Towards Optimal Robustness of Network Controllability: An Empirical Necessary Condition

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Abstract—To better understand the correlation between network topological features and the robustness of network controllability in a general setting, this paper suggests a practical approach to searching for optimal network topologies with given numbers of nodes and edges. Since theoretical analysis is impossible at least in the present time, exhaustive search based on optimization techniques is employed, firstly for a group of small-sized networks that are realistically workable, where exhaustive means 1) all possible network structures with the given numbers of nodes and edges are computed and compared, and 2) all possible node-removal sequences are considered. An empirical necessary condition (ENC) is observed from the results of exhaustive search, which shrinks the search space to quickly find an optimal solution. ENC shows that the maximum and minimum in- and out-degrees of an optimal network structure should be almost identical, or within a very narrow range, i.e., the network should be extremely homogeneous. Edge rectification towards the satisfaction of the ENC is then designed and evaluated. Simulation results on large-sized synthetic and real-world networks verify the effectiveness of both the observed ENC and the edge rectification scheme. As more operations of edge rectification are performed, the network is getting closer to exactly satisfying the ENC, and consequently the robustness of the network controllability is enhanced towards optimum.

Index Terms—network controllability, robustness, empirical necessary condition, node degree, optimization

I. INTRODUCTION

Complex networks have gained growing popularity and accelerating momentum since late 1990s, becoming a self-contained discipline integrating network science, systems engineering, statistical physics, applied mathematics, social sciences and the like [1]–[4]. The ultimate goal of understanding complex networks is to control them for utilization. In this regard, whether or not they can be controlled is essential, which leads to the fundamental concept of network controllability. Consequently, network controllability has become a focal issue in the studies of complex networks [5]–[15], where the concept of controllability refers to the ability of a network in moving from any of its initial state to any desired target state under an admissible control input within a finite duration of time.

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It was shown [5] that identifying the minimum number of external control inputs (recalled driver nodes) to achieve a full control of a directed network requires searching for a maximum matching of the network, which quantifies the network structural controllability. Practically, however, finding a maximum matching of a large-scale network is computationally time-consuming or even impossible. Along the same line of research, in [6], an efficient measure to assess the state controllability of a large-scale sparse network is suggested, based on the rank of the controllability matrix of the network.

It has been quite a long time for people to understand the intrinsic relation between topology and controllability of a general directed network. In [7], it demonstrates that clustering and modularity have no discernible impact on the network controllability, while underlying degree correlations have certain effects. In [8], it reveals that random networks of any topology are controllable by an infinitesimal fraction of driver nodes, if both of its minimum in- and out-degrees are greater than two. The underlying hierarchical structure of such a network leads to an effective random upstream (or downstream) attack, which removes the hierarchical upstream (or downstream) node of a randomly-picked one, since this attack strategy would remove more hubs than a random attack strategy does [16]. In [16], a control centrality is defined to measure the importance of nodes, discovering that the upstream (or downstream) neighbors of a node are usually more (or less) important than the node itself. Interestingly, it is recently found that the existence of special motifs such as loops and chains is beneficial for enhancing the robustness of the network controllability [17]–[19]. The network controllability of some canonical graph models is studied and compared quite thoroughly in [20]. As for growing networks, the evolution of network controllability is investigated in [21]. Moreover, the controllability of multi-input/multi-output networked systems is studied in [10], [22], with necessary and sufficient conditions derived. A comprehensive overview of the subject is presented in a recent survey [15].

On the other hand, random failures and malicious attacks on complex networks have become concerned issues today [16], [23]–[27]. To resist attacks, strong robustness is desirable and even necessary for a practical network. A measure for the network controllability is quantified by the number of external control inputs needed to recover or to retain the network controllability after the occurrence of an attack, while its robustness is quantified by a sequence of values that record the remaining levels of the network controllability after a sequence of attacks. To optimize the network robustness, one aims to enhance and maintain a highest possible connectedness.
of the network against various attacks [25]. Given the degree-preserving requirement or constraint (i.e., the degree of each node remains unchanged through the process of optimization), an edge-rewiring method is proposed in [28] to increase the number of edges between high-degree nodes, thus generating a new network with a highest $k$-shell component. In [29], the structure of a network is modified by degree-preserving edge-rewiring, where spectral measures are used as the objective for optimization. By optimizing a specified spectral measure of the network through random edge-rewiring, the robustness of the resultant network is accordingly enhanced. It is however noticed that, although widely used as an estimator of the robustness for real-world networks, the correlation between spectral measures and the robustness remains unclear [30]. Nevertheless, given a reliable predictive measure or indicator of the network robustness, optimization algorithms can be applied [31], [32]; while if there are more than one predictive measures, multi-objective optimization schemes can be applied instead [33]. In [34], it is shown that both edge-robustness and node-robustness (i.e., the robustness against edge- and node-removals, respectively) can be enhanced simultaneously. A common observation is that heterogeneous networks with onion-like structure are robust against attacks [25], [35]–[37]. The evolution of alternative attack and defense is studied in [38], where attack means edge-removal and defense means edge-replenishment. The connectedness of the largest-sized connected cluster is the typically-used measure for such robustness [25]. It should be noted that, for the study to be presented in this article, although the robustness of network connectedness has a certain positive correlation with the robustness of network controllability, they have very different measures and objectives.

Regarding the controllability of a complex network, it refers to a static property that reflects how well the network can be controlled. Yet, the robustness of network controllability is a dynamic process that reflects how well the network can maintain its controllability against destructive attacks by means of node-removal or edge-removal. Reportedly, intentional degree-based node-removal attacks in the sense of removing nodes with highest degrees are more effective than random attacks on network structural controllability over directed random-graph networks and also directed scale-free networks [39]. In [40], the optimization of robustness of controllability is transformed into the transitivity maximization for control routes. In [41], edge directionality is considered as the only operation to enhance the robustness of controllability, preserving the underlying topology meanwhile. In [42], the change of controllability of random networks and scale-free networks in the processes of cascadings failures is studied. For networks with different topologies, the results show that the robustness of network controllability will become stronger through allocating different control inputs and edge capacities.

Both random and intentional edge-removal attacks have also been studied by many. In [43], for example, it shows that the intentional edge-removal attack by removing highly-loaded edges is very effective in reducing the network controllability. It is further observed, in e.g. [44], that intentional edge-based attacks are usually able to trigger cascadings failures in scale-free networks but not necessarily in random-graph networks. These observations have motivated some recent in-depth analysis of the robustness of the network controllability [17]. In this regard, both random and intentional attacks as well as both node-removal and edge-removal attacks were investigated. Specifically, for a random upstream (or downstream) attack that removes the upstream (or downstream) node of a randomly-picked one, the upstream and downstream relationship is determined by the underlying hierarchical structure of the network. This type of random attack has a non-uniform distribution, since the hub nodes are more likely being attacked in this scenario [16]. In particular, it was found that redundant edges, which are not included in any of the maximum matchings, can be rewired or re-directed so as to possibly enlarge a maximum matching such that the needed number of driver nodes is reduced [45], [46].

Although the relations between network topology and network controllability have been investigated in some studies, there is no prominent theoretical indicator or performance index that can well describe the robustness of network controllability with a measures based on such relations. Under different attacks, the robustness of network controllability behaves differently. The nature of the attack methods leads to different measures of the importance of a node (or an edge) in a network. Generally, degree and betweenness are two commonly-used measures for the importance [39].

This paper continues the above investigations to further explore the network topological properties that affect or even determine the optimal robustness of both state and structural controllability, against random node-removal attack. First, an exhaustive search is performed on a group of small-sized networks. Then, an empirical necessary condition (ENC) is observed and summarized. A simple yet effective edge rectification strategy, namely the random edge rectification (RER), is proposed for modifying the network topology to satisfy the ENC, so that the robustness of network controllability is enhanced. Similarly to [47], where the optimal network topology with best possible synchronizability is observed and summarized through extensive empirical experiments, the observed ENC is confirmed by extensive numerical simulations here, since it is impossible to theoretically prove, and probably no one could do so at this time. Finally, both ENC and RER are verified by optimizations of a number of synthetic and real-world networks with different properties.

The rest of the paper is organized as follows. Section II reviews the network controllability and its robustness against various destructive attacks. Section III introduces the ENC and the RER. Section IV investigates both ENC and RER by extensive numerical simulations, on both synthetic and real-world networks. Section V concludes the investigation.

II. NETWORK CONTROLLABILITY AND ITS ROBUSTNESS

A. Network Controllability and Criteria

Consider a linear time-invariant (LTI) networked system described by $\dot{x} = Ax + Bu$, where $A$ and $B$ are constant matrices of compatible dimensions, $x$ is the state vector, and $u$ is the control input. The system is state controllable if and
only if the controllability matrix \([B \ AB \ A^2B \ \ldots \ A^{N-1}B]\) has a full row-rank, where \(N\) is the dimension of \(A\). The concept of \textit{structural controllability} is a slight generalization dealing with two parameterized matrices \(A\) and \(B\), in which the parameters characterize the structure of the underlying networked system: if there are specific parameter values that can ensure the system described by the two parameterized matrices be state controllable, then the system is structurally controllable. In case the system is controllable, its state vector \(x\) can be driven from any initial state to any target state in the state space within finite time by a suitable control input \(u\).

The controllability of a network, or networked system, is measured by the density of the controlled nodes, \(n_D\), defined by

\[
n_D = \frac{N_D}{N}, \tag{1}
\]

where \(N_D\) is the number of external control inputs (driver nodes) needed to retain the network controllability after the occurrence of an attack to the network, while the denominator \(N\) is the current network size that ensures the controllability. This measure \(n_D\) allows networks with different sizes can be compared. The network size does not change during an edge-removal attack but would be reduced by a node-removal attack. It is noted that the smaller the \(n_D\) value is, the better the network controllability will be.

Generally, there are two ways to calculate the number \(N_D\) of driver nodes, for structural controllability and exact (state) controllability, respectively. To introduce these two criteria, first recall from graph theory that in a directed network, a matching is a set of edges that do not share common start nodes or common end nodes. A maximum matching is a matching that contains the largest possible number of edges, which cannot be further extended in the network. A node is matched if it is the end of an edge in the matching; otherwise, it is unmatched. A perfect matching is a (maximum) matching that matches all nodes in the network.

According to the \textit{minimum inputs theorem} [5], when a maximum matching is found, the number \(N_D\) of driver nodes is determined by the number of unmatched nodes, i.e.,

\[
N_D = \max\{1, N - |E^*|\}, \tag{2}
\]

where \(|E^*|\) is the number of edges in the maximum matching \(E^*\). If a network has a perfect matching, then the number of driver nodes is \(N_D = 1\) and the control input can be put at any node; otherwise, \(N_D = N - |E^*|\) control inputs are needed, which should be put at those unmatched nodes.

As for exact controllability, if a network is sparse, its number \(N_D\) of driver nodes can be calculated by \(N_D = \max\{1, N - \text{rank}(A)\}\). Here, a network is considered to be sparse if the number of edges \(M\) (i.e., the number of nonzero elements of the adjacency matrix) is much smaller than the possible maximum number of edges, \(M_{\text{max}} = N \cdot (N - 1)\). Usually, if \(M/M_{\text{max}} \leq 0.05\), then it is considered as a sparse network.

\section*{B. Robustness of Network Controllability}

The robustness of network controllability is evaluated after a node or an edge is removed, one by one, yielding a sequence of values that reflect how robust (or vulnerable) a networked system is against the destructive attacks. Different attack strategies result in different damages to the network topology and also its controllability. An attack strategy is chosen according to the “importance” of nodes or edges in the network, but there are different concepts of importance in applications. In this paper, the importance is the controllability of the network.

Generally, there are two types of attacks, namely intentional and random node-removal attacks. An intentional attack aims at removing a node that is the most important to maintain the network controllability; for example, the node with the largest degree or betweenness. A random attack removes a randomly-picked node at each time step. In this paper, only \textit{random node-removal} attacks are considered, while intentional node-removal can be similarly discussed.

The comparison of robustness of network controllability among different networks will be performed by 1) observing the resultant curves of the controllability matrices, and 2) comparing the robustness measure \(R_c\) [18], [25], [27], [48], defined as follows:

\[
R_c = \frac{1}{N-1} \sum_{i=1}^{N-1} f(i), \tag{3}
\]

where, as an extension of the robustness measure defined in [25], \(f(i)\) can be the density of the required driver nodes [27], [48] or the rank of the comparison of controllability [18], when a total of \(i\) nodes are removed. In both cases, a smaller value of \(R_c\) means better robustness against attacks.

\section*{III. Empirical Necessary Condition for Optimal Topology}

In this section, the relation between topological structure and robustness of controllability is first studied, by observing the attack simulations on some very small-sized networks. In this case, an exhaustive attack strategy can be applied. Then, the observations are summarized as the ENC, as presented by Eq. (5) in Section III-B. To rectify an arbitrarily given network towards the satisfaction of ENC, a simple rectification strategy is proposed in Section III-C.

\subsection*{A. Exhaustive Attack}

To understand a full picture of the controllability change under all possible node-removal attacks, an exhaustive attack to a set of small-sized networks is first simulated and evaluated.

Given a network of \(N\) nodes, there are \((N-1)!\) permutations of the node-removal sequence, e.g., 1, 2, \ldots, \(N - 1\), and 3, \(N - 1\), \ldots, 5, etc. Note that an intentional attack (e.g., a degree-based attack) is a specific case in such (permuted) sequences. By performing a node-removal sequence, it generates a resultant curve of controllability values (denoted by \(\delta\)), which is the controllability measure for the remaining network after a total of \(i\) \((i = 1, 2, \ldots, N - 1)\) nodes were removed sequentially. The robustness of controllability of a network under the exhaustive attack is then obtained by averaging all
these \((N - 1)!\) curves, i.e., a mean curve denoted by \(\bar{\delta}\) as follows:
\[
\bar{\delta} = \frac{1}{(N - 1)!} \sum_{k=1}^{(N-1)!} \delta_k,
\]
where \(\delta_k\) represents the \(k\)-th resultant curve of controllability values. The exhaustive attack strategy considers all the sequences equally. Thus, the mean resultant curve of the exhaustive attack is equivalent to the mean of random attacks when the number of repeated runs is large enough. Each node is considered of equal importance in the network controllability study, where each node \(i\) \((i = 1, 2, \ldots, N)\) has an equal probability to be removed at the \(j\)th \((j = 1, 2, \ldots, N - 1)\) step within any attack sequence.

Table I shows the results of performing the exhaustive attack on small-sized networks, where the network size is set to 4, 5, and 6 only. In the table, ‘PI’ represents the number of possible instances with given \(N\) and \(M\), after filtering out isomorphs. For example, when \(N = 5\) and \(M = 10\), there are 1665 possible combinations to form a unique network instance. For each instance, all \((N - 1)!\) attack sequences are implemented and recorded. In the table, ‘ENC’ represents the number of network instances that exactly satisfy the ENC (5) in Section III-B); ‘O’ represents the number of optimal robustness instances. The topology of the optimal instance presented in Table I can be found in Figs. S1–S3 of the Supplementary Information (SI). A phenomenon can be clearly observed from Table I and the optimal instance presented in SI, as summarized in Fig. 1. Empirically, it is observed that the optimal instance set is a subset of the instances that exactly satisfy the ENC, which is a subset of the full set of all possible network instances with the given values of \(N\) and \(M\).

### TABLE I: Results of performing exhaustive attack on small-sized networks. PI represents the number of possible network instances with given \(N\) and \(M\). ENC represents the number of network instances that satisfy Eq. (5); O represents the number of optimal robustness instances. The relationships of PI, O, and ENC sets are shown in Fig. 1.

| \(N\) | \(M\) | PI | ENC | O |
|------|------|----|-----|---|
| 4    | 4    | 22 | 5   | 1 |
| 5    | 5    | 37 | 5   | 1 |
| 6    | 6    | 47 | 12  | 2 |
| 7    | 7    | 38 | 5   | 1 |
| 8    | 8    | 27 | 2   | 1 |
| 9    | 9    | 13 | 3   | 2 |
| 10   | 10   | 5  | 3   | 2 |
| 11   | 11   | 1  | 1   | 1 |

| \(N\) | \(M\) | PI | ENC | O |
|------|------|----|-----|---|
| 4    | 5    | 108| 1   | 1 |
| 5    | 6    | 326| 10  | 1 |
| 6    | 7    | 607| 47  | 2 |
| 7    | 8    | 112| 69  | 2 |
| 8    | 9    | 147| 26  | 1 |
| 9    | 10   | 1665| 5  | 1 |
| 10   | 11   | 1489| 26 | 1 |
| 11   | 12   | 1154| 70 | 2 |

**B. Empirical Necessary Condition**

It returns \((N - 1)!\) controllability curves after the exhaustive attack is performed. The mean curve is calculated to be the average robustness performance. An illustrative example is given in Fig. 2, where the means and standard deviations are given. Then, the robustness measure \(R_c\) of each network is calculated according to Eqs. (3) and (4). In this example, network Net1 is recognized to have better robustness of controllability than Net2, since Net1 has a lower mean curve.

Since both the number of possible network instances and the number of attack sequences increase drastically as network size increases, only very small-sized networks are examined, with results presented in Table I. For given \(N\) and \(M\), the number of instances with optimal robustness is much fewer than the number of all possible instances. Considering together the reported observations [17]–[19], it can be concluded that an optimal instance has the following characteristics: 1) it contains a directed global loop that connects all the \(N\) nodes; 2) both the in- and out-degrees are extremely-homogeneously distributed with extremely small differences, if any. Here, the first observation may be integrated into the second. Since the in- and out-degrees of nodes in a directed loop are both extremely-homogeneously distributed, each node has in-degree one and out-degree one. This observation is also consistence with the observations reported earlier in [17]–[19], where it was found that multiple-loop and multiple-chain structures enhance the robustness of network controllability. Therefore, based on all these observations, for a directed network with \(N\) nodes and \(M\) edges, the network topology with optimal robustness of controllability (against exhaustive or random
node attacks) should satisfy the following condition:

\[ \frac{M}{N} \leq k_i^{\text{in/out}} \leq \left\lceil \frac{M}{N} \right\rceil, \quad i = 1, 2, \ldots, N, \quad (5) \]

where \( k_i^{\text{in/out}} \) means both in- and out-degrees, in which as a standard notation the floor function \( \lfloor x \rfloor \) returns the greatest integer less than or equal to \( x \), and the ceiling function \( \lceil x \rceil \) returns the least integer greater than or equal to \( x \).

Equation (5) suggests that the degree distribution of optimal instances should be allocated in a very narrow slot in the plot. For example, as illustrated by Fig. 3, given \( N \) nodes and \( N \) edges, the only instance satisfying Eq. (5) is a directed global loop (Fig. 3(A)), where each node has in-degree one and out-degree one, and any tree structure (Fig. 3(B)) or reverse edge in a ring-shaped structure (Fig. 3(C)) does not belong to the global loop hence will significantly alter the extremely-homogeneous distribution of node degrees. This is also obvious from Table I, where for each case of \( M = N = 4, 5, 6 \), there is only one instance satisfying the ENC, which is also the optimal instance.

![Fig. 3: [Color online] Given equal numbers of nodes and edges, possible topologies include: (A) a directed global loop, (B) a tree, and (C) a ring-shaped network with a reverse edge.](image)

Empirically, it is observed that all instances with optimal robustness of controllability satisfy the ENC. But, for a network instance satisfying ENC, it is not necessarily optimal, as illustrated by Fig. 1. Therefore, this is only a necessary condition.

With the restriction of ENC, the number of candidate instances in searching for optimal instances is significantly reduced. For example, as can be seen from Table I, given \( N = 5 \) and \( M = 10 \), the probability for a random network instance has the optimal robustness is 1/1665. By searching only the instances that satisfy ENC, the probability increases to 1/5. Thus, the probability of success is largely improved and the computational cost is significantly reduced.

It can also be observed from Table I that, as \( N \) and \( M \) increase, the number of instances satisfying ENC remains relatively small, compared to the total number of possible instances. Thus, with the objective of searching for the optimal instances, many instances that do not satisfy ENC can be eliminated from the candidate pool. When \( N \) and \( M \) are not very small, the number of possible instances could be tremendously huge. Therefore, the ENC provides an efficient means of improving the performance of searching for optimal instances from a large pool of candidates.

### C. Edge Rectification

Since it is computational impossible to review all the possible instances when \( N \) and \( M \) are large, a simple yet effective strategy called the random edge rectification (RER) is proposed here to rectify a synthetic or real-world network for its satisfaction of the ENC. It is a variant network, one with the same \( N \) and \( M \) but different topology. On the other hand, it is also impossible to apply exhaustive attacks on a large-sized network, so a random attack is applied with many repeated runs instead.

For any node \( i \), if its in- or out-degree does not satisfy Eq. (5), edge rectification is needed. There are four possible edge rectification operations:

1. If \( k_i^{\text{out}} < \lfloor M/N \rfloor \), then find another node \( k \) with out-degree greater than \( \lfloor M/N \rfloor \), and randomly pick one of its out-edges, \( A_{k,i} \). Delete this edge \( A_{k,i} \) and add an edge \( A_{k,i} \). This increases \( k_i^{\text{out}} \) by one and decreases \( k_k^{\text{out}} \) by one.
2. If \( k_i^{\text{out}} > \lfloor M/N \rfloor \), then randomly pick one of its out-edges \( A_{i,j} \), and find another node \( k \) with out-degree less than \( \lfloor M/N \rfloor \). Delete this edge \( A_{i,j} \) and add an edge \( A_{k,j} \). This decreases \( k_i^{\text{out}} \) by one and increases \( k_k^{\text{out}} \) by one.
3. If \( k_i^{\text{in}} < \lfloor M/N \rfloor \), then find another node \( k \) with in-degree greater than \( \lfloor M/N \rfloor \), and randomly pick one of its in-edges \( A_{l,k} \). Delete this edge \( A_{l,k} \) and add an edge \( A_{l,k} \). This increases \( k_i^{\text{in}} \) by one and decreases \( k_k^{\text{in}} \) by one.
4. If \( k_i^{\text{in}} > \lfloor M/N \rfloor \), then randomly pick one of its in-edges \( A_{j,i} \), and find another node \( k \) with in-degree less than \( \lfloor M/N \rfloor \). Delete this edge \( A_{j,i} \) and add an edge \( A_{j,k} \). This decreases \( k_i^{\text{in}} \) by one and increases \( k_k^{\text{in}} \) by one.

An execution of any of the above four rectifications is said to be an RER operation. Specifically, the RER strategy is defined as follows: pick a random operation of the four edge rectification operations, until the stop criterion is met. The stop criterion is either “the maximum number of RER operations is reached” or “the network has satisfied the ENC”.

Given two networks, the one requiring less number of RER operations to exactly satisfy the ENC is said to be closer to satisfying ENC.

### IV. Experimental Studies

In this section, the RER strategy is applied to several different complex network topologies, including six synthetic and two real-world networks, to improve their robustness of controllability. The influences of RER is investigated on 1) modifying the networks’ degree distributions towards satisfaction of ENC, 2) enhancing the robustness of controllability, and 3) enhancing the robustness of connectedness.

Six typical directed synthetic network models are adopted for simulation, namely the Erdős–Rényi random graph (ER) [49], Newman–Watts small-world (SW) network [50], generic scale-free (SF) network [39], [51], [52], q-snapback network (QSN) [17], [19], random triangle network (RTN) [18], and random rectangle network (RRN) [18].
Two real-world networks are used for verification, namely the email-Eu-core (EE)\(^1\) network and the Gnutella peer-to-peer (GP)\(^2\) network, which will be detailed in Section IV-D.

In the following, the generation methods and parameters of the six synthetic networks are introduced.

1) Erdős–Rényi Random Graph Networks: An ER network is generated as follows:
- Start with \(N\) isolated nodes.
- Pick up all possible pairs of nodes from the \(N\) given nodes, denoted by \(i\) and \(j\) (\(i \neq j, i,j = 1,2,\ldots,N\)), once and only once. Connect each pair of nodes by a directed edge with probability \(p_{RG} \in [0,1]\), where the edge has the same probability directing from \(i\) to \(j\), or \(j\) to \(i\).

Given the numbers of \(N\) and \(M\), let \(p_{RG} = \frac{M}{N(N-1)}\). To exactly control the number of generated edges to be \(M\), uniformly-randomly adding or removing edges can be performed. Here, when adding an edge, the direction can be random.

2) Newman–Watts Small-world Networks: An SW network is generated as follows:
- Start with a directed \(N\)-node loop having \(K\) connected nearest-neighbors on each side of each node.
- Additional edges with random directions are added without removing any existing edges.

Set \(K = 2\) in the following, namely, a node \(i\) is connected to its two nearest neighbors on each side, with nodes \(i - 1, i + 1, i - 2\) and \(i + 2\), via edges \(A_{i-1,i}, A_{i,i+1}, A_{i-2,i}\) and \(A_{i,i+2}\).

3) Scale-Free Networks: An SF network is generated as follows:
- Start with \(N\) isolated nodes.
- A weight \(w_i = (i + \theta)^{-\sigma}\) is assigned to node \(i\), with \(\sigma \in [0, 1]\) and \(\theta \ll N\).
- Two nodes \(i\) and \(j\) (\(i \neq j, i,j = 1,2,\ldots,N\)) are randomly picked from the pool with a probability proportional to the weights \(w_i\) and \(w_j\), respectively. Then, an edge \(A_{ij}\) from \(i\) to \(j\) is added (if the two nodes are already connected, do nothing).
- Repeat Step 3), until \(M\) edges have been added.

The resulting network has a power-law distribution \(k^{-\gamma}\) with \(\gamma = 1 + \frac{\theta}{\sigma}\), where \(k\) is the degree variable, which is independent of \(\theta\). Here, \(\sigma\) is set to 0.999, and thus \(\gamma = 2.001\).

4) q-Snapback Networks: Consider a q-snapback network (QSN) with only one layer \(r_{QSN}\) for simplicity. This QSN is generated as follows:
- Start with a directed chain of \(N\) nodes, where each node \(i = 1, 2, \ldots, N - 1\) has an edge \(A_{i,i+1}\).
- For each node \(i = r_{QSN} + 1, r_{QSN} + 2, \ldots, N\), it connects backward to the previously-appeared nodes \(i - l \times r_{QSN}\) (\(l = 1, 2, \ldots, \lfloor i/r_{QSN}\rfloor\)), with the same probability \(q \in [0,1]\).

In the following experimental study, \(r_{QSN}\) is set to 2. Given \(N = 1000\) and \(M = 5000\), \(q\) is estimated to be 0.008 for fair comparisons. To exactly generate \(M\) edges, uniformly-randomly edge-adding with random direction should be applied.

5) Random Triangle Networks: Triangular structure, which has been observed benefit to the robustness of controllability [17] and network stability [53], [54], is frequently observed in real-life situations.

A directed random triangle network (RTN) is generated as follows:
- Start with \(N - 3\) isolated nodes, with the other 3 nodes connected in a directed triangle.
- Randomly pick up two nodes, \(i\) and \(j\), without edge \(A_{ij}\) or \(A_{ji}\) (otherwise, do nothing). Then, randomly pick up a node \(k\) from all the neighbors of node \(j\). If there is an edge \(A_{jk}\), then add two edges \(A_{ij}\) and \(A_{ik}\) (e.g., with an edge \(A_{kj}\)), add two edges \(A_{ji}\) and \(A_{ik}\).
- Repeat Step 2), until \(M\) edges have been added.

6) Random Rectangle Networks: The above directed RTN is extended to a random rectangle network (RRT), as follows:
- Start with \(N - 4\) isolated nodes, and the other 4 nodes are connected in a directed rectangle.
- Randomly pick up three nodes, \(i\), \(j\), \(k\), \(w\), without edges between any pair of them (otherwise, do nothing). Then, randomly pick up a node \(w\) from the neighbors of node \(k\). If there is an edge \(A_{kw}\), then add edges \(A_{w, i}, A_{ij}\), and \(A_{jk}\); otherwise (e.g., with an edge \(A_{uk}\)), add edges \(A_{ki}, A_{ij}\), and \(A_{uw}\).
- Repeat Step 2), until \(M\) edges have been added.

Since at each time step, two edges are added into RTN, and three edges are added into RRN, uniformly-randomly adding or removing edges can be performed to control the number of edges exactly.

In the simulation below, the network size is \(N = 1000\) with average out-degree \((K^{\text{out}}) = 5\), i.e., \(M = 5000\). To minimize the influence of stochasticity, for each configuration with the given \(N\), \(M\), and the number RER operations, referred to as a network instance, repeat 30 independent runs. For each network, the random attack is performed 50 times independently. Thus, each statistic datum is averaged from 1500 runs. Simulation results with different network sizes \(N = \{500, 2000\}\), and different average out-degrees of \((K^{\text{out}}) = \{3, 8\}\), are shown in Figs. S6–S13 of the SI.

A. Towards Satisfaction of the ENC

Figure 4 presents the boxplot of the needed number of RER operations for a network to exactly satisfy the ENC. In a boxplot, the blue box indicates that the central 50% samples lie within this section; the red bar inside the box is the median; the upper and lower black bars are the greatest and least values, excluding outliers; and finally the red pluses represent the outliers. It can be seen from the figure that, for a network configuration with \(N = 1000\) and \(M = 5000\), ER, SW, QSN, RTN, and RRN require a median of rounds of \(0.8 \times 10^4\) to \(0.9 \times 10^4\) for rectification, while SF requires rounds of \(1 \times 10^4\) to \(1.1 \times 10^5\). SW is the closest to satisfying the ENC, while SF is the farthest. Referring to Fig. 5(A), SW shows the best robustness of controllability, while SF shows the worst. Or,
Simply put, a network with better robustness of controllability needs less number of RER operations towards satisfaction of the ENC. Given different values of $N$ and $M$, the needed number of RER operations for ER and SF can be found in Fig. S14 of the SI.

**B. Towards Optimal Robustness of Controllability**

Now, the change of robustness of controllability is studied, as the number of RER operations changes.

First, note from Fig. 4 that it requires about ten thousands of RER operations for a network with $N = 1000$ and $M = 5000$ to satisfy the ENC.

Then, to see the changes, the following four situations are compared: 1) no RER operation is implemented, 2) 1000 RER operations are implemented, which are around one tenth of the number of the needed RER operations to exactly satisfy the ENC, 3) 5000 RER operations are implemented, which are around a half of the number of operations to exactly satisfy the ENC, and 4) unlimited RER operations (denoted by Inf) until the ENC is exactly satisfied.

Figure 5 shows that the robustness of structural controllability of the six networks is enhanced as the number of RER operations increases. In Fig. 5(A), case 1), shows different curves of controllability; case 2), the robustness of all networks is improved and the performance difference becomes smaller; cases 3) and 4), the robustness is significantly enhanced and the difference of curves becomes indistinguishable, for which although there is not guarantee that the rectified networks have optimal robustness of controllability, it is obvious that the robustness is significantly enhanced.

Figures 6 and 7 show the change of heterogeneity of out- and in-degrees (HO and HI), against the proportion of removed nodes. It can be seen from the figures that both HO and HI increase as nodes are gradually removed. As can also be seen from Figs. 6(A) and 7(A), the original SF network has the highest HO and HI, suggesting that low HO and HI values imply better robustness of controllability.

As the number of RER operations increases (Figs. 6(B,C) and 7(B,C)), both HO and HI are reduced, finally resulting in extremely-homogeneous networks (Figs. 6(D) and 7(D)), which show the best robustness of controllability.

Since connectedness is also important in the regard of network controllability and other issues, the proportion of node-removals needed to disconnect a network, namely, the minimum proportion of nodes to be removed in order to break the network into disjoint components, under random attacks, is examined next.

As can be seen from Fig. 8(A), different networks show different behaviors against random attacks, where SF is the easiest to be disconnected among the six networks, while SW is the hardest. This phenomenon is consistent with what was presented in Fig. 4(A), where SF shows the worst robustness against attacks, while SW has the best. In Fig. 8(B), the proportion of node-removals to disconnect all networks is increased, meaning that 1000 RER operations improve the connectedness of all networks against attacks. Finally, in Fig. 8(C,D), the value of $P_N$ is further increased. Fig. 8 demonstrates that the robustness of network connectedness is improved as the number of RER operations increases.

**C. Extensive Simulations on ER and SF**

Next, only ER and SF are discussed. A small step length of RER increase is set, such that the subtle influences of RER on the robustness of both controllability and connectedness can be clearly evaluated.

Figure 9 shows the curves of the robustness of controllability of ER and SF, as the number of RER operations increases, namely, with RER = {0, 100, 200, 500, 1000, 2000, 5000, Inf}. The results are averaged on 100 repeated runs. It is obvious that increasing the number of RER operations significantly enhances the robustness of controllability. The curves are distinguishable even when 100 RER operations are performed on the networks, showing that the operations have clear impacts.

Figure 10 shows the proportion of random node-removals to disconnect a network, against the number of RER operations. The data are averaged on 100 repeated runs. In this figure, a higher $P_N$ value means more node-removals is needed to disconnect the network, namely, the network has better robustness of connectedness. For both ER and SF, the robustness of connectedness is improved as the number RER operations increases.

As shown in Figs. 6 and 7, the operation of RER makes a network gradually become homogeneous. Fig. 11 shows the change of out-degree distributions of ER and SF. Fig. 11(A) shows that the out-degree distribution of the original ER is Poisson, but as the number of RER operations increases, the out-degree distribution becomes concentrated at $M/N$ ($M/N = 5$ in the figure). Fig. 11(B) shows that the original power-law distribution of SF also concentrates at $M/N$. Unlimited number of RER operations make both ER and SF (and any other network) become extremely homogeneous.

**D. Two real-world Networks**

Consider two real-world networks, namely email-Eu-core (EE) network and Gnutella peer-to-peer (GP) network [55]. Their parameters and brief descriptions are presented in Table II.
The original EE and GP (with RER = 0) are compared to the settings with RER = \{100, 1000, 5000, 10000, \text{Inf}\}. The controllability curves are shown in Fig. 12. A phenomenon similar to the simulations on synthetic networks is observed: the robustness of controllability is improved as the number of RER operations increases. The controllability curves of the original EE and GP (with RER = 0) are far away from the curves that exactly satisfy the ENC (with RER = \text{Inf}). This clearly shows that real-world networks are far away from having optimal robustness of controllability.

In Fig. 13, the boxplot presents the proportion of node-
removals needed to break the network into disjoint components, for EE and GP respectively. It can be observed that the original real-world networks are quite fragile, but after rectified with RER operations, their robustness of connectedness is significantly improved.

V. CONCLUSIONS

This paper presents a search for the network configuration with optimal robustness of controllability against random node-removal attacks. Since analytical approach is impossible at least in this time, the exhaustive attack strategy that applies all possible attack sequences is applied. Since this too is

Fig. 8: [Color online] Proportion of random node-removals (denoted by $P_N$) to disconnect a network: (A) without any rectification; (B) with 1000 operations; (c) with 5000 RER operations; (D) with RER operations until ENC is exactly satisfied.

Fig. 9: [Color online] Robustness of structural controllability of (A) ER, and (B) SF. $n_D$ represents the density of controlled-nodes calculated by Eq. (1); $P_N$ represents the proportion of removed nodes. (Robustness of exact controllability can be found in Fig. S5 of the SI.)

Fig. 10: [Color online] Proportion of random node-removals (denoted by $P_N$) against the number of RER operations to disconnect a network: (A) ER, and (B) SF.

Fig. 11: [Color online] Out-degree distribution changes as the number of RER operations increases: (A) ER, and (B) SF. (In-degree distribution can be found in Fig. S15 of the SI.)

Fig. 12: [Color online] Robustness of structural controllability of (A) EE, and (B) GP. $n_D$ represents density of controlled-nodes calculated by Eq. (1); $P_N$ represents the proportion of removed nodes.

Fig. 13: [Color online] Proportion of random node-removals (denoted by $P_N$) against the number of RER operations to disconnect a network: (A) EE, and (B) GP.
an intractable attempt even for the numerical approach, the work is performed on some very small-size networks. This nevertheless yields clear determined patterns of optimal solutions, which suggests an empirical necessary condition (ENC), indicating that the optimal instance of network configuration should be extremely homogeneous. ENC rules out the network instances that would not be candidates having optimal robustness of controllability. A random edge rectification (RER) strategy is then proposed to rectify synthetic and real-world networks towards exact satisfaction of the ENC, which also provides a way to enhance the robustness of controllability. The observed ENC may be useful in designing future network models. The phenomenon observed in this paper has an important implication that real-world networks as well as the commonly-used synthetic models are actually far away from the topologies with optimal robustness of controllability. Future work along the same line may be extended to other scenarios of malicious attacks, e.g., edge-removal and intentional attacks.

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Supplementary Information for the Paper
“Towards Optimal Robustness of Network Controllability: 
An Empirical Necessary Condition”

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1 Optimal Topology

Figures S1, S2, and S3 show the optimal network instances of small-sized networks. The number of nodes N and number of edges M are shown in Table S1, together with the number of possible instances (PI), and the number of instances with optimal robustness of controllability (O).

Table S1: N and M represent the number of nodes and edges, respectively. PI represents the number of possible network instances with given N and M. O represents the number of optimal robustness instances.

| N | M | PI | O |
|---|---|----|---|
| 4 | 4 | 22 | 1 |
| 4 | 5 | 37 | 1 |
| 4 | 6 | 47 | 2 |
| 4 | 7 | 27 | 1 |
| 4 | 8 | 38 | 2 |
| 4 | 9 | 27 | 1 |
| 4 | 10 | 13 | 1 |
| 4 | 11 | 5 | 1 |
| 4 | 12 | 1 | 1 |
| 4 | 13 | 2 | 2 |
| 4 | 14 | 2 | 2 |
| 4 | 15 | 1 | 1 |
| 4 | 16 | 2 | 2 |
| 4 | 17 | 1 | 1 |
| 4 | 18 | 2 | 2 |
| 4 | 19 | 1 | 1 |

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Figure S1: Optimal network topology of very small-sized networks (Part I).
Figure S2: Optimal network topology of very small-sized networks (Part II).

(A) N=5 M=12 (1)  (B) N=5 M=12 (2)  (C) N=5 M=13 (1)  (D) N=5 M=13 (2)

(E) N=5 M=14  (F) N=5 M=15  (G) N=5 M=16 (1)  (H) N=5 M=16 (2)

(I) N=5 M=16 (3)  (J) N=5 M=17 (1)  (K) N=5 M=17 (2)  (L) N=5 M=17 (3)

(M) N=5 M=18 (1)  (N) N=5 M=18 (2)  (O) N=5 M=19  (P) N=6 M=6

(Q) N=6 M=24 (1)  (R) N=6 M=24 (2)  (S) N=6 M=25 (1)  (T) N=6 M=25 (2)
Figure S3: Optimal network topology of very small-sized networks (Part III).
2 Robustness of Exact Controllability

Figure S4: Robustness of exact controllability of the six networks: (A) without any rectification; (B) with 1000 RER operations; (C) with 5000 RER operations; (D) with RER operations until ENC is satisfied. $n_D$ represents density of control-nodes calculated in terms of exact controllability. $P_N$ represents the proportion of removed nodes.

Figure S5: Robustness of exact controllability of (A) ER and (B) SF, when the number of RER varies from 0 to infinity. $n_D$ represents density of control-nodes; $P_N$ represents the proportion of removed nodes.
3 Average Out-degree $\langle k^{\text{out}} \rangle = \{3, 8\}$

Figure S6: Number of RER operations to rectify a network to satisfy the ENC. The network configuration is $\langle k^{\text{out}} \rangle = 3$ and $\langle k^{\text{out}} \rangle = 8$; the number of repeated runs is 100.

Figure S7: Robustness of structural controllability of the six networks: (A) without any rectification; (B) with 500 RER operations; (C) with 1000 RER operations; (D) with RER operations until ENC is satisfied. $n_D$ represents density of control-nodes; $P_N$ represents the proportion of removed nodes.

Figure S8: Robustness of exact controllability of the six networks: (A) without any rectification; (B) with 500 RER operations; (C) with 1000 RER operations; (D) with RER operations until ENC is satisfied. $n_D$ represents density of control-nodes; $P_N$ represents the proportion of removed nodes.
4 Network Size \( N = \{500, 2000\} \)

Figure S10: Number of RER operations to rectify a network to satisfy the ENC. The network configuration is \( N = 500 \) and \( N = 2000 \); the number of repeated runs is 100.

Figure S11: Robustness of structural controllability of the six networks: (A) without any rectification; (B) with 500 RER operations; (C) with 1000 RER operations; (D) with RER operations until ENC is satisfied. \( n_D \) represents density of control-nodes; \( P_N \) represents the proportion of removed nodes.
Figure S12: Robustness of exact controllability of the six networks: (A) without any rectification; (B) with 500 RER operations; (C) with 1000 RER operations; (D) with RER operations until ENC is satisfied. \( n_D \) represents density of control-nodes; \( P_N \) represents the proportion of removed nodes.

Figure S13: Proportion of random node-removals (denoted by \( P_N \)) to disconnect a network: (A) without any rectification; (B) with 500 RER operations; (C) with 1000 RER operations; (D) with RER operations until ENC is satisfied.
5 Other Supplementary Information

Figure S14: Average number of RER operations to rectify a network to full satisfy the ENC: (A) ER and (B) SF. $\langle k^{\text{out}} \rangle$ represents the average out-degree; $N$ represents network size. The number of repeated runs is 100.

Figure S15: In-degree distribution changes as the number of RER increases: (A) ER and (B) SF.