Research on Centralities Based on von Neumann Entropy for Nodes and Motifs

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Abstract. When analyzing the statistical and topological characteristics of complex networks, an effective and convenient way is to compute the centralities for recognizing influential and significant nodes or structures. Centralities for nodes are widely researched to depict the networks from a certain perspective and perform great efficiency, yet most of them are restricted to local environment or some specific configurations and hard to be generalized to structural patterns of networks. In this paper we propose a new centrality for nodes and motifs by the von Neumann entropy, which allows us to investigate the importance of nodes or structural patterns in the view of structural complexity. By calculating and comparing similarities of this centrality with classical ones, it is shown that the von Neumann entropy node centrality is an all-round index for selecting crucial nodes, and able to evaluate and summarize the performance of other centralities. Furthermore, when the analysis is generalized to motifs to achieve the von Neumann entropy motif centrality, the all-round property is kept, the structural information is sufficiently reflected by integrating the nodes and connections, and the high-centrality motifs found by this mechanism perform greater impact on the networks than high-centrality single nodes found by classical node centralities. This new methodology reveals the influence of various structural patterns on the regularity and complexity of networks, which provides us a fresh perspective to study networks and performs great potentials to discover essential structural features in networks.

1. Introduction

Networks provide us a useful tool to analyze a wide range of complex systems, including WWW, the social structure, the economic behaviors, and the biochemical reactions. Since the 1990s, a great number of interdisciplinary studies involving network both in theories and empirical work, have come up and developed new techniques and models to shed a light on the complex structure behind the particular subjects.

Among these studies, centrality which indicts the most important nodes in networks has received considerable attention. Many centralities have been proposed to describe and measure the importance of nodes in certain aspect to perform their specific
explanations for importance. The closeness centrality [1, 2] is defined as the average of shortest pathes from the node to all the other nodes in the whole network and aims to find the center based on pathes and node geological positions. Freeman [3] introduced the betweenness centrality to measure the controlling ability of nodes on communication between each pair of nodes and help find the nodes that control the information flow in the network. Bonacich [4] proposed the eigenvector centrality which takes into account the influence of powerful neighbors when evaluating node importance, and based on this the PageRank is established by Larry Page et al. [5] to work as the core websites-ranking algorithm of Google. Piraveenan et al. [6] proposed the percolation centrality to measure the node importance in aiding percolation of networks and considered that the values of nodes centrality depend on their states, which is widely implemented in percolation networks like contagion and computer virus spreading processes. These methods promote the application of network researches and deeper our understanding in complex systems.

However, when measuring node importance, one single node centrality is not always perfect since all the centralities only describe networks by a specific perspective. A huge number of real-world data is complex and requires multiple or comprehensive description. For example in a social network [39], nodes with high degrees or high betweenness centrality could have significant yet different effects on the network. In this situation it is necessary to make sure that an all-round description about the nodes importance could be presented. Also, it has been shown that single node is not sufficient to depict the complete structure and function of networks. Since nodes are the smallest elements in networks, their centrality can not exactly capture the global correlation of the whole network. The significant structural connection or combination patterns among a small number of nodes provide a simplified framework which could describe the organization of networks with less information lost. These patterns can be used to help understand the dynamics of networks in information dissemination and networks functional models insightfully. Thus the centrality of these small connected structure will work as a clear and quantified measurement of importance of network sub-structure in mesoscopic level and provide more information than node centralities.

Till now, most studies on complex network focus on graph theory, which mostly focuses on local structure and heuristic strategies such as centrality and modularity, and entropy provides an alternative way to measure the global characterization and had won great success in many researching fields. The von Neumann entropy (or quantum entropy) has shown great success in qualifying the organization structure and levels in networks, and can be applied in networks as an index to quantify the network heterogeneous characteristics. Passerini et al. [14] used the normalized combinational Laplacian matrix of networks to study the quantum state and von Neumann entropy of networks, and proved that the regular graphs and complete graphs have maximum entropy while networks with the same number of nodes and edges which contain large cliques have the minimum entropy. According to this result the von Neumann entropy could reflect the regularity of networks. By defining a rank-1 operator in the bipartite
tensor product space \[15\], Beaudrap et al. provided an interpretation of von Neumann entropy, and regarded the von Neumann entropy as the measurement of quantum entanglement between two systems corresponding to edges and nodes respectively. Han et al. \[16\] developed a simplified von Neumann entropy which could be computed using nodes degree statistics, compared it with Estrada’s heterogeneity index of node \[17\], and concluded that the von Neumann entropy can be used to measure the network complexity. The von Neumann entropy describes networks integrally and allows us to combine it with other concepts.

Recently some new fundamental concepts are proposed to help us understand networks topology and predict their functions. In 2002, Alon et al. \[7\] introduced the idea of motif when they were studying the gene network, which is defined as the recurring, significant sub-networks and patterns in a network, and it is discovered that the frequencies of some specific motifs in realistic networks are much more significant by comparing with random networks \[8\]. Triangular motifs (Figure 5a, \(M_3^1\)-\(M_3^7\)), which were obtained in sociogram, are crucial in understanding social network \[9\]. Mangan et al. proved the feed-forward loop (Figure 5a, \(M_3^3\)), one of the most significant motif structures, plays a fundamental role in transcription regulation network \[10\]. J. Honey et al. found that in the large-scale cortical network, the structure hubs tend to participate in open bidirectional wedges \(M_3^{13}\) (Figure 5a, \(M_3^{13}\)). Milo et al. found that in a food web the bi-parallel motif (Figure 5b), which illustrates two species who prey on a common creature may have one common predator, emerges a lot more than in random networks with the same nodes and degrees \[8\]. These concepts uncover the basic building blocks of networks and provide an interpretable view of network structure.

To analyze data better and understand the inherent structure and organization of networks, we make use of the von Neumann entropy to establish a new measurement and apply it with motifs to study the centrality. In section 2 the von Neumann entropy of networks is introduced, and the von Neumann entropy node centrality for networks is defined. Then some specific examples are analyzed and this node centrality is compared to other classical node centralities in the view point of similarity. Next in section 3 motifs are introduced and the von Neumann entropy motif centrality is defined and compared with other centralities. These researches extend the centrality to the small and regular structure in networks and demonstrate their superior in deciding the importance of nodes.

2. Node Centrality Based on von Neumann Entropy

2.1. The von Neumann Entropy of Networks

To introduce the von Neumann entropy, we first introduce the Laplacian matrix and the computation of von Neumann entropy of networks. Given an undirected network \(G(V, E)\), \(V\) (or \(V(G)\)) is a finite set whose elements are nodes of the network \(G\) and \(E\) (or \(E(G)\)) is the edges set. \(E\) is composed of unordered pairs of nodes who belong to
V, namely, when \((v_i, v_j) \in E\), we have \((v_j, v_i) \in E\) and \(v_i, v_j \in V\). The edge in the form of \((v_i, v_i)\) is called a self-loop. In this paper we only talk about the networks without self-loops. The adjacency matrix is an \(n \times n\) matrix, where \(|V| = n\). Using \(A(G)\) to denote the adjacency matrix of \(G\), the columns and rows of \(A(G)\) are labeled by the vertices of \(G\), and the \((i, j)\) entry of \(A(G)\) is 1 if and only if \((v_i, v_j) \in E(G)\), namely the adjacency matrix \(A(G)\) could be defined as follows:

\[
\begin{align*}
[A(G)]_{i,j} &= \begin{cases} 
1 & \text{if } (v_i, v_j) \in E(G) \\
0 & \text{if } (v_i, v_j) \notin E(G).
\end{cases}
\end{align*}
\]

(1)

The degree of a vertex \(v_i \in G\), denoted as \(d_G(v_i)\), is the total number of edges this vertex has. The degree-sum of network \(G\) is defined as the sum of degrees of all vertices, namely \(d(G) = \sum_{i \in V(G)} d_G(v_i)\). Note here \(d(G) = 2|E(G)|\). In this way we could define the degree matrix which is an \(n \times n\) diagonal matrix and denoted as \(D(G)\). The entries in the degree matrix are defined as follows:

\[
[D(G)]_{i,j} = \begin{cases} 
d_G(v_i) & \text{if } i = j \\
0 & \text{if } i \neq j.
\end{cases}
\]

(2)

The combinatorial Laplacian matrix (for short, Laplacian) \(L(G)\) could be define as \(L(G) = D(G) - A(G)\). For a weighted network with weight matrix \(W\), assume that the weights are assigned to edges and every weight is positive. Then the \(L(G)\) could be still defined as

\[
[L(G)]_{i,j} = \begin{cases} 
-w_{i,j} & \text{if } i \neq j \\
\sum_k w_{i,k} & \text{if } i = j.
\end{cases}
\]

(3)

It is worth noting that the Laplacian matrix will not change if the self-loop is added or deleted. As we can see, the Laplacian matrix is a diagonally dominant Hermite matrix, thus it is positive semi-defined \([20]\). With the Laplacian matrix scaled by the degree-sum, the density matrix of network \(G\) is defined as

\[
\rho(G) = \frac{L(G)}{d(G)} = \frac{1}{d(G)}(D(G) - A(G)).
\]

(4)

Evidently the density matrix is also positive semi-defined. According to the properties of positive semi-defined matrix and \(\rho(G) \cdot 1 = 0\), let \(0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n \leq 1\) be the \(n\) ordered eigenvalues of \(\rho(G)\). Thus the von Neumann entropy of network \(G\), denoted by \(S_E(G)\), is defined as \([21]\)

\[
S_E(G) = - \sum_{1 \leq i \leq n} \lambda_i \log \lambda_i,
\]

(5)

where \(\lambda \log \lambda = 0\) when \(\lambda = 0\).

The structural complexity is one of the most important properties in a complex network. Many classical properties, like degree and clustering coefficient, are local parameters and only capture microscopic features. Some other indices like betweenness and closeness centralities only depict parts of behavior of nodes and do not perform integral properties of networks. Global and computational efficient parameters are
needed necessarily to help analyze the networks and measure the complexity and regularity. Researchers have found a lot of indices to measure the structural complexity of networks. Xiao et al. [25] explored to use the trace of heat kernel to measure similarity and clustering of networks. Estrada [17] designed a heterogeneity index based on the variation of degree functions of all pairs of linked nodes, and gave bounds for this index when quantifying the heterogeneity of different networks. Most of these measurements and parameters are based on the Laplacian matrix of networks. The Laplacian matrix is symmetric and holds the complete characterizations of networks since it could be used to restore network. For the Laplacian matrix, the most important quantities are the eigenvalues, e.g., the second largest eigenvalue of Laplacian of a network helps determine the lower bound on the vertex connectivity of networks [22]. From the definitions above, it could be observed that the von Neumann entropy integrates the total values and properties of all the eigenvalues and thus could reflect structural features.

2.2. Definition of von Neumann Entropy Node Centrality

Let \( s \) be a subnetwork of \( G \), and denote \( G \setminus s \) to be the network remained after deleting the nodes in \( s \) and edges linked with these nodes. There are many researches related to von Neumann entropy and its function in describing the network structure, which receive quite a lot of attention. Combining with centrality, some preliminary studies on this entropy [43] could be found. Accordingly, the centrality of node \( v \) can be defined as the variation of von Neumann Entropy when removing the node and edges related to it from the network. Using \( C_E(v) \) to denote the von Neumann entropy node centrality, we have

\[
C_E(v) = |S_E(G) - S_E(G \setminus v)|. \tag{6}
\]

According to known researches related to von Neumann entropy, the \( S_E \) can reflect the regularity and complexity of the network and is effective to characterize the global structure of networks. When a node is removed, the network will change, which leads to the change of the Laplacian matrix and its eigenvalues, thus the von Neumann entropy of the network will finally change. If deleting node \( x \) brings larger change of \( S_E \) than deleting node \( y \), it proves that deleting node \( x \) could cause more significant change on the eigenvalues and network structure. For example, if deleting one node increases the von Neumann entropy largely, it means the network becomes more homogeneous since the von Neumann entropy reflects the irregularity, and this node is sufficient to be regarded as an important one. If the deleting decreases the von Neumann entropy greatly, it makes the network uneven, and it could be inferred that this node may bridge the network in its distribution and perform transitional function in the structure, thus this node should be viewed as a prominent one. In this way, when removing a node from the network, the change in von Neumann entropy will present the impact of this node on the whole network structure, which makes the von Neumann entropy a great parameter to build centrality.
Since the von Neumann entropy measures the irregularity of networks and deleting nodes could possibly increase or decrease the irregularity, it is natural that deleting nodes would make a network more uneven or more balancing. It is discovered that in some scale-free networks, deleting highest-degree nodes will not always certainly increase or decrease the von Neumann entropy and their specific statuses in networks, centers or transitions, can not be judged directly by degree. An example is shown in Figure 1.

**Figure 1.** One example of network with 200 nodes and 520 edges. It is a scale-free network generated by preferential attachment principle: firstly a small random network is generated; then new nodes are added to the network and the original nodes which have higher degrees are more likely to connect with the new nodes. Node $v_9$ has the highest degree 38 and node $v_{37}$ has the second highest degree 35. When removing nodes $v_9$, the von Neumann entropy will increase; when deleting node $v_{37}$, the von Neumann entropy will decrease.

### 2.3. Examples on von Neumann Entropy Centrality

To illustrate the efficiency of von Neumann entropy centrality, some specific networks are used to perform and compare different node centralities. The results of betweenness, closeness, degree and von Neumann entropy node centralities of Padgett Florentine families network and the gift-giving network are shown in Figure 2.

The Padgett Florentine families network is a network of marital ties among Renaissance Florentine families [37, 38]. This network is built based on historical documents and an edge between two nodes means there existed marriage alliance between the two corresponding families. The network includes families who were involved in the struggle for the control of the city in politics around 1430s. 16 families are contained in the network and there is a major component consisted by 15 of them. As we could see, all the node centralities rank the Medici as the most influential one. This actually coincides with historical fact since the Medici family is one of the most famous families in history who reached peak in Italian upper classes during Renaissance. The von Neumann entropy centrality is able to find out the most influential families correctly as other node centralities: all the first five families in the $C_E$ sort appear in
Figure 2. (a.) Padgett Florentine families marital ties network. 16 nodes and 20 edges are contained in this network. The Pucci family did not have marital tie with others, so the major part of the network is a component with 15 nodes. (b.) The gift-exchange network in a Papuan village. There are 22 nodes and 39 edges. Each node stands for a household and each edge stands for gift exchange. (c, d.) The two toy networks.

other three centrality sorts and the Medici family has the highest centrality. This proves that the von Neumann entropy centrality could work as a reasonable and accurate new centrality and can exactly capture the nodes which work as the most influential ones and are crucial to the whole network.

The other example, the gift-giving network, shows the gift exchange relations among 22 households in a Papuan village [35, 36]. In this network, if two households exchange gifts, there will be an edge between them. In this village, the gift-exchanging is significant because it is regarded as a method to request political and economic assistance
from others and works as the pristine market. Although there may exist deep contents and meanings behind the whole process in the network, yet it is natural to realize that the family who exchanges gifts with more persons and have high degrees may have larger influence on the whole village. At the same time, since the exchange process could be long and complicated, like the family $A$ may ask family $B$ to ask family $C$ to assist $A$, the betweenness centrality and closeness centrality will also point out influential households or persons in the network. Thus it is incomplete to evaluate the network with only one single centrality. Multiple centralities are required to help understand the structure and information behind the network better. As shown in the figure, the von Neumann entropy centrality performs its potential to be an all-round node-importance index: the first five nodes in $C_E$ sort have highest ranks in other centralities sorts, like node 11 ranks first in $C_B$ sort and $C_C$ sort, node 5 ranks the second in $C_D$ sort. The von Neumann entropy centrality could be viewed as a combination of other centralities and the all-round property of $C_E$ allows us to find more meaningful information in the network.

To further explain and understand the all-round feature of $C_E$, we present centralities of two toy networks. The network in Figure 2 is symmetric and node 4 obviously has highest betweenness centrality. Removing node 4 will break the network into two components and undermine the connectivity of this network. However, when choosing the most significant node in the network, betweenness centrality would not lead to the best choice since removing node 3 (or node 5) will not only undermine the connectivity, but also destroy the triangular structure on the left (or right). In this deciding process, $C_B$ and $C_D$ should work as signs of importance at the same time. As shown in the table, the von Neumann entropy centrality performs its all-round property and is able to combine the results of $C_B$ and $C_D$ and give out a more reasonable and complete result comparing to other centralities.

The network in Figure 2 is also symmetric where node 1, node 2 and node 3 have the highest closeness centrality, and combining with the $C_D$ sort, node 2 and node 3 are regarded to be the most significant nodes. When node 2 or 3 got deleted, node 6 or 7 would become a single node and the structure of the network would be destroyed greatly, and the von Neumann entropy centrality gets the same conclusion. Since deleting node 4 or 5 has no effect on the connectivity of the whole network and they rank lower in $C_C$ sort than node 1, it is not natural to understand why node 4 and node 5 rank higher than node 1. It can be inferred that the reason is that the remainder networks after deleting corresponding nodes are different: when node 1 is deleted, the degrees of remainder nodes are $(1, 1, 2, 2, 2, 2)$; when deleting node 4 or 5, remainder nodes degrees are $(1, 1, 1, 2, 2, 3)$; the later is more uneven than the former. As the von Neumann entropy is a measure of regularity, deleting node 4 or 5 will lead to larger decreasing in von Neumann entropy, and in $C_E$ sort node 4 and node 5 rank higher than node 1. This phenomenon supports the idea that the von Neumann entropy centrality is a global measure of network regularity and $C_E$ could reflect the statuses of nodes on the network topological structure.
From networks above, it can be concluded that one single classical centrality is not enough to depict and measure the importance of nodes sufficiently. The von Neumann entropy centrality is a combination of traditional centralities and could be viewed as a comprehensive measure of node importance. The \( C_E \) takes the global network structure into account and has performed its superior in selecting significant nodes in network.

2.4. Comparison with Other Centralities

To compare von Neumann entropy centrality with others, we attempt to compare the nodes sequences ordered by corresponding centralities. Firstly define \( Or(v_i, C_B) \) to be the position of node \( v_i \) in the node sequence ordered by the betweenness centrality decreasingly, and the set \( S(l, C_B) \) of betweenness centrality to be the set of nodes whose positions are at the first \( l \) of all ordered nodes, namely, \( S(l, C_B) = \{ v_i | 1 \leq i \leq N, Or(v_i, C_B) \leq l \} \). Thus for degree centrality, closeness centrality and von Neumann entropy node centrality above, we get \( Or(v_i, C_D), S(l, C_D), Or(v_i, C_C), S(l, C_C), Or(v_i, C_E) \) and \( S(l, C_E) \) separately. After these definitions, let \( I(l, C_1, C_2) \) be the intersect set of the first \( l \) nodes ordered by centralities \( C_1 \) with \( C_2 \), that is to say, \( I(N, 1, C_1, C_2) = \{ v_i | 1 \leq i \leq N, v_i \in S(l, C_1) \cap S(l, C_2) \} \). Define \( Sim_l(C_1, C_2) = \frac{|I(N, 1, C_1, C_2)|}{l} \) as the similarity of two centralities \( C_1 \) and \( C_2 \) at order \( l \), and the similarity for two centralities \( C_1 \) and \( C_2 \) can be obtained as

\[
Sim(N, C_1, C_2) = w(N) \sum_{l=1}^{N} Sim_l(C_1, C_2) \frac{1}{l},
\]

where \( \sum_{l=1}^{N} 1/l = \frac{1}{\ln(N)} \). Evidently, \( Sim = 1 \) requires the two nodes sequences ordered by centralities \( C_1 \) and \( C_2 \) are totally the same, and this similarity for centralities is a proper measurement to reveal their correlations. An example with detailed computation is shown in Figure 3.

Using the similarity defined above, it could be concluded that the von Neumann entropy centrality is able to characterize networks. The similarities of \( C_E \), \( C_B \), \( C_C \), and \( C_D \) for five network models are calculated: ER, scale-free Barabási-Albert random model (SFBA) \cite{28,29}, scale-free random model with gene duplication and divergence (SF-GD) \cite{30}, geometric random model (GEO) \cite{31}, geometric random model with gene duplication (GEO-GD) \cite{32}. Results are shown in Figure 4 and Table 1. Each value is the average over 100 networks.

Firstly use Erdős-Rényi (ER) \cite{27} networks to investigate the von Neumann entropy node centrality. ER is viewed as a uniformly randomly interacted network, and the probability of adding links between any pair of nodes is identical and independent. In Figure 4, 100 ER networks with 200 nodes and 500 edges are generated and the sizes of intersect sets of von Neumann entropy centrality and other centralities in Figure are given. For a specific node centrality \( C_{node} \), the box-size of \( Sim_l(C_E, C_{node}) \) is small and these two centralities are consistent, which suggests that the von Neumann entropy does make sense when it works as a centrality. At the same time, as the values of
Figure 3. An example of network containing 6 nodes with detailed computation of similarity. The similarity between degree centrality $C_D$ and closeness centrality $C_C$ is shown on the right where the values of $Sim_i(C_C, C_D)$ and $Sim(6, C_C, C_D)$ are given out.

$Sim_i(C_E, C_{node})$ are lower than 0.3, the von Neumann entropy centrality is different from betweenness centrality, closeness centrality and degree centrality.

Figure 4. The boxplots of $Sim_i(C_E, C_{node})$, when $C_{node}$ is betweenness centrality, closeness centrality or degree centrality. Each boxplot is drawn by generating 100 ER networks. Each network contains 200 nodes and 500 edges. For each centrality we give out the first 60 nodes to compare. (a.) The intersect set of von Neumann entropy node centrality and betweenness centrality. The y-axis is $Sim_i(C_E, C_B)$. (b.) The intersect set of von Neumann entropy node centrality and closeness centrality. The y-axis is $Sim_i(C_E, C_C)$. (c.) The intersect set of von Neumann entropy node centrality and degree centrality. The y-axis is $Sim_i(C_E, C_D)$.

Since SFBA is generated by preferential attachment principle, nodes with higher degrees at beginning tend to get more edges when adding new nodes, which allows them to gather together and have higher centralities, including higher degree, betweenness and closeness centralities. Thus no matter which one of network features like degree, shortest paths or entropy is used to measure the nodes importance, the values of similarities of SFBA networks are higher than others. According to the computation of similarity, in all the five models, the betweenness centrality has higher similarity with von Neumann
entropy node centrality than others, which suggests that the betweenness centrality may measure some key structural features and its bridging effect may play a more important role in describing complexity of the whole networks. For instance, GEO could be regraded as the networks presenting the distance relationship of uniformly distributed nodes in Euclidean space, so the $C_B$ and $C_C$ perform higher similarity to $C_E$. For lattice networks, the similarity values are quite similar, which is a reasonable result because the lattice network is a highly homogeneous network and nodes are quite similar from any perspective. From these results it can be concluded that different network models perform distinct similarity patterns and von Neumann entropy centrality could be used to work as indicator of structural characterizations in networks.

| Similarity | Betweenness | Closeness | Degree |
|------------|-------------|-----------|--------|
| SFBA       | 0.3752      | 0.2664    | 0.3251 |
| SF-GD      | 0.2770      | 0.1727    | 0.2066 |
| GEO        | 0.2100      | 0.1527    | 0.1502 |
| GEO-GD     | 0.2288      | 0.1403    | 0.1727 |
| Lattice    | 0.0765      | 0.0787    | 0.0787 |

### 3. Motif Centrality Based on von Neumann Entropy

#### 3.1. The Subtle Structure: Motif

Motifs are defined as small subgraphs and connection patterns that appear in networks frequently and they are regarded as the building blocks of complex networks and useful tools to uncover the structural design principles of network. The 13 three-node motifs in directed networks are shown in Figure 5a. In undirected networks, there are 2 three-node motifs and 6 four-node motifs, which are shown in Figure 5c and denoted as $M_1$-$M_8$. In this paper we mainly focus on undirected three-node and four-node motifs.

In graph theory, if there is a bijection $\phi$ between two graphs $X$ and $Y$ from $V(X)$ to $V(Y)$, such that nodes $x$ and $y$ in $X$ are neighbors if and only if $\phi(x)$ and $\phi(y)$ in $Y$ are neighbors, then $\phi$ is an isomorphism from $X$ to $Y$ and $X$ and $Y$ are isomorphic, written as $X \cong Y$. For a motif $m_0 \in T$, if there is a subgraph $s$ of $G$ which is isomorphic to motif $m_0$, namely $s \cong m_0$, it is said that there exists motif $m_0$ structure in network $G$.

Use $T$ to denote the set of motifs and $T(i)$ be the set of all $i$-node motifs, and they are searched using the enumeration algorithm. To find all the three-node motifs, all the edges between a node and its first order neighbors need to be checked. For a node $v$ with degree $k$, let $v_1$ and $v_2$ be two of its first-order neighbors. By checking the connection patterns among $v$, $v_1$ and $v_2$, the specific motif pattern will be determined
Figure 5. (a.) All the 13 three-node motifs in directed networks. (b.) The bi-parallel motif. This structure frequently shows up in the food chain network. (c.) The 2 three-node motifs and 6 four-node motifs in undirected networks.

and the number of 3-node motifs found by this way is \( \binom{k}{2} \), which equals to \( \frac{1}{2}(k^2 - k) \). Repeating the same procedure for all nodes in the network will find all the 3-node motifs contained in the network. Thus for a network with \( N \) nodes and \( M \) edges, the number of three-node motifs in this network is \( \frac{N}{2}(\langle k^2 \rangle - \langle k \rangle) \), where \( \langle k^n \rangle \) is the \( n \)-th moment of the degree distribution, and the searching time is proportional to the total motifs number.

To calculate \( \langle k \rangle \) and \( \langle k^2 \rangle \), given the generating function of the degree distribution

\[
G_0(x) = \sum_{i=0}^{\infty} p_i x^i, \quad (8)
\]

where \( p_i \) is the probability of a node having degree \( i \), the average degree of all nodes in the network is

\[
\langle k \rangle = \sum_i i p_i = G'_0(1). \quad (9)
\]

Using the results of higher moments of degree distribution derived from generating function \( G_0(x) \), we have the second moment of the degree distribution

\[
\langle k^2 \rangle = \sum_i i^2 p_i = ((x \frac{d}{dx})^2 G_0(x))|_{x=1}. \quad (10)
\]

In this way, to find all the 3-node motifs in the whole network, the calculation complexity
is $O(N(\langle k^2 \rangle - \langle k \rangle))$. Since
\[
\langle k^2 \rangle - \langle k \rangle = \left. \left( (x \frac{d}{dx} G_0(x)) \right) \right|_{x=1} - G'_0(1)
\]
\[
= \left. \left( x (G'_0(x) + xG''_0(x)) \right) \right|_{x=1} - G'_0(1)
\]
\[
= G''_0(1), \tag{11}
\]
the calculation complexity of finding all three-node motifs is $O(N G''_0(1))$.

For four-node motifs, it can be started from one edge $e$ with its two end nodes $v_m$ and $v_n$. Let $v_{m_1}$ be one of the neighbors of $v_m$ and $v_{n_1}$ be one of the neighbors of $v_n$. Studying the connection among $v_m$, $v_n$, $v_{m_1}$ and $v_{n_1}$ will determine which motif this four-node subgraph is. This works for $M_3$, $M_4$ and $M_6$-$M_8$ and their number is $k'_m \times k'_n$, where $k'_m$ and $k'_n$ are the degrees of $v_m$ and $v_n$ except $e$. To find all $M_5$ motifs it is sufficient to check the connection among the two end node $v_m$, $v_n$ and two neighbors $v_{m_1}$ and $v_{m_2}$ of $v_m$ or $v_{n_1}$ and $v_{n_2}$ of $v_n$. The number of $M_5$ in the network is $\frac{1}{2} k'_m (k'_m - 1) + \frac{1}{2} k'_n (k'_n - 1)$. The generating function of distribution of $k'_m$ or $k'_n$ is
\[
G'_1(x) = \sum_{i=0}^{\infty} q_i x^i, \tag{12}
\]
where $q_i = \frac{(i+1)p_{i+1}}{(k'_m)_{i+1}}$. Similar to $G_0(x)$, the average degree above satisfies $\langle k'_m \rangle = \langle k'_n \rangle = \langle k' \rangle = G'_1(1)$ and $\langle k^2' \rangle - \langle k' \rangle = G''_1(1)$. Then to find all the four-node motifs, the complexity is $O(M(G'_1(1) + G''_1(1)))$. It is worth noting that there exist replicated motifs, and after the searching, the list of motifs should be checked to delete repeated ones.

As the elemental construction blocks of networks, motifs play significant and meaningful roles in networks, and researches on motifs will help reveal the key structures and characterizations. Firstly the specific motif concept will help us concentrate on the local structure and connection patterns instead of single nodes. Then this method is flexible and expandable, i.e. we could choose to study motifs composed by any number of nodes and in any shapes. At the same time it allows us to focus on any one or some of the specific network connection structures. All of these make the motif a convenient tool to study networks.

### 3.2. Definition and Similarity of Motif Centrality

We have shown the definition of node centrality based on the von Neumann entropy and the performance of von Neumann entropy centrality as an all-round measurement of node importance. However, it is hard to get deeper understanding in the topology structure and function only by single nodes, since nodes are the smallest objects in networks and concern little specific structural information. Centralities should not be confined to single nodes, and it is necessary to study the structural connection patterns, such as motifs, graphlets \[11,12\] and cliques \[42\]. In this section it is aimed to investigate motifs using von Neumann entropy.
Motif has been widely accepted and researched, yet there are only a few researches about motif centrality. Piraveenan et al. [26] researched the four-node motif centrality on metabolic networks. They calculated the average node betweenness centrality and closeness centrality on four-node motif which appear frequently, and found that for some motifs, the average centrality of nodes on these motifs is much higher than the average centrality of global nodes. This result suggests that some dominant motifs do play important roles, like hubs or gathering centers, which shows the potential of motif centrality.

Let \( M(G, T) \) be the set containing all the motifs that belong to \( T \) and could be found in network \( G \), namely, 
\[
M(G, T) = \{ m | m \subset G, \exists m_0 \in T, m \cong m_0 \}.
\] (13)

Generalizing the definition from node centrality, for motif \( m \in M(G, T) \), the von Neumann entropy motif centrality can be defined as 
\[
C^M_E(m) = |S_E(G) - S_E(G \setminus m)|.
\] (14)

In this paper \( C \) is used to denote node centrality and \( C^M \) motif centrality.

Until now, most researches concerning motif centrality are actually the generalizations of node centrality, like marketing centrality motifs [40] and average betweenness centrality of each motif [26], which deeply rely on node centralities. Since motifs emphasize on the structure and connection pattern which could not be found by only observing single nodes, these concepts could not capture the structural characterizations completely. For many node centralities, like eigenvector centrality and closeness centrality, they are hard to be generalized to motifs directly. Von Neumann entropy provides an access to evaluate and measure the impact of specific structure on the global network and a new perspective to study network structural features.

To compare with other motif centralities, we use average node centrality of each motif, and the motif betweenness centrality \( C^M_B \), motif closeness centrality \( C^M_C \) and motif degree centrality \( C^M_D \) are calculated as the average of corresponding centralities of nodes this motif contains, i.e. \( C^M_i(m) = \sum_{v_j \in m} C_i(v_j) / |m| \). Or \( (m_i, C^M_i) \) could still be defined for motifs instead of nodes, and the set of motifs whose ranks in motif centrality sort are less than \( l \) is written as 
\[
S^M(l, C^M_i, T) = \{ m | m \in M(G, T), Or(m, C^M_i) \leq l \}.
\] (15)

The intersect set of von Neumann entropy motif centrality \( C^M_E \) with other motif centrality \( C^M_i \), written as \( I^M(l, C^M_E, C^M_i, T) \), is the set of nodes appeared in both the first \( l \) motifs ordered by \( C^M_E \) and the motif centrality \( C^M_i \), i.e., 
\[
I^M(l, C^M_E, C^M_i, T) = \{ v_j | 1 \leq j \leq N, \exists m_1 \in S^M(l, C^M_E, T), m_2 \in S^M(l, C^M_i, T), s.t. v_j \in m_1 \cap m_2 \}.
\] (16)

Similar to that of node centralities, similarity of motif centralities can be investigated. \( I^M(l, C^M_{1,2}, T(n)) \) is denoted as \( Sim^M_i(C^M_1, C^M_{2}, T(n)) \) and the motif
Table 2. Values of $\text{Sim}^M(C^M_E, C^M_B, T(3))$, $\text{Sim}^M(C^M_E, C^M_C, T(3))$ and $\text{Sim}^M(C^M_E, C^M_D, T(3))$ for SFBA, SF-GD, GEO and GEO-GD network. These similarity values are averaged over 100 networks.

| Similarity | Betweenness | Closeness | Degree |
|------------|-------------|-----------|--------|
| SFBA       | 0.5666      | 0.4807    | 0.5143 |
| SF-GD      | 0.4219      | 0.3689    | 0.3323 |
| GEO        | 0.3025      | 0.2572    | 0.1699 |
| GEO-GD     | 0.3205      | 0.2195    | 0.2138 |

Figure 6. $\text{Sim}^M_i(C^M_E, C^M_i, T(3))$ for each motif centrality computed by average of node centralities and von Neumann entropy motif centrality. We use GEO, SFBA, SFGD and GEO-GD to generate networks. Each network contain 200 nodes and about 500 edges. Since it is random to add a node or an edge, in these models, it is hard to control the number of edges to be 500 exactly, thus in these four models we set the number of edges to be 480-520 when using them to generate networks. Each curve presents the average result of 100 networks. (a.) The intersect set of von Neumann entropy motif centrality and betweenness node centrality. The y-axis is $\text{Sim}^M_i(C^M_E, C^M_B, T(3))$. (b.) The intersect set of von Neumann entropy motif centrality and closeness node centrality. The y-axis is $\text{Sim}^M_i(C^M_E, C^M_C, T(3))$. (c.) The intersect set of von Neumann entropy motif centrality and degree node centrality. The y-axis is $\text{Sim}^M_i(C^M_E, C^M_D, T(3))$.

The similarity between $C^M_1$ and $C^M_2$ for $T(n)$ is defined as

$$
\text{Sim}^M(C^M_1, C^M_2, T(n)) = w(|M(G, T(n))|) \sum_{l=1}^{[M(G, T(n))]} \frac{\text{Sim}^M_i(C^M_1, C^M_2, T(n))}{l}.
$$

In this subsection several networks are generated to observe the similarity for the 3-motif set $T(3)$. Values of $\text{Sim}^M(C^M_E, C^M_B, T(3))$, $\text{Sim}^M(C^M_E, C^M_C, T(3))$ and $\text{Sim}^M(C^M_E, C^M_D, T(3))$ of networks generated from SFBA, SF-GD, GEO and GEO-GD are computed, which are shown in Table 2. It could be observed that the values of SFBA are larger than others, which is in accordance with node similarity values and could be explained by preferential attachment principle and high-degree nodes gathering. These results are also reflected in Figure 6 where curves of $\text{Sim}^M_i(C^M_E, C^M_B, T(3))$, $\text{Sim}^M_i(C^M_E, C^M_C, T(3))$ and $\text{Sim}^M_i(C^M_E, C^M_D, T(3))$ with $1 \leq l \leq 500$ are drawn, and
the SFBA curves are higher than others. The same happens to another scale-free model SF-GD, and since in its generating process the “parent” nodes are randomly selected and independent to degrees, the high-degree nodes are not so highly centralized and the values of SF-GD are a bit lower than SFBA. The GEO model is based on space distances in Euclidean space, so the centralities related to geometrical positions of nodes play more important roles in the network, and the $\text{Sim}^M(C_E^M, C_B^M, T(3))$, $\text{Sim}^M(C_E^M, C_C^M, T(3))$ are higher than $\text{Sim}^M(C_E^M, C_D^M, T(3))$, which is also demonstrated by curves in Figure 6. This phenomenon could also be observed in the GEO-GD model, which uses GEO model as the original network when generated. All these results illustrate that the von Neumann entropy motif centrality is still an all-round index of network structural features and the similarity patterns vary when the structure of networks changes.

3.3. The Superiority of von Neumann Entropy Motif Centrality

To compare the von Neumann entropy motif centrality with other centralities including node centralities and other motif centralities, von Neumann entropy is used to measure the changes of networks and the efficiency of different centralities. Here, our aim is to observe the impacts of deleting motifs or nodes by investigating the entropy variation for all the centralities we study in this paper. To make it a fair comparison, the numbers of nodes deleted for different centralities should be made the same.

Undoubtedly, deleting motifs with highest orders in $C_E^M$ sort leads to larger changes of von Neumann entropy than deleting motifs with highest orders in $C_B^M$, $C_C^M$ or $C_D^M$ sorts, and deleting nodes with highest $C_E$ values would cause larger changes of von Neumann entropy than deleting nodes with highest $C_B$, $C_C$ or $C_D$. Viewing a three-node motif as three single nodes combined, the entropy variation caused by deleting the motif is the same as deleting the three single nodes one by one, so the von Neumann entropy has an accumulation property and deleting three single nodes with highest $C_E$ causes larger change in von Neumann entropy than deleting any three-node motif. Then, the rest work for us is to determine whether the motifs with the highest $C_E^M$ could lead to more structural changes than nodes with highest other centralities, and in this section the efficiency of $C_E^M$ comparing with the classical node centralities $C_B$, $C_C$ and $C_D$ will be analyzed.

The changes of entropy variation for different centralities are plotted in Figure 7 and the ER, GEO and SFBA models are used to generate networks. To compare the entropy variations, we keep the numbers of nodes deleted with highest $C_B$, $C_C$ and $C_D$ to be the same with the number of nodes contained in the motifs deleted with the highest $C_E^M$. As we could see, the results of three-node motif are quite similar to the results of four-node motif for the same network models, and the SFBA model performs more significant variations then other models. It is obvious that removing significant motifs could lead to larger changes in von Neumann entropy than removing the same number of significant single nodes. This suggests that the von Neumann entropy motif centrality is able to capture the topology information contained in the subtle structure which
cannot be presented by classical node centralities, and there exists great potentials of von Neumann motif centrality in revealing the underlying topology structure of network.

Figure 7. The comparison of change in von Neumann entropy when deleting motifs or single nodes ordered by node centrality. The x-axis is the number of motifs deleted. The y-axis is \((S_E(G) - S_E(G \setminus S'))/S_E(G)\) where \(S'\) is the nodes set deleted. When comparing the change of entropy, the same number of nodes is deleted from the original networks to keep the sizes of networks the same. We use ER, GEO and SFBA models to generate networks, and each network contains 200 nodes and 480-520 edges. The result in the figures is the average of 100 networks, and the results of von Neumann entropy motif centrality, node betweenness, node closeness and node degree centralities are drawn on the figure. (a. and d.) Changes of von Neumann entropy when deleting nodes or motifs in ER networks. (b. and e.) Changes of von Neumann entropy when deleting nodes or motifs in GEO networks. (c. and f.) Changes of von Neumann entropy when deleting nodes or motifs in SFBA networks. (a), (b) and (c) are changes of von Neumann entropy with \(T(3)\) and (d), (e) and (f) with \(T(4)\).

For the investigation of node and motif importance/centrality, the purpose is to locate the key nodes or microscopic patterns in the structure and functions of network. Our researches provide a new and useful tool for network research since motifs characterize the networks at multiple scales and help us understand and control networks better. To control or destroy a network, a direct target is the nodes found by classical centralities. In the language of network attack or defense, the most important hubs should be additionally protected to avoid the attack from hackers for destroying the network; in disease spreading, the fragile important spreaders should be specially protected and controlled to interrupt the transmission. However, since usually these high-centrality nodes are not closely related in geographical positions or functionally, the cost in controlling or destroying some of these nodes could be very high. Locating and protecting the dispersedly distributed hubs takes cost a huge number of time and budgets; isolating and curing the key single spreaders could lead to the separation of precious medical and human resources. By our research, aiming at connected nodes
group will improve the efficiency and lower the cost at the same time. The von Neumann entropy motif centrality shows great potentials in networks structure researches and provides us a new perspective to research networks deeply and apply conclusions of networks into practice.

4. Conclusion and Discussion

In this paper the node and motif centralities based on von Neumann entropy are discussed, which makes it possible to study the importance of nodes or motifs in the perspective of structural regularity and complexity. By comparing von Neumann entropy node centrality with classical node centrality, it is shown that the $C_E$ is an all-round measurement of node importance, and can be applied to evaluate other node centralities, which is also performed in comparing von Neumann entropy motif centrality with other motif centralities. By comparing the changes of von Neumann entropy when deleting motifs with high $C^M_E$ or nodes with high node centralities, it is concluded that the motifs have greater impact on the global networks than single nodes and von Neumann motif centrality can capture the significant structural patterns.

Since a great number of real-world data is directed, it is worth defining and researching the von Neumann entropy on directed networks. Chung provided a definition of Laplacian matrix on directed networks [23] using Perron-Frobenius Theorem [20] and based on this work, Ye et al. [24] proposed a method to approximate the von Neumann entropy of directed networks, which allows us to compute the von Neumann entropy in terms of in-degree and out-degree of nodes simply. However, these results only work on strongly-connected directed networks. Another definition involving incidence matrix [22], loses the direction information when calculating the Laplacian. It is still an open problem to define the von Neumann entropy on directed networks generally.

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