Optimal k-centers of a graph: a system-theoretic approach

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Abstract

In a network consisting of n nodes, this paper's goal is to identify the 'most central' k nodes with respect to the definitions of centrality proposed in this paper. This concept finds applications in various scenarios, ranging from multi-agent problems where external communication (or leader nodes) must be identified, to more classical use cases like ambulance or facility location problems. Depending on the specific application, there exist several notions of quantifying k-centrality, and the set of best k nodes obviously varies based on the chosen definition. Closely related to graphs, we also explore notions of k-centrality within stochastic matrices. In this paper, we formulate two new metrics and establish connections to a well-studied metric from the literature (that was proposed and more studied for stochastic matrices, and then extended to graph-Laplacians). We prove that these three notions match for path-graphs and formulate an explicit expression for the metric both in general and at optimality. Some of the results extend to graphs more general than path-graphs, and the agreement among the three metrics is later analyzed for randomly generated general graphs, where we also include a few other system-theoretic notions and consider these too in the comparison.

The first metric proposed in this paper involves maximizing the smallest eigenvalue of the graph Laplacian matrix after an appropriate diagonal entry perturbation. This maximization can be interpreted as minimizing the time constant of discharge when a corresponding RC circuit is provided a leakage across various combinations of k capacitors. The second metric focuses on minimizing the Perron root of a substochastic matrix that is a principal submatrix of a stochastic matrix: an idea proposed and interpreted in the literature linking it to 'manufacturing consent'. The third one explores minimizing the Perron root of a perturbed (now super-stochastic) matrix, which can be seen as minimizing the impact of added stubborn-ness. The first of these metrics is linked to time-constant of a dynamical system and dominance is formalized through k-centrality; later in this paper, we compare these metrics with other system-theoretic notions, namely, observability Gramian and port-centrality in terms of maximum energy extraction from a uniformly charged circuit-system (using the Riccati theory).

It is important to emphasize that we consider applications (for example, facility location) when the notions of central nodes are such that the set of the 'best' k nodes does not necessarily contain the set of the $k-1$ nodes: this distinguishes these notions from the well-studied ranking-based metrics. We apply the proposed k-centrality notions to various network structures.
Keywords: Graph centers, Laplacian matrices, Stochastic matrices, Fiedler vector, Matrix perturbation, k-centrality.
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1. Introduction

Optimal/central nodes selection involves determining the most appropriate or ideal nodes within a system or network to serve specified goals. This process pinpoints one or more highly significant nodes in the network, determined by a criterion of centrality. Optimal node selection has wide-ranging applications in fields such as networking, electrical circuits, logistics, transportation, data centers and social media/influencer networks. Its significance extends to efficient/fastest communication, network resilience, resource allocation, security, influence and control.

In this paper, we consider only simple undirected, unweighted graphs, i.e., with no self-loops and no multiple edges between any pairs of the vertices. Node centrality is a well-explored topic in the literature. Various centrality measures, including degree centrality [20], closeness centrality [19], betweenness centrality [2], eigenvector centrality [4], and Page-Rank [17], are used to rank nodes based on different aspects of the network. In most of these centrality measures, due to a ranking based process, the set of 'best' k ports, denoted as S_k, includes the 'best' $k-1$ ports, set S_{k-1}. However, in many practical notions of centrality, as pursued in this paper, the inclusion of S_{k-1} in S_k is neither assumed nor required. We consider an example to demonstrate this after we describe one of the proposed notions of centrality. Metrics that have this feature have been studied, see for example [10], but these have been more of discrete/combinatorial optimization, which do not easily allow extensions to the case of weighted graphs. On the contrary, the notion proposed in [5, 6] is well-suited for weighted graphs too, and we compare our results closely with this notion.

In this paper we propose two new notions of choosing the best k ports within a network and compare these two notions with an existing one. One of the proposed notions analyzes the change in the smallest eigenvalue of the Laplacian matrix when the matrix is subjected to a perturbation in the diagonal entry; we call this the Maximized Laplacian matrix Smallest Eigenvalue (*Definition 2.1[i](MaxLSE)*). The other two definitions and the rest of this paper are compared/related to this notion and hence we include this construction as a definition for easy referencing. We point out that this notion is closely linked to the time-constant of a system, namely the dominant pole, i.e. the pole that is nearest to the imaginary axis; this system-theoretic interpretation of this metric, together with two others, namely observability Gramian and the Riccati-theory based method of identifying those ports as central which allow maximum energy extraction from a uniformly charged circuit-system (elaborated in Section 4) connect structural graph theory with systems theory.

Definition 1.1. *Consider an undirected, unweighted simple graph G of n nodes and m edges. Index the nodes as 1 to n. Associate an RC circuit with n capacitors (each of unit capacitance) and m resistors (each of unit resistance) with this graph as follows: each edge of the graph is a resistor connected between the corresponding nodes of that edge. Each of the n nodes is connected to one terminal of a capacitor; the capacitors are indexed by nodes 1 to n based on this terminal's node-index. The other terminals of all the n capacitors are connected together: these terminals form the ground-node (say node-0).*

With respect to this RC circuit associated to the graph, a node of the graph now refers to a port across the corresponding capacitor.

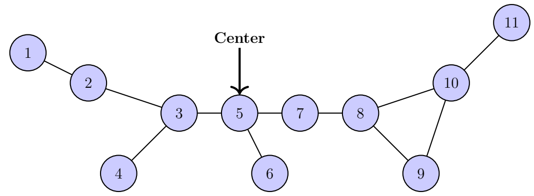
The significance of the RC circuit with the graph's Laplacian is straightforward: if $v(t) \in \mathbb{R}^n$ is the vector of capacitor voltages, then the capacitor voltages evolve as per the first order differential equation: $\frac{d}{dt}v(t) = -Lv(t)$. Further, addition of an amount $\epsilon > 0$ at a diagonal entry of L (say $(j,j)^{\text{th}}$ entry) corresponds to attaching a 'leakage resistance' across the capacitor of index j: the leakage resistance being equal to $1/\epsilon$. If the graph G is connected, then the sole eigenvalue of L at the origin is now displaced to a small and positive value $\lambda_1(j)$, thus making the perturbed Laplacian matrix positive *definite*, and further, the displacement in the eigenvalue being dependent on the node-choice j. Clearly, given that the graph is connected, and thanks to the leakage resistance introduced, the RC circuit is now able to discharge to the zero state from any initial state of capacitor voltages. A natural question arises as to which is the capacitor j such that introducing the leakage resistance across it leads to the fastest discharge, equivalently, perturbing which diagonal entry (j,j) of the Laplacian matrix (by adding $\epsilon > 0$) results in the maximum increase of the smallest eigenvalue of the perturbed Laplacian matrix.

Given that identifying the central node with respect to the Definition 2.1[i](MaxLSE) is regarding identifying the 'port' where introducing the leakage-resistance results in smallest time-constant, we use central-'port' and central-node interchangeably throughout this paper. Thus after identifying the central node (or set of k-central nodes), we speak about an optimally perturbed Laplacian matrix, and equivalently an RC circuit that has been placed with leakage resistance optimally at the central port (or set of k central ports).

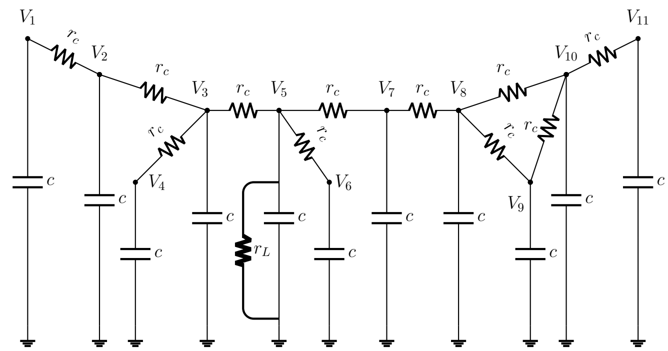
The RC circuit for a graph, together with the leakage-resistance at one/two ports, are shown for an example in Figure 1: in which a graph of 11 nodes and the corresponding RC network are considered.

By brute-force calculation (and also fairly intuitively), the single-best center node is node-5 and the best two central nodes are nodes 3 and 8 (w.r.t. the notion described above and more precisely defined below within Definition 2.1[i](MaxLSE)). Thus, in this example, the best single-center is not amongst the best pair of centers; this is typical in many facility location problems for instance.

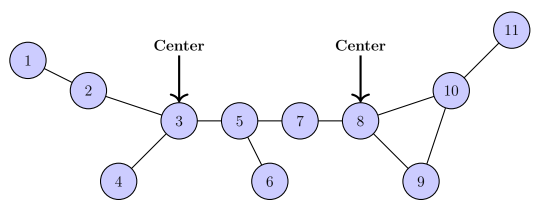
Further, in this paper, we compare the notion introduced in Definition 2.1[i](MaxLSE) with one other metric proposed/pursued for stochastic matrices (in [5, 6]) and later extended to Laplacian matrices (called the 'grounded Laplacian', see [24]). Remarks 2.2 and 2.3 give an interpretation of these metrics. Finally, we formulate a notion of centrality for stochastic matrices that captures the extent to which stubborn-ness introduced at a node can be diffused. Remark 2.3 elaborates more on this interpretation of k-centrality.



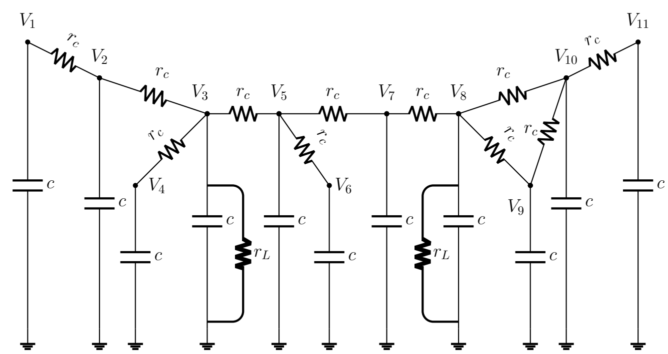
(a) Graph G with one center 5 (center w.r.t. *Definition 2.1[i](MaxLSE))*



(b) An analogous RC network of G and leakage resistances across capacitors at node 5 and the ground.



(c) Graph G with two centers 3 & 8 (centers w.r.t. *Definition 2.1[i](MaxLSE))*



(d) An analogous RC network of G and leakage resistances across capacitors at nodes $3, 8$ and the ground.

Figure 1: Choosing best k-ports in Graph G

This paper deals with both:

- Laplacian matrices for unweighted, undirected graphs, and
- symmetric stochastic matrices: a doubly stochastic version of the Laplacian matrix (see [14]).

In this context, we define $Z_n := I - \tau L_n$, for a sufficiently small $\tau > 0$, as in equation (1). It can be interpreted as a discretized version (a doubly stochastic version of the Laplacian matrix) of the continuous-time system $\dot{x} = -Lx$, with L as the Laplacian of the unweighted, undirected graph G. For this paper we assume

$$Z_n := I - \tau L_n \quad \text{where} \quad 0 < \tau < \frac{1}{\Delta(G)} \quad \text{and} \quad \Delta(G) := \text{max. degree of the graph } G. \tag{1}$$

This assumption on τ ensures that $I - \tau L$ is a stochastic matrix: the exact value of τ is not relevant any more for the rest of this paper's results. We do use the property that if L is symmetric, tridiagonal and unreduced[1] then Z_n too is symmetric, tridiagonal and unreduced.

1.1. Notation

The notation we follow is standard: the sets of real and complex numbers are denoted respectively by $\mathbb{R}$ and $\mathbb{C}$. We use $|S|$ to denote the cardinality of a set S. Given an undirected, unweighted simple[2] graph G, the number of vertices/nodes are usually n, out of which k best nodes are to be selected: usually $k < n/2$. We index the nodes from 1 to n and, when dealing with the path graph P_n, the indexing is linear from one end to the other. The eigenvalues of the Laplacian matrix of the network graph $L(G)$ (or any symmetric matrix in $\mathbb{R}^{n \times n}$) are denoted and numbered as $\lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_n$, i.e. $\lambda_1 = \lambda_{\min}$ and $\lambda_n = \lambda_{\max}$. The matrix Z is usually the doubly stochastic version of Laplacian matrix L, as in equation (1). The minimum eigenvalue of the Laplacian matrix $\lambda_{\min}$ is central in this paper: its dependence is investigated w.r.t. different parameters: the number of centers sought (i.e. k), the number of nodes, the perturbation ϵ, port-index p (or port-indices p_1 and p_2); and depending on the context, we write explicitly only some of its arguments and do not write explicitly $\lambda_{\min}(k, n, \epsilon, p_1, p_2)$ each time: the context helps in disambiguation.

1.2. Organization of this paper

The paper is organized as follows: the subsequent section (Section 2) defines the k-centrality notions that are pursued throughout the paper. This is succeeded by the section on the main results (Section 3), which contains the principal findings of the study pertaining to the path graph and also some results for general graphs. In the following section, i.e. Section 4, some heuristics are presented for identifying central nodes in general graphs with a few more system-theoretic k-centrality notions and a comparison amongst various notions is also included in this section. Section 5 contains concluding remarks and deliberates on some future directions. After the references, two appendices follow: the first one (Section 6) contains some auxiliary results and additional new results that support or augment the main outcomes. The second appendix contains proofs of all the results of this paper, both main and auxiliary.

[1] A tridiagonal matrix is called unreduced if each of the super-diagonal and sub-diagonal entries are nonzero.

[2] A graph G is called simple if there are no self-loops and G has at most one edge between any pair of nodes.

2. Definitions of k-centrality and possible inter-relations

In the definition below, we propose three metrics for best k-ports selection, one of which (Definition 2.1[ii] (MinSubLE)) has been quite well-studied in the literature; see [5, 6] and also [24].

Definition 2.1. *Consider an undirected, unweighted simple graph G_1 of n nodes and the corresponding Laplacian matrix $L_n \in \mathbb{R}^{n\times n}$. Let $Z_n \in \mathbb{R}^{n\times n}$ be the corresponding doubly stochastic matrix as defined in equation (1). For a subset $S \subset \{1, 2, \dots, n\}$, with $|S| = k < n$, and for a sufficiently small $\epsilon > 0$, construct[3] matrices ${}^S\tilde{L}_n$ and ${}^S\tilde{Z}_n \in \mathbb{R}^{n\times n}$ as follows:*

$$ {}^S\tilde{L}_n := L_n - \epsilon \sum_{j\in S} e_j e_j^T \quad \text{and} \quad {}^S\tilde{Z}_n := Z_n + \epsilon \sum_{j\in S} e_j e_j^T. \tag{2} $$

Also define the principal submatrix ${}^S\hat{Z} \in \mathbb{R}^{(n-k)\times(n-k)}$ obtained by removing[4] the k rows and k columns indexed by the set S from the matrix Z_n. Define the three metrics and the corresponding sets[5] of k-centers S^* w.r.t. each metric as follows.

*[i] Maximize **Laplacian's** Smallest-Eigenvalue (MaxLSE): The best k nodes are defined as the subset S^*_{MaxLSE} which maximizes $\lambda_{\min}({}^S\tilde{L}_n)$, i.e.*

$$ S^*_{MaxLSE} := \arg \max_{\substack{\text{all subsets } S \\ \text{with } |S| = k}} \lambda_{\min}({}^S\tilde{L}_n). $$

*[ii] [5, 6] Minimize **Sub**-stochastic Largest-Eigenvalue (MinSubLE): The best k nodes is defined as the subset $S^*_{M\textbf{Sub}\text{-}LE}$ that minimizes $\lambda_{\max}({}^S\hat{Z})$ of the principal submatrix ${}^S\hat{Z} \in \mathbb{R}^{(n-k)\times(n-k)}$ corresponding to S, with the k rows/columns indexed by S removed from Z:*

$$ S^*_{M\textbf{Sub}\text{-}LE} := \arg \min_{\substack{\text{all subsets } S \\ \text{with } |S| = k}} \lambda_{\max}({}^S\hat{Z}). $$

*[iii] Minimize **Super**-stochastic Largest Eigenvalue (MinSupLE): The best k nodes is defined as the subset $S^*_{M\textbf{Sup}\text{-}LE}$: that minimizes the largest eigenvalue of the super-stochastic matrix ${}^S\tilde{Z}_n \in \mathbb{R}^{n\times n}$ obtained by the perturbation defined in equation (2):*

$$ S^*_{M\textbf{Sup}\text{-}LE} := \arg \min_{\substack{\text{all subsets } S \\ \text{with } |S| = k}} \lambda_{\max}({}^S\tilde{Z}_n). $$

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[3]For sufficiently small positive ϵ, the subset S^* depends only on the Laplacian matrix L and the graph. This too is elaborated later below.

[4]This is same as that proposed in [5, 6] and also similar to the notion of grounded-Laplacian pursued in [24, 15].

[5]Of course, for each of the set-optimization problems within the definitions, the argument of the maximization/minimization need not be unique. In each of the results in this paper, we explicitly assume conditions that ensure the uniqueness of the argument.

The link/interpretation of Definition 2.1[i](MaxLSE) with its corresponding RC circuit, and the discharging through leakage resistances introduced at the k-nodes indexed by S, is elaborated within and soon after Definition 1.1. We relate the 3 definitions, and in particular the first one, with the facility/ambulance location problem and the maximal covering location problem later below in Remark 3.4.

Definition 2.1[ii](MinSubLE) is familiar and well-studied in the literature [5], the principal sub-stochastic matrix largest eigenvalue minimization based selection. The following remark provides an interpretation (based on [5]) of Definition 2.1[ii](MinSubLE) in the sense of 'manufacturing consent' i.e. how fast influence can be diffused.

Remark 2.2. *The notion of best k-nodes for a stochastic matrix in the sense of 'manufacturing consent' (i.e. Definition 2.1[ii](MinSubLE)) was proposed in [5, 6] and is also closely related to that of the 'grounded Laplacian' (see [15, 24]). In this definition, given a stochastic matrix Z_n and given a subset S of cardinality k, the corresponding k rows and k columns are removed thus making the resulting matrix sub-stochastic (or positive definite, in the case of the grounded Laplacian). The minimization of the largest eigenvalue of the principal submatrix ${}^S\hat{Z} \in \mathbb{R}^{(n-k)\times(n-k)}$ is interpreted as, loosely speaking, how quickly the influence through the k nodes over-rides onto the rest $n-k$ nodes compared to the influence due to the $n-k$ nodes on themselves. Further, loosely speaking again, the minimization of the largest eigenvalue results in fastest convergence to steady state or equilibrium, i.e. the smallest 'mixing-time' in the context of the corresponding Markov chain.*

The following remark discusses an interpretation of Definition 2.1[iii](MinSupLE) as stubborn-ness (or influence diffusion) measure.

Remark 2.3. *The Definition 2.1[iii](MinSupLE) can be understood as follows. The addition of a small and positive value of ϵ at diagonal elements of Z corresponding to S may be interpreted as introducing a small amount of 'stubborn-ness' at those nodes. The addition of an amount $\epsilon > 0$ to a diagonal entry can cause an increase of the largest eigenvalue beyond 1 by varying amounts (the increase being between 0 and ϵ): the nodes that are quite central are able to 'diffuse' this stubborn-ness to (or influence) their neighbouring nodes much better than nodes which are isolated or near to isolated. Minimizing the largest eigenvalue of the super-stochastic matrix (as the proposed notion in Definition 2.1[iii](MinSupLE)) amounts to finding nodes where the introduced stubborn-ness diffuses the most: thus more influential nodes can diffuse this stubborn-ness better.*

We pursue with the above three definitions in the following section, which contains the main results of this paper.

3. Main results: k centrality and inter-relations

In this section, we formulate the main results of this paper. The proofs of the results in this section need further results which have been formulated and proved in the following sections. Most of the main results pertain to path graphs for which we prove the optimality of the same set of k-central nodes w.r.t. the different definitions listed in Definition 2.1[MaxLSE, MinSubLE, MinSupLE]. Closed-form expressions are also formulated and proved for the case of path graphs on n-nodes. Some results in this section are about general graphs, i.e. not necessarily path graphs; Theorems 3.5 and 3.6 are respectively about a close relation between two of the definitions and about a certain independence of the first order term w.r.t. number of edges and the graph. Pursuing further about general graphs, as far as k-centers are concerned, the metrics and heuristics do not agree 100% and later in Section 4 we include computational experiments on randomly generated graphs of various orders: both trees and graphs with cycles.

3.1. Central nodes for path graph

Our first main result obtains a single central node for the path graph w.r.t. all three Definition 2.1(MaxLSE, MinSubLE, MinSupLE).

Theorem 3.1. *Let n be odd with $n \geqslant 3$, and consider the path graph P_n on n nodes and consider L_n the corresponding Laplacian matrix. Suppose v_F is the Fiedler eigenvector, i.e. the eigenvector corresponding to λ_2. Define $Z_n := I_n - \tau L_n$ for sufficiently small and positive τ (as in equation (1)). Let $p \in \{2, 3, \cdots, n-1\}$ and consider the perturbed Laplacian matrix $\tilde{L}_n := L_n + \epsilon e_p e_p^T$. Define[6] $p^* := \frac{n+1}{2}$. Then the following hold regarding the single node centrality w.r.t. Definition 2.1[MaxLSE, MinSubLE, MinSupLE].*

(a) The smallest eigenvalue of $\tilde{L}_n$, upto 2^{nd} order in ϵ, is

$$\lambda_{\min}(\epsilon, p) = \frac{\epsilon}{n} - \frac{\epsilon^2}{12n^2}\left\{(n^2-1) + 12(p-p^*)^2\right\}.$$

(b) The smallest eigenvalue $\lambda_{\min}$ of perturbed Laplacian matrix (upto 2^{nd} order in ϵ) is maximized at $p = p^*$, and $\max_p \lambda_{\min}(\tilde{L}_{n,\epsilon}, p)$ equals $\frac{\epsilon}{n} - \frac{\epsilon^2}{12n^2}(n^2-1)$ and also equals

$$\frac{\epsilon}{n} - \frac{\epsilon^2}{4n}\sum_{j=2}^{n} \frac{\cos^2\left(\pi(j-1)/2\right)}{\sin^2\left(0.5\pi(j-1)/n\right)\left\{\sum_{i=1}^{n}\cos^2\left(\pi(j-1)(i-0.5)/n\right)\right\}}. \tag{3}$$

(c) The node indexed at p^* is center w.r.t. all three definitions within Defn 2.1[MaxLSE, MinSubLE, MinSupLE] (upto 2^{nd} order approximation in ϵ).

(d) [3] Further, if $v_2 \in \mathbb{R}^n$ is the eigenvector corresponding to the eigenvalue λ_2 (the Fiedler value) of L_n, and $v_2(j)$ is the j^{th} component of v_2, then $\quad v_2(j) = 0 \iff j = p^*$.

[6] With n odd, p^* is the traditional physical center of the path graph P_n.

See the appendix for the proof. An interesting fact about the dependence of $\lambda_{\min}(\epsilon, p)$ on $p \in \mathbb{R}$, instead of $p \in \mathbb{Z}$, is as follows. While $p^* = \frac{n+1}{2}$ is expected to be the maximizer for $\lambda_{\min}$ when $p \in \mathbb{Z}$, it is noteworthy that for $p \in \mathbb{R}$, the point p^* is a local minimizer: see Lemma 6.2 for a more precise formulation and the proof. Figure 2 shows a plot of $\lambda_{\min}$ versus p revealing the local minimum (though p indicates the port index and is thus to be considered an integer). This fact makes the above theorem significant.

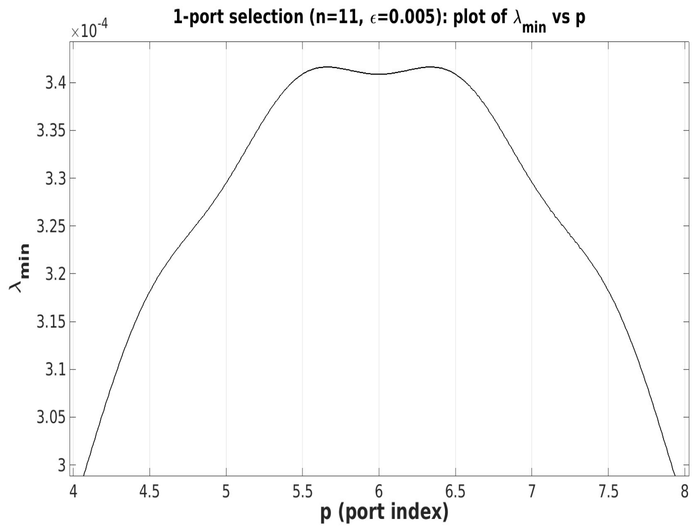

Figure 2: Plot of smallest eigenvalue $\lambda_{\min}(L_{11})$ (the Laplacian of path graph P_{11}) versus port index p (for continuum variable $p \in \mathbb{R}$) showing local minima at the 'physical center' $p^* = 6$, though for integers p, a global maxima is indeed as expected at p^*: Theorem 3.1

The following result obtains two central nodes for the path graph w.r.t. Definition 2.1[MaxLSE, MinSubLE, MinSupLE]: here too the 3 definitions coincide, and further, a certain 'independence' of the effects due to the two central nodes (formulated in statement (a)) is revealed; this is elaborated in Remark 3.4.

Theorem 3.2. *Let n be even, with $\frac{n}{2}$ odd and $n \geqslant 6$. Consider the path graph P_n and its corresponding Laplacian matrix L_n and define the perturbed Laplacian matrix, $\approx{L}_n := L_n + \epsilon e_{p_1} e_{p_1}^T + \epsilon e_{p_2} e_{p_2}^T$ with $p_1, p_2 \in \{1, 2, , \ldots, n\}$ and assume [7] $p_1 < \frac{n}{2} < p_2$. Define $p_1^* := \dfrac{n+2}{4}$ and $p_2^* := \dfrac{3n+2}{4}$: the 'physical centers' of the two halves (see Footnote 6) of the path graph P_n. Then, the following hold about the 2-central nodes w.r.t. Definition 2.1[MaxLSE, MinSubLE, MinSupLE] when considering only upto 2nd order in ϵ.*

(a) The smallest eigenvalue of $\approx{L}_n$ equals

$$\lambda_{\min}(\epsilon, p_1, p_2) = \frac{2\epsilon}{n} - \frac{\epsilon^2}{12n^2}\left[(n^2 - 4) + 24(p_1 - p_1^*)^2 + 24(p_2 - p_2^*)^2\right].$$

[7] The assumption $p_1 < \frac{n}{2} < p_2$ merely ensures that the ports are being searched in the two different halves: this assumption is fairly reasonable and helps simplify the proofs.

(b) $\lambda_{\min}(\epsilon, p_1, p_2)$ *gets maximized uniquely at* $p_1 = p_1^*$, $p_2 = p_2^*$ *and* $\max_{p_1,p_2} \lambda_{\min}(\approx{L}_{n,\epsilon}, p_1, p_2)$ *equals* $\frac{2\epsilon}{n} - \frac{\epsilon^2}{12n^2}(n^2-4)$ *and also equals*

$$\frac{2\epsilon}{n} - \frac{\epsilon^2}{4n}\sum_{j=2}^{n} \frac{\Big\{\cos\left(\pi(j-1)/4\right) + \cos\left(3\pi(j-1)/4\right)\Big\}^2}{\sin^2\left(0.5\pi(j-1)/n\right)\left\{\sum_{i=1}^{n}\cos^2\left(\pi(j-1)(i-0.5)/n\right)\right\}} \quad . \tag{4}$$

(c) *The nodes indexed at* p_1^* *and* p_2^* *are centers w.r.t. all 3 Definitions 2.1[MaxLSE, MinSubLE, MinSupLE].*

(d) *Further, if* v_3 *is the eigenvector corresponding to the eigenvalue* λ_3 *of* L_n*, and suppose* $v_3(j)$ *denotes the* j^{th} *component of* v_3*. Then,* $v_3(j) = 0 \iff$ *either* $j = p_1^*$ *or* $j = p_2^*$.

See the appendix for the proof. The last statement above and the following theorem (of k-central nodes) are a generalization (for path graphs) of Statement (d) of Theorem 3.1, the Fiedler vector based center (see [3] for this celebrated result): the replacement being that for k-centers, we consider the eigenvector corresponding to $(k+1)^{\text{th}}$ smallest eigenvalue of the Laplacian matrix for path graphs. The following theorem also quantifies the shift in the zero eigenvalue (for the path graph Laplacian) due to perturbation at diagonal entries indexed by set S with cardinality k. The centers with respect to only Definition 2.1[ii](MinSubLE) is proved (as the physical centers of the k-equal parts); proving that the k-centers for path-graph coincide with the other two notions of k-centers is a matter of future work.

Theorem 3.3. *Let* $S \subset \{1, 2, \ldots, n\}$ *with* $|S| = k < n$ *and let* $S = \{p_1, p_2, \ldots, p_k\}$*. Suppose* L_n*, the Laplacian matrix for* P_n*, is perturbed to* ${}^{S}\tilde{L}_n := L_n + \epsilon \sum_{j\in S} e_{p_i} e_{p_i}^T$ *for small* $\epsilon > 0$ *and with* e_{p_i} *the* p_i^{th} *column of the identity matrix. Then,*

(a) *the smallest eigenvalue of the Laplacian matrix is given by:*

$$\lambda_{\min}({}^{S}\tilde{L}_n) = \frac{k\epsilon}{n} - \frac{\epsilon^2}{4n}\sum_{j=2}^{n} \frac{\Big\{\sum_{i=1}^{k}\cos\big(\pi(j-1)(p_i-0.5)/n\big)\Big\}^2}{\sin^2\left(0.5\pi(j-1)/n\right)\left\{\sum_{i=1}^{n}\cos^2\left(\pi(j-1)(i-0.5)/n\right)\right\}} + O(\epsilon^3). \tag{5}$$

Further, suppose n *is divisible by* k *and let* n/k *be odd. Define the* k *nodes* $p_i^* := \dfrac{(2i-1)n+k}{2k}$ *where* $i = 1, 2, \ldots, k$*: these are the physical centers of the* k *equal parts of* P_n*. Then,*

(b) $p_1^*,\ p_2^*, \ldots, p_k^*$ *form the unique central nodes w.r.t. Definition 2.1[ii](MinSubLE) and the corresponding optimal value of* $\lambda_{\max}({}^{S^*}\hat{Z}) = \cos(k\pi/n)$.

(c) *Let* $v_{k+1} \in \mathbb{R}^n$ *be the eigenvector corresponding to the eigenvalue* λ_{k+1} *of* L_n *and let* $v_{k+1}(j)$ *denote the* j^{th} *component of* v_{k+1}*. Then,* $v_{k+1}(j) = 0 \iff j \in \{p_1^*,\ p_2^*, \ldots, p_k^*\}$.

See the appendix for the proof. As mentioned just before Theorem 3.2, a fairly unintuitive property is the seeming mutual independence of the optimality of the best two ports. This is demonstrated in Table 1 and later elaborated in Remark 3.4.

Table 1: $\lambda_{\min}$(scaled by multiplying by 10^2) vs port indices: 2-ports selection in P_{14}: $p_1 \in \{1, \ldots, 7\}$ are indices along the rows and $p_2 \in \{8, \ldots, 14\}$ are indices along the columns; value of $\epsilon = -10^{-2}$.

Port #	8	9	10	11	12	13	14
1	-1.455	-1.450	-1.447	**-1.446**	-1.447	-1.450	-1.455
2	-1.450	-1.445	-1.442	**-1.441**	-1.442	-1.445	-1.450
3	-1.447	-1.442	-1.439	**-1.438**	-1.439	-1.442	-1.447
4	**-1.446**	**-1.441**	**-1.438**	**-1.437**	**-1.438**	**-1.441**	**-1.446**
5	-1.447	-1.442	-1.439	**-1.438**	-1.439	-1.442	-1.447
6	-1.450	-1.445	-1.442	**-1.441**	-1.442	-1.445	-1.450
7	-1.455	-1.450	-1.447	**-1.446**	-1.447	-1.450	-1.455

The following remark discusses about the mutual independence of one port selection of the other port w.r.t. Definition 2.1[i](MaxLSE).

Remark 3.4. *An interesting and significant consequence of Theorem 3.2(a), under mild/reasonable assumptions (see Footnote 7), is the independence of the roles that j_1 and j_2 play in the contributions towards the second order effect in the shift of the minimum eigenvalue. When using the RC circuit and leakage resistance analogy elaborated above, this independence points out that choice of one node for leakage does not affect the optimality of the other: this distinguishes the RC circuit leakage resistance placement problem from the ambulance location problem that is well-studied in the facility location literature; see [16] for a recent paper and its references, and also [7] for a classic paper initiating such work as a maximal covering location problem.*

The following theorem states the equivalence of Definition 2.1[i](MaxLSE) and [iii](MinSupLE) for a general simple graph G. This result holds for not just for path graphs but also for general graphs, though the definitions and interpretations for the two definitions are fairly different (one about RC circuit's quick discharge, while the other about diffusion of added stubborn-ness.

Theorem 3.5. *Consider a general simple graph G with n nodes having Laplacian matrix L_n and the stochastic matrix $Z_n = I_n - \tau L_n$. Let $|S| = k$ and suppose the Laplacian matrix L_n is perturbed to ${}^S\tilde{L}_n := L_n - \epsilon \sum_{j\in S} e_j e_j^T$ and the stochastic matrix Z_n is perturbed to ${}^S\tilde{Z}_n := Z_n + \epsilon \sum_{j\in S} e_j e_j^T$.*
Then, the set S_1^* that maximizes the smallest eigenvalue of perturbed Laplacian matrix as in Definition 2.1[i](MaxLSE) and the set S_3^* that minimizes the largest eigenvalue of ${}^S\tilde{Z}_n$ as in Definition 2.1[iii]

(MinSupLE), are the same [8] *k-centers of the network i.e.*

$$\arg \max_{\substack{\textit{all subsets } S \\ \textit{with } |S|=k}} \lambda_{\min}({}^S\tilde{L}_n) = \arg \min_{\substack{\textit{all subsets } S \\ \textit{with } |S|=k}} \lambda_{\max}({}^S\tilde{Z}_n). \tag{6}$$

See the appendix for the proof.

3.2. First order approximation of the perturbed Laplacian matrix smallest eigenvalue: general graphs

Theorems 3.1, 3.2 and Theorem 3.3 reveal that the first order approximation of the smallest eigenvalue of the perturbed Laplacian matrix is $\frac{k\epsilon}{n}$ for a path graph: independent of the port indices at which perturbation is carried out. Extending this result to tree or general graph, we formulate the following theorem: the first order approximation is independent of not just the port-indices, but also both the graph G_n and the number of edges (provided the graph G_n is connected).

Theorem 3.6. *Let $S \subset \{1, 2, \ldots, n\}$ for $|S| = k < n$ and let G_n be any undirected and unweighted simple connected graph. Perturb L_n, the Laplacian matrix for G_n, to ${}^S\tilde{L}_n := L_n + \epsilon \sum_{j \in S} e_j e_j^T$ for a sufficiently small $\epsilon > 0$, where e_j is the j^{th} column of the identity matrix. Then, for any G_n satisfying the above assumptions, upto the first order in ϵ, the smallest eigenvalue $\lambda_{\min}$ of ${}^S\tilde{L}_n$*

- *is independent of the number of edges in the graph G_n,*
- *is independent of the port indices (i.e. independent of set S), and*
- *satisfies $\lambda_{\min} = k\epsilon/n$.*

See the appendix for the proof.

3.3. Scaling with respect to number ports and number of nodes

We saw in the previous subsection that the linear approximation is independent of the port index for an undirected, unweighted, general simple graph (i.e. path graph, general tree and also for graphs with cycles). Thus the 2^{nd} order term plays the key role about optimality of port indices. In this subsection, we first observe through an example in Figure 3 that a certain convexity exists in the way the function $\lambda_{\min}$ depends on number of ports at respective port optimality. More precisely, from Figure 3, we see that $\lambda^*_{\min}(k)$ at optimal k-ports is greater than k times $\lambda^*_{\min}(1)$ at optimal 1-port for the case of P_{21}, the path graph on 21 nodes.

For the special case of $k = 1$ and $k = 2$, we use Theorem 3.1 and Theorem 3.2 to formulate the theorem below. To avoid divisibility constraints/assumptions, we assume n to be sufficiently large.

[8] In case of non-uniqueness of the optimization in LHS/RHS in equation (6), the equation is to be understood as the sets which maximise $\lambda_{\min}({}^S\tilde{L}_n)$ is same as the sets which minimise $\lambda_{\max}({}^S\tilde{Z}_n)$.

Theorem 3.7. *Consider a path graph of sufficiently large order n and let $k < n$. Let $\lambda_{\min}(k)$ be the optimal shift in the smallest eigenvalue as per Defn 2.1[i](MaxLSE) for the optimal choice of k-ports. Then, $\lambda_{\min}(2) > 2 \times \lambda_{\min}(1)$ for upto 2^{nd} order approximation in ϵ.*

See the appendix for the proof.

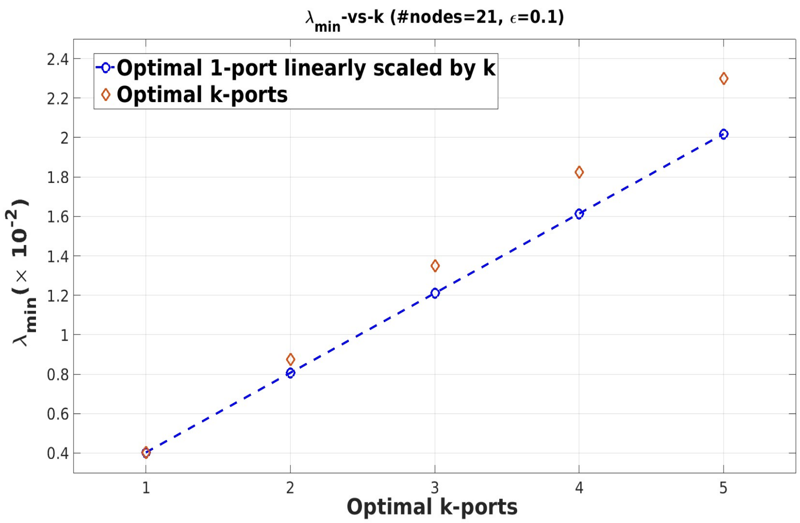

Figure 3: Path graph with multiple (optimal) ports, say k, and the shift achieved is more than k times the shift due to a single port

Remark 3.8. *Figure 3 shows the shift in $\lambda_{\min}$ with respect to the k-optimal ports, and it compares this shift with that of one optimal port linearly scaled to k ports: the optimal k-port perturbation yields a greater shift than k times 1-port perturbation. Thus, in this example, $\lambda_{\min}(k)$ is a convex function of k. In contrast with the law of diminishing returns, here we have more than proportionate return with additional 'investment' in introducing leakage resistances. In a circuit analogy interpretation, k-port perturbation represents k different passages for discharge, enabling the capacitor to discharge from the nearest leakage resistance, and thus faster. Consequently, discharge through the k-optimal ports is faster compared to a single passage scaled by k. Thus, an RC circuit helps explain the convexity. Further, the circuit interpretation also explains a plausible reason as to why we have a case opposite to the 'law of diminishing returns'.*

3.4. Relation between 1-optimal port and 2-optimal ports: path graphs

In the path graph network, P_n and P_{2n}, we investigate the question: if we select 1-optimal port and 2-optimal ports respectively, what is the relationship between the smallest eigenvalue shifts that occur in both cases? From a circuit's viewpoint, when connecting two circuits in, loosely speaking, "cascade", the question is: will the larger circuit discharge faster or slower? The following theorem claims an equality between the smallest eigenvalue of the perturbed Laplacian matrix for one port selection (for n-node path graph) and two ports selection (for a $2n$ node path graph) at respective optimalities.

Theorem 3.9. *Let n be odd, consider an n-nodes path graph Laplacian L_n. Suppose L_n is perturbed optimally for a 1-port selection to get: $\tilde{L}_n := L_n + \epsilon e_{p^*} e_{p^*}^T$, with $p^* = \dfrac{(n+1)}{2}$. Similarly, suppose a $2n$-nodes path graph Laplacian L_{2n} is perturbed optimally for 2-ports selection to get: $\tilde{\tilde{L}}_{2n} := L_{2n} + \epsilon\{e_{p_1^*} e_{p_1^*}^T + e_{p_2^*} e_{p_2^*}^T\}$, with $p_1^* = \dfrac{n+2}{4}$ and $p_2^* = \dfrac{3n+2}{4}$. Then, $\lambda_{\min}(\tilde{L}_n) = \lambda_{\min}(\tilde{\tilde{L}}_{2n})$.*

See the appendix for the proof. In the above theorem, using the Cauchy interlacing theorem[9] [18, Theorem 10.1.1], it is easy to see that $\lambda_{\min}(\tilde{L}_n) \geqslant \lambda_{\min}(\tilde{\tilde{L}}_{2n})$, given that $\tilde{L}_n$ is a principal submatrix of $\tilde{\tilde{L}}_{2n}$; the above theorem proves equality for the smallest eigenvalues of $\tilde{L}_n$ and $\tilde{\tilde{L}}_{2n}$. The above result might not be too surprising from a circuit's viewpoint given the symmetry in the network for the slowest mode. The result below about the remaining eigenvalues also is true, though the proof is quite tedious; due to paucity of space and due to a lack of clear motivation/significance, we include the statement below as only an 'observation' and we do not pursue a proof in this paper. This result below relates other eigenvalues of $\tilde{L}_n$ and $\tilde{\tilde{L}}_{2n}$.

Observation 3.10. *Let n be odd, consider an n-nodes path graph Laplacian L_n. Suppose L_n is perturbed by arbitrary ϵ for an optimal 1-port selection: $\tilde{L}_n := L_n + \epsilon e_{p^*} e_{p^*}^T$, with $p^* = \dfrac{(n+1)}{2}$. Denote the eigenvalues of the perturbed Laplacian matrix $\tilde{L}_n$ as $\lambda_1 < \lambda_2 < \cdots < \lambda_n$. Further, suppose a $2n$-nodes path graph Laplacian L_{2n} is perturbed by arbitrary ϵ for 2-ports selection: ($\tilde{\tilde{L}}_{2n} := L_{2n} + \epsilon(e_{p_1^*} e_{p_1^*}^T + e_{p_2^*} e_{p_2^*}^T)$, with $p_1^* = \dfrac{n+2}{4}$ and $p_2^* = \dfrac{3n+2}{4}$). Denote the eigenvalues of the perturbed Laplacian matrix $\tilde{\tilde{L}}_{2n}$ as $\mu_1 < \mu_2 < \cdots < \mu_{2n}$.*
Then the following equalities/inequalities hold between the eigenvalues of $\tilde{L}_n$ and $\tilde{\tilde{L}}_{2n}$:

$$\lambda_1 = \mu_1 < \mu_2 < \lambda_2 = \mu_3 < \mu_4 < \lambda_3 = \mu_5 < \cdots < \lambda_n = \mu_{2n-1} < \mu_{2n}.$$

The above observation is obvious for $\epsilon = 0$ (as per (ii) of Proposition 6.1 from P_n to P_{2n} the eigenvalues are merely interpolated): the significance is that the claim is in fact true for $\epsilon \neq 0$ too. As a separate extension/generalization of Theorem 3.9, the following conjecture points towards the independence of the $\lambda_{\min}$ with respect to edge addition after the optimal port selection: the edge addition being arbitrary as long as the addition connects the two disjoint path-graphs. The mutual independence of optimality of the two ports (Remark 3.4) is another motivation to check about the question of arbitrarily connecting of two 'optimally-leaked' RC circuits that are constructed from path graphs P_n and its effect on the smallest eigenvalue (i.e. time-constant corresponding to the discharge rate).

[9] The eigenvalues of a real symmetric $n \times n$ matrix are interlaced, with a non-strict inequality, with the eigenvalues of any of its $(n-1) \times (n-1)$ sized principal sub-matrix.

Conjecture 3.11. *Let n be odd, consider a path graph P_n Laplacian matrix L_n. Suppose for optimal 1-port selection L_n is perturbed to $\tilde{L}_n := L_n + \epsilon e_{p^*} e_{p^*}^T$, with $p^* = \frac{(n+1)}{2}$. Denote the optimal perturbed RC circuit as P_n^*. Suppose an RC circuit is formed as $P_n^* \cup P_n^*$ and suppose one edge (i.e. one unit-resistance) is added between any pair of nodes of the graph $P_n^* \cup P_n^*$ such that the resulting graph is connected: denote the resulting connected graph on $2n$ nodes as T_{2n}. Then, $\lambda_{\min}(P_n^*) = \lambda_{\min}(P_n^* \cup P_n^*) = \lambda_{\min}(T_{2n})$.*

4. Comparison of proposed metrics with other system-theoretic measures: general graphs

Except Theorems 3.5 and 3.6, most results in this paper pertain to path graphs. In this section, we investigate using randomly generated graphs, both trees and graphs with cycles, the extent to which we have agreement amongst the various metrics this paper proposes. We also pursue two more system-theoretic measures. Of course, each of these measures have different significances and they are not expected to agree 100%. Taking Definition 2.1[i] MaxLSE as the base metric and using this for comparing with the other formulated metrics, Table 2 contains the percentages of agreement with the base metric (i.e. (MaxLSE). The number of ports considered for the experiments tabulated in Table 2 are one, two and three; in case of two and three ports, we consider as 'matched' only if all elements in the optimal sets match when comparing any two definitions.

We now elaborate on two more notions, both having a system-theoretic relevance, that are also tabulated in Table 2.

- **ARE solution** $K_{\min}$: Consider the RC circuit again associated to a graph, and instead of introducing a leakage resistance at one or more of the chosen ports, one can consider charging the circuit externally and in this situation, if i is the current provided through the chosen ports, and v is the vector of voltages across these ports respectively, then $v^T i$ is the total power provided to the circuit (total across all the chosen ports, with the appropriate load convention for v and for i). A natural optimal control question of relevance in system theory in general and passivity studies in particular is that of maximizing $\int_0^\infty -v^T i \, dt$ over all trajectories starting from the vector of all capacitor voltages equal to 1 V (i.e. vector $\mathbf{1} \in \mathbb{R}^n$) at $t = 0$, and ending finally at the vector 0, i.e. the fully discharged circuit (at $t = +\infty$). When choosing k ports, one can define those k ports as central where this energy that can be extracted from the circuit uniformly charged (i.e. the voltage vector $\mathbf{1} \in \mathbb{R}^n$) is maximized over all combinations of k ports: this amounts to studying different Algebraic Riccati Equations (ARE) for each of the choice of k ports, and maximizing $\mathbf{1}^T K_{\min} \mathbf{1}$ over all such choices of k ports; $K_{\min}$ being the minimum ARE solution w.r.t. the passivity supply rate for the RC circuit corresponding to the particular choice of k ports.

- **Observability Gramian** Q: Consider again the RC circuit associated to the graph. In this measure, we ask the question: how much energy can be extracted from the chosen ports, say k of them, from a given initial condition voltage vector v_0? Those k ports are called central for which the energy that can be extracted is maximum (over all choices of k ports): further the maximization is done w.r.t. the initial condition voltage vector equal to $\mathbf{1}$: this vector corresponding to the so-called 'consensus' vector. See [26, 22], for example, for more details.
- **Laplacian eigenvector:** Various results in the earlier section indicate (for path graphs) about how a certain eigenvector of the Laplacian matrix has components zero exactly for those nodes which are k-central. In our opinion, this result is a generalization (albeit only for path graphs) of the well-known fact that, for trees, the Fiedler vector components increase in magnitude as one moves along branches away from the 'characteristic block': see [3]. Thus, while the characteristic node (when one exists) is the center for trees, our results for path graphs indicate that eigenvectors for larger eigenvalues also contain information about k centers. More precisely, when identifying the central k-nodes for a graph on n nodes, then the eigenvector v_{k+1}, corresponding to eigenvalue λ_{k+1} (assuming that this eigenvalue is not repeated), has magnitude smallest at those k-nodes which are central in the graph. This observation agrees for path graphs, as formulated and proved in the theorems in the main section. In Tables 2, we check the extent to which this agrees with other metrics for general graphs: both trees and graphs with cycles. The column marked 'Eigenvector' corresponds to picking those nodes which are smallest in magnitude in the eigenvector v_{k+1} of the Laplacian matrix, and checking agreement about this set with the k-centers identified by MaxLSE.

Table 2: Comparison of various metrics for general graphs, taking into account choices of upto three ports.

Graphs	**n**	% **match with Max*LSE*** ($\epsilon = 0.01$) for 100 graphs				
		Min*Sup*LE	**Min*Sub*LE**	**Laplacian eigenvector**	$\mathbf{1}^{\mathbf{T}} K_{\min} \mathbf{1}$	$\mathbf{1}^{\mathbf{T}} Q \mathbf{1}$
Path	11	100%	100%	100%	100%	100%
Tree	7	100%	97.67%	66%	97%	59%
Tree	9	100%	91%	69.67%	99.67%	63%
General	7	100%	78.15%	40.74%	90%	80.37%
General	9	100%	70.5%	33.34%	97.92%	90.63%

A comparison of the 5 metrics with Definition 2.1[i] MaxLSE as the base is tabulated in Table 2. Of course, MinSupLE and MaxLSE agree completely as expected: see Theorem 3.5 for the statement and proof. When comparing with others, it is interesting that the column corresponding to $\mathbf{1}^T K_{\min} \mathbf{1}$ shows maximum agreement with the MaxLSE metric: both have very clear system-theoretic significances; one (the base metric, i.e. MaxLSE) indicates the time-constant of discharge with the more central nodes resulting in smallest time-constant. The other metric ($\mathbf{1}^T K_{\min}\mathbf{1}$) captures that the more central nodes allow more extraction of the energy stored in the capacitors.

5. Concluding remarks and future directions

In this paper, we introduced two new measures, Maximized Laplacian Smallest Eigenvalue (MaxLSE) and Minimized Super-stochastic Largest Eigenvalue (MinSupLE), for selecting the best k ports in a graph. We further proved that the results obtained above metrics perfectly aligned with the results obtained using the existing metric, Minimized Sub-stochastic Largest Eigenvalue (MinSubLE) for the path graph.

We proved that the smallest eigenvalue of the Laplacian matrix for a path graph P_n is equal to the smallest eigenvalue of a path graph P_{2n} at optimal selection of one and two ports respectively. Additionally, we observed that the eigenvalues of the Laplacian matrix $\tilde{L}_n$ for the n-node path graph are all present as eigenvalues in the Laplacian matrix $\tilde{\tilde{L}}_{2n}$ of the 2n-node path graph. These eigenvalues are interlaced with the other n eigenvalues of the matrix. Furthermore, we showed that the smallest eigenvalue of the perturbed Laplacian matrix of the general graph, considering only upto the first-order approximation in ϵ depends only on n and k: thus proving independence of the graph, the port-indices of the k chosen ports and the number of edges.

When selecting two ports, we showed that the choice of one optimal port is independent of the other in the path graph. We also proved that the shift in the minimum eigenvalue ($\lambda_{\min}$) with respect to the 2-optimal ports exceeds the shift obtained by linearly scaling a single optimal port to 2 ports. Furthermore, our observation indicates that an optimal k-ports perturbation results in a larger shift than k times the shift caused by a 1-port perturbation. Consequently, the function $\lambda_{\min}(k)$ is convex and provides a greater return than the scaled investment (in contrast to the law of diminishing returns).

For future directions, we aim to demonstrate the independence of selecting one optimal port from another when choosing k-ports in the path graph. We aim to prove $\lambda_{\min}(k)$ convexity for k-ports selection. We plan to globally prove the selection of k optimal ports for the path graph using all three metrics (MaxLSE, MinSubLE, and MinSupLE). Our future work will focus on globally proving the selection of k optimal ports for general graphs using our two metrics (MaxLSE and MinSupLE).

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6. Appendix A1: Auxiliary results

This section contains results from the literature (called propositions) and (new) auxiliary results, using which we prove the main results stated in Section 3. The auxiliary results proofs are in the appendix.

The following proposition (from [21]) states an expression for eigenvalues and the corresponding eigenvector of the path graph P_n of order n. Also shown there is the fairly nontrivial identity (equation (7)) about the norm of each of the eigenvectors; the relevance of the identity is more trigonometric than the focus of this paper. This result is used in this paper to prove Theorems 3.1, 3.2 and 3.3.

Proposition 6.1. *[21, Lemma 6.6.1] Let L_n be the Laplacian matrix of the path graph P_n of order n. Then the (ordered) eigenvalues $\lambda_j \in \mathbb{R}$ and corresponding eigenvectors, $v_j \in \mathbb{R}^n$ of the Laplacian matrix L_n satisfy the following.*

i) The eigenvalues λ_j are distinct and $0 \leqslant \lambda_j < 4$.

ii) The j-th eigenvalue λ_j equals $2 - 2\cos\big(\pi(j-1)/n\big)$.

iii) The p^{th} component of the corresponding eigenvector $v_j \in \mathbb{R}^n$ satisfies $v_j(p) = \cos\big(\pi(j-1)(p-0.5)/n\big)$.

iv) The eigenvector $v_j \in \mathbb{R}^n$ formulated in (iii) above satisfies: $\|v_j\|_2 = \sqrt{\frac{n}{2}}$, i.e.

$$\sum_{p=1}^{n} \cos^2\left(\frac{\pi p(j-1)}{n} - \frac{\pi(j-1)}{2n}\right) = \frac{n}{2}. \tag{7}$$

The eigenvalues of the path graph are distinct as evident from the above proposition: this provides the uniqueness of the eigenvector (of course, upto scaling by a non-zero scalar). The following lemma provides an expression of the smallest eigenvalue of the Laplacian matrix of the path graph after a rank-one perturbation at one of the diagonal entries. This lemma helps in proof of Theorem 3.1.

Lemma 6.2. *Let n be odd and let L_n be the Laplacian matrix for the path graph of P_n. Suppose L_n is perturbed to $L_n + \epsilon e_p e_p^T$ for sufficiently small ϵ with e_p, the p^{th} column of the identity matrix.*

a) Then, the smallest eigenvalue of the perturbed Laplacian matrix, $\tilde{L}_n := L_n + \epsilon e_p e_p^T$ is given by:

$$\lambda_{\min}(\tilde{L}_{n,\epsilon}, p) = \frac{\epsilon}{n} - \frac{\epsilon^2}{4n} \sum_{j=2}^{n} \frac{\cos^2\big(\pi(j-1)(p-0.5)/n\big)}{\sin^2\left(0.5\pi(j-1)/n\right)\left\{\sum_{i=1}^{n}\cos^2\left(\pi(j-1)(i-0.5)/n\right)\right\}} + O(\epsilon^3)$$

b) Assume $p \in \mathbb{R}$ (instead of $p \in \mathbb{Z}$) and consider only upto 2nd-order terms in ϵ. Then $\lambda_{\min}(\tilde{L}_{n,\epsilon}, p)$ is locally minimized at $p^* = \frac{n+1}{2}$.

See appendix for the proof. The following lemma provides an expression of the smallest eigenvalue of the Laplacian matrix of the path graph after perturbation at two of its diagonal entries: proof of Theorem 3.2 uses this lemma.

Lemma 6.3. *Let L_n, the Laplacian matrix for the path graph of n nodes, with n even and $\dfrac{n}{2}$ odd, be perturbed to $\approx{L}_n = L_n + \epsilon e_{p_1} e_{p_1}^T + \epsilon e_{p_2} e_{p_2}^T$ for small $\epsilon > 0$ and e_{p_1}, e_{p_2} are the p_1^{th} and p_2^{th} columns of identity matrix. Then the smallest eigenvalue of the perturbed Laplacian matrix, is given by:*

$$\lambda_{\min}(\approx{L}_{n,\epsilon}, p_1, p_2) = \frac{2\epsilon}{n} - \frac{\epsilon^2}{4n} \sum_{j=2}^{n} \frac{\left\{\cos\big(\pi(j-1)(p_1-0.5)/n\big) + \cos\big(\pi(j-1)(p_2-0.5)/n\big)\right\}^2}{\sin^2\left(0.5\pi(j-1)/n\right)\left\{\sum_{i=1}^{n}\cos^2\left(\pi(j-1)(i-0.5)/n\right)\right\}} + O(\epsilon^3).$$

See appendix for the proof. In addition to what is formulated and proved in the above lemma, what is also true, but perhaps not worth the space for a proof, is that, like Lemma 6.2(b), for the minimum eigenvalue $\lambda_{\min}(p_1^*, p_2^*)$, the pair of best 2-centers of P_n too form a local minima for real values of p_1 and p_2, in addition to the global-maxima over all integer pairs.

The following proposition (from [8]) formulates an expression for the eigenvector of a symmetric matrix perturbed by another small symmetric matrix. The proof of Theorem 3.3 utilizes this result.

Proposition 6.4. *[8] Let $A \in \mathbb{R}^{n\times n}$ be a symmetric matrix with n distinct eigenvalues λ_j, and corresponding eigenvector v_j. Let $P \in \mathbb{R}^{n\times n}$ be a symmetric matrix. Consider $\tilde{A} := A + \epsilon P$, a perturbation of A, where $\epsilon \in \mathbb{R}$ is small in magnitude.*
Then, the perturbed eigenvector $\hat{v}_j$ is:

$$\hat{v}_j := v_j + \epsilon \sum_{k=1, k\neq j}^{n} \frac{v_j^T P v_k}{\lambda_j - \lambda_k} v_k + O(\epsilon^2). \tag{8}$$

The following lemma deals with the dependence of the smallest eigenvalue of the perturbed Laplacian matrix of the path graph P_n (and also P_{2n}) on the value of n; the perturbation being at first diagonal entry for L_n (respectively, first and last diagonal entries for L_{2n}). It also proves equality between the smallest eigenvalue of the perturbed Laplacian matrix of the path graph P_{2n}, perturbed at first and last diagonal entries and P_n, perturbed at first diagonal entry. The proof of Theorem 3.3 utilizes this result too.

Lemma 6.5. *Consider a path graph of n nodes, and perturb its Laplacian matrix L_n to $\tilde{L}_n := L_n + e_1 e_1^T$, defined as T^{po}, say. Also consider a path graph of $2n$ nodes, and perturb its Laplacian matrix L_{2n} to $\overset{\approx}{L}_{2n} := L_{2n} + e_1 e_1^T + e_{2n} e_{2n}^T$, defined as T^o, say.. Then, the following hold.*

(a) $\lambda_{\min}(L_n + e_1 e_1^T) = \lambda_{\min}(L_{2n} + e_1 e_1^T + e_{2n} e_{2n}^T) = 2 - 2\cos\left(\dfrac{\pi}{2n+1}\right)$.

(b) The smallest eigenvalue of $\tilde{L}_n$ (which is also equal to smallest eigenvalue of $\overset{\approx}{L}_{2n}$) is monotonically strictly decreasing with respect to n.

See appendix for the proof. In addition to being tridiagonal, the matrices $\overset{\approx}{L}_{2n}$ and $\tilde{L}_n$ also are Toeplitz and pseudo-Toeplitz[10] matrices respectively, and we use these facts, together with results from [12], to

[10] A square matrix T^o is called Toeplitz if the (i,j)-th entry of T^o, i.e. $T^o_{i,j}$ satisfies $T^o_{i,j} = T^o_{i+1,j+1}$ for all i, j. Since we restrict ourselves to only tridiagonal matrices in this context, in the notation of Proposition 6.9 for the entries along the diagonal, sub-diagonal and super-diagonal, Toeplitz-property translates to $a_i = a_j$ for $i, j \in \{1, \ldots, n\}$, and similarly for b_i and c_k. A square matrix T^{po} is called pseudo-Toeplitz if only the first diagonal entry is possibly unequal from the other diagonal entries. In the notation of Proposition 6.9, when dealing with tridiagonal matrices, pseudo-Toeplitz property translates to just the a_1 value being possibly unequal to the other a_i, while all other a_i are equal to each other.

prove Theorem 3.3. The following lemma provides an approximation of a root of the polynomial obtained as the sum of two polynomials one of which is scaled by a small ϵ. This lemma plays a key role in the proof of Theorem 3.1.

Lemma 6.6. *Let $a(s)$ and $b(s)$ be two finite-degree polynomials with $a(s) = a_0 + a_1 s + a_2 s^2 + \cdots + s^n$ and $b(s) = b_0 + b_1 s + b_2 s^2 + \cdots + b_{n-1} s^{n-1}$. Suppose $a_0 = 0$, $a_1 \neq 0$, and $b_0 \neq 0$. Define the polynomial $p_\epsilon(s) := a(s) + \epsilon b(s)$ and consider the root $\lambda = 0$ of $a(s)$ and dependence of $\lambda(\epsilon)$ on ϵ. Expand $\lambda(\epsilon)$ about $\epsilon = 0$ in a series in ϵ as: $\lambda(\epsilon) = \beta_1 \epsilon + \beta_2 \epsilon^2 + \beta_3 \epsilon^3 + \cdots$. Then,*

$$\beta_1 = \frac{-b_0}{a_1} \qquad \text{and} \qquad \beta_2 = \frac{a_1 b_1 b_0 - a_2 b_0^2}{a_1^3}. \tag{9}$$

See appendix for the proof. The following lemma, an extension of the above lemma, provides approximation of a root of the polynomial obtained as the sum of three polynomials two of which are scaled by small values: ϵ and ϵ^2 respectively. The root is represented in powers of ϵ.

Lemma 6.7. *Let polynomials $a(s)$, $b(s)$ and $c(s)$ be such that $a(s) = a_0 + a_1 s + a_2 s^2 + \cdots + s^n$, $b(s) = b_0 + b_1 s + b_2 s^2 + \cdots + b_{n-1} s^{n-1}$ and $c(s) = c_0 + c_1 s + c_2 s^2 + \cdots + c_{n-2} s^{n-2}$. Suppose $a_0 = 0$, $a_1 \neq 0$, $b_0 \neq 0$ and $c_0 \neq 0$. Define the polynomial $p_\epsilon(s) := a(s) + \epsilon b(s) + \epsilon^2 c(s)$ and consider the root $\lambda = 0$ of $a(s)$ and dependence of $\lambda(\epsilon)$ on ϵ. Expand $\lambda(\epsilon)$ about $\epsilon = 0$ in a series in ϵ as: $\lambda(\epsilon) = \beta_1 \epsilon + \beta_2 \epsilon^2 + \beta_3 \epsilon^3 + \cdots$. Then,*

$$\beta_1 = \frac{-b_0}{a_1} \qquad \text{and} \qquad \beta_2 = \frac{(a_1 b_1 b_0 - a_2 b_0^2 - a_1^2 c_0)}{a_1^3}. \tag{10}$$

See appendix for the proof. The proposition (from [1]) below formulates the characteristic equation of $-L_n$, where L_n is the Laplacian matrix of the path graph; this is helpful for proofs of Theorems 3.1 and 3.2.

Proposition 6.8. *[1, p. 645] Let $n \geqslant 2$ and consider the undirected, unweighted path graph P_n on n nodes and its Laplacian matrix L_n. The characteristic polynomial[11] of $-L_n$ is:*

$$\det(sI + L_n) = ns + \frac{n(n^2-1)}{6} s^2 + \frac{n(n^2-1)(n^2-4)}{120} s^3 + \cdots + 2(n-1)s^{n-1} + s^n. \tag{11}$$

The proposition below provides a recursive characteristic polynomial relation for a generic tridiagonal matrix. This result plays a key role for proving Propositions 6.10 and 6.11, and also for proving Lemma 6.12.

[11]We consider $-L_n$ instead of L_n merely to circumvent the book-keeping of the sign-changes in the coefficients.

Proposition 6.9. *[12, eq(9)] Let $Q_m \in \mathbb{R}^{m\times m}$ be a tridiagonal matrix of the following form:*

$$Q_m = \begin{bmatrix} a_1 & c_2 & 0 & 0 & \dots & 0 \\ b_2 & a_2 & c_3 & 0 & \dots & 0 \\ 0 & b_3 & a_3 & c_4 & 0\dots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & b_{m-1} & a_{m-1} & c_m \\ 0 & \dots & \dots & 0 & b_m & a_m \end{bmatrix} \text{ where } a_i,\ b_i,\ c_i \in \mathbb{R}$$

Let $\psi_m(s)$ be the characteristic polynomial of Q_m and let $m \geqslant 2$. Define $\psi_0 = 1,\ \psi_1 = (s - a_1)$. Then, $\psi_m = (s - a_m)\psi_{m-1} - b_m c_m \psi_{m-2}$.

The proposition below is an adaptation of the tridiagonal matrix characteristic polynomial (Proposition 6.9) to path graph for a single rank perturbation of the Laplacian matrix. This result is needed to prove Lemma 6.13.

Proposition 6.10. *Let $n \geqslant 2$ and consider the undirected, unweighted path graph P_n on n nodes and its Laplacian L_n. Define $\tilde{L}_n := L_n + \epsilon e_p e_p^T$ for some $p \in \{1, 2, \dots, n\}$. Let $\psi_m(s)$ be the characteristic polynomial of the tridiagonal matrix of size m, with $m \geqslant 2$: see Proposition 6.9. Then the characteristic polynomial of $\tilde{L}_n$ is*

$$\det(sI - \tilde{L}_n) = (s - 2 - \epsilon)\psi_{p-1}\psi_{n-p} - \psi_{p-2}\psi_{n-p} - \psi_{p-1}\psi_{n-p-1} \tag{12}$$

where $\psi_p = (s-2)\psi_{p-1} - \psi_{p-2}$, for $2 < p \leqslant n$ with $\psi_0 = 1$, $\psi_1 = (s-1)$ and $\psi_2 = (s-1)(s-2)$.

The following proposition is an adaptation of the tridiagonal matrix characteristic polynomial (Proposition 6.9) to the path graph Laplacian with a rank-two perturbation.

Proposition 6.11. *Let $n \geqslant 6$ and consider the undirected, unweighted path graph P_n on n nodes and its Laplacian L_n. Define $\tilde{\tilde{L}}_n := L_n + \epsilon e_{p_1} e_{p_1}^T + \epsilon e_{p_2} e_{p_2}^T$ for $p_1,\ p_2 \in \{1, 2, \dots, n\}$ with $1 \leqslant p_1 < n/2 < p_2 \leqslant n$. Let $\psi_m(s)$ be the characteristic polynomial of the tridiagonal matrix of size $m \in \mathbb{Z}$ (refer Proposition 6.9). Define $\psi_p := (s-2)\psi_{p-1} - \psi_{p-2}$, for $2 < p \leqslant n$ with $\psi_0 = 1$, $\psi_1 = (s-1)$, $\psi_2 = (s-1)(s-2)$. Then, the characteristic polynomial of $\tilde{\tilde{L}}_n$ is*

$$\begin{aligned} \det(sI - \tilde{\tilde{L}}_n) = {} & (s-2-\epsilon)^2 \psi_{p_1-1}\psi_{p_2-p_1-1}\psi_{n-p_2} \\ & - (s-2-\epsilon)\Big\{\psi_{p_1-1}\psi_{p_2-p_1-1}\psi_{n-p_2-1} + \psi_{p_1-1}\psi_{p_2-p_1-2}\psi_{n-p_2} + \psi_{p_1-2}\psi_{p_2-p_1-1}\psi_{n-p_2} \\ & + \psi_{p_1-1}\psi_{p_2-p_1-2}\psi_{n-p_2}\Big\} \\ & + \Big\{\psi_{p_1-2}\psi_{p_2-p_1-1}\psi_{n-p_2-1} + \psi_{p_1-1}\psi_{p_2-p_1-3}\psi_{n-p_2} + \psi_{p_1-1}\psi_{p_2-p_1-2}\psi_{n-p_2-1}\Big\}. \end{aligned}$$

The above result is a careful use of the recursive relation and hence included here as a proposition. The following lemma obtains the characteristic equation of the perturbed Laplacian of the path graph after perturbation at any one of the diagonal location of the matrix with coefficient of s in the perturbation.

Lemma 6.12. *Consider an odd integer $n \geqslant 3$ and let L_n be the Laplacian matrix of the path graph P_n. Define $p^* := (n+1)/2$ and $\tilde{L}_n := L_n + \epsilon e_j e_j^T$ for $j \in \{1, 2, \ldots, n\}$. Also let $a(s) := \det(sI - L_n)$ and $b_j(s) := -1 + s(\frac{(n-1)^2+2(n-1)}{4} + (j - p^*)^2)$ + (terms in s^2 & higher). Then, the characteristic polynomial of $\tilde{L}_n$ is*

$$\det(sI - L_n + \epsilon e_j e_j^T) = a(s) + \epsilon b_j(s).$$

The proof of Lemma 6.12 follows by a careful and straight-forward use of mathematical induction, in which Proposition 6.10 and the tridiagonal structure are both recursively utilized and the terms corresponding to ϵ^0 and ϵ^1 are meticulously collected (only for terms with degree in s at most 2). Since the proof is primarily careful book-keeping along these lines, we skip the proof.

The following lemma obtains the characteristic equation of the perturbed Laplacian of the path graph after perturbation at any two of the diagonal locations of the matrix. This result is useful for proving Theorem 3.2.

Lemma 6.13. *Consider an even integer $n \geqslant 6$ such that $n/2$ is odd and let L_n be the Laplacian matrix for the path graph P_n. Let j_1 and j_2 satisfy $1 \leqslant j_1 < n/2 < j_2 \leqslant n$ and define $p_1^* := \dfrac{n+2}{4}$ and $p_2^* := \dfrac{3n+2}{4}$. Define $a(s) := \det(sI - L_n)$, and $b_{j_1,j_2}(s) := 2 - (\frac{3n^2-4}{8} - \frac{n(j_1-j_2)}{2} + (j_1 - p_1^*)^2 + (j_2 - p_2^*)^2)s +$ (terms in s^2 & higher). Further, let $c_{j_1,j_2}(s) := (j_2 - j_1) +$ (terms in s & higher). Consider the perturbed Laplacian matrix $\approx{L}_n := L_n + \epsilon e_{j_1} e_{j_1}^T + \epsilon e_{j_2} e_{j_2}^T$. Then, the characteristic polynomial of $\approx{L}_n$ is $\det(sI - \approx{L}_n) = a(s) + \epsilon b_{j_1,j_2}(s) + \epsilon^2 c_{j_1,j_2}(s)$.*

Just like the proof of Lemma 6.12, the proof of Lemma 6.13 too follows by a careful and straight-forward application of mathematical induction and Proposition 6.11 and the tridiagonal structure are both utilized and the terms corresponding to ϵ^0, ϵ^1 and ϵ^2 are collected (for terms with degree in s at most 2); we skip this proof too for the same reason as for Lemma 6.12.

7. Appendix A2: Proofs of main and auxiliary results

In this section, we use the auxiliary results of Section 6 and also the results from the literature included in that section to prove the main results of this paper. The proofs of the auxiliary results too are contained later within this section.

Proof of Theorem 3.1: **Part a)** Using the results from Lemma 6.12 and Proposition 6.8 for n odd, we have:

$$a_1 = n, \quad a_2 = \frac{-n(n^2-1)}{6}, \quad b_0 = -1, \quad b_1 = \{\frac{(n-1)^2 + 2(n-1)}{4} + (j - p^*)^2\}.$$

Further from equation (9) of Lemma 6.6, we have
$\beta_1 = \dfrac{-b_0}{a_1} = \dfrac{1}{n}$ and $\beta_2 = \dfrac{a_1b_1b_0 - a_2b_0^2}{a_1^3} = \dfrac{-n\{\frac{(n-1)^2+2(n-1)}{4} + (j-p^*)^2\} + \frac{n(n^2-1)}{6}}{n^3}$. Simplifying this expression we get $\beta_2 = \dfrac{n^2-1}{6n^2} + \dfrac{\frac{(n-1)^2+2(n-1)}{4} + (j-p^*)^2}{n^2} = -\{\dfrac{(n^2-1)+12(j-p^*)^2}{12n^2}\}$.

Finally, we substitute values of $\beta_1,\ \beta_2$ in $\lambda_{\min} = \beta_1\epsilon + \beta_2\epsilon^2$ (upto 2^{nd} order in ϵ) to get

$$\lambda_{\min}(\epsilon, j) = \frac{\epsilon}{n} - \epsilon^2\left[\frac{(n^2-1)+12(j-p^*)^2}{12n^2}\right]$$

This proves part (a).

Part b) Considering just the linear and quadratic orders in ϵ, the expression

$$\lambda_{\min}(\epsilon, j) = \frac{\epsilon}{n} - \epsilon^2\left[\frac{(n^2-1)+12(j-p^*)^2}{12n^2}\right],$$

for a fixed ϵ and varying j, when plotted against varying j, is a clearly a parabola that peaks at $j = p^*$. Thus $j = p^*$ globally maximizes the $\lambda_{\min}(\epsilon, j)$ and the corresponding maximum value (upto 2^{nd} order in ϵ) is

$$\lambda_{\min}(\epsilon, p^*) = \frac{\epsilon}{n} - \epsilon^2\left[\frac{n^2-1}{12n^2}\right].$$

We now show that $\lambda_{\min}(\epsilon, p^*)$ also equals the other expression, i.e. equation (3) within Theorem 3.1, i.e.

$$\lambda_{\min}(p) = \frac{\epsilon}{n} - \frac{\epsilon^2}{4n}\sum_{j=2}^{n}\frac{\cos^2\left(\dfrac{\pi(j-1)p}{n} - \dfrac{\pi(j-1)}{2n}\right)}{\sin^2(0.5\pi(j-1)/n)\left\{\sum_{p=1}^{n}\cos^2\left(\frac{\pi p(j-1)}{n} - \frac{\pi(j-1)}{2n}\right)\right\}} + O(\epsilon^3) \text{ terms}$$

In order to avoid space, this expression is formulated and proved in more generality for k-ports instead of one-port: we thus merely substitute $k = 1$ in the expression obtained within Theorem 3.3. This proves part (b).

Part c) Using Theorem 3.3 that considers the k-central ports w.r.t., Definition 2.1[ii](MinSubLE), we have that $p_i^* = \dfrac{(2i-1)n+k}{2k}$ with $i = 1, 2, \ldots, k$ being the optimal k ports (under the divisibility assumption). As a special case, for $k = 1$, we get that $p = p^* = \frac{n+1}{2}$ is the center as per this definition, and this coincides with as Defn 2.1[i](MaxLSE) as proved in part (b) above. Further, Theorem 3.5 shows the equivalence between definitions[i] MaxLSE and [ii] MinSupLE. Thus, $p = p^*$, is the center w.r.t. all three Defn 2.1, thus proving part (c) of the theorem.

Part d) Proposition 6.1 contains the following general expression for the eigenvectors of the path graph Laplacian:

$$v_q(p) = \cos\Big(\frac{\pi(q-1)p}{n} - \frac{\pi(q-1)}{2n}\Big) \quad \text{with} \quad q = \{1, 2, \ldots, n\}.$$

Choosing the Fiedler vector $v_2(p)$, for 1-port selection, from Proposition 6.1, we see that part (d) follows and thus completes the proof of Theorem 3.1. □

Proof of Theorem 3.2: **Part a)** Using results from Lemmas 6.13 and Proposition 6.8 for n even, we have: $a_1 = -n, \quad a_2 = \dfrac{n(n^2-1)}{6}, \quad c_0 = (j_2 - j_1)$, and also $b_0 = 2, \quad b_1 = -\Bigg(\dfrac{3n^2-4}{8} - \dfrac{n(j_1-j_2)}{2} + (j_1 - p_1^*)^2 + (j_2 - p_2^*)^2\Bigg)$. Further, from equation (10) of Lemma 6.7, we also have $\beta_1 = \dfrac{-b_0}{a_1} = \dfrac{-2}{-n} = \dfrac{2}{n}$ and $\beta_2 = \dfrac{b_1 b_0}{a_1^2} - \dfrac{a_2 b_0^2}{a_1^3} - \dfrac{c_0}{a_1} = \dfrac{n(j_1-j_2) - 2(j_1-p_1^*)^2 - 2(j_2-p_2^*)^2 - \frac{3n^2-4}{4}}{n^2} + \dfrac{2(n^2-1)}{3n^2} + \dfrac{j_2 - j_1}{n}$. Simplifying this expression, we get $\beta_2 = \left[\dfrac{n^2-4}{-12n^2} - 2\left\{\dfrac{(j_1-p_1^*)^2 + (j_2-p_2^*)^2}{n^2}\right\}\right]$.

Substituting β_1 and β_2 in $\lambda_{\min}(\epsilon, j_1, j_2) = \beta_1\epsilon + \beta_2\epsilon^2$ (upto 2^{nd} order in ϵ), we get

$$\lambda_{\min}(\epsilon, j_1, j_2) = \frac{2\epsilon}{n} - \epsilon^2\left[\frac{(n^2-4) + 24\left\{(j_1-p_1^*)^2 + (j_2-p_2^*)^2\right\}}{12n^2}\right], \text{ thus proving part (a).}$$

Part b) In the above expression, pursuing further with just upto the above 2nd order approximation, we first note that p_1 occurs in just one term: within the quadratic term, while p_2 occurs in just one other term: within the quadratic term: this clearly indicates (considering the signs) that a maximization of $\lambda_{\min}(\epsilon, j_1, j_2)$ is achieved jointly at $p_1 = p_1^*$ and $p_2 = p_2^*$. Substituting these values, we get the maximum value is (upto 2^{nd} order in ϵ) as

$$\lambda_{\min}(\epsilon, p_1^*, p_2^*) = \frac{2\epsilon}{n} - \epsilon^2\left[\frac{n^2-4}{12n^2}\right]$$

We next show that $\lambda_{\min}(\epsilon, p_1^*, p_2^*)$ also equals the other expression: within Statement (b) of Theorem 3.2 (namely equation (4)):

$$\lambda_{\min}(\widetilde{\widetilde{L}}, p_1, p_2, \epsilon) = \frac{2\epsilon}{n} - \frac{\epsilon^2}{4n}\sum_{j=2}^{n} \frac{\left\{\cos\Big(\frac{\pi(j-1)p_1}{n} - \frac{\pi(j-1)}{2n}\Big) + \cos\Big(\frac{\pi(j-1)p_2}{n} - \frac{\pi(j-1)}{2n}\Big)\right\}^2}{\frac{n}{2}\sin^2\left(0.5\pi(j-1)/n\right)}.$$

Next, similar to the single-port case, here too we note that this expression is a special case of Theorem 3.3(a) with $k = 2$, and we substitute $p_1 = p_1^* = \frac{n+2}{4}$, $p_2 = p_2^* = \frac{3n+2}{4}$ in equation (5) to get:

$$\max_{p_1,p_2} \lambda_{\min}(\tilde{\tilde{L}}_{n,\epsilon}, p_1, p_2) = \lambda_{\min}(\tilde{\tilde{L}}_{n,\epsilon}, p_1, p_2)\Bigg|_{p_1=p_1^*, p_2=p_2^*} = \frac{2\epsilon}{n} - \epsilon^2 \left[\frac{n^2-4}{12n^2}\right]$$

$$= \frac{2\epsilon}{n} - \frac{\epsilon^2}{4n} \sum_{j=2}^{n} \frac{\Big\{\cos\left(\pi(j-1)/4\right) + \cos\left(3\pi(j-1)/4\right)\Big\}^2}{\frac{n}{2}\sin^2\left(0.5\pi(j-1)/n\right)}$$

This proves part (b) of the theorem.

Part c) In the context of Defn 2.1[ii](MinSubLE) for k-ports selection, from Theorem 3.3 we have that $p_i^* = \dfrac{(2i-1)n + k}{2k}$ with $i = 1, 2, \ldots, k$, are optimal k-centers for the path graph (subject to the divisibility assumptions listed there). As a special case, for $k = 2$, $p_1 = p_1^* = \frac{n+2}{4}$, $p_2 = p_2^* = \frac{3n+2}{4}$ which is same as that by Defn 2.1[i](MaxLSE) as shown in part (a). Further, Theorem 3.5 shows the equivalence between the Definitions 2.1[i](MaxLSE) and 2.1[iii](MinSupLE) for general graphs. This proves that $p_1 = p_1^* = \frac{n+2}{4}$, $p_2 = p_2^* = \frac{3n+2}{4}$ are the centers w.r.t. all three Defn 2.1 and thus proves part (c).

Part d) From Proposition 6.1, the eigenvectors of the path graph.

$$v_q(p) = \cos\left(\frac{\pi(q-1)p}{n} - \frac{\pi(q-1)}{2n}\right) \quad \text{with} \quad q = \{1, 2, \ldots, n\}$$

Choosing $q = 3$, the eigenvector $v_3 \in \mathbb{R}^n$ (for 2-ports selection) and equating $\dfrac{\pi(q-1)p}{n} - \dfrac{\pi(q-1)}{2n} = \dfrac{\pi}{2}$ and $\dfrac{3\pi}{2}$, we get part (d) and this completes proof of part (d) and also of Theorem 3.2. □

Proof of Theorem 3.3: For proof of part (a) statement, we proceed as follows. From Proposition 6.1 we use that for path graph, the ordered eigenvalues λ_j, for $j = \{1, 2, \ldots, n\}$, equal $2 - 2\cos\left(\dfrac{\pi(j-1)}{n}\right)$. The corresponding eigenvector, $v_j(p) = \cos\left(\dfrac{\pi p(j-1)}{n} - \dfrac{\pi(j-1)}{2n}\right)$. The eigenvector, normalized to 2-norm equal to 1, is

$$\hat{v}_j(p) = \cos\left(\frac{\pi p(j-1)}{n} - \frac{\pi(j-1)}{2n}\right) \Big/ \mathcal{N}_j$$

with the denominator $\mathcal{N}_j$ within the above equation shown to be equal to $\sqrt{\frac{n}{2}}$ (see Proposition 6.1(iv)).

Using the expressions of v_j and λ_j in equation (8) of Proposition 6.4 (specialized to L_n of path graph), we get the perturbed eigenvector upto 2^{nd} order in ϵ:

$$\hat{\hat{v}}_1(\epsilon) = \hat{v}_1 + \epsilon \sum_{j=2}^{n} \frac{\sum_{i=1}^{k} \cos\left(\dfrac{\pi(j-1)p_i}{n} - \dfrac{\pi(j-1)}{2n}\right)}{-2n\sqrt{2}\ \sin^2\left(0.5\pi(j-1)/n\right)} \hat{v}_j + \epsilon^2\psi = \hat{v}_1 + \epsilon\mathcal{X} + \epsilon^2\psi \tag{13}$$

with $\chi, \psi \in \mathbb{R}^n$, and the first-order coefficient

$$\chi = \sum_{j=2}^{n} \frac{\sum_{i=1}^{k} \cos\left(\frac{\pi(j-1)p_i}{n} - \frac{\pi(j-1)}{2n}\right)}{-2n\sqrt{2}\ \sin^2\left(0.5\pi(j-1)/n\right)} \hat{v}_j.$$

Similarly, consider the perturbed eigenvalue upto 2^{nd} order in ϵ: $\tilde{\lambda}_1 = \lambda_1 + \epsilon\beta_1 + \epsilon^2\beta_2$ for the perturbed Laplacian matrix: $\tilde{L}_n = L_n + \epsilon V = L_n + \epsilon \sum_{i=1}^{k} e_{p_i} e_{p_i}^T$. Considering the eigenvalue and corresponding eigenvector for this perturbed Laplacian matrix we have: $\tilde{L}_n \hat{\tilde{v}}_1(\epsilon) = \tilde{\lambda}_1 \hat{\tilde{v}}_1(\epsilon)$. Substituting $\tilde{L}_n$, $\hat{\tilde{v}}_1(\epsilon)$, and $\tilde{\lambda}_1$, we obtain:

$$(L_n + \epsilon V)(\hat{v}_1 + \epsilon\chi + \epsilon^2\psi) = (\lambda_1 + \epsilon\beta_1 + \epsilon^2\beta_2)(\hat{v}_1 + \epsilon\chi + \epsilon^2\psi). \tag{14}$$

Upon simplifying the above equation:

$$L_n\hat{v}_1 + \epsilon L_n\chi + \epsilon^2 L_n\psi + \epsilon V\hat{v}_1 + \epsilon^2 V\chi + \epsilon^3 V\psi =$$
$$\lambda_1\hat{v}_1 + \epsilon\lambda_1\chi + \epsilon^2\lambda_1\psi + \epsilon\beta_1\hat{v}_1 + \epsilon^2\beta_1\chi + \epsilon^3\beta_1\psi + \epsilon^2\beta_2\hat{v}_1 + \epsilon^3\beta_2\chi + \epsilon^4\beta_2\psi$$

On comparing 'ϵ' terms: $L_n\chi + V\hat{v}_1 = \lambda_1\chi + \beta_1\hat{v}_1$. Since, $\lambda_1(L_n) = 0$ and $\hat{v}_1^T L_n = 0$.
On pre-multiplying both sides by $\hat{v}_1^T$, we get

$$\beta_1 = \hat{v}_1^T V \hat{v}_1 = \hat{v}_1^T \left(\sum_{i=1}^{k} e_{p_i} e_{p_i}^T\right) \hat{v}_1 \quad \Longrightarrow \quad \beta_1 = \frac{k}{n} \tag{15}$$

Similarly, on comparing 'ϵ^2' terms: $L_n\psi + (\sum_{i=1}^{k} e_{p_i} e_{p_i}^T)\chi = \lambda_1\psi + \beta_1\chi + \beta_2\hat{v}_1$.
Since, for symmetric matrix eigenvector corresponding to distinct eigenvalues are orthogonal, $\hat{v}_1^T v_j = 0$ for $j = \{2, 3, \ldots, n\} \implies \hat{v}_1^T\chi = 0$. Also, $\lambda_1(L_n) = 0$ and $\hat{v}_1^T L_n = 0$.
On pre-multiplying both sides by $\hat{v}_1^T$, we get

$$\hat{v}_1^T (\sum_{i=1}^{k} e_{p_i} e_{p_i}^T)\chi = \hat{v}_1^T \beta_2 \hat{v}_1 \quad \Longrightarrow \beta_2 = \hat{v}_1^T (\sum_{i=1}^{k} e_{p_i} e_{p_i}^T)\chi$$

Using the value of χ in above equation, we get

$$\beta_2 = \hat{v}_1^T (\sum_{i=1}^{k} e_{p_i} e_{p_i}^T) \sum_{j=2}^{n} \frac{\sum_{i=1}^{k} \cos\left(\frac{\pi(j-1)p_i}{n} - \frac{\pi(j-1)}{2n}\right)}{-2n\sqrt{2}\ \sin^2\left(0.5\pi(j-1)/n\right)} \hat{v}_j.$$

Using value of $\hat{v}_1$, we get

$$\beta_2 = \frac{1}{\sqrt{n}} (\sum_{i=1}^{k} e_{p_i}^T) \sum_{j=2}^{n} \frac{\left\{\sum_{i=1}^{k} \cos\left(\frac{\pi(j-1)p_i}{n} - \frac{\pi(j-1)}{2n}\right)\right\}}{-2n\sqrt{2}\ \sin^2\left(0.5\pi(j-1)/n\right)} \hat{v}_j.$$

On simplifying and using the value of $\hat{v}_j$, we get

$$\beta_2 = \frac{1}{n^2}\sum_{j=2}^{n} \frac{\left\{ \sum_{i=1}^{k} \cos\left(\frac{\pi(j-1)p_i}{n} - \frac{\pi(j-1)}{2n} \right) \Big/ \mathcal{N}_{j_i} \right\}^2}{-2\sin^2\left(0.5\pi(j-1)/n\right)} \tag{16}$$

Hence, $\lambda_{\min}(\tilde{L}_{n,\epsilon}, p) = \tilde{\lambda}_1 = \lambda_1 + \epsilon\beta_1 + \epsilon^2\beta_2$

Using values of β_1 and β_2 from equation (15), (16) and $\lambda_1(L_n) = 0$, we get:

$$\lambda_{\min}(\tilde{L}_{n,\epsilon}, p) = \frac{k\epsilon}{n} - \frac{\epsilon^2}{2n^2}\sum_{j=2}^{n} \frac{\left\{ \sum_{i=1}^{k} \cos\left(\frac{\pi(j-1)p_i}{n} - \frac{\pi(j-1)}{2n} \right) \right\}^2}{\sin^2\left(0.5\pi(j-1)/n\right)},$$

thus completing the proof of part (a).

Part b) This part of the proof consists of two parts:

- that p_i^* forming the set S^* indeed achieves $\lambda_{\max}({}^{S^*}\hat{Z})$,
- any other $S \subset \bar{n}$, $|S| = k$ result in $\lambda_{\max}({}^{S}\hat{Z}) > \lambda_{\max}({}^{S^*}\hat{Z})$.

We first begin by noting that $\arg \max_{\substack{\text{all subsets } S \\ \text{with } |S|=k}} \lambda_{\min}({}^{S}\tilde{L}_n) = \arg \min_{\substack{\text{all subsets } S \\ \text{with } |S|=k}} \lambda_{\max}(-{}^{S}\tilde{L}_n)$ each of which is the same as $\arg \min_{\substack{\text{all subsets } S \\ \text{with } |S|=k}} \lambda_{\max}(-{}^{S}\tilde{L}_n\tau)$. Definition 2.1(ii) involves removal of k rows and k columns from $Z_n = I_n - \tau\, {}^{S}\tilde{L}_n$ when searching for the $\min_{|S|=k} \lambda_{\max}({}^{S}\hat{Z})$. Notice first the fact that for a subset S of a specified cardinality k, due to the eventual removal of the k rows and k columns corresponding to S, the operation of getting $\hat{L}$ from $\hat{\hat{L}}$ becomes redundant; in other words, S^* minimizes $\lambda_{\max}(\hat{Z})$ over all S if and only if S^* minimizes $\lambda_{\min}(\hat{\hat{L}}_n)$ over all S.

Further, assuming[12] consecutive rows/columns are not removed, after removing k rows and k columns from $\tilde{L}_n$, we obtain an $\hat{\hat{L}}_n$ which is a block diagonal matrix; and this block diagonal matrix is comprised of $k+1$ tridiagonal blocks, of which $k-1$ tridiagonal Toeplitz matrices of the form as T^o (using the notation of Lemma 6.5), and two tridiagonal pseudo-Toeplitz matrices of the form as T^{po} (using again the notation of Lemma 6.5).

Using Lemma 6.5, and in particular, $\lambda_{\min}(T^o_{2\ell}) = \lambda_{\min}(T^{po}_{\ell})$, we note that to maximize $\lambda_{\min}$, we require the tridiagonal Toeplitz matrix T^o and the two tridiagonal pseudo-Toeplitz matrix T^{po} of sizes 2ℓ and ℓ respectively ($\ell \in \mathbb{Z}$).

[12] This assumption is reasonable after noting that it is easier to prove non-optimality of the set S when it contains consecutive integers: using the two statements of Lemma 6.5.

We next note that after k rows and k columns removal, we get an $(n-k)\times(n-k)$ size matrix which is block diagonal; the sizes of these blocks and their total are $\ell + \underbrace{2\ell + 2\ell + \cdots + 2\ell}_{k-1} + \ell = n-k$, with ℓ being the size of the first and last blocks T^{po} while 2ℓ being the size of all the remaining blocks T^{o}. This implies that $\ell = \dfrac{n-k}{2k}$. Thus the optimal locations are at $p_1^* = \ell + 1 = \dfrac{n-k}{2k} + 1 = \dfrac{n+k}{2k}$. Similarly, $p_2^* = p_1^* + 2\ell + 1 = \dfrac{n+k}{2k} + 2\dfrac{n-k}{2k} + 1 = \dfrac{3n+k}{2k}$, and so on. Hence, in general $p_i^* = \dfrac{(2i-1)n+k}{2k}$ with $i = 1, 2, \ldots, k$.

At optimality, ${}^{S^*}\hat{Z}$ is tridiagonal Toeplitz matrix whose largest eigenvalue using formula from [11, p. 116] for $a = c = 1/2$ and $b = 0$ for block of size $2\ell \times 2\ell$, we get
$\lambda_{\max}({}^{S^*}\hat{Z}) = \cos(\pi/(2\ell+1)) = \cos(k\pi/n)$.

Since optimality provides for only two sizes of the block diagonal sub-matrices, we first deduce that removal of k rows and k columns at <u>any</u> of the other locations would lead to at least one of the following two cases:

- Case 1) At least one of the $k-1$ tridiagonal Toeplitz matrices T^{o} is of size strictly smaller than $\frac{n-k}{k}$. This would result in $\lambda_{\min}(\tilde{L}) < \lambda_{\min}(\tilde{L}^*)$ (see Lemma 6.5).
- Case 2) At least one of the 2 tridiagonal pseudo-Toeplitz matrices T^{po} is of size strictly smaller than $\frac{n-k}{2k}$. This would also result in $\lambda_{\min}(\tilde{L}) < \lambda_{\min}(\tilde{L}^*)$ (see Lemma 6.5).

Since each of the two cases results in $\lambda_{\min}(\tilde{L}) < \lambda_{\min}(\tilde{L}^*)$, we note that the 2^{nd} part of the proof of part (b) is complete.

Part c) From Proposition 6.1, the eigenvectors $v_q \in \mathbb{R}^n$ of the path graph for eigenvalue λ_q Choosing $q = k+1$, the eigenvector $v_{k+1}(p)$, for k-ports selection in Proposition 6.1, we get

$$\frac{k\pi p}{n} - \frac{k\pi}{2n} = \frac{\pi(2i-1)}{2} \text{ for } i \in \mathbb{N} \iff (2p-1)k = n(2i-1) \iff p = \frac{n(2i-1)+k}{2k}.$$

(Note: $p's \in \mathbb{N}$, $\frac{n}{k}$ is odd).

So, $v_{k+1}(j) = 0 \iff j \in \{p_1^*, p_2^*, \ldots p_k^*\}$.
This completes, the proof of part (c) of the theorem. This completes the proof of Theorem 3.3. □

Proof of Theorem 3.5: The Laplacian matrix L_n of path graph P_n is perturbed as:
${}^{S}\tilde{L}_n := L_n - \epsilon \sum_{j\in S} e_j e_j^T$ where $S \subset \{1, 2, \ldots, n\}$, with $|S| = k < n$ and $\epsilon > 0$.

${}^{S}\tilde{Z}_n := Z_n + \epsilon \sum_{j\in S} e_j e_j^T$ where $Z_n = I_n - \tau L_n$, where $\tau < \Delta^{-1}$ with Δ: the maximum degree of graph.

Definition 2.1[i](MaxLSE) identifies nodes as center if at these k nodes $\lambda_{\min}(\tilde{L}_n)$ gets maximized.

Definition 2.1[iii](MinSupLE) identifies nodes as center if at these k nodes $\lambda_{\max}(\tilde{Z}_n = I_n - \tau\tilde{L}_n)$ get minimized.

Now obtain stochastic matrix Z_n corresponding to L_n as: $Z_n = I_n - \tau L_n$.

${}^S\tilde{Z}_n = I_n - {}^S\tilde{L}_n\tau = Z_n + \tau\epsilon\sum_{j\in S} e_j e_j^T$.

Since scaling a matrix by $\tau > 0$ only scales the eigenvalues, we first note

$$\arg\max_{\substack{\text{all subsets } S\\ \text{with } |S|=k}} \lambda_{\min}({}^S\tilde{L}_n) = \arg\max_{\substack{\text{all subsets } S\\ \text{with } |S|=k}} \lambda_{\min}({}^S\tilde{L}_n\tau), \tag{17}$$

and noting the negative sign, any of the above also equals

$$\arg\min_{\substack{\text{all subsets } S\\ \text{with } |S|=k}} \lambda_{\max}(-{}^S\tilde{L}_n\tau).$$

In addition, we observe that the operation $P \to P + cI$ merely shifts the eigenvalues accordingly; this gives

$$\arg\min_{\substack{\text{all subsets } S\\ \text{with } |S|=k}} \lambda_{\max}(-\tau\ {}^S\tilde{L}_n) = \arg\min_{\substack{\text{all subsets } S\\ \text{with } |S|=k}} \lambda_{\max}(I_n - {}^S\tilde{L}_n\tau). \tag{18}$$

Hence, from equations (17-18):

$$\arg\max_{\substack{\text{all subsets } S\\ \text{with } |S|=k}} \lambda_{\min}({}^S\tilde{L}_n) = \arg\min_{\substack{\text{all subsets } S\\ \text{with } |S|=k}} \lambda_{\max}(I_n - {}^S\tilde{L}_n\tau).$$

Thus, Definition 2.1[i](MaxLSE) and [ii](MinSupLE) result in the same k nodes being identified as the k-centers.

This completes the proof of Theorem 3.5. □

Proof of Theorem 3.6: Consider Laplacian is perturbed at any of the k-diagonal entry at ϵ, $|S| = k$: ${}^S\tilde{L}_n = L_n + \epsilon\sum_{i\in S} e_i e_i^T = L_n + \epsilon V$.

Let perturbed smallest eigenvalue (upto first order approx in ϵ) be $\hat{\lambda}_1 = \lambda_1 + \epsilon\beta_1$

and using Proposition 6.4, the corresponding eigenvector (upto first order approx in ϵ) be $\hat{v}_1(\epsilon) = v_1 + \epsilon\sum_{j=2,}^{n} \frac{v_1^T V v_j}{\lambda_1 - \lambda_j} v_j$. For ease of manipulation, define the coefficient of ϵ as $\chi := \sum_{j=2,}^{n} \frac{v_1^T V v_j}{\lambda_1 - \lambda_j} v_i$ with $\chi \in \mathbb{R}^n$, using which we express $\hat{v}_1 = v_1 + \epsilon\chi$. Thus, for perturbed Laplacian matrix eigenvalue, eigenvector equation, we have:

$$(L_n + \epsilon V)(v_1 + \epsilon\chi) = (\lambda_1 + \epsilon\beta_1)(v_1 + \epsilon\chi).$$

Upon simplifying the above equation, we get

$$L_n v_1 + \epsilon L_n\chi + \epsilon V v_1 + \epsilon^2 V\chi = \lambda_1 v_1 + \epsilon\lambda_1\chi + \epsilon\beta_1 v_1 + \epsilon^2\beta_1\chi.$$

On equating the terms of 1^{st} order in ϵ, we get

$$L_n\chi + Vv_1 = \lambda_1\chi + \beta_1 v_1,$$

$$L_n \sum_{j=2,}^{n} \frac{v_1^T V v_j}{\lambda_1 - \lambda_j} v_j + \sum_{i\in S} e_i e_i^T v_1 = \lambda_1 \sum_{j=2,}^{n} \frac{v_1^T V v_j}{\lambda_1 - \lambda_j} v_j + \beta_1 v_1.$$

On pre-multiplying both sides by v_1^T in above equation and using orthogonality of eigenvectors of symmetric matrix, $v_1^T v_j = 0$ for $j = 2, 3, \dots, n$, we get:

$$\beta_1 v_1^T v_1 = v_1^T \sum_{i\in S} e_i e_i^T v_1 \implies \beta_1 = \frac{v_1^T \sum_{i\in S} e_i e_i^T v_1}{v_1^T v_1} = \frac{k}{n}.$$

Thus the first order approx of $\hat{\lambda}_1 = \lambda_1 + \epsilon\frac{k}{n}$ is independent of port indices and also independent of the number of edges in the graph G_n. □

Proof of Theorem 3.7: For 1 optimal port selection, for n nodes from Theorem 3.1, we have

$$\lambda^*_{\min}(1) = \frac{\epsilon}{n} - \epsilon^2\left[\frac{n^2-1}{12n^2}\right]. \tag{19}$$

For 2 optimal ports selection for n nodes from Theorem 3.2, we have

$$\lambda^*_{\min}(2) = \frac{2\epsilon}{n} - \epsilon^2\left[\frac{n^2-4}{12n^2}\right]. \tag{20}$$

On multiplying equation (19) by 2 for linear scaling and subtracting from equation (20), we get:

$$\lambda^*_{\min}(2) - 2\lambda^*_{\min}(1) = \frac{2\epsilon}{n} - \epsilon^2\left[\frac{n^2-4}{12n^2}\right] - \frac{2\epsilon}{n} + \epsilon^2\left[\frac{(n^2-1)}{6n^2}\right] = \epsilon^2\frac{(n^2+2)}{12n^2} > 0.$$

Thus, $\lambda^*_{\min}(2) > 2\lambda^*_{\min}(1)$ by considering upto 2^{nd} order terms in ϵ; this completes the proof of Theorem 3.7. □

Proof of Theorem 3.9: Consider a path graph P_n, Laplacian L_n with n odd is perturbed optimally for 1-port selection:

$\tilde{L}_n := L_n + \epsilon e_{p^*} e_{p^*}^T$, with $p^* = \dfrac{(n+1)}{2}$.

Further, path graph P_{2n}, Laplacian L_{2n} with n odd is perturbed optimally for 2-ports selection:

$\approx{L}_{2n} := L_{2n} + \epsilon\{e_{p_1^*} e_{p_1^*}^T + e_{p_2^*} e_{p_2^*}^T\}$, with $p_1^* = \dfrac{n+2}{4}$ and $p_2^* = \dfrac{3n+2}{4}$.

From Theorem 3.1, we have: $\lambda_{\min}(\tilde{L}_{n,\epsilon}, p)\Big|_{p=p^*} = \lambda^*_{\min}(\tilde{L}_n) = \dfrac{\epsilon}{n} - \epsilon^2\left[\dfrac{n^2-1}{12n^2}\right]$.

Further from Theorem 3.2, we have:

$$\lambda_{\min}(\overset{\approx}{L}_{n,\epsilon}, p_1, p_2)\Big|_{p_1=p_1^*, p_2=p_2^*} = \lambda^*_{\min}(\overset{\approx}{L}_n) = \frac{2\epsilon}{n} - \epsilon^2\left[\frac{n^2-4}{12n^2}\right].$$

Thus, for size n in $\tilde{\tilde{L}}_{2n}$, replacing n by $2n$, we get:

$$\lambda^*_{\min}(\tilde{\tilde{L}}_{2n}) = \frac{2\epsilon}{2n} - \epsilon^2 \left[\frac{4n^2-4}{12\times 4n^2}\right] = \frac{\epsilon}{n} - \epsilon^2\left[\frac{n^2-1}{12n^2}\right] = \lambda^*_{\min}(\tilde{L}_n)$$

This completes the proof of Theorem 3.9. □

Proof of Lemma 6.2: Suppose Laplacian matrix L_n of path graph P_n is perturbed to: $\tilde{L}_n = L_n + \epsilon e_j e_j^T$ where $j \in \{1,2,3,\ldots n\}$ and small $|\epsilon|$.

Part a) From Theorem 3.3(a), for $k-$ports selection, we have:

$$\lambda_{\min}({}^S\tilde{L}_n) = \frac{k\epsilon}{n} - \frac{\epsilon^2}{4n}\sum_{j=2}^{n} \frac{\left\{\sum_{i=1}^{k}\cos\left(\frac{\pi(j-1)p_i}{n} - \frac{\pi(j-1)}{2n}\right)\right\}^2}{\sin^2(0.5\pi(j-1)/n)\left\{\sum_{p=1}^{n}\cos^2\left(\frac{\pi p(j-1)}{n} - \frac{\pi(j-1)}{2n}\right)\right\}} + O(\epsilon^3).$$

For $1-$port selection, using $k=1$ in above equation, we get:

$$\lambda_{\min}(\tilde{L}_{n,\epsilon},p) = \frac{\epsilon}{n} - \frac{\epsilon^2}{4n}\sum_{j=2}^{n} \frac{\cos^2\left(\frac{\pi(j-1)p}{n} - \frac{\pi(j-1)}{2n}\right)}{\sin^2(0.5\pi(j-1)/n)\left\{\sum_{p=1}^{n}\cos^2\left(\frac{\pi p(j-1)}{n} - \frac{\pi(j-1)}{2n}\right)\right\}} + O(\epsilon^3) \text{ terms.}$$

This completes the part a) of the proof.

Part b) We have upto 2^{nd} order of ϵ:

$$\hat{\lambda}_{\min}(\tilde{L}_{n,\epsilon},p) = \frac{\epsilon}{n} - \frac{\epsilon^2}{4n}\sum_{j=2}^{n} \frac{\cos^2\left(\frac{\pi(j-1)p}{n} - \frac{\pi(j-1)}{2n}\right)}{\sin^2(0.5\pi(j-1)/n)\left\{\sum_{i=1}^{n}\cos^2\left(\frac{\pi i(j-1)}{n} - \frac{\pi(j-1)}{2n}\right)\right\}}.$$

Derivative of $\hat{\lambda}_{\min}(\tilde{L}_n,p)$ w.r.t. p:

$$\frac{d\hat{\lambda}_{\min}(\tilde{L}_n,p)}{dp} = \frac{\epsilon^2}{4n}\sum_{j=2}^{n} \frac{\sin\left(\frac{2\pi(j-1)p}{n} - \frac{\pi(j-1)}{n}\right)\left(\frac{\pi(j-1)}{n}\right)}{\sin^2(0.5\pi(j-1)/n)\left\{\sum_{i=1}^{n}\cos^2\left(\frac{\pi i(j-1)}{n} - \frac{\pi(j-1)}{2n}\right)\right\}}.$$

Derivative of $\hat{\lambda}_{\min}(\tilde{L}_n,p)$ at $p = \frac{n+1}{2}$:

$$\frac{d\hat{\lambda}_{\min}(\tilde{L}_n,p)}{dp} = \frac{\epsilon^2}{4n}\sum_{j=2}^{n} \frac{\sin\left(\frac{\pi(j-1)(n+1)}{n} - \frac{\pi(j-1)}{n}\right)\left(\frac{\pi(j-1)}{n}\right)}{\sin^2(0.5\pi(j-1)/n)\left\{\sum_{i=1}^{n}\cos^2\left(\frac{\pi i(j-1)}{n} - \frac{\pi(j-1)}{2n}\right)\right\}}$$

$$= \frac{\epsilon^2}{4n}\sum_{j=2}^{n} \frac{\sin\left(\pi(j-1)\right)\left(\frac{\pi(j-1)}{n}\right)}{\sin^2(0.5\pi(j-1)/n)\left\{\sum_{i=1}^{n}\cos^2\left(\frac{\pi i(j-1)}{n} - \frac{\pi(j-1)}{2n}\right)\right\}} = 0.$$

Thus, $p = \dfrac{n+1}{2}$ is a stationary point.

We now check 2^{nd} derivative condition. The second derivative of $\hat{\lambda}_{\min}(\tilde{L}_n, p)$ w.r.t. p:

$$\frac{d^2}{dp^2}\hat{\lambda}_{\min}(\tilde{L}_n, p) = \frac{\epsilon^2}{2n}\sum_{j=2}^{n}\frac{\cos\left(\dfrac{2\pi(j-1)p}{n} - \dfrac{\pi(j-1)}{n}\right)\left(\dfrac{\pi(j-1)}{n}\right)^2}{\sin^2\left(0.5\pi(j-1)/n\right)\left\{\sum_{i=1}^{n}\cos^2\left(\frac{\pi i(j-1)}{n} - \frac{\pi(j-1)}{2n}\right)\right\}}.$$

Evaluating the second derivative of $\hat{\lambda}_{\min}(\tilde{L}_n, p)$ w.r.t. p at $p = \dfrac{n+1}{2}$:

$$\begin{aligned}\frac{d^2}{dp^2}\hat{\lambda}_{\min}(\tilde{L}_n, p) &= \frac{\epsilon^2}{2n}\sum_{j=2}^{n}\frac{\cos\left(\dfrac{\pi(j-1)(n+1)}{n} - \dfrac{\pi(j-1)}{n}\right)\left(\dfrac{\pi(j-1)}{n}\right)^2}{\sin^2\left(0.5\pi(j-1)/n\right)\left\{\sum_{i=1}^{n}\cos^2\left(\frac{\pi i(j-1)}{n} - \frac{\pi(j-1)}{2n}\right)\right\}}\\ &= \frac{\epsilon^2}{2n}\sum_{j=2}^{n}\frac{\cos\Big(\pi(j-1)\Big)\left(\dfrac{\pi(j-1)}{n}\right)^2}{\sin^2\left(0.5\pi(j-1)/n\right)\left\{\sum_{i=1}^{n}\cos^2\left(\frac{\pi i(j-1)}{n} - \frac{\pi(j-1)}{2n}\right)\right\}}.\end{aligned}$$

gives, upon substitution and upon using Proposition 6.1,

$$\left.\frac{d^2}{dp^2}\hat{\lambda}_{\min}(\tilde{L}_n, p)\right|_{p=\frac{n+1}{2}} = \frac{\epsilon^2}{n^2}\sum_{j=2}^{n}\frac{(-1)^{j-1}\left(\dfrac{\pi(j-1)}{n}\right)^2}{\sin^2\left(0.5\pi(j-1)/n\right)}.$$

Since n is odd, the above sum is a sum of $\frac{n-1}{2}$ pairs of successive differences:

$$\frac{d^2\hat{\lambda}_{\min}(\tilde{L}_n, p)}{dp^2} = \frac{4\epsilon^2}{n^2}\sum_{q=1}^{\frac{n-1}{2}}\left\{\frac{\left(\dfrac{\pi 2q}{2n}\right)^2}{\sin^2\left(\dfrac{\pi 2q}{2n}\right)} - \frac{\left(\dfrac{\pi(2q-1)}{2n}\right)^2}{\sin^2\left(\dfrac{\pi(2q-1)}{2n}\right)}\right\}. \quad (21)$$

Each of the $(n-1)/2$ pairs is positive since for $q \in \{1, 2, \ldots \frac{n-1}{2}\}$, we use that $\frac{x}{\sin(x)}$ is monotonically increasing[13] for $x \in (0, \frac{\pi}{2})$. This helps conclude that $\dfrac{d^2\hat{\lambda}_0}{dp^2} > 0$ for $p = p^*$. Therefore, p^* is a local minimizer (considering $p \in \mathbb{R}$). This completes the part b) of the proof and thus this completes the proof of Lemma 6.2. □

[13] We use the fact that the $\dfrac{x}{\sin(x)}$ is a monotonically increasing function in the interval $[0, \frac{\pi}{2})$ and that this expression is of the form $\dfrac{x_2^2}{\sin^2(x_2)} < \dfrac{x_1^2}{\sin^2(x_1)}$ for $0 < x_1 < x_2 < \frac{\pi}{2}$.

Proof of Lemma 6.3: From Theorem 3.3(a), we have:

$$\lambda_{\min}({}^{S}\tilde{L}_n) = \frac{k\epsilon}{n} - \frac{\epsilon^2}{2n^2}\sum_{j=2}^{n} \frac{\left\{\sum_{i=1}^{k}\cos\left(\frac{\pi(j-1)p_i}{n} - \frac{\pi(j-1)}{2n}\right)\right\}^2}{\sin^2\left(0.5\pi(j-1)/n\right)} + O(\epsilon^3)$$

For 2-ports selection, using $k=2$ in the above equation, we get that $\lambda_{\min}(\approx{\tilde{L}}_{n,\epsilon}, p_1, p_2) =$

$$\frac{2\epsilon}{n} - \frac{\epsilon^2}{2n^2}\sum_{j=2}^{n} \frac{\left\{\cos\big(\pi(j-1)(p_1-0.5)/n\big) + \cos\left(\frac{\pi(j-1)p_2}{n} - \frac{\pi(j-1)}{2n}\right)\right\}^2}{\sin^2\left(0.5\pi(j-1)/n\right)} + O(\epsilon^3),$$

thus completing the proof. □

Proof of Lemma 6.5: Consider $\tilde{L}_n := L_n + e_1e_1^T$ which is a tridiagonal pseudo-Toeplitz matrix; see Footnote 10 for the definition. Using the result from [12], we get $\lambda(\tilde{L}_n) = 2 - 2\cos\left(\frac{\pi k}{2n+1}\right)$, where $k = 1, 2, \ldots, n$. For $k = 1$, we have $\lambda_1(\tilde{L}_n) = \lambda_{\min}(\tilde{L}_n) = 2-2\cos\left(\frac{\pi}{2n+1}\right)$. Consider $\approx{\tilde{L}}_{2n} = L_{2n}+e_1e_1^T+e_{2n}e_{2n}^T$ which is a tridiagonal Toeplitz matrix (see Footnote 10). Hence, again from [12], we get $\lambda(T_n) = 2 - 2\cos\left(\frac{\pi k}{n+1}\right)$ where $k = 1, 2, \ldots, n$. Therefore for $2n \times 2n$: $\lambda(\approx{\tilde{L}}_{2n}) = 2 - 2\cos\left(\frac{\pi k}{2n+1}\right)$ where $k = 1, 2, \ldots, 2n$. Thus, for $k = 1$, $\lambda_1(\approx{\tilde{L}}_{2n}) = \lambda_{\min}(\approx{\tilde{L}}_{2n}) = 2 - 2\cos\left(\frac{\pi}{2n+1}\right) = \lambda_{\min}(\tilde{L}_n)$.
Hence, $\lambda_{\min}(\tilde{L}_n)$ and $\lambda_{\min}(\approx{\tilde{L}}_{2n})$ are equal.

We next prove that we have monotonically strict decrease in the smallest eigenvalue of the modified Laplacian $\tilde{L}_n$ when n increases. Though n is only integer, we prove that even when considering $n \in \mathbb{R}$ and $n \geqslant 1$, we have monotonically strict decrease, and hence this would then prove for $n \in \mathbb{Z}$ (and $n \geqslant 1$) too. On differentiating $\lambda_{\min}(\tilde{L}_n) = 2 - 2\cos\left(\frac{\pi}{2n+1}\right)$ w.r.t. n, we get

$$\frac{\partial\lambda_{\min}(\tilde{L}_n)}{\partial n} = \frac{-4\pi}{(2n+1)^2}\sin\left(\frac{\pi}{2n+1}\right)$$

which is negative for $n \geqslant 1$. This proves $\lambda_{\min}(\tilde{L}_n)$ is monotonically decreasing w.r.t. n and completes the proof of Lemma 6.5. □

Proof of Lemma 6.6: Consider the polynomials $a(s) = a_0 + a_1s + a_2s^2 + \cdots + s^n$ and $b(s) = b_0 + b_1s + b_2s^2 + \cdots + b_{n-1}s^{n-1}$ be two finite-degree polynomials with $a_0 = 0$, $a_1 \neq 0$, and $b_0 \neq 0$.
Define the polynomial $p_\epsilon(s) := a(s) + \epsilon b(s)$. Clearly $s = 0$ is a root of $p_\epsilon(s)$ for $\epsilon = 0$.
In addition consider the dependence $\lambda_{\min}$ on ϵ; expand $\lambda_{\min}(\epsilon)$ about the origin in a series expansion: $\lambda_{\min}(\epsilon) = \beta_1\epsilon + \beta_2\epsilon^2 + \beta_3\epsilon^3 + \cdots$.

Rearrange $a(s) + \epsilon b(s) = 0$, to get $\epsilon(s) = \frac{a(s)}{b(s)}$, and to make the dependence of ϵ on s more explicit, express $\epsilon(s) = \frac{-a(s)}{b(s)} = \alpha_1 s + \alpha_2 s^2$ (upto the 2nd order term in s). Next, evaluating $\frac{d\epsilon}{ds}$ at $s = 0$, we obtain: $\left.\frac{d\epsilon}{ds}\right|_{s=0} = \alpha_1 = \frac{-a_1}{b_0}$. Further, evaluating for the 2nd-derivative, $\frac{d^2\epsilon}{ds^2}$ at $s = 0$, we obtain: $\left.\frac{d^2\epsilon}{ds^2}\right|_{s=0} = 2\alpha_2 = \frac{2a_1b_1 - 2a_2b_0}{b_0^2}$ which implies that $\alpha_2 = \frac{a_1b_1 - a_2b_0}{b_0^2}$.

Now consider, $s = \lambda_{\min}(\epsilon) \approx \beta_1\epsilon + \beta_2\epsilon^2$. Using standard formulae (see [25]) that relate the coefficients in the Taylor series expansions of $f(\cdot)$ and $f^{-1}(\cdot)$, we get the desired relations in equation (9) by performing the following manipulations. Use $\beta_1 = \frac{1}{\alpha_1}$ and $\beta_2 = -\frac{\alpha_2}{\alpha_1^3}$ to get $\beta_1 = \frac{-b_0}{a_1}$ and $\beta_2 = \frac{a_1b_1 - a_2b_0}{b_0^2} \times \frac{b_0^3}{a_1^3} = \frac{a_1b_1b_0 - a_2b_0^2}{a_1^3}$. This completes the proof. □

Proof of Lemma 6.7: Consider polynomials $a(s) = a_0 + a_1s + a_2s^2 + \cdots + s^n$, $b(s) = b_0 + b_1s + b_2s^2 + \cdots + b_{n-1}s^{n-1}$ and $c(s) = c_0 + c_1s + c_2s^2 + \cdots + c_{n-2}s^{n-2}$ such that $a_0 = 0$, $a_1 \neq 0$, $b_0 \neq 0$ and $c_0 \neq 0$. Define the polynomial $p_\epsilon(s) := a(s) + \epsilon b(s) + \epsilon^2 c(s)$.

In addition consider the root $\lambda_{\min}$ and the dependence of this root on ϵ. Further, note $\lambda_{\min}(0) = 0$. Expand $\lambda_{\min}(\epsilon)$ about the origin in a series expansion: $\lambda_{\min}(\epsilon) = \beta_1\epsilon + \beta_2\epsilon^2 + \beta_3\epsilon^3 + \cdots$ and also consider the series expansion of $\epsilon(s)$: about $\epsilon = 0$

$$\epsilon(s) = \alpha_1 s + \alpha_2 s^2 + \alpha_3 s^3 + \cdots . \tag{22}$$

On differentiating $p_\epsilon(s)$ w.r.t. s, (and denoting such differentiation operation by $\cdot'$) we get $p'_\epsilon(s) = 0$, using which we get $a' + \epsilon b' + \epsilon^2 c' + \epsilon' b + 2\epsilon\epsilon' c = 0$, which in turn results in $\epsilon' = \frac{-(a' + \epsilon b' + \epsilon^2 c')}{b + 2\epsilon c}$.

Next, using the above expression and (22), $\alpha_1 = \epsilon'(0) = \frac{-a_1}{b_0}$. Further, on differentiating $p_{\epsilon^2}(s)$ twice w.r.t. s, we get $a'' + \epsilon b'' + \epsilon'' b + 2\epsilon' b' + 4\epsilon\epsilon' c' + 2(\epsilon')^2 c + \epsilon^2 c'' + 2\epsilon\epsilon'' c = 0$. This implies that $\epsilon''(0) = 2\frac{a_1b_1b_0 - a_2b_0^2 - a_1^2c_0}{b_0^3}$. Now using equation (22), we obtain $\alpha_2 = \frac{\epsilon''(0)}{2} = \frac{a_1b_1b_0 - a_2b_0^2 - a_1^2c_0}{b_0^3}$. We next use that $s = \lambda_{\min}(\epsilon) \approx \beta_1\epsilon + \beta_2\epsilon^2$. Using standard formulae (see [25], for example) that relate the coefficients in the Taylor series expansions of $f(\cdot)$ and $f^{-1}(\cdot)$, we get the desired relations in equation (10) as follows. While using these formulae, we note that $\beta_1 = \frac{1}{\alpha_1}$ and $\beta_2 = -\frac{\alpha_2}{\alpha_1^3}$. Next, using values of α_i, we get $\beta_1 = \frac{-b_0}{a_1}$ and $\beta_2 = \frac{(a_1b_1b_0 - a_2b_0^2 - a_1^2c_0)}{b_0^3} \times \frac{b_0^3}{a_1^3}$ which simplified gives the desired relation $\beta_2 = \frac{(a_1b_1b_0 - a_2b_0^2 - a_1^2c_0)}{a_1^3}$. This completes the proof of Lemma 6.7. □