Decreasing the spectral radius of a graph by link removals

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Abstract

The decrease of the spectral radius, an important characterizer of network dynamics, by removing links is investigated. The minimization of the spectral radius by removing m links is shown to be an NP-complete problem, which suggests to consider heuristic strategies. Several greedy strategies are compared and several bounds on the decrease of the spectral radius are derived. The strategy that removes that link $l = i \sim j$ with largest product $(x_1)_i (x_1)_j$ of the components of the eigenvector x_1 belonging to the largest adjacency eigenvalue is shown to be superior to other strategies in most cases. Furthermore, a scaling law where the decrease in spectral radius is inversely proportional to the number of nodes N in the graph is deduced. Another sublinear scaling law of the decrease in spectral radius versus the number m of removed links is conjectured.

1 Introduction

The largest eigenvalue $\lambda_1(A)$ of the adjacency matrix A, called the spectral radius of the graph, plays an important role in dynamic processes on graphs, such as e.g. virus spread [1]. In a SIS type of network infection, the steady-state[1] infection of the network is determined by a phase transition at the epidemic threshold $\tau_c = \frac{1}{\lambda_1(A)}$: when the effective infection rate $\tau > \tau_c$, the network is infected, whereas below τ_c, the network is virus-free. Beside virus spread, the same type of phase-transition threshold [2] in the coupling strength $g_c \sim \frac{1}{\lambda_1(A)}$ occurs in a network of coupled oscillators.

Motivated by a $\frac{1}{\lambda_1(A)}$ threshold separating two different phases of a dynamic process on a network, we want to change the network in order to enlarge the network's epidemic threshold τ_c, or, equivalently, to lower $\lambda_1(A)$. Removing nodes is often too drastic[2], and, therefore, we concentrate here mainly on the problem of removing m links from a graph G with N nodes and L links. We are searching for

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[1] In the exact SIS model, the steady-state is the healthy state, which is the only absorbing state in the Markov process. However, in networks of realistic size N, this steady-state is only reached after an unrealistically long time. The steady-state in the N-intertwined virus spread model refers to the meta-stable state, which is reached exponentially rapidly and which reflects real epidemics more closely.

[2] The influence of the addition of a node in G to the spectrum of A is discussed in [3, art. 60].

a strategy so that, after removing m links, λ_1 is minimal. Earlier, Restrepo *et al.* [4] have initiated an instance of this problem: "How does λ_1 decrease when links are removed?" They introduced a new graph metric, called the dynamical importance $I_x = \frac{\lambda_1(A)-\lambda_1(A\backslash\{x\})}{\lambda_1(A)}$, where x either denotes the removal of a link $x = l$ or of a node $x = n$. The dynamical importance was further investigated by Milanese *et al.* [5]. Both Restrepo *et al.* and Milanese *et al.* have approached the problem by using perturbation theory. However, they did not consider optimality of their removal strategy.

In this paper, we complement their study by first showing in Section 2 that the *Link Spectral Radius Minimization (LSRM) problem and the Nodal Spectral Radius Minimization (NSRM) problem*, defined in Problem 1 and Problem 3, are NP-hard, which means in practice, that an optimal solution in a large network cannot be computed and that good approximate algorithms or heuristics need to be devised. The NP-completeness of LSRM and NSRM is demonstrated by reducing the problem to an equivalent problem, namely finding a Hamiltonian path in a graph, that is known to be NP-complete [6]. Since LSRM and NSRM are NP-complete, we cannot hope to find exact analytic formulae for the decrease in the spectral radius. However, in Section 3, we provide a general analytic description, bounds, several lemmas and we study the effect of node and link removal on closed walks and the influence of assortativity on the spectral radius. This developed theory direct us to find good heuristics. Section 4 proposes eight different strategies (or heuristics) for removing one link in a network and these strategies are benchmarked with the optimal strategy via extensive simulations. The removal of the link l between nodes i and j with highest product $(x_1)_i\,(x_1)_j$ of the eigenvector components belonging to the largest eigenvalue $\lambda_1(A)$ of the adjacency A is demonstrated to be the best heuristic. However, it is not always the best heuristic when more than one link is removed as illustrated in Fig. 1-3. The scaling law (18) for removing one link in Section 5 demonstrates, presumably for all graphs, that a decrease in λ_1 is inversely proportional to the size N of the graph. Hence, small graphs show the effect of link removals on λ_1 more clearly than large graphs. The scaling law (15) is much less accurately known, but indicates a sublinear decrease in λ_1 with the number m of removed links. We also claim that the optimal way to remove m links is to make the resulting graph as regular as possible, because a regular graph has the lowest spectral radius among all graphs with N nodes and L links.

Another type of strategy to prevent the outbreak of a virus is to quarantine infected nodes. Omic *et al.* [7] have studied immunization via modularity partitioning, where inter-community links are removed such that intra-community communication is preserved. Taylor and Restrepo [8] investigated the effect of adding a subgraph to a network on its largest adjacency eigenvalue λ_1. Inspired by network synchronization, Watanabe and Masuda [9] have investigated a similar problem as the NSRM but with a different object function: remove nodes in a graph to maximize the second smallest eigenvalue of the Laplacian of the graph, also coined the algebraic connectivity [3]. They have presented several strategies comparable to ours, and also found that the eigenvector strategy performed overall the best. Related to [9], but based on a weighted, asymmetric Laplacian of a graph, Nishikawaa and Mottera [10] point to the non-trivial effect of link removals on network synchronization.

2 The *Spectral Radius Minimization problem* is NP-hard

In this section, we prove that optimally decreasing the largest adjacency eigenvalue (the spectral radius) of a graph by a fixed number of link removals is NP-hard. It is widely believed that NP-hard problems cannot be solved exactly in a time complexity that is upper bounded by a polynomial function of the relevant input parameters (N and L). Let us first formulate the *Link Spectral Radius Minimization (LSRM) problem* precisely:

Problem 1 (Link Spectral Radius Minimization (LSRM) problem) *Given a graph $G(\mathcal{N}, \mathcal{L})$ with N nodes and L links, spectral radius $\lambda_1(G)$, and an integer number $m < L$. Which m links from the graph G need to be removed, such that the spectral radius of the reduced graph G_m of $L - m$ links has the smallest spectral radius out of all possible graphs that can be obtained from G by removing m links?*

Theorem 1 *The LSRM problem is NP-hard.*

To prove this theorem, we rely on the following lemmas, but first we need the definition of a path P_h with h hops or links. A path P_h with h hops starting from a node n_0 and ending at node n_h is defined as $P_h = n_0 \sim n_1 \sim n_2 \sim \ldots \sim n_{h-1} \sim n_h$, where each link $n_i \sim n_j$ between nodes n_i and n_j as well as each node n_i occurs once in the sequence defining the path P_h, in contrast to a walk $W_h = n_0 \sim n_1 \sim n_2 \sim \ldots \sim n_{h-1} \sim n_h$ with h hops, where a node n_i can appear more than once.

Lemma 1 *The path P_{N-1} visiting N nodes has a strictly smaller spectral radius than all other connected graphs with N nodes. Furthermore, $\lambda_1(P_{N-1}) = 2\cos\left(\frac{\pi}{N+1}\right)$.*

Proof: [11, p. 21][3, p. 125] □

Lemma 2 *The eigenvalues of a disconnected graph are composed of the eigenvalues (including multiplicities) of its connected components.*

Proof: [3, art. 80, p. 73-74] □

Lemma 3 *Among all possible graphs of N nodes and $N - 1$ links, the path P_{N-1} visiting N nodes has the smallest spectral radius.*

Proof: A connected graph of N nodes and $N-1$ links is a tree, of which the path is a special case. According to Lemma 1 the path has a spectral radius strictly smaller than 2, which is the smallest spectral radius possible in connected graphs. Hence, we need to demonstrate that the Lemma also holds for disconnected graphs. For ease of presentation, we assume that the disconnected graph consists of two connected components A_1 and A_2: A_1 of x nodes and A_2 of $N - x$ nodes. Our arguments also apply to multiple connected components. Now, A_1 contains at least $x - 1$ links, otherwise it is not a connected component, and A_2 contains at least $N - x - 1$ links. Since the sum of these links equals $N - 2$, either A_1 or A_2 must contain one extra link, thereby creating a cycle in that component. A graph that contains a cycle (i.e., which is not a tree) has a spectral radius larger than or equal to two. This component will, according to Lemma 2, contribute to an overall spectral radius that is larger than that of a path, which is smaller than 2. □

To prove Theorem 1, we will use the NP-complete Hamiltonian path problem [6].

Problem 2 (Hamiltonian path problem) *Given a graph $G(\mathcal{N}, \mathcal{L})$ with N nodes and L links, a Hamiltonian path is a path that visits every node exactly once. The Hamiltonian path problem is to determine if G contains a Hamiltonian path.*

We are now ready to prove Theorem 1:

Proof: In our proof we will demonstrate that if we could solve the LSRM problem in polynomial time, then we would also be able to settle the NP-complete Hamiltonian path problem. Assume we have a graph G of $L = N - 1 + m$ links. Removing m links will result in a graph G_m of $N - 1$ links. According to Lemma 3, a path is the only graph structure of $N - 1$ links that has the smallest largest adjacency eigenvalue and that eigenvalue equals $\lambda_1 = 2\cos\left(\frac{\pi}{N+1}\right)$. Moreover, a path of $N - 1$ links in a graph of N nodes, is a Hamiltonian path. If, after solving the LSRM problem we obtain $\lambda_1 = 2\cos\left(\frac{\pi}{N+1}\right)$ (smaller is not possible) then we have found a Hamiltonian path (G_m). If $\lambda_1 > 2\cos\left(\frac{\pi}{N+1}\right)$, then the original graph G does not contain a Hamiltonian path. The LSRM problem is therefore at least as hard as the Hamiltonian path problem. □

We have to interpret Theorem 1 with care. Computing the largest eigenvalue can be done in polynomial time. Consequently, the number of possible combinations $\binom{L}{m}$ of m links that we could check (by computing in polynomial time the largest eigenvalue of the graph G_m resulting after the removal of that specific set of links) is bounded by $O(L^m)$, which is a polynomial function in L. For instance, if $m = 1$, by checking the spectral radius reduction induced by the removal of each of the L links, we can obtain a solution with a complexity of L times the complexity of computing the largest eigenvalue. However, in that case m is fixed and not part of the input N, L, m as defined in problem 1. In other words, m should have been replaced with a fixed integer number in the problem definition to make it clear that m is not part of the input and that its fixed value holds for all problem instances. In problem 1, m is part of the input and, as in our proof, may for instance depend on the number of nodes and links (it makes sense to remove more links in larger networks). The previous argument therefore does not apply to problem 1, which is NP-hard as proved in Theorem 1. In fact, in our proof $m = L - N + 1$ so that the worst-case complexity of checking all possibilities is $O(L^{L-N+1})$, which is now clearly non-polynomial in the input N, L, m. Similar NP-complete problems, in which the input does not only rely on N and L, but also on another metric k, are the Independent Set problem (defined in problem 4 below) and the Disjoint Connecting Paths problem [6], where k mutually node-disjoint paths need to be found between k corresponding source-destination pairs. This problem also can be solved in polynomial time if k is fixed and thus not part of the input [12], while it is NP-complete if k is part of the input. In general, NP-complete problems that can be solved by algorithms, that are exponential only in the size of a fixed parameter while polynomial in the size of the (remaining) input, are called *fixed-parameter tractable*, because those problems can be solved efficiently for small values of the fixed parameter.

As an example to illustrate the NP-completeness of the LSRM problem, Fig. 1-3 show, in a topology of $N = 10$ nodes and $m = 3$ link removals, that the "best single step strategy" is not always optimal in the end. The "best single step strategy" consists of removing the link that lowers $\lambda_1(A) - \lambda_1(A_1) = y_1$ most in the first step. Next, in the second step, the link that lowers $\lambda_1(A_1) - \lambda_1(A_2) = y_2$ most is removed and finally, in the third step, the link that lowers $\lambda_1(A_2) - \lambda_1(A_3) = y_3$ most is removed. The optimal situation depicts the removal of $m = 3$ for which $\lambda_1(A) - \lambda_1(A_3) = y^*$ is maximal. Hence,

$y_1 + y_2 + y_3 \leq y^*$.

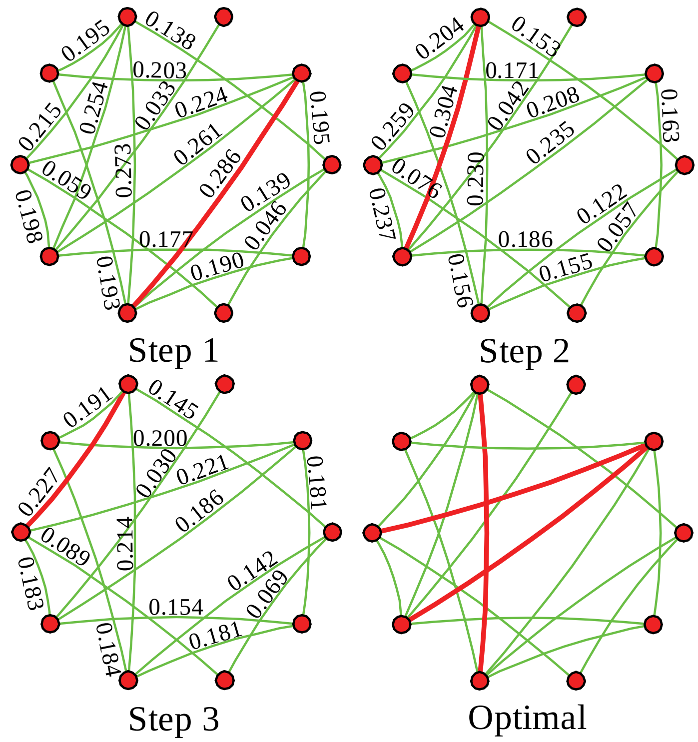

Figure 1: (Color online) An example of a graph with $N = 10$ nodes, where *none* of the links in the greedy approach appears in the optimal set of links. The numbers indicate the change in largest eigenvalue $\lambda_1(A) - \lambda_1(A \backslash \{l\})$ after removal of link l.

In addition, 10^6 instances of Erdős-Rényi (ER) random graphs with $N = 10$ and link density $p = \frac{2 \ln N}{N}$ have been generated. In each instance, the "best single step strategy" and the global optimum have been computed. In 63185 (6,3%) instances, there was no overlap in links, in 332262 (33,2%) ER graphs, there was one link in common, in 97944 (9,8%) ER graphs, we found 2 links in common and in the remaining 506609 (50,7%) ER graphs, all 3 links in the "best single step strategy" were the same as in the global optimum. Moreover, Fig. 4 illustrates that the global optimum is not always unique. The global optimum may not be unique, as it is possible that the removals of different sets of m links will lead to cospectral or even isomorphic smaller graphs, as indicated in Fig. 4.

The minimum number m of links that need to be removed from G to ensure that λ_1 in G_m is lowered below some given value ξ is

$$m \leq L - \frac{\xi^2 + N - 1}{2}$$

which is derived from the bound [3, (3.48) on p. 54], due to Yuan Hong [13],

$$\lambda_1 \leq \sqrt{2L - N + 1} \tag{1}$$

for connected graphs, else $\lambda_1 \leq \sqrt{2L\left(1 - \frac{1}{N}\right)}$.

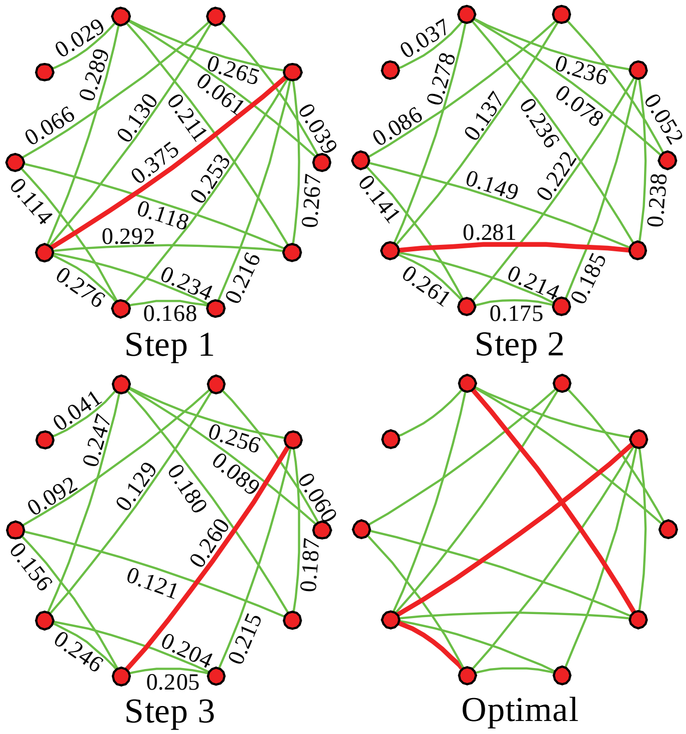

Figure 2: (Color online) An example of a graph with $N = 10$ nodes, where only 1 link in the greedy approach appears in the optimal set of links.

2.1 Link versus node removal

Removing nodes to maximally lower the largest eigenvalue may seem an easier problem than removing links. For, when we remove the highest degree node, $\lambda_1(A)$ is likely reduced most (because L is reduced most). This suggestion follows from bounds in [3, p. 48] and the bounds

$$\frac{2L}{N}\sqrt{1+\frac{\mathrm{Var}[D]}{(E[D])^2}} \leq \lambda_1 \leq \min\left\{\sqrt{\frac{2L(N-1)}{N}}, d_{\max}\right\} \tag{2}$$

where D is the degree of an arbitrary node in G. Unfortunately, this intuition is wrong. The eigenvalues of the adjacency matrix $A_{l(G)}$ of the line graph $l(G)$ of G and A are related [3, (2.9) on p. 20]. Since links in G are nodes in $l(G)$, and since there is a one-to-one relation between $l(G)$ and G, removing nodes in $l(G)$ according to a certain strategy, results in a corresponding strategy for removing links in G. Since the link spectral radius minimization (LSRM) problem is NP-hard (Theorem 1), the problem of removing m nodes from a graph G is NP-hard as well. We will provide a proof for general graphs and subsequently demonstrate that it is also NP-complete in the subclass of line graphs. Let us first formally define the problem:

Problem 3 (Nodal Spectral Radius Minimization (NSRM) problem) *Given a graph $G(\mathcal{N},\mathcal{L})$ with N nodes and L links, spectral radius $\lambda_1(G)$, and an integer number $m < N$. Which m nodes from the graph G need to be removed, such that the spectral radius of the reduced graph G_m of $N-m$ nodes has the smallest spectral radius out of all possible graphs that can be obtained from G by removing m nodes?*

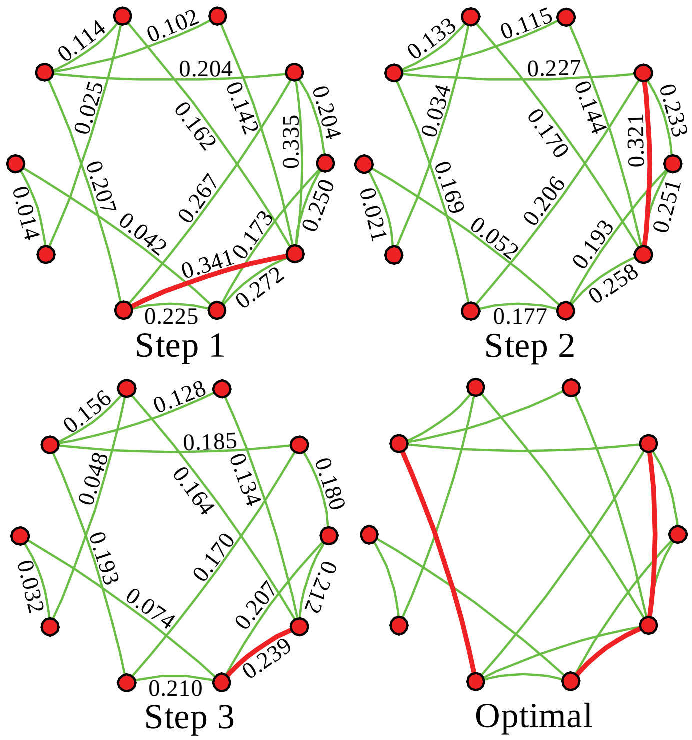

Figure 3: (Color online) An example of a graph with $N = 10$ nodes, where *two* links in the greedy approach appear in the optimal set of links.

Theorem 2 *The NSRM problem is NP-hard.*

We provide a proof by reducing the NP-complete independent set problem [6] to NSRM.

Problem 4 (Independent set problem) *Given a graph $G(\mathcal{N}, \mathcal{L})$ with N nodes and L links and a positive integer $k \leq N$, is there a subset $\mathcal{N}' \subseteq \mathcal{N}$, such that $|\mathcal{N}'| \geq k$ and such that no two nodes in $\mathcal{N}'$ are joined by a link in $\mathcal{L}$?*

Proof of Theorem 2: The lowest spectral radius of a graph equals $\lambda_1(G) = 0$, which is obtained for a graph without any links. Removing nodes that are not part of an independent set, will result in an independent set of nodes that are not linked to each other. Hence, to solve the independent set problem it suffices to remove $m = N - k$ nodes from the graph G, such that the spectral radius of the reduced graph G_m is smallest possible. If we get $\lambda_1(G_m) = 0$, then G_m constitutes an independent set of k nodes. If $\lambda_1(G_m) > 0$, then no independent set with at least k nodes exists. $\square$

Line graphs are a specific class of graphs and not all problems that are NP-complete for general graphs are also NP-complete for line graphs (e.g., according to Roussopoulos [14], the clique problem is not hard in line graphs, while it is an NP-complete problem in general). Hence, we proceed to demonstrate that the NSRM problem remains NP-hard in line graphs. We use similar arguments as for the proof of Theorem 1. A Hamiltonian path in the graph G corresponds to a path of $N - 1$ nodes in the line graph $l(G)$ of G. A line graph $l(G)$ contains L nodes and can be generated in polynomial time from G. According to Lemma 1, the graph structure of $N - 1$ nodes that has the smallest largest

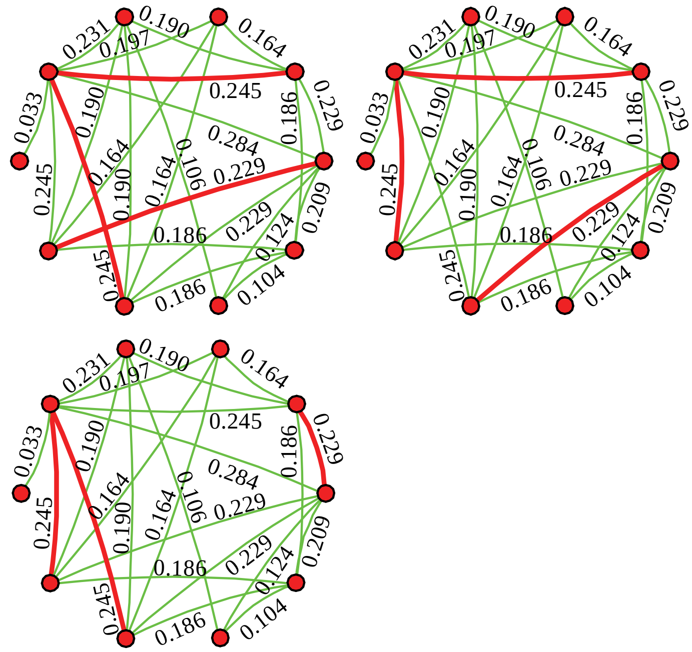

Figure 4: (Color online) An example where the global optimum is not unique. The original $\lambda_1(A) = 5.065310$ and, after removal of three links, the smallest largest eigenvalue is $\lambda_1(A_3) = 4.312414$. Consequently, the largest $\lambda_1(A) - \lambda_1(A_3) = 0.752896$ is obtained after removal of the three red links.

eigenvalue is the path. Hence, removing $L-N+1$ nodes from the line graph $l(G)$ such that the spectral radius is reduced most, should correspond to a path of $N-1$ nodes (if it exists), which corresponds to a Hamiltonian path in G. Solving the NSRM problem in a line graphs $l(G)$ is therefore as hard as finding Hamiltonian paths in the corresponding graph G.

Finally, let l be the removed link that maximizes $\lambda_1(G) - \lambda_1(G\backslash\{l\})$. Let the node n be the transform of link l in the line graph $l(G)$. Then, $\lambda_1(l(G)) - \lambda_1(l(G)\setminus\{n\})$ is not always the maximum. Simulations on 100 Erdős-Rényi random graphs show the "success rate", the percentage of graphs in which the best link l in G corresponds to the best node n in $l(G)$ in the table 1.

p / N	0.1	0.2	0.3
10	67%	80%	83%
20	65%	76%	81%
30	59%	76%	81%
40	70%	79%	81%
50	63%	75%	82%
60	67%	82%	86%

Table 1: Success rate in line graphs.

3 Spectral graph theory

We derive a theoretical underpinning to deduce the best heuristic for the LSRM problem. We first introduce the notation. Let x_1 be the eigenvector of A belonging to $\lambda_1(A)$ in the original graph G and normalized such that $x_1^T x_1 = 1$. The graph G contains N nodes and L links. Let $\mathcal{M}_m$ denote the set of the m links that are removed from G and $G_m = G \backslash \mathcal{M}_m$ is the resulting graph after the removal of m links from G. We denote the adjacency matrix of G_m by A_m, which is still a symmetric matrix. Similarly, let w_1 be the normalized eigenvector of A_m corresponding to $\lambda_1(A_m)$ in the graph G_m. By the Perron-Frobenius theorem [3], all components of x_1 and w_1 are non-negative (positive if the corresponding graph is connected).

Let e_j be a base vector in the N-dimensional space, where the i-th component equals $(e_j)_i = \delta_{ij}$ and δ_{ij} is the Kronecker delta, i.e. $\delta_{ij} = 1$ if $i = j$ and otherwise, $\delta_{ij} = 0$. Then, the adjacency matrix that represents the single link between nodes i and j equals

$$\hat{A}_{ij} = e_i e_j^T + e_j e_i^T \tag{3}$$

Thus, $\hat{A}_{ij}$ equals the zero matrix, except that $\left(\hat{A}_{ij}\right)_{ij} = \left(\hat{A}_{ij}\right)_{ji} = 1$. Clearly, $\det\left(\hat{A}_{ij} - \lambda I\right) = (-1)^N \lambda^{N-2}\left(\lambda^2 - 1\right)$, such that the largest eigenvalue of $\hat{A}_{ij}$ is 1. Also, for any vector z,

$$z^T \hat{A}_{ij} z = z^T\left(e_i e_j^T + e_j e_i^T\right) z = z^T e_i e_j^T z + z^T e_j e_i^T z = 2 z_i z_j \tag{4}$$

By invoking $0 \leq (z_i - z_j)^2$, we observe that $2 z_i z_j \leq z_i^2 + z_j^2 \leq \sum_{i=1}^N z_i^2 = z^T z$. Hence, when considering normalized vectors such that $z^T z = \|z\|_2^2 = 1$, we obtain the upper bound

$$2 z_i z_j \leq 1$$

After these preliminaries, we now embark on the problem.

3.1 The difference $\lambda_1(A) - \lambda_1(A_m)$

With the normalization $x_1^T x_1 = 1$ and $w_1^T w_1 = 1$, the Rayleigh relations [3] become

$$\lambda_1(A) = x_1^T A x_1$$
$$\lambda_1(A_m) = w_1^T A_m w_1$$

Writing out the quadratic form

$$\lambda_1(A) = x_1^T A x_1 = \sum_{i=1}^N \sum_{j=1}^N a_{ij} (x_1)_i (x_1)_j = 2 \sum_{i=1}^N \sum_{j=i+1}^N a_{ij} (x_1)_i (x_1)_j \tag{5}$$
$$= 2 \sum_{l=(i\sim j)\in\mathcal{L}} (x_1)_i (x_1)_j = 2 \sum_{l=1}^L (x_1)_{l^+} (x_1)_{l^-}$$

where a link l joins the nodes l^+ and l^-, shows that $\lambda_1(A)$ can be written as a sum of positive products over all links in the graph G.

We now provide a general bound on the difference between the largest eigenvalues in G and $G_m = G \backslash \mathcal{M}_m$, where m links are removed.

Lemma 4 *For any graph G and $G_m = G\backslash\mathcal{M}_m$, it holds that*

$$2\sum_{l\in\mathcal{M}_m}(w_1)_{l^+}(w_1)_{l^-} \leq \lambda_1(A) - \lambda_1(A_m) \leq 2\sum_{l\in\mathcal{M}_m}(x_1)_{l^+}(x_1)_{l^-} \tag{6}$$

where x_1 and w_1 are the eigenvectors of A and A_m corresponding to the largest eigenvalues $\lambda_1(A)$ and $\lambda_1(A_m)$, respectively, and where a link l joins the nodes l^+ and l^-.

Proof: Since $A_m = A - \sum_{l\in\mathcal{M}_m}\hat{A}_{l^+l^-}$ where the left-hand side (or start) of the link l is the node l^+ and the right-hand side (or end) of the link l is the node l^- and with the normalization $x_1^T x_1 = 1$, the Rayleigh relations [3] yield

$$\begin{aligned}\lambda_1(A) = x_1^T A x_1 &= x_1^T\left(A_m + \sum_{l\in\mathcal{M}_m}\hat{A}_{l^+l^-}\right)x_1\\ &= x_1^T A_m x_1 + \sum_{l\in\mathcal{M}_m} x_1^T\hat{A}_{l^+l^-}x_1\end{aligned}$$

Using (4) yields $x_1^T\hat{A}_{l^+l^-}x_1 = 2(x_1)_{l^+}(x_1)_{l^-}$ and we arrive at

$$\lambda_1(A) = x_1^T A_m x_1 + 2\sum_{l\in\mathcal{M}_m}(x_1)_{l^+}(x_1)_{l^-}$$

The Rayleigh principle states that, for any normalized vector w with $w^T w = 1$, it holds that $w^T A w \leq \lambda_1(A)$ and equality is only attained if w equals the eigenvector of A belonging to $\lambda_1(A)$. Since x_1 is not the eigenvector of A_m belonging to $\lambda_1(A_m)$, we have that $x_1^T A_m x_1 \leq \lambda_1(A_m)$ and

$$\lambda_1(A) = x_1^T A_m x_1 + 2\sum_{l\in\mathcal{M}_m}(x_1)_{l^+}(x_1)_{l^-} \leq \lambda_1(A_m) + 2\sum_{l\in\mathcal{M}_m}(x_1)_{l^+}(x_1)_{l^-}$$

from which the upper bound in (6) is immediate. When repeating the analysis from the point of view of A_m rather than from A, then

$$\begin{aligned}\lambda_1(A_m) = w_1^T A_m w_1 &= w_1^T\left(A - \sum_{l\in\mathcal{M}_m}\hat{A}_{l^+l^-}\right)w_1\\ &= w_1^T A w_1 - 2\sum_{l\in\mathcal{M}_m}(w_1)_{l^+}(w_1)_{l^-}\end{aligned}$$

By invoking the Rayleigh principle again, we arrive at the lower bound. □

For connected graphs G and G_m, it is known that $\lambda_1(A) - \lambda_1(A_m) > 0$ (see Lemma 7 in [3]). The same conclusion also follows from Lemma 4 because the Perron-Frobenius theorem [3] states that all vector components of w_1 (and x_1) are positive in a connected graph G_m. Lemma 4 indicates that, when those m links are removed that maximize $2\sum_{l\in\mathcal{M}_m}(x_1)_{l^+}(x_1)_{l^-}$, then the upper bound in (6) is maximal, which may lead to the largest possible difference $\lambda_1(A) - \lambda_1(A_m)$. However, those removed links do not necessarily also maximize the lower bound $2\sum_{l\in\mathcal{M}_m}(w_1)_{l^+}(w_1)_{l^-}$. Hence, the greedy strategy of removing consecutively the link l with the highest product $(x_1)_{l^+}(x_1)_{l^-}$ is not necessarily guaranteed to lead to the overall optimum. The fact that the SRM problem is NP-hard, as proved in Section 2, underlines this remark.

Lemma 8 in [3] states that

$$\lambda_1(A) - \lambda_1(A_m) \leq \lambda_1(A - A_m)$$

Since $A - A_m = \sum_{l\in\mathcal{M}_m} \hat{A}_{l^+l^-}$, it remains to find a close upper bound for $\lambda_1\left(\sum_{l\in\mathcal{M}_m} \hat{A}_{l^+l^-}\right)$. Using the bounds [3, (3.48) on p. 54], gives

$$\lambda_1\left(\sum_{l\in\mathcal{M}_m} \hat{A}_{l^+l^-}\right) \leq \min\left(\sqrt{2m-N+1}, d_{\max}(A-A_m)\right) 1_{\{A-A_m \text{ is a connected graph}\}}$$
$$+\min\left(\sqrt{2m-\frac{2m}{N}}, d_{\max}(A-A_m)\right) 1_{\{A-A_m \text{ is not a connected graph}\}}$$

In general, it is difficult to find sharper bounds (see e.g. [15],[16]). If $m=2$, then $\lambda_1\left(\sum_{l\in\mathcal{M}_2} \hat{A}_{l^+l^-}\right) = \sqrt{2}$ when the two links are connected and $\lambda_1\left(\sum_{l\in\mathcal{M}_2} \hat{A}_{l^+l^-}\right) = 1$ when the two links are disconnected. If $m=1$, then $\lambda_1\left(\hat{A}_{l^+l^-}\right) = 1$ and we obtain

$$\lambda_1(A) - \lambda_1(A_1) \leq 1 \tag{7}$$

Lemma 5 *For $m=1$ link removed from G, equality in (7) is only attained for the graph consisting of the complete graph K_N with $N=2$ nodes and a set of disjoint nodes.*

Proof: Equality in (7) combined with (6) in Lemma 4 implies that

$$1 = \lambda_1(A) - \lambda_1(A_1) \leq 2(x_1)_{l^+}(x_1)_{l^-}$$

Next, from $2(x_1)_{l^+}(x_1)_{l^-} \leq (x_1)_{l^+}^2 + (x_1)_{l^-}^2 \leq x_1^T x_1 = 1$, we conclude that the equality in (7) holds if and only if $(x_1)_{l^+} = (x_1)_{l^-} = 1/\sqrt{2}$. Since in such case $(x_1)_{l^+}^2 + (x_1)_{l^-}^2 = 1$, we conclude that all other components of the eigenvector x_1 are equal to zero. Recall that x_1 is the principle eigenvector which, according to the Perron-Frobenius Theory, is positive if G is a connected graph. If G has more than two nodes ($N>2$), the above argument shows that G must be disconnected with K_2 being the unique component with the largest spectral radius. Therefore, the remaining components must be isolated nodes. □

3.1.1 Application of perturbation theory to m link removals

Let $\lambda_1 > \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of A, with $x_1, x_2, \ldots, x_n$ the corresponding eigenvectors, which form an orthonormal basis. We apply the general perturbation formulae [17]

$$x(\zeta) = x_1 + \zeta\sum_{k=2}^{N}\frac{x_k^T B x_1}{\lambda_1-\lambda_k}x_k + \zeta^2\sum_{m=2}^{N}\left\{\frac{\left(x_1^T B x_1\right)\left(x_m^T B x_1\right)}{\lambda_1-\lambda_m} - \sum_{k=2}^{N}\frac{\left(x_k^T B x_1\right)\left(x_m^T B x_k\right)}{\lambda_1-\lambda_k}\right\}\frac{x_m}{\lambda_m-\lambda_1} + O\left(\zeta^3\right) \tag{8}$$

$$\lambda(\zeta) = \lambda_1 + \zeta x_1^T B x_1 + \zeta^2\sum_{k=2}^{N}\frac{\left(x_k^T B x_1\right)^2}{\lambda_1-\lambda_k} + \tag{9}$$
$$+\zeta^3\sum_{m=2}^{N}\left\{\left(x_m^T B x_m\right) - \left(x_1^T B x_1\right)\right\}\left(\frac{x_1^T B x_m}{\lambda_1-\lambda_m}\right)^2 + 2\zeta^3\sum_{m=2}^{N}\sum_{k=2}^{m-1}\frac{\left(x_1^T B x_m\right)\left(x_m^T B x_k\right)\left(x_k^T B x_1\right)}{\left(\lambda_1-\lambda_m\right)\left(\lambda_1-\lambda_k\right)} + O\left(\zeta^4\right)$$

for the matrix $A(\zeta) = A + \zeta B$ by using $B = \sum_{l=1}^{m} \hat{A}_{l+l-}$ and $\zeta = -1$. We remark that $|\zeta| = 1$ is large for a perturbation to be effective in general.

Using the definition (3) of the matrix $\hat{A}_{l+l-}$, we obtain

$$x_k^T \hat{A}_{l+l-} x_q = x_k^T e_{l+} e_{l-}^T x_q + x_k^T e_{l-} e_{l+}^T x_q = (x_k)_{l+} (x_q)_{l-} + (x_k)_{l-} (x_q)_{l+}$$

and

$$x_k^T B x_q = \sum_{l=1}^{m} x_k^T \hat{A}_{l+l-} x_q = \sum_{l=1}^{m} \left\{ (x_k)_{l+} (x_q)_{l-} + (x_k)_{l-} (x_q)_{l+} \right\}$$

where x_k denotes the eigenvector of A belonging to eigenvalue λ_k. From (8), the first order perturbation for the eigenvector of A_m is

$$x_1(\zeta) \simeq x_1 - \sum_{k=2}^{N} \sum_{l=1}^{m} \frac{(x_k)_{l+} (x_q)_{l-} + (x_k)_{l-} (x_q)_{l+}}{\lambda_1 - \lambda_k} x_k$$

and from (9) the corresponding eigenvalue perturbation, up to second order, is

$$\lambda_1(\zeta) = \lambda_1(A) - 2 \sum_{l=1}^{m} (x_1)_{l+} (x_1)_{l-} + \sum_{k=2}^{N} \frac{\left(\sum_{l=1}^{m} \left\{ (x_k)_{l+} (x_1)_{l-} + (x_k)_{l-} (x_1)_{l+} \right\} \right)^2}{\lambda_1 - \lambda_k}$$

Since $\lambda_1(\zeta) = \lambda_1(A_m)$, the difference in largest eigenvalues equals approximately

$$\lambda_1(A) - \lambda_1(A_m) \simeq 2 \sum_{l=1}^{m} (x_1)_{l+} (x_1)_{l-} - \sum_{k=2}^{N} \frac{\left(\sum_{l=1}^{m} \left\{ (x_k)_{l+} (x_1)_{l-} + (x_k)_{l-} (x_1)_{l+} \right\} \right)^2}{\lambda_1(A) - \lambda_k(A)} \tag{10}$$

Of course, we can also apply the perturbation formula to A_m and add m links so that $\zeta = 1$. The difference in largest eigenvalues equals approximately

$$\lambda_1(A) - \lambda_1(A_m) \simeq 2 \sum_{l=1}^{m} (w_1)_{l+} (w_1)_{l-} + \sum_{k=2}^{N} \frac{\left(\sum_{l=1}^{m} \left\{ (w_k)_{l+} (w_1)_{l-} + (w_k)_{l-} (w_1)_{l+} \right\} \right)^2}{\lambda_1(A_m) - \lambda_k(A_m)} \tag{11}$$

The proof of Lemma 4 indicates that the difference between the largest eigenvalues is

$$\lambda_1(A) - \lambda_1(A_m) = x_1^T A_m x_1 - w_1^T A_m w_1 + 2 \sum_{l \in \mathcal{M}_m} (x_1)_{l+} (x_1)_{l-}$$

which, since A_m and A are symmetric, also can be written as

$$\lambda_1(A) - \lambda_1(A_m) = (x_1 - w_1)^T A_m (x_1 + w_1) + 2 \sum_{l \in \mathcal{M}_m} (x_1)_{l+} (x_1)_{l-} \tag{12}$$

or as

$$\lambda_1(A) - \lambda_1(A_m) = (x_1 - w_1)^T A (x_1 + w_1) + 2 \sum_{l \in \mathcal{M}_m} \left(w_1^T \right)_{l+} (w_1)_{l-} \tag{13}$$

The Perron-Frobenius theorem [3] implies that there is at least one component in $x_1 - w_1$ that is negative (because $x_1^T x_1 = w_1^T w_1 = 1$).

The expansions (10) and (11) should be compared with the exact expressions (12) and (13), respectively. Moreover, they lead to a second proof of Lemma 4, provided a second order perturbation is accurate enough. Since the sum in (11), as well as in (10), is positive and all components w_1 and x_1

are positive when G is connected, comparison with (12) and (13) suggests (provided a second order perturbation is accurate enough), for connected graphs, that

$$(x_1 - w_1)^T A (x_1 + w_1) > 0$$

while

$$(x_1 - w_1)^T A_m (x_1 + w_1) < 0$$

For large graphs, where $\lambda_1 = O(N)$, the expansion up to second order, thus ignoring terms of $O(\zeta^3)$ in (8) and (9), can be already good. This is the approach of Restreppo *et al.* [4] and verified numerically by Milanese *et al.* [5].

3.2 Closed walks in subgraphs

Let G be a connected graph with adjacency matrix A. From the decomposition [3, art. 156 on p. 226]

$$A = \sum_{i=1} \lambda_i x_i x_i^T,$$

using $x_i^T x_j = 0$ for $i \neq j$ and $x_i^T x_i = 1$ for any i, we have that

$$A^k = \sum_{i=1}^{n} \lambda_i^k x_i x_i^T.$$

When $k \to \infty$, the most important term in the sum above is $\lambda_1^k x_1 x_1^T$, provided that G is nonbipartite[3]. In such case, we have $\lambda_1 > |\lambda_i|$ for $i = 2, \ldots, n$, and so, for any two nodes u, v of G,

$$\lim_{k\to\infty} \frac{(A^k)_{uv}}{\lambda_1^k (x_1)_u (x_1)_v} = \lim_{k\to\infty} \frac{\sum_{i=1}^n \lambda_i^k (x_i)_u (x_i)_v}{\lambda_1^k (x_1)_u (x_1)_v} = 1 + \sum_{i=2}^{n} \frac{(x_i)_u (x_i)_v}{(x_1)_u (x_1)_v} \left(\frac{\lambda_i}{\lambda_1}\right)^k = 1.$$

In view of the above, we will deliberately resort to the following *approximation*:

$$\text{For large } k: (A^k)_{uv} \approx \lambda_1^k (x_1)_u (x_1)_v .$$

Under such approximation, the total number of closed walks of large length k in G is

$$\sum_{u\in V(G)} (A^k)_{uu} \simeq \sum_{u\in V(G)} \lambda_1^k (x_1)_u (x_1)_u = \lambda_1^k \sum_{u\in V(G)} (x_1)_u^2 = \lambda_1^k.$$

We will demonstrate that removing the node u or the link $u \sim v$ with highest vector component $(x_1)_u$ or highest vector component product $(x_1)_u (x_1)_v$ will decrease $\lambda_1(A)$ most.

[3] In case G is bipartite, let (U, V) be the bipartition of nodes of G. Then $\lambda_n = -\lambda_1$, $(x_n)_u = (x_1)_u$ for $u \in U$ and $(x_n)_v = -(x_1)_v$ for $v \in V$. Both λ_1 and λ_n are simple eigenvalues, so that $\lambda_1 > |\lambda_i|$ for $i = 2, \ldots, n-1$. Similarly as above we get

$$\lim_{k\to\infty} \frac{(A^k)_{u,v}}{\lambda_1^k (x_1)_u (x_1)_v} = 1 + \lim_{k\to\infty} (-1)^k \frac{(x_n)_u (x_n)_v}{(x_1)_u (x_1)_v}.$$

Obviously, the limit above exists if we restrict k to range over odd or even numbers only, in which case the limit is either 0 or 2, depending on whether u and v belong to the same or different parts of the bipartition. This suggests that the same strategy will extend to bipartite graphs as well, except that the argument will have to take into account the nonexistence of odd closed walks.

3.2.1 Node removal

In order to find the node whose deletion reduces λ_1 most, we will consider the *equivalent* question: which deleted node u reduces the number of closed walks in G for some large length k most?

Of course, the number of closed walks of length k which start at node u is equal to $(A^k)_{uu} \approx \lambda_1^k (x_1)_u^2$. When we delete node u from G, then, besides the closed walks which start at u, we also destroy the closed walks which start at another node v, but which contain u as well. Any such closed walk that starts at v may contain several occurrences of u.

For fixed u, k and v, let W_t denote the number of closed walks of length k which start at v and which contain u at least t times, $t \geq 1$. Suppose that in such a walk, node u appears after l_1 steps, after $l_1 + l_2$ steps, after $l_1 + l_2 + l_3$ steps, and so on, the last appearance accounted after $l_1 + \cdots + l_t$ steps. Here $l_1, \ldots, l_t \geq 1$. Moreover, u must appear for the last time after at most $k-1$ steps (after k steps we are back at v), thus we may also introduce $l_{t+1} = k - (l_1 + \cdots + l_t)$ and ask that $l_{t+1} \geq 1$. Then, we have

$$\begin{aligned} W_t &= \sum_{l_1,\ldots,l_{t+1}} (A^{l_1})_{vu} (A^{l_2})_{uu} \ldots (A^{l_t})_{uu} (A^{l_{t+1}})_{uv} \\ &\simeq \sum_{l_1,\ldots,l_{t+1}} \lambda_1^k (x_1)_v^2 (x_1)_u^{2t} = \lambda_1^k (x_1)_v^2 (x_1)_u^{2t} \sum_{\sum_{j=1}^{t+1} l_j = k; l_j \geq 1} 1. \end{aligned}$$

Introducing $l_1' = l_1 - 1, \ldots, l_{t+1}' = l_{t+1} - 1$, the last sum is equal to the number of nonnegative solutions to

$$l_1' + l_2' + \cdots + l_t' + l_{t+1}' = k - t - 1,$$

which is, in turn, equal to $\binom{(k-1-t)+t}{t} = \binom{k-1}{t}$. Therefore,

$$W_t \simeq \binom{k-1}{t} \lambda_1^k (x_1)_v^2 (x_1)_u^{2t}.$$

Consider now a closed walk of length k starting at v which contains u exactly j times. Such walk is counted j times in W_1, $\binom{j}{2}$ times in W_2, $\binom{j}{3}$ times in W_3, $\ldots$, $\binom{j}{j}$ times in W_j, and using the well-known equality

$$1 = \sum_{t \geq 1} (-1)^{t-1} \binom{j}{t}$$

we see that this closed walk is counted exactly once in the expression

$$W^v = W_1 - W_2 + W_3 - \cdots + (-1)^{t-1} W_t + \ldots$$

Thus, W^v represents the number of closed walks of length k starting at v which will be affected by deleting u. From the above expression for W_t, we have

$$\begin{aligned} W^v &\simeq \sum_{t \geq 1} (-1)^{t-1} \binom{k-1}{t} \lambda_1^k (x_1)_v^2 (x_1)_u^{2t} \\ &= -\lambda_1^k (x_1)_v^2 \sum_{t \geq 1} \binom{k-1}{t} \left(-(x_1)_u^2\right)^t \\ &= \lambda_1^k (x_1)_v^2 \left[1 - (1 - (x_1)_u^2)^{k-1}\right] \end{aligned}$$

Therefore, the total number of closed walks of length k destroyed by deleting u is equal to

$$\begin{aligned}
W &\simeq \lambda_1^k \left(x_1\right)_u^2 + \sum_{v\neq u} W^v \\
&= \lambda_1^k \left(x_1\right)_u^2 + \lambda_1^k \sum_{v\neq u} \left(x_1\right)_v^2 \left[1-(1-\left(x_1\right)_u^2)^{k-1}\right] \\
&= \lambda_1^k \left[\left(x_1\right)_u^2 + (1-\left(x_1\right)_u^2)\left[1-(1-\left(x_1\right)_u^2)^{k-1}\right]\right] \\
&= \lambda_1^k \left[1-(1-\left(x_1\right)_u^2)^{k}\right].
\end{aligned}$$

The last function is increasing in $\left(x_1\right)_u$ in the interval $[0,1]$, and so we conclude that most closed walks are destroyed when we remove the node with the largest principal eigenvector component. Hence, the spectral radius (see (5)) is decreased the most in such case as well.

3.2.2 Link removal

Similarly as in previous section, we want to find out the deletion of which link $u \sim v$ mostly reduces the number of closed walks in G of some large length k?

For fixed u, v and k, let W_t denote the number of closed walks of length k which start at some node w and contain the link $u \sim v$ at least t times, $t \geq 1$. Suppose that in such walk, the link $u \sim v$ appears at positions $1 \leq l_1 \leq l_2 \leq \cdots \leq l_t \leq k$ in the sequence of links on the walk, and let $u_{i,0}$ and $u_{i,1}$ be the first and the second node of the ith appearance of uv in the walk. Obviously, either $(u_{i,0}, u_{i,1}) = (u, v)$ or $(u_{i,0}, u_{i,1}) = (v, u)$. Then

$$\begin{aligned}
W_t &= \sum_{w\in V} \sum_{l_1\leq\cdots\leq l_t} (A^{l_1-1})_{wu_{1,0}} \left(\prod_{i=2}^{t} (A^{l_i-l_{i-1}-1})_{u_{i-1,1}u_{i,0}}\right) (A^{k-l_t-1})_{u_{t,1}w} \\
&\simeq \sum_{w\in V} \sum_{l_1\leq\cdots\leq l_t} \lambda_1^{l_1-1} \left(x_1\right)_w \left(x_1\right)_{u_{1,0}} \left(\prod_{i=2}^{t} \lambda_1^{l_i-l_{i-1}-1} \left(x_1\right)_{u_{i-1,1}} \left(x_1\right)_{u_{i,0}}\right) \lambda_1^{k-l_t-1} \left(x_1\right)_{u_{t,1}} \left(x_1\right)_w \\
&= \sum_{w\in V} \left(x_1\right)_w^2 \sum_{l_1\leq\cdots\leq l_t} \lambda_1^{k-t} \prod_{i=1}^{t} (\left(x_1\right)_{u_{i,0}} \left(x_1\right)_{u_{i,1}})^2 \\
&= \binom{k}{t} \lambda_1^{k-t} (2\left(x_1\right)_u \left(x_1\right)_v)^t.
\end{aligned}$$

The term $2\left(x_1\right)_u \left(x_1\right)_v$ appears in the last equation because there are two ways to choose $(x_{u_{i,0}}, x_{u_{i,1}})$ for each $i = 1, \ldots, t$.

Now, the number of walks affected by deleting the link $u \sim v$ is equal to

$$\begin{aligned}
W^{uv} &= \sum_{t\geq 1} (-1)^{t-1} W_t \\
&= \sum_{t\geq 1} (-1)^{t-1} \binom{k}{t} \lambda_1^{k-t} (2\left(x_1\right)_u \left(x_1\right)_v)^t \\
&= \lambda_1^k - \sum_{t\geq 0} (-1)^{t} \binom{k}{t} \lambda_1^{k-t} (2\left(x_1\right)_u \left(x_1\right)_v)^t \\
&= \lambda_1^k - (\lambda_1 - 2\left(x_1\right)_u \left(x_1\right)_v)^k.
\end{aligned}$$

The last function is increasing in $(x_1)_u (x_1)_v$ in the interval $[0, \lambda_1/2]$, and so most closed walks are destroyed when we remove the link with the largest product of principal eigenvector components. Thus, the spectral radius is decreased the most in such case as well.

3.3 Assortativity and lower bounds for λ_1

A lower bound of the largest adjacency eigenvalue $\lambda_1 \geq \frac{N_3}{N_2}$ has been proved in [18], where N_k is the total number of walks of length k. The lower bound $\frac{N_3}{N_2}$ appeared earlier as an approximation in [19] of the largest adjacency eigenvalue λ_1, and it is a perfect linear function of assortativity ρ_D [18].

Let us first look at the decrease of $\frac{N_3}{N_2}$ by a link removal. We know [18] that

$$\frac{N_3}{N_2} = \frac{\sum_{i=1}^{N} d_i^3 - \sum_{i \sim j} (d_i - d_j)^2}{\sum_{i=1}^{N} d_i^2}$$

We denote N_3 and N_3' as the number of 3 hop walks in the original graph G and in the graph $G \backslash \{l_{ij}\}$ with one link $l = i \sim j$ less, respectively. Then, we have that

$$\begin{aligned}
\Delta_3 &= N_3 - N_3' \\
&= d_i^3 + d_j^3 - (d_i - 1)^3 - (d_j - 1)^3 - (d_i - d_j)^2 - \sum_{l \in \mathcal{N}(i), l \neq j} (d_l - d_i)^2 - (d_l - d_i + 1)^2 \\
&\quad - \sum_{l \in \mathcal{N}(j), l \neq i} (d_l - d_j)^2 - (d_l - d_j + 1)^2
\end{aligned}$$

where d_i is the degree of node i in the original graph G and $\mathcal{N}(i)$ is the set of the neighbors of node i. The decrease Δ_3 can be simplified as

$$\begin{aligned}
\Delta_3 &= 2 - 3(d_i + d_j) + 3(d_i^2 + d_j^2) - (d_i - d_j)^2 + \sum_{l \in \mathcal{N}(i), k \neq j} (2d_l - 2d_i + 1) + \sum_{l \in \mathcal{N}(j), l \neq i} (2d_l - 2d_j + 1) \\
&= 2(d_i^2 + d_j^2) + 2d_i d_j + 2 - 3(d_i + d_j) + (d_i + d_j - 2) - 2d_i(d_i - 1) - 2d_j(d_j - 1) \\
&\quad + \sum_{l \in \mathcal{N}(i), k \neq j} 2d_l + \sum_{l \in \mathcal{N}(j), k \neq i} 2d_l \\
&= 2d_i d_j + \sum_{l \in \mathcal{N}(i), k \neq j} 2d_l + \sum_{l \in \mathcal{N}(j), k \neq i} 2d_l \\
&= 2d_i d_j + 2(s_i + s_j) - 2(d_i + d_j)
\end{aligned}$$

where

$$s_i = \sum_{l \in \mathcal{N}(i)} d_l \tag{14}$$

is the total degree of all the direct neighbors of a node i. Similarly, the decrease in the number of two hop walks is denoted as

$$\Delta_2 = N_2 - N_2' = 2(d_i + d_j - 1)$$

Note that Δ_2 and Δ_3 are only functions of a local property, i.e. the degree d_i and d_j of the two end nodes of a link l_{ij}. The complexity of computing Δ_3 or Δ_2 for all linked node pairs is $O(N^2)$ in a dense graph, which is the worst case.

4 Strategies to minimize the largest eigenvalue by link removal

This section discusses and compares various strategies in Fig. 5, denoted by S.

The first strategy, as suggested in Section 3, is to remove the link with maximum product of the eigenvector components. Specifically, this strategy is denoted by $S = x_i x_j$ instead of $S = (x_1)_i (x_1)_j$ to simplify the notation in the figures, and it removes that link $l = i \sim j$ for which $(x_1)_i (x_1)_j$ is maximal.

Section 3.3 hints that the spectral radius is possibly decreased the most by a link removal that either reduces $S = \frac{N_3}{N_2}$ or the assortativity $S = \rho_D$ the most. Strategy $S = \frac{N_3}{N_2}$ will remove the link such that $\frac{N_3 - \Delta_3}{N_2 - \Delta_2}$ is minimized.

The other considered strategies $S = d_i d_j$ and $S = d_i + d_j$ remove that link $l = i \sim j$ with largest sum or product of the degrees of the link's end points, whereas the strategies $S = s_i + s_j$ and $S = s_i s_j$ remove the link with the largest sum or product of the total degree s_i of the neighbors at both end points. Finally, we also considered the strategy $S =$ betweenness, that removes the link with highest link betweenness, i.e. the number of shortest paths between all node pairs that traverse the link.

We define the performance measure Ξ_S of a particular link removal strategy S by

$$\Xi_S = (\lambda_1(A) - \lambda_1(A_1))_{\text{optimal}} - (\lambda_1(A) - \lambda_1(A_1))_{\text{Strategy } S}$$

Fig. 5 compares the above explained strategies. Fig. 5 confirms that strategy $S = x_i x_j$ is superior to all other strategies. There is a very small difference between the strategies $S = d_i + d_j$ and $S = d_i d_j$ and between $S = s_i + s_j$ and the corresponding product $S = s_i s_j$. In both cases the product strategy is slightly better (but the difference is not observable from Fig. 5).

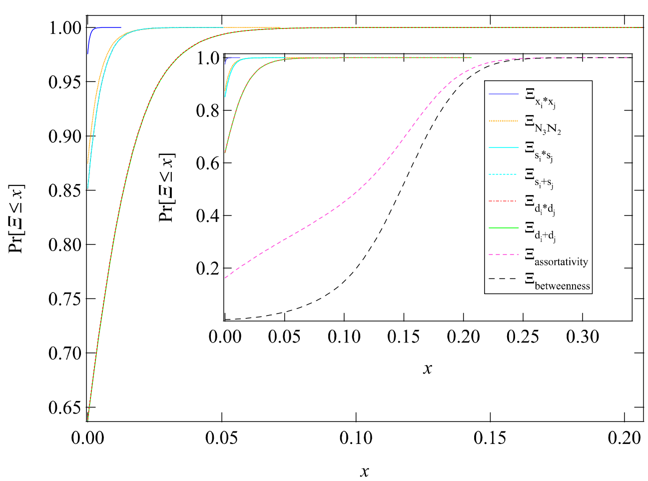

Figure 5: (Color online) Various strategies applied to 10^6 instances of ER graphs with $N = 20$ and $p = 2 \ln N / N$. The insert shows two additional strategies "assortativity" and "betweenness" that are clearly worse than the others.

Another strategy is to remove the link that possibly disconnects the graph G into two disjoint graphs G_1 and G_2. However, this strategy is not always optimal as illustrated in Fig. 6. Only when

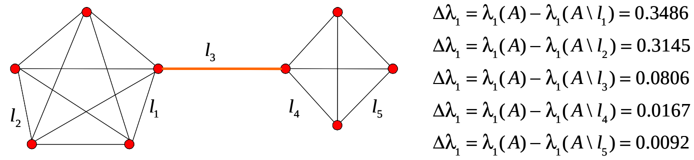

Figure 6: (Color online) All possible $\Delta\lambda_1$ are computed when one link is removed.

both G_1 and G_2 are the same, we found that the removal of the connecting link induces the largest decrease in $\Delta\lambda_1$. Since this strategy cannot be applied always, we have further ignored this strategy.

4.1 Removing $m > 1$ links

In this section, we investigate the behavior of the several strategies when more than one link is removed. We generated 10^4 Erdős-Rényi graphs with $N = 10$ nodes and $L = 20$ links, of which about two percent are disconnected. From each of the generated graphs, all the links are removed one by one following the different "greedy" strategies. We compare the decrease in λ_1 for each strategy to the optimal solution found by removing all possible combinations of m links. In Fig. 7, the percentage of agreement between the greedy strategies and the optimal strategy is shown.

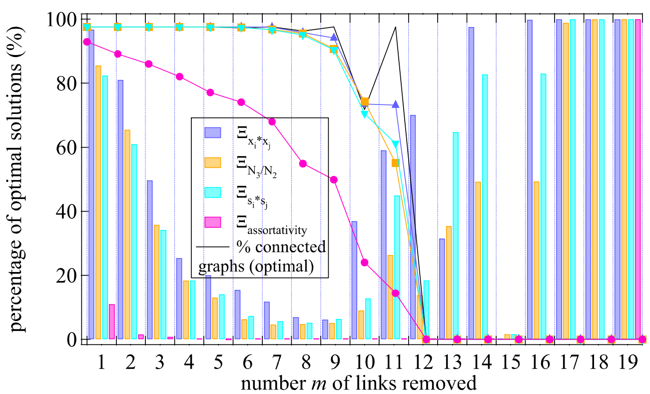

Figure 7: (Color online) Four strategies compared with the global optimum as a function of the number m of removed links in ER random graphs with $N = 10$ nodes and $L = 20$ links, where 10^4 instances are generated. The lines show the percentage of connected graphs per strategy after the removal of m links.

Fig. 7 illustrates that strategy $S = \max_{1 \leq (i,j) \leq N} (x_1)_i (x_1)_j$ is nearly always (except for $m = 13$) superior to strategy $S = N_3/N_2$ and $S = s_i s_j$, which agrees with the theory in Section 3. Fig. 7 exhibits a regime change from $m = 10$ on, where the connectivity of the graphs starts to decrease rapidly.

The peculiar regime for $m > 10$ can be understood as follows. The optimal solution for $m = 10$ removals is a circuit, if the original graph contains a single connected circuit on $N = 10$ nodes. If strategy $S = \max_{1 \leq (i,j) \leq N} (x_1)_i (x_1)_j$ finds the optimal solution for $m = 10$ removals, the only possible solution for $m = 11$ removals is to cut the circuit to form a path. This is also the optimal solution.

The eigenvector components of a path graph are symmetrical around the node(s) in the middle of the path and are maximal for the center node(s). Strategy $S = \max_{1\leq(i,j)\leq N}(x_1)_i(x_1)_j$ will, for the next link removal, cut the path in the middle. The resulting graph is also the optimal solution. In the next step, however, the strategy will cut one of the paths in two, resulting in three paths of lengths one, two and four links, respectively. The optimal solution for $m = 13$ link removals consists of a graph with three paths of lengths two and one of length three. This graph can never be formed by strategy $S = \max_{1\leq(i,j)\leq N}(x_1)_i(x_1)_j$ starting from a circuit. The optimal solution for $m = 14$ consists of two paths of length two and two paths of length one, which can be obtained in many different ways, including cutting the longest path of the solution for $m = 13$. In almost 98% of the cases this solution is found by strategy $S = \max_{1\leq(i,j)\leq N}(x_1)_i(x_1)_j$. The high success rate means, at the same time, that the optimal solution for $m = 15$ is almost never found because it cannot be reached from the optimal solution of $m = 14$ by another link removal, regardless of the followed strategy. The weaker performance of strategy $S = s_is_j$ for $m = 12$ can be explained by considering the optimal solution for $m = 11$ which is a path of nine links. Strategy $S = s_is_j$ removes the link that has the maximum product of the one hop neighbors of its endpoints. Since a path has an even degree distribution, except for the endpoints, the five links that form the center of the path have an equal probability of being removed. Consequently, the optimal solution for $m = 11$ will result in the optimal solution for $m = 12$ only one in five times. The other four possibilities lead to a graph with either a combination of a path of length two and a path of length six or a combination of a path of length three and a path of length five. Both these graphs will give the optimal solution for $m = 13$ link removals, which explains the increased succes rate for $m = 13$.

At $m = 15$, the graph consists of 5 links and $N = 10$ nodes, configured in separated "cliques" K_2 (i.e. line segments) and the largest eigenvalue is minimal at $\lambda_1 = 1$. For $m > 15$, the strategies are all the same: a clique K_2 (i.e. disjoint link) is removed.

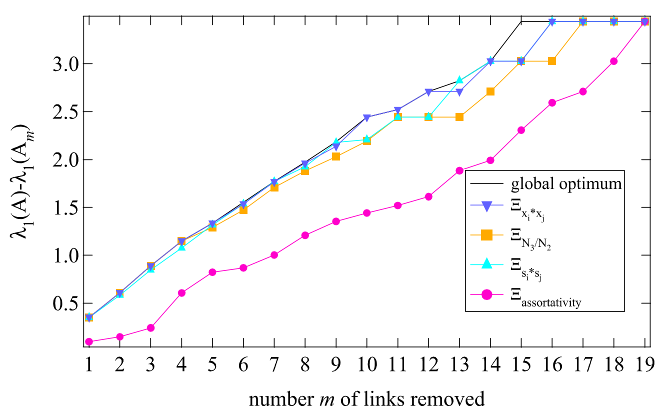

Figure 8: (Color online) The performance $\lambda_1(A) - \lambda_1(A_m)$ of four strategies versus m link removals in a typical instance of a graph with $N = 10$ and $L = 20$ links.

Fig. 8 illustrates four strategies on a typical instance of a network with $N = 10$ and $L = 20$ links. While the strategy $S =$ assortativity clear underperforms, the three other strategies $S = x_ix_j$, $S = N_3/N_2$ and $S = s_is_j$ are competitive: for small m, the strategy $S = x_ix_j$ excels (as shown in

Fig. 7), but for larger m the others can outperform. Again, this phenomenon is characteristic for an NP-complete problem, where the whole previous history of links removals affects the current link removal. The considered strategies (except for the global optimum one) are greedy and only optimize the current link removal, irrespective of the way in which the current graph G_m is obtained previously.

5 Scaling Law of $(\lambda_1(A) - \lambda_1(A_m))_{\text{optimal}}$

Another observation from Fig. 8 is that

$$\Delta\lambda_m|_{\text{optimal}} = \lambda_1(A) - \lambda_1(A_m)|_{\text{optimal}} = O\left(m^\beta\right) \tag{15}$$

where $\beta \leq 1$. In other words, we conjecture that the scaling of $\lambda_1(A) - \lambda_1(A_m)$ with m is sublinear in m (for non-regular graphs) and that the coefficient β is likely a function of the type of graph. Obviously, $\Delta\lambda_m = 0$, when $m = 0$. Applying the upper bound (1) to $\lambda_1(A_m)$ shows that

$$\begin{aligned}\Delta\lambda_m &\geq \lambda_1(A) - \sqrt{1-\frac{1}{N}}\sqrt{2L-2m} \\ &\geq \lambda_1(A) - \sqrt{1-\frac{1}{N}}\sqrt{2L} + \sqrt{1-\frac{1}{N}}\sqrt{2m} = O\left(m^{1/2}\right)\end{aligned}$$

On the other hand, if G_m is a regular graph, then

$$\Delta\lambda_m = \lambda_1(A) - \frac{2L-2m}{N} = O(m)$$

In particular, if G and G_m are regular graphs, then

$$\Delta\lambda_m = \frac{2m}{N} \tag{16}$$

These arguments illustrate that $\frac{1}{2} < \beta \leq 1$. Fig. 8 shows that $\lambda_1(A) - \lambda_1(A_m)|_{\text{optimal}}$ is likely close to $\beta = 1$, which suggests that the optimal way to remove m links is to make G_m as regular as possible, because the lowest possible $\lambda_1(A_m)$ with given N and $L-m$ is obtained for a regular graph (as follows from the Rayleigh inequality $\lambda_1(A) \geq \frac{2L}{N}$).

While the law (15) is difficult to prove in general, we provide evidence by computing the decrease in λ_1 when m random links are removed in the class of Erdős-Rényi random graphs $G_p(N)$. For sufficiently large Erdős-Rényi random graphs $G_p(N)$, we know [3] that

$$E[\lambda_1] = (N-2)p + 1 + O\left(\frac{1}{\sqrt{N}}\right)$$

When m random links are removed from $G_p(N)$, we again obtain an Erdős-Rényi random graph with link density

$$p^* = \frac{L-m}{\binom{N}{2}}$$

Hence,

$$\begin{aligned}E[\Delta\lambda_m] &= E[\lambda_1(G_p(N))] - E[\lambda_1(G_{p^*}(N))] \\ &= (N-2)(p-p^*) + R_p(N)\end{aligned}$$

where the error term $R_p(N)$ is unknown. Assuming that $R_p(N)$ is negligibly small, we find, for sufficiently high N,

$$E[\Delta\lambda_m] \simeq \frac{(N-2)\,m}{\binom{N}{2}} = \frac{2m}{N} - \frac{2m}{N(N-1)}$$

Thus, the average decrease in $\lambda_1(A) - \lambda_1(A_m)$ after removing m random links in $G_p(N)$ is approximately, for large N,

$$E[\Delta\lambda_m] \simeq \frac{2m}{N} \tag{17}$$

which is close to (16) for regular graphs.

For $m = 1$, simulations on various types of graphs in Fig. 9 and Fig. 10 suggest the scaling law

$$(\lambda_1(A) - \lambda_1(A_1))_{\text{optimal}} = \frac{\alpha}{N} \tag{18}$$

where α is graph specific. In other words, $N\Delta\lambda_1 = \alpha$ is independent of the size of the graph.

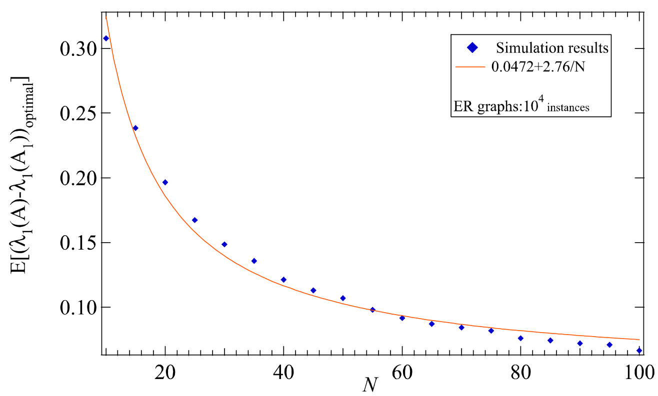

Figure 9: (Color online) The scaling law of $(\lambda_1(A) - \lambda_1(A_1))_{\text{optimal}}$ for ER random graphs as a function of N.

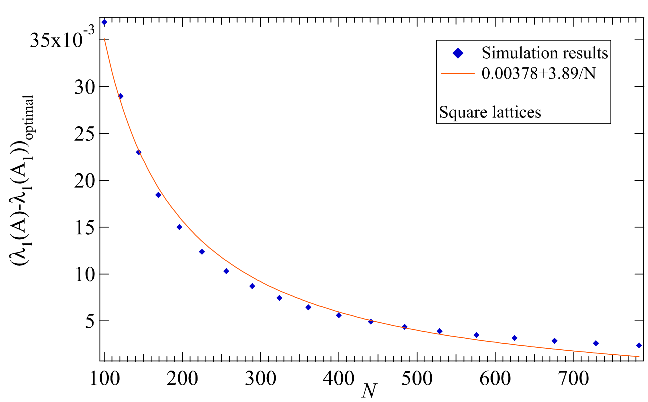

Figure 10: (Color online) The scaling law of $(\lambda_1(A) - \lambda_1(A_1))_{\text{optimal}}$ for square lattices as a function of N.

Ignoring the asymptotic nature of the analysis that led to (17), we observe that, for $m = 1$, a maximum occurs at $N = 2$. Fig. 11 shows the pdf of $\Delta\lambda$ for Erdős-Rényi random graphs, where for each curve 10^6 ER graphs have been created in which one random link was removed. The simulations agree with $E[\Delta\lambda] \simeq \frac{2}{N}$ and indicate that $\text{Var}[\Delta\lambda] \simeq 13 + 2E[\Delta\lambda]$. Since a random link removal is inferior to the removal of the optimal link, Fig. 9 indeed illustrates that the coefficient of the inverse N scaling law $\alpha_{G_p(N)} \simeq 2.75 > 2$. Fig. 10 shows that $\alpha_{lattice} \simeq 3.9 > \alpha_{G_p(N)} \simeq 2.75$, which may indicate that deviations from regularity causes λ_1 to decrease more.

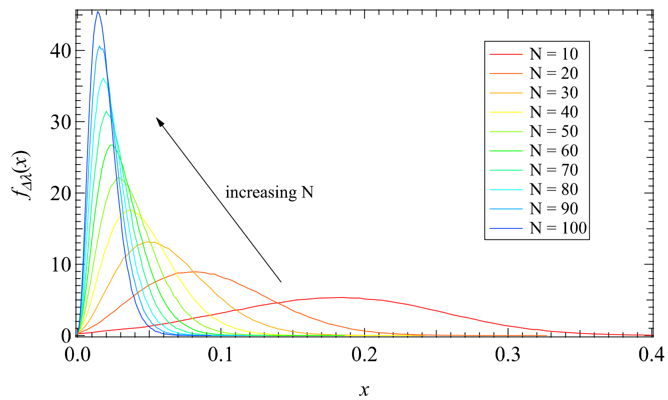

Figure 11: (Color online) The probability density function of $\Delta\lambda_1$ for ER random graphs of several sizes N.

6 Conclusions

The spectral radius is both fundamental in graph theory as well as in many dynamic processes in complex networks such as epidemic spreading, synchronization and reaching consensus [3, p. 200]. We have shown that the spectral radius minimization problem (for both link as node removals) is an NP-hard problem, which opens the race to find the best heuristic. In particular, in large infrastructures such as transportation networks, where removing links can be very costly, a near to optimal strategy is desirable. We have shown that an excellent strategy is $S = x_i x_j$: on average, this strategy outperforms most other heuristics, but it does not beat them at all times. Beside graph theoretic bounds and arguments that underline the goodness of the heuristic $S = x_i x_j$, two scaling laws (15) and (18) are found: these laws may help to estimate the decrease in spectral radius as a function of the number N of nodes and/or the number m of link removals. It may be worthwhile that further investigations compute or estimate the scaling parameters β in (15) as well as α in (18).

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