the language of graph theory. It then discusses two popular algorithms, followed by their implementation and scaling results. Enhanced implementation was carried out by using the PyPy interpreter which achieved significant speedup compared to regular Python. While this is the last iteration for the course, the report unfortunately is still incomplete.

Future work is summarized below.

- Testing the running times on more benchmark and real-world networks.
- Getting the C++ parallel version of spectral clustering to work and benchmarking it.

1.13 Response to Reviews

- Corrected grammar in several places of the text
- Added a section on the graph Laplacian
- Re-wrote certain parts of the pseudocodes to make it more coherent

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