

Correlation Analysis between Maximal Clique Size and Centrality Metrics for Random Networks and Scale-Free Networks

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Received: March 5, 2016

Accepted: March 20, 2016

Online Published: March 30, 2016

doi:10.5539/cis.v9n2p41

URL: <http://dx.doi.org/10.5539/cis.v9n2p41>

The research is financed by the NASA EPSCoR sub award (#: NNX14AN38A) from University of Mississippi.

Abstract

The high-level contribution of this paper is a comprehensive analysis of the correlation levels between node centrality (a computationally light-weight metric) and maximal clique size (a computationally hard metric) in random network and scale-free network graphs generated respectively from the well-known Erdos-Renyi (ER) and Barabasi-Albert (BA) models. We use three well-known measures for evaluating the level of correlation: Product-moment based Pearson's correlation coefficient, Rank-based Spearman's correlation coefficient and Concordance-based Kendall's correlation coefficient. For each of the several variants of the theoretical graphs generated from the ER and BA models, we compute the above three correlation coefficient values between the maximal clique size for a node (maximum size of the clique the node is part of) and each of the four prominent node centrality metrics (degree, eigenvector, betweenness and closeness). We also explore the impact of the operating parameters of the theoretical models for generating random networks and scale-free networks on the correlation between maximal clique size and the centrality metrics.

Keywords: complex network graphs, correlation coefficient, centrality metrics, maximal clique size, scale-free networks, random networks

1. Introduction

Network Science (a.k.a. Complex Network Analysis) is an emerging area of interest in the big data paradigm and corresponds to analyzing complex real-world networks and theoretical model-based networks from a graph theory point of view. Among the various measures used for complex network analysis, node centrality is a prominently used measure of immense theoretical interest and practical value. The centrality of a node is a link statistics-based quantitative measure of the topological importance of the node with respect to the other nodes in the network (Newman, 2010). Applications for node centrality metrics could be for example to identify the most influential persons in a social network, the key infrastructure nodes in an internet, the super-spreaders of a disease, etc. The existing centrality metrics could be broadly classified into two categories (Newman, 2010): neighbor-based and shortest path-based. Degree centrality (DegC) and Eigenvector centrality (EVC; Bonacich, 1987) are well-known measures for neighbor-based centrality, while Betweenness centrality (BWC; Freeman, 1977) and Closeness centrality (CIC; Freeman, 1979) are well-known measures for shortest path-based centrality. Various time-efficient and space-efficient algorithms (e.g., Brandes, 2001; Kang et al., 2011) have been proposed in the literature to determine each of the above centrality metrics. Hence, we refer to node centrality as a computationally light-weight measure.

In addition to node centrality, there exists several other informative measures for quantitatively assessing the importance of a node in a complex network - some of which are too time consuming to determine. We consider one such measure in this paper - the maximal clique size for a node. The maximal clique size for a node is defined as the largest size clique the node is part of (Cormen et al., 2009). A "clique" in a graph is a subset of the vertices such that there exists an edge between any two vertices in the subset (Cormen et al., 2009). The size of a clique is the number of vertices that are part of the clique. Each node in a graph could be part of one or more cliques of different sizes. The largest size clique that a node is part of is of interest for community detection in

complex networks (in order to identify nodes that are highly modular). A community of vertices is a subset of the vertices in a graph such that there are more links among vertices within this subset and relatively fewer links to vertices outside this subset (Newman, 2010). The effectiveness of the partitioning of a network into communities is evaluated using a metric called the modularity score (Newman, 2006). The larger the number of vertices within a community and larger the number of links between these vertices, the larger the modularity score for the community. Hence, it is of logical interest to identify vertices that are highly modular and design algorithms for community detection involving such vertices.

Unfortunately, the problem of determining the maximal clique size for a vertex is NP-hard (Cormen et al., 2009) and we refer to it as a computationally hard measure. One would have to rely on either time consuming exact algorithms or sub optimal (but relatively less time consuming) approximation heuristics to determine the maximal clique size for a vertex. Also, the focus of the research community has been mostly on developing exact algorithms and approximation heuristics (e.g., Carraghan & Pardalos, 1990; Ostergard, 2002; Pattabiraman et al., 2013) for a related problem called the maximum clique size, which is the largest clique size for the entire graph. The maximal clique size for one or more vertices could correspond to the maximum clique size for the graph; but not all vertices are likely to be part of the maximum clique. There could be several vertices in a graph for which the maximal clique size would be less than the maximum clique size.

Our contributions in this paper are as follows: We identify one or more computationally light-weight centrality metrics that have a high correlation with that of the maximal clique size (a computationally hard measure). In this pursuit, we run the most time-efficient algorithms for each of the four centrality metrics (DegC, EVC, BWC and CIC) and an adapted version of the exact algorithm originally proposed for maximum clique size (Pattabiraman et al., 2013) to determine the maximal clique size of the vertices in complex networks. We run these algorithms on random networks and scale-free networks generated respectively from the well-known Erdos-Renyi (Erdos & Reny, 1959) and Barabasi-Albert (Barabasi & Albert, 1999) theoretical models. We evaluate the correlation between maximal clique size for a node and each of the four centrality metrics using three well-known correlation measures (Triola, 2012): (i) Pearson's product-moment based correlation coefficient, (ii) Spearman's rank based correlation coefficient and (iii) Kendall's concordance based correlation coefficient. We identify the centrality metrics that have the highest correlation as well as the lowest correlation with the maximal clique size with respect to each of the above three correlation measures for random networks and scale-free networks. We also identify the correlation measures for which we incur the largest and smallest values for the correlation coefficient for different combinations of the centrality metrics and the theoretical networks. In addition, we evaluate the impact of the operating parameters of the theoretical models on the nature of the correlation observed between each of the four centrality metrics and maximal clique size.

The rest of the paper is organized as follows: Section 2 introduces the maximal clique size of a graph and describes an exact algorithm to determine the same. Section 3 reviews the two neighbor-based centrality metrics (DegC and EVC) and the two shortest path-based centrality metrics (BWC and CIC) and briefly describes an efficient algorithm to determine each of them. Section 4 introduces the three measures for evaluating the correlation coefficient between node centrality and maximal clique size per node. Sections 5 and 6 respectively present the results for correlation coefficient analysis on random network graphs (generated from the Erdos-Renyi model) and scale-free network graphs (generated from the Barabasi-Albert model). Section 7 reviews related work on correlation studies involving centrality metrics and maximal/maximum clique size. Section 8 concludes the paper. Throughout the paper, the terms 'node' and 'vertex' as well as 'link' and 'edge' are used interchangeably. Likewise, a vertex might be referred to either as i or v_i . They mean the same. We model all the theoretical-model generated graphs as undirected graphs.

2. Maximal Clique Size

The maximal clique size of a node is the largest size clique that the node is part of. The maximal clique size of a node is a measure of the level of modularity of the node and could be used to identify seed nodes (for a community detection algorithm) around which communities could evolve. In spite of its importance for identifying highly modular nodes in complex networks, most of the research focus in the literature has been on a related measure called the maximum clique size - the size of the largest clique in a graph. As the problems of determining both the maximum clique size and maximal clique size are NP-hard (Cormen et al., 2009), we decided to adapt an exact algorithm for determining maximum clique size in a graph to determine the maximal clique size for the vertices in the graph. We choose the recently proposed exact algorithm by Pattabiraman et al (Pattabiraman et al., 2013) for maximum clique size of a graph and slightly modify it to determine the maximal clique size of the individual vertices in a graph.

2.1 Original Exact Algorithm to Determine Maximum Clique Size for a Graph

The original exact algorithm by Pattabiraman et al (2013) follows a branch and bound approach of searching through all possible cliques and limiting the exploration only to vertices whose agglomeration has scope of being larger than the size of the largest clique known until then. Figure 1 illustrates the pseudo code of the exact algorithm for maximum clique size. As one can notice, the algorithm uses a variable *max* to keep track of the largest size clique determined during the search process. The procedure MAXCLIQUE proceeds in iterations, and in the i^{th} iteration, the algorithm explores whether a clique of size greater than the current value of *max* could be determined involving vertex v_i (the vertices are considered in the increasing order of their IDs) and its neighbors. For each such vertex v_i , a candidate set of vertices U is constructed involving v_i 's neighbors (each of whose degree is at least the value of *max*) and is passed to the sub routine CLIQUE along with a variable *size* whose value at any time during the execution of the sub routine represents the size of the largest clique known until then involving vertex v_i and its neighbors.

```

Procedure MAXIMUMCLIQUE ( $G = (V, E)$ )
   $max \leftarrow 0$ 
  for  $i : 1$  to  $|V|$  do
    if  $\text{degree}(v_i) \geq max$  then
       $U \leftarrow \phi$ 
      for each  $v_j \in \text{Neighbor}(v_i)$  do
        if  $\text{degree}(v_j) \geq max$  then
           $U \leftarrow U \cup \{v_j\}$ 
          CLIQUE( $G, U, 1$ )

Subroutine CLIQUE( $G = (V, E), U, size$ )
  //  $size$  is the size of clique found so far
  if  $U = \phi$  then
    if  $size > max$  then
       $max \leftarrow size$ 
    return
  while  $|U| > 0$  do
    if  $size + |U| \leq max$  then
      return
    select any vertex  $u$  from  $U$ 
     $U \leftarrow U \setminus \{u\}$ 
     $N'(u) := \{w | w \in \text{Neighbor}(u) \wedge \text{degree}(u) \geq max\}$ 
    CLIQUE( $G, U \cap N'(u), size + 1$ )

```

Figure 1. Exact Algorithm to Determine Maximum Clique Size for a Graph (adapted from Pattabiraman et al., 2013)

The sub routine CLIQUE expands the size of the clique involving v_i with one vertex at a time (starting with v_i itself) through a combination of iterations and recursions. In each such iteration, a random node u is removed from the set U passed to the sub routine and the set U is filtered to retain only those vertices that are also neighbors of the node u ; the value of *size* is incremented by 1 to account for the inclusion of node u to the clique and a recursive call to CLIQUE is made with the updated U and value of *size*. A recursive call to the sub routine CLIQUE runs as long as the current value of *max* is less than the sum of the size of the set U passed to the sub routine and the *size* of the current clique found until then. During the sequence of returns from the recursive calls, it is also possible that a different neighbor node u of v_i gets selected and the size of the clique involving the new node u and its neighbors along with v_i could be larger the current value of *max*. Also, during any such recursive call to CLIQUE, if the size of the set U reaches zero, the algorithm terminates the sequence of recursions and updates the value of *max* if it is less than the *size* of the clique found until then involving vertex v_i and its neighbors.

The efficiency of the algorithm is severely impacted by the order the vertices are considered for the iterations. A labeling of the vertices in the decreasing order of their degree increases the chances of finding the maximum size clique much earlier than a random labeling of the vertices (Pattabiraman et al., 2013). If the maximum size clique is found in the earlier iterations itself, the subsequent iterations could end up to be mere pruning operations if the vertices involved in these iterations have a degree smaller than the maximum size clique determined until then.

2.2 Modified Exact Algorithm to Determine Maximal Clique Size for a Vertex

Figure 2 illustrates the pseudo code that we propose for a modified exact algorithm to determine the maximal clique size for any vertex in a given graph. Unlike the procedure MAXIMUMCLIQUE (discussed in Section 2.1), we can no longer discard vertices with degree lower than the maximum clique size found until then for the entire graph. We need to run the procedure for every vertex to determine the maximal clique size involving the

vertex.

For each vertex v_i , to start with, the maximal clique size known until then is 0; so, we construct the candidate set of vertices (U) involving all the neighbors of v_i and pass them to the sub routine CLIQUE. We could retain all the pruning strategies (discussed in Section 2.1) in the sub routine CLIQUE: we need not explore node u (chosen from the set U) and its neighbors if their degree is smaller than the value of $size$ (the maximal clique size involving vertex v_i) known until then. For speedup, we list the neighbors of a vertex v_i in the initial set U passed from the procedure MAXIMAL CLIQUE to the sub routine CLIQUE in the decreasing order of their degree.

Procedure MAXIMALCLIQUE ($G = (V, E)$)

```

for  $i : 1$  to  $|V|$  do
     $maximalCliqueSize[v_i] \leftarrow 0$ 
     $U \leftarrow \phi$ 
    for each  $v_j \in Neighbor(v_i)$  do
         $U \leftarrow U \cup \{v_j\}$ 
    CLIQUE( $G, v_i, U, 1$ )
    
```

Subroutine CLIQUE($G = (V, E), v_i, U, size$)

// $size$ is the size of clique found so far for vertex v_i

```

if  $U = \phi$  then
    if  $size > maximalCliqueSize[v_i]$  then
         $maximalCliqueSize[v_i] \leftarrow size$ 
    return
    while  $|U| > 0$  do
        if  $size + |U| \leq maximalCliqueSize[v_i]$  then
            return
        select any vertex  $u$  from  $U$ 
         $U \leftarrow U \setminus \{u\}$ 
         $N'(u) := \{w \mid w \in Neighbor(u) \wedge degree(w) \geq maximalCliqueSize[v_i]\}$ 
        Clique( $G, v_i, U \cap N'(u), size + 1$ )
    
```

Figure 2. Exact Algorithm to Determine Maximal Clique Size for a Vertex (adapted from Pattabiraman et al., 2013)

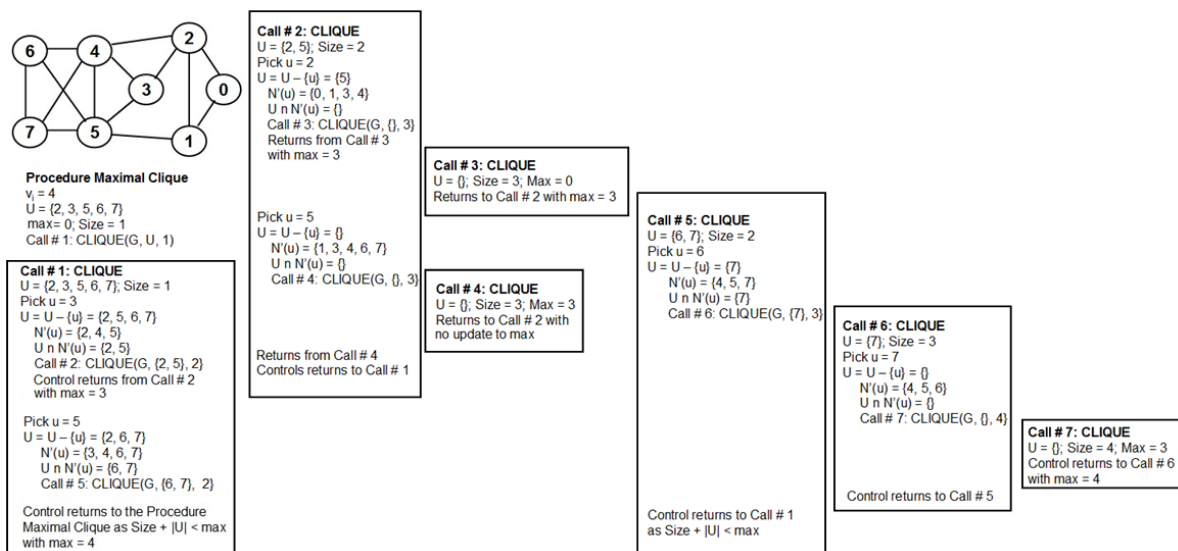


Figure 3. Example to Illustrate Execution of the Exact to Determine Maximal Clique Size for a Vertex

Figure 3 presents an example to illustrate the execution of the modified exact algorithm to determine the maximal clique size for a vertex. We consider vertex $v_i = 4$ as the vertex for which we want to find the maximal

clique size. We identify each recursive call to the sub routine CLIQUE with a unique identification number (Call # 1, 2, etc) so that it is easy trace the execution of the algorithm. The first few recursive calls (Call #s 1 - 2 - 3 - 4) lead to the identification of clique {4, 2, 3} of size 3. However, the next set of recursive calls (Call #s: 1 - 5 - 6 - 7) lead to the identification of the maximal size clique {4, 5, 6, 7} involving vertex 4. Figure 4 illustrates the maximal clique size of all the vertices in the sample graph used in Figure 3.

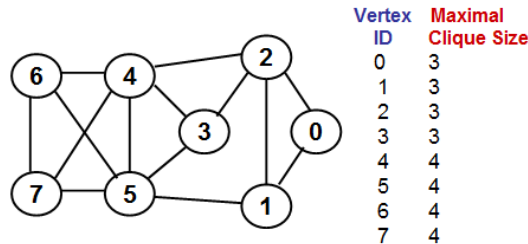


Figure 4. Maximal Clique Size of the Vertices in a Sample Graph

3. Maximal Clique Size

We now review the centrality metrics that are used for the correlation coefficient analysis studies in this paper. These are the neighbor-based degree centrality (DegC) and eigenvector centrality (EVC) metrics and the shortest path-based betweenness centrality (BWC) and closeness centrality (CIC) metrics.

3.1 Degree Centrality

The degree centrality of a vertex is the number of neighbors for the vertex in the graph and can be easily computed by counting the number of edges incident on the vertex. If A is the $n \times n$ adjacency matrix for a graph such that $A[i, j] = 1$ if there is an edge connecting v_i to v_j (for undirected graphs) and $A[i, j] = 0$ if there is no edge connecting v_i and v_j . The degree centrality of a vertex v_i is defined quantitatively as follows:

$$DegC(v_i) = \sum_{j=1}^n A[i, j] \tag{1}$$

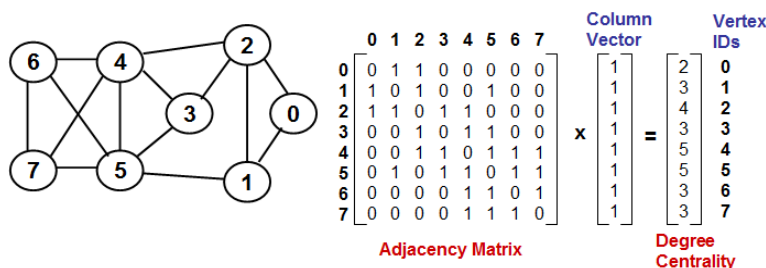


Figure 5. Example to Illustrate the Computation of Degree Centrality

Figure 5 illustrates an example for computing the degree centrality of all the vertices in a graph as the product of the adjacency matrix of the graph and a unit column vector of 1s corresponding to the number of vertices in the graph.

3.2 Eigenvector Centrality

The eigenvector centrality (EVC) of a vertex is a quantitative measure of the degree of the vertex as well as the degree of its neighbors. A vertex that has a high degree for itself as well as located in the neighborhood of high-degree vertices is likely to have a larger EVC. The EVC values of the vertices in a graph correspond to the entries for the vertices in the principal eigenvector of the adjacency matrix of the graph. An $n \times n$ adjacency matrix has n eigenvalues and the corresponding eigenvectors. The principal eigenvector is the eigenvector corresponding to the largest eigenvalue (principal eigenvalue) of the adjacency matrix, A . Moreover, if all the entries in a square matrix are positive (i.e., greater than or equal to zero), the principal eigenvalue as well as the entries in the principal eigenvector are also positive (Lay, 2011).

We determine the EVC of the vertices using the Power-iteration method (Lay, 2011). According to this method,

we start with a unit vector $X_0 = [1 \ 1 \ 1 \ 1 \dots 1 \ 1]$ of all 1s corresponding to the number of vertices in the graph and go through a sequence of iterations. The tentative eigenvector computed during the $(i+1)^{th}$ iteration is given as: $AX_i / \|AX_i\|$, where $\|AX_i\|$ is the normalized value of the vector resulting from the product of the adjacency matrix and the tentative eigenvector computed during the i^{th} iteration. We continue the iterations until the normalized value $\|AX_i\|$ does not change significantly and converges to a constant value (when rounded to the second decimal). The normalized value at this juncture also corresponds to the principal eigenvalue of the adjacency matrix and the tentative eigenvector computed with this normalized value corresponds to the principal eigenvector of the adjacency matrix. We illustrate the execution of the Power-iteration method with the example shown in Figure 6. As can be noticed from Figure 6, even though both vertices 4 and 5 have the same larger degree (five) - the EVC of vertex 4 is larger than the EVC of vertex 5 - this could be attributed to the degree distribution $\{3, 3, 3, 4, 5\}$ of the neighbors of vertex 4 vis-a-vis the degree distribution $\{3, 3, 3, 2, 5\}$ of the neighbors of vertex 5.

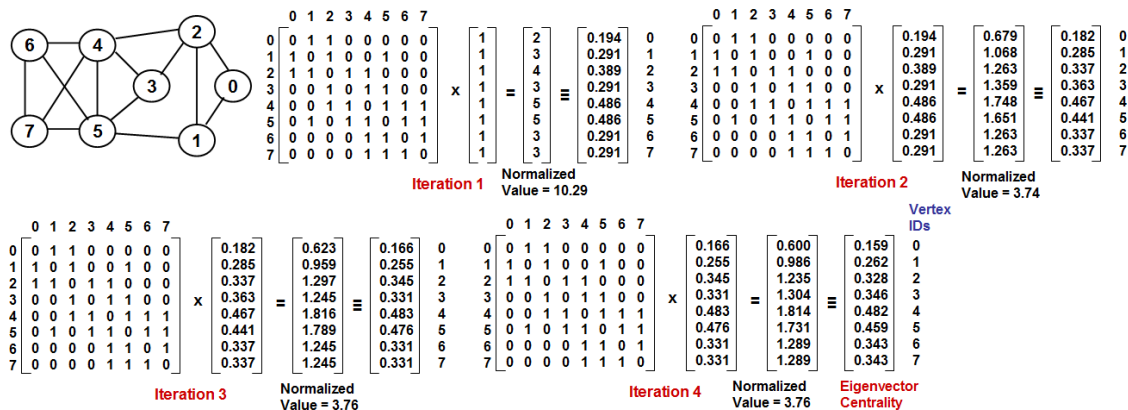


Figure 6. Example to Illustrate the Calculation of Eigenvector Centrality using Power Iteration Method

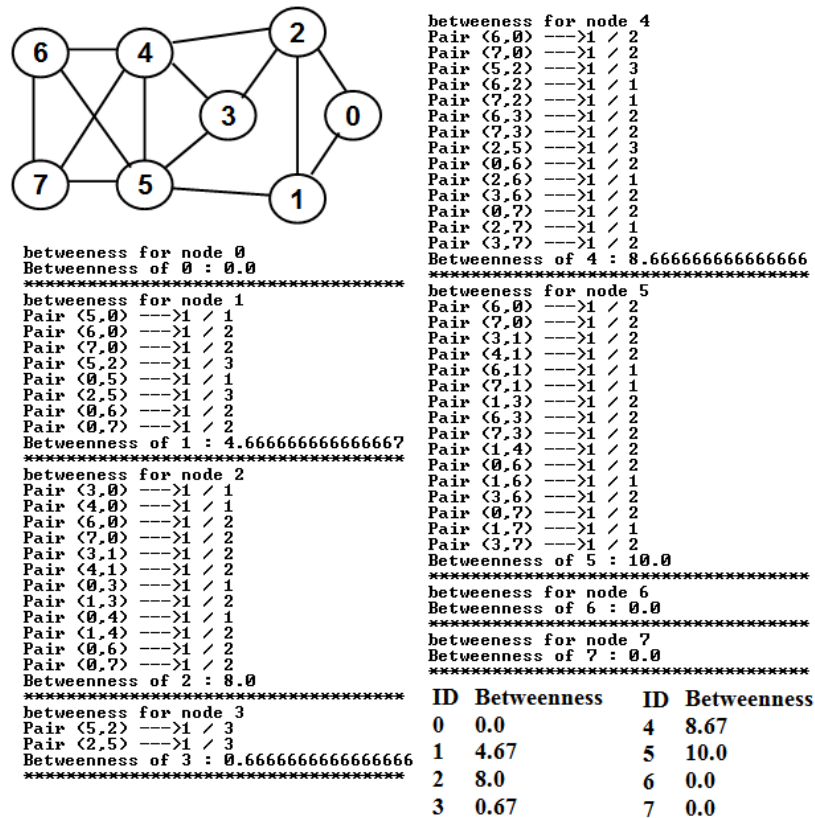


Figure 7. Example to Illustrate the Calculation of Betweenness Centrality

3.3 Betweenness Centrality

The betweenness centrality (BWC) of a vertex is the sum of the fraction of shortest paths going through the vertex between any two vertices, considered over all pairs of vertices. In this paper, we determine the BWC of the vertices using the Breadth First Search (BFS)-variant of the well-known Brandes algorithm (Brandes, 2001). We run the BFS algorithm on each vertex in the graph and determine the level of each vertex (the number of hops/edges from the root) in each of these BFS trees. The root of a BFS tree is said to be at level 0 and the number of shortest paths from the root to itself is 1. On a BFS tree rooted at vertex r , the number of shortest paths for a vertex i at level l ($l > 0$) from the root r is the sum of the number of shortest paths from the root r to each the neighbors of vertex i (in the original graph) that are at level $l-1$ in the BFS tree.

Since we are working on undirected graphs, the total number of shortest paths from vertex i to vertex j (denoted sp_{ij}) is simply the number of shortest paths from vertex i to vertex j in the shortest path tree rooted at vertex i or vice-versa. The number of shortest paths from a vertex i to a vertex j that go through a vertex k (denoted $sp_{ij}(k)$) is the maximum of the number of shortest paths from vertex i to vertex k in the shortest path tree rooted at i and the number of shortest paths from vertex j to vertex k in the shortest path tree rooted at vertex j .

$$BWC(k) = \sum_{\substack{k \neq i \\ k \neq j}} \frac{sp_{ij}(k)}{sp_{ij}} \tag{2}$$

Figure 7 illustrates an example to calculate the BWC of vertices in the same graph used in Figures 3-6. We can observe the betweenness values for vertices 0, 6 and 7 are zero each, because no shortest path between any two vertices go through them. We observe that even though vertices 4 and 5 have the same larger degree, the average degree of the neighbors of vertex 5 is slightly lower than the average degree of the neighbors of vertex 4. As a result, vertex 5 is more likely to occupy a relatively larger fraction of the shortest path between any two vertices and incur a relatively larger BWC value compared to vertex 4 (even though vertex 4 has a larger EVC value). Also, even though vertex 3 has a larger degree than vertex 1, the BWC of vertex 1 is significantly larger than that of vertex 3. This could be attributed to vertex 1 lying on the shortest path from vertices 0 and 2 to vertices 4, 5, 6 and 7; on the other hand, vertex 3 lies only on the shortest path between 2 and 5.

3.4 Closeness Centrality

The closeness centrality (CIC) of a vertex is the inverse of the sum of the number of shortest paths from the vertex to every other vertex in the graph. We determine the CIC of the vertices by running the BFS algorithm on each vertex and summing the number of shortest paths from the root vertex to every other vertex in these BFS trees. Figure 8 illustrates an example to compute the CIC of the vertices. We observe vertices with a larger degree are more likely to have shortest paths of lower hop count to the rest of the vertices, leading to a larger CIC value.

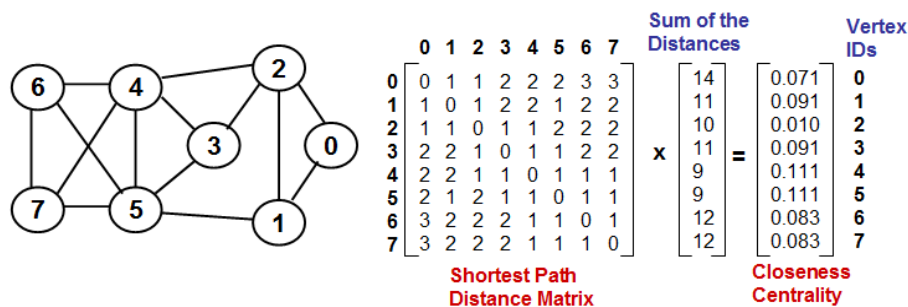


Figure 8. Example to Illustrate the Calculation of Closeness Centrality

4. Correlation Coefficient Measures

We now discuss the three well-known correlation coefficient measures that are used to evaluate the correlation between maximal clique size and the four centrality metrics presented in Section 3. These are the Product-moment based Pearson's correlation coefficient, Rank based Spearman's correlation coefficient and Concordance based Kendall's correlation coefficient. All the three measures evaluate the extent of the degree of linear dependence (Triola, 2012) between two datasets or performance metrics (in our case, the maximal clique size and each of the four centrality metrics).

The correlation coefficient values obtained for all the three measures range from -1 to 1. Correlation coefficient values closer to 1 indicate a stronger positive correlation between the two metrics considered (i.e., a vertex having a larger value for one of the two metrics is more likely to have a larger value for the other metric too), while values closer to -1 indicate a stronger negative correlation (i.e., a vertex having a larger value for one of the two metrics is more likely to have a smaller value for the other metric). Correlation coefficient values closer to 0 indicate no correlation (i.e., the values incurred by a vertex for the two metrics are independent of each other). We will adopt the ranges (rounded to two decimals) proposed by Evans (1995) to indicate the various levels of correlation, shown in Table 1. For simplicity, we refer to the two datasets as *M* and *C* respectively corresponding to the maximal clique size and centrality. We will use the results from Figures 4-8 to illustrate examples for the computation of the correlation coefficient under each of the three measures.

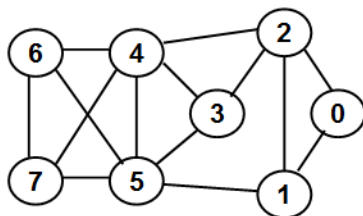
Table 1. Range of Correlation Coefficient Values and the Corresponding Levels of Correlation

Range of Correlation Coefficient Values	Level of Correlation	Range of Correlation Coefficient Values	Level of Correlation
0.80 to 1.00	Very Strong Positive	-1.00 to -0.80	Very Strong Negative
0.60 to 0.79	Strong Positive	-0.79 to -0.60	Strong Negative
0.40 to 0.59	Moderate Positive	-0.59 to -0.40	Moderate Negative
0.20 to 0.39	Weak Positive	-0.39 to -0.20	Weak Negative
0.00 to 0.19	Very Weak Positive	-0.19 to -0.01	Very Weak Negative

4.1 Pearson's Product-Moment Correlation Coefficient

The Pearson's product moment-based correlation coefficient for two datasets is defined as the covariance of the two datasets divided by the product of their standard deviation (Triola, 2012). Let M_{avg} and C_{avg} denote the average values for the maximal clique size and a centrality metric for a graph of n vertices and let M_i and C_i denote respectively the values for the maximal clique size and the centrality metric of interest incurred for vertex i . The Pearson's correlation coefficient (indicated PCC) is quantitatively defined as shown in equation (3). The term product moment is associated with the product of the mean (first moment) adjusted values for the two metrics in the numerator of the formulation. Figure 9 presents the calculation of the PCC for the maximal clique size (M) and degree centrality (C) values obtained for the example graph used in Figures 3-8. We obtain a Correlation Coefficient value of 0.5 (see Figure 9) indicating a moderately positive correlation between the two metrics for the example graph.

$$PCC(M, C) = \frac{\sum_{i=1}^n (M_i - M_{avg})(C_i - C_{avg})}{\sqrt{\sum_{i=1}^n (M_i - M_{avg})^2 \sum_{i=1}^n (C_i - C_{avg})^2}} \tag{3}$$



Vertex	M	C (DegC)	M - M _{avg}	C - C _{avg}	(M - M _{avg}) * (C - C _{avg})	(M - M _{avg}) ²	(C - C _{avg}) ²
0	3	2	-0.5	-1.5	0.75	0.25	2.25
1	3	3	-0.5	-0.5	0.25	0.25	0.25
2	3	4	-0.5	0.5	-0.25	0.25	0.25
3	3	3	-0.5	-0.5	0.25	0.25	0.25
4	4	5	0.5	1.5	0.75	0.25	2.25
5	4	5	0.5	1.5	0.75	0.25	2.25
6	4	3	0.5	-0.5	-0.25	0.25	0.25
7	4	3	0.5	-0.5	-0.25	0.25	0.25
Avg	3.5	3.5		Sum	2	2	8

Correlation Coefficient = $2 / \sqrt{(2 \cdot 8)} = 0.5$

Figure 9. Example to Illustrate the Computation of Pearson's Correlation Coefficient (between Maximal Clique Size: *M* and Degree Centrality: *C*)

4.2 Spearman's Rank-Based Correlation Coefficient

Spearman's rank correlation coefficient (SCC) is a measure of how well the relationship between two datasets (variables) can be assessed using a monotonic function (Triola, 2012). To compute the SCC of two datasets M and C , we convert the raw scores M_i and C_i for a vertex i to ranks m_i and c_i and use formula (2) shown below, where $d_i = m_i - c_i$ is the difference between the ranks of vertex i in the two datasets. We follow the convention of assigning the rank values from 1 to n for a graph of n vertices, even though the vertex IDs range from 0 to $n-1$. To obtain the rank for a vertex based on the list of values for a performance metric, we first sort the values (in ascending order). If there is any tie, we break the tie in favor of the vertex with a lower ID; we will thus be able to arrive at a tentative, but unique, rank value for each vertex with respect to the performance metric. We determine a final ranking of the vertices as follows: For vertices with unique value of the performance metric, the final ranking is the same as the tentative ranking. For vertices with an identical value for the performance metric, the final ranking is assigned to be the average of their tentative rankings. Figure 10 illustrates the computation of the tentative and final ranking of the vertices based on their maximal clique size and degree centrality values in the example graph used in Figures 3-9 as well as illustrates the computation of the Spearman's rank-based correlation coefficient.

$$SCC(M, C) = 1 - \frac{6 \sum_{i=1}^n d_i^2}{n(n^2 - 1)} \quad (4)$$

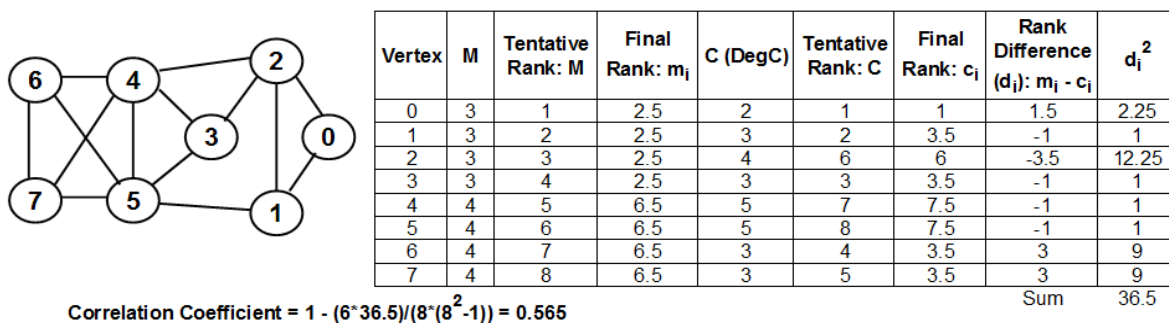


Figure 10. Example to Illustrate the Computation of Spearman's Correlation Coefficient (between Maximal Clique Size: M and Degree Centrality: C)

In Figure 10, we observe ties among vertices with respect to both the maximal clique size and degree centrality. The tentative ranking is obtained by breaking the ties in favor of vertices with lower IDs. In the case of maximal clique size (M), we observe the four vertices 0-3 have an identical M value of 3 each and their tentative rankings are 1-4; the final ranking (2.5) of each of these four vertices is thus the average of 1, 2, 3 and 4. Likewise, the four vertices 4-7 have an identical M value of 4 each and their tentative rankings are 5-8; the final ranking (6.5) of each of these four vertices is thus the average of 5, 6, 7 and 8. In the case of degree centrality (D), we observe ties among vertices with degree 3 (tentative rankings of 2, 4 and 5; final ranking: 3.5 - average of 2, 4 and 5) and among vertices with degree 5 (tentative rankings of 7 and 8; final ranking: 7.5 - average of 7 and 8). The Spearman's rank-based correlation coefficient (SCC) computed for maximal clique size and degree centrality for the example graph used from Figures 3-9 is 0.565. We observe the SCC value to be slightly larger than the PCC value obtained in Figure 9 for the same graph; but, the level of correlation for both the measures still falls in the range of moderately positive correlation.

4.3 Kendall's Concordance-Based Correlation Coefficient

Kendall's concordance-based correlation coefficient (KCC) for any two performance metrics (say, M and C) is a measure of the similarity (a.k.a. concordance) in the ordering of the values for the metrics incurred by the vertices in the graph (Triola, 2012). We define a pair of distinct vertices v_i and v_j as concordant if $\{M_i > M_j \text{ and } C_i > C_j\}$ or $\{M_i < M_j \text{ and } C_i < C_j\}$. In other words, a pair of vertices v_i and v_j are concordant if either one of these two vertices strictly have a larger value for the two metrics M and C compared to the other vertex. We define a pair of distinct vertices v_i and v_j as discordant if $\{M_i > M_j \text{ and } C_i < C_j\}$ or $\{M_i < M_j \text{ and } C_i > C_j\}$. In other words, a pair of vertices v_i and v_j are discordant if a vertex has a larger value for only one of the two performance

metrics. A pair of distinct vertices v_i and v_j are neither concordant nor discordant if either $\{M_i = M_j\}$ or $\{C_i = C_j\}$ or $\{M_i = M_j \text{ and } C_i = C_j\}$. The Kendall's concordance-based correlation coefficient is simply the difference between the number of concordant pairs (denoted $\#conc.pairs$) and the number of discordant pairs ($\#disc.pairs$) divided by the total number of pairs considered. For a graph of n vertices, KCC is calculated as shown in formulation (5).

$$KCC(M, C) = \frac{\#conc.pairs - \#disc.pairs}{\frac{1}{2}n(n-1)} \tag{5}$$

Figure 11 illustrates the calculation of the Kendall's correlation coefficient between maximal clique size and degree centrality for the example graph used in Figures 3-9. For a graph of 8 vertices, the total number of distinct pairs that could be considered is $8(8-1)/2 = 28$ and out of these, 10 pairs are classified to be concordant and 2 pairs as discordant. The remaining 16 pairs are neither concordant nor discordant (denoted as N/A) in the figure. We get a correlation coefficient of 0.286, falling in the range of weakly positive correlation, and it is lower than the correlation coefficient values (falling in the range of moderately positive correlation) obtained with the Pearson's and Spearman's measures. The KCC is also observed to return the lowest correlation coefficient values for all our experiments with the random networks and scale-free networks (Section 5-6). Thus, the KCC could be construed to provide a lower bound for the correlation coefficient values and the level of correlation between maximal clique size and the centrality metric considered.

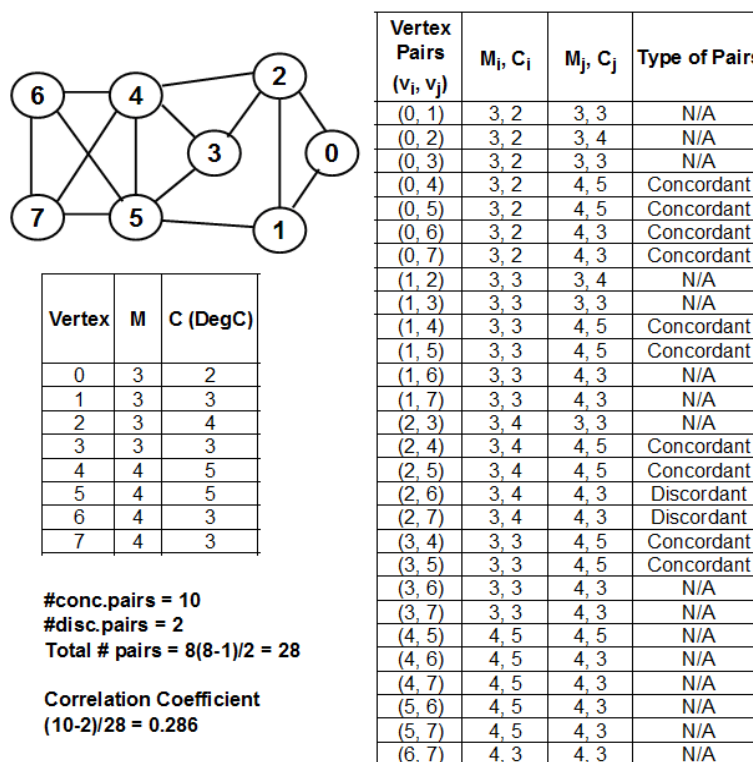


Figure 11. Example to Illustrate the Computation of Kendall's Correlation Coefficient (between Maximal Clique Size: M and Degree Centrality: C)

5. Random Network Graphs

In this section, we discuss the results of our correlation analysis studies for maximal clique size vs. centrality metrics on the random network graphs generated from the well-known Erdos-Renyi (ER) model (Erdos & Renyi, 1959). Under the ER model, there could exist a link between any two nodes in the network with a probability p_{link} . We conduct the simulations for a network of 100 nodes and vary the p_{link} values from 0.01 to 0.50. For each p_{link} value, we run 100 runs of the simulations and average the results for the correlation coefficient with

maximal clique size for each centrality metric under each of the three correlation measures. For a given p_{link} value, we consider all pairs of nodes in the network and set up a link between any two nodes if the random number (in the range 0...1) generated for the pair of nodes is less than or equal to p_{link} .

The larger the p_{link} value, the larger the number of links generated in a random network and lower the variation in node degree, measured in terms of the spectral radius ratio for node degree, denoted λ_{sp} (Meghanathan, 2014). The spectral radius ratio for node degree for a graph is the ratio of the principal eigenvalue of the adjacency matrix of the graph to that of the average node degree. The λ_{sp} values are always greater than or equal to 1.0. The larger the value, the larger the variation in node degree. Random networks exhibit a Poisson-style degree distribution and have a lower variation in node degree; their λ_{sp} values are typically closer to 1.0. Scale-free networks have a larger variation in node degree (especially those with a few hubs - high degree nodes, and the rest of the nodes are of relatively much lower degree) - incurring a larger λ_{sp} value. With a larger number of links for a fixed number of nodes, the robustness of the network (with regards to disconnection due to link failures) also increases (as is measured in terms of the algebraic connectivity of the network). The algebraic connectivity (Maia de Abreu, 2007) of a connected network is the second smallest eigenvalue of the Laplacian matrix (Triola, 2012) of a graph. If \mathbf{A} and \mathbf{D} are respectively the adjacency matrix and degree matrix of a graph, the Laplacian matrix \mathbf{L} is simply $\mathbf{A} - \mathbf{D}$. The degree matrix is also a square matrix whose non-diagonal entries are all zeros and the diagonal entries correspond to the degree of the vertices. From Figure 12, we observe the spectral radius ratio for node degree to show a sharp decrease (a power-law style decrease) with increase in p_{link} , where as the algebraic connectivity exhibits a moderate rate of increase with increase in p_{link} .

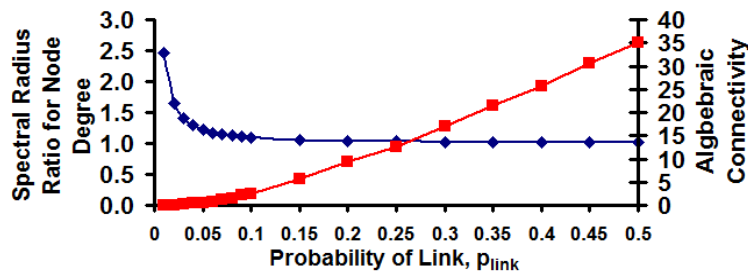
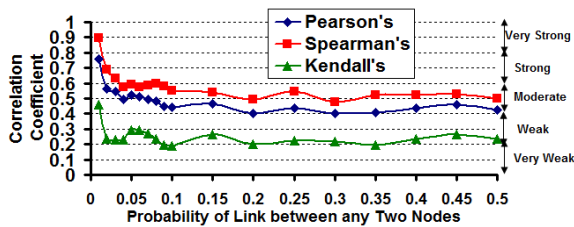
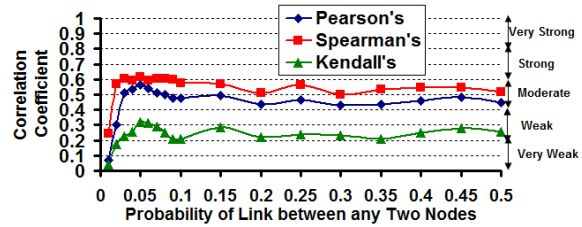


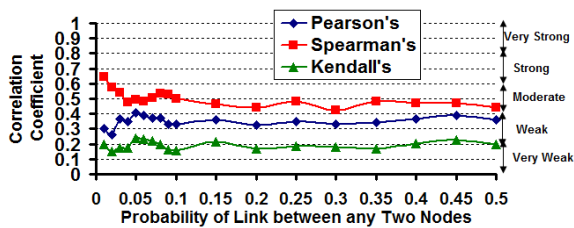
Figure 12. Spectral Radius and Algebraic Connectivity of Random Networks under the ER Model



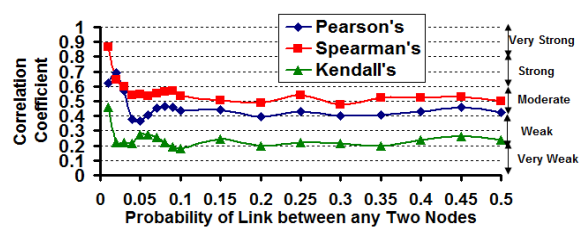
Maximal Clique Size vs. Degree Centrality



Maximal Clique Size vs. Eigenvector Centrality



Maximal Clique Size vs. Betweenness Centrality

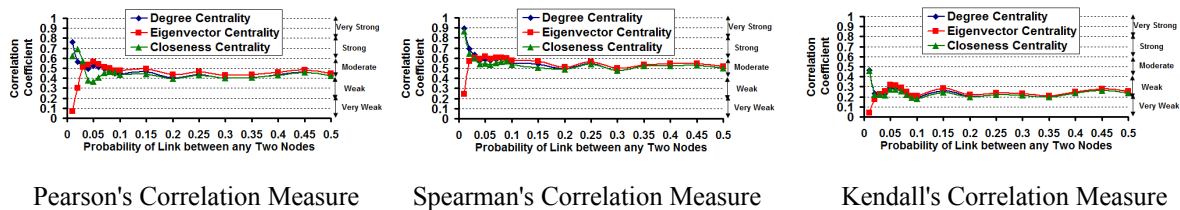


Maximal Clique Size vs. Closeness Centrality

Figure 13. Distribution of the Correlation Coefficient Values for the ER Model based-Random Networks (from the Correlation Measures Viewpoint)

With respect to the correlation measures used, from Figure 13, we observe the Spearman's rank-based correlation and Kendall's concordance-based correlation measures to respectively serve as an upper bound and lower bound

for the level of correlation. All the four centrality metrics incur relatively closer values for the correlation coefficient under the Pearson's and Spearman's correlation measures to an extent that the level of correlation between a centrality metric and maximal clique size is the same under both the measures for a majority of the p_{link} values. The betweenness centrality incurs the lowest correlation coefficient values with maximal clique size under all the three correlation measures. Hence, when we just plot the correlation coefficient values of the three centrality metrics under a particular correlation measure (Figure 14), for p_{link} values greater than or equal to 0.05 (referred to as the fully connected regime: see the discussion below), we observe a negligible difference in the level of correlation for DegC, EVC and CIC with maximal clique size, with the EVC incurring slightly larger correlation coefficient values (the maximum difference is within 0.05 for $p_{link} \geq 0.1$).



Pearson's Correlation Measure Spearman's Correlation Measure Kendall's Correlation Measure
Figure 14. Distribution of the Correlation Coefficient Values for Random Networks (from the Centrality Metrics Viewpoint)

From Figure 13, we observe that for random networks with p_{link} values starting from 0.05, the level of correlation (for any centrality metric with the maximal clique size under any of the three correlation measures) is at best moderately positive. The degree centrality and closeness centrality metrics exhibit strong-very strong positive correlation (a decrease in the level of correlation as p_{link} increases) for p_{link} values ranging from 0.01 to 0.04 (scenarios when the variation in node degree is larger, and the connectivity of the network is low). The eigenvector centrality metric exhibits weak-moderate positive correlation (an increase in the level of correlation as p_{link} increases) for p_{link} values ranging from 0.01 to 0.04 and the level of correlation remains the same for p_{link} values greater than or equal to 0.05. The betweenness centrality metric exhibits a relatively higher level of correlation for p_{link} values 0.01 to 0.09, compared to the level of correlation observed for p_{link} values greater than or equal to 0.1. Thus, for at least three of the four centrality metrics, the transition from a relatively higher or lower level of positive correlation to at best a moderately positive level of correlation (that remains the same henceforth) occurs at p_{link} value of 0.05 (for a network of $n = 100$ nodes, $p_{link} = 0.05 \approx \ln(n)/n$) and this could be termed as the critical probability at which the random network is considered to be in the fully connected regime (Christensen et al., 1998) and have a single giant component with no isolated nodes or clusters. For $p_{link} \geq 1/n$ (i.e., $p_{link} \geq 0.01$ for $n = 100$ nodes) and $p_{link} < \ln(n)/n$, we could refer to the random network to be in the supercritical regime (Christensen et al., 1998) with a single giant component, but with one or more isolated nodes or clusters. Hence, for a random network under evolution according to the ER model, we could conclude that the centrality metrics exhibit at best a moderately positive correlation with the maximal clique size in the fully connected regime; whereas the degree centrality and closeness centrality metrics exhibit a strong-very strong positive correlation with the maximal clique size in the supercritical regime.

6. Scale-Free Network Graphs

In this section, we discuss the results of correlation analysis obtained for scale-free network graphs generated from the well-known Barabasi Albert (BA) model (Barabasi & Albert, 1999). The BA model for network evolution is based on the notion of preferential attachment: i.e., a newly introduced node prefers to attach itself to nodes with relatively larger degree. In addition to the total number of nodes (n) in the network, the BA model works based on two parameters: the initial number of nodes (n_0) and the initial number of links added per node introduction (m_0). We start with a network of n_0 nodes (identified with ids $1, \dots, n_0$) such that there exists at least one link incident on each node. We then start introducing new nodes to the network, one node at a time, and these nodes are identified based on the time of their introduction. The first node is considered to be introduced at time n_0+1 , the second node at time n_0+2 , ..., and the last node is considered to be introduced at time n . Let $k_i(t)$ denoted the degree of node i (introduced at time i) at some time instant t (such that $t \geq i$). When a new node is to be introduced at time $t+1$, the probability for node i to be considered for a link to the newly introduced node is:

$$\frac{k_i(t)}{\sum_{j=1}^t k_j(t)} \quad (6)$$

$A_{[j,t+1]}=0$

All the existing nodes (to which the newly introduced node at time instant $t+1$ does not have a link yet; i.e. $A_{[j,t+1]} = 0$ for $j = 1, \dots, t$, where A is the adjacency matrix of the network graph) are considered while computing the above probability formulation for adding each of the m_0 links to the newly introduced node.

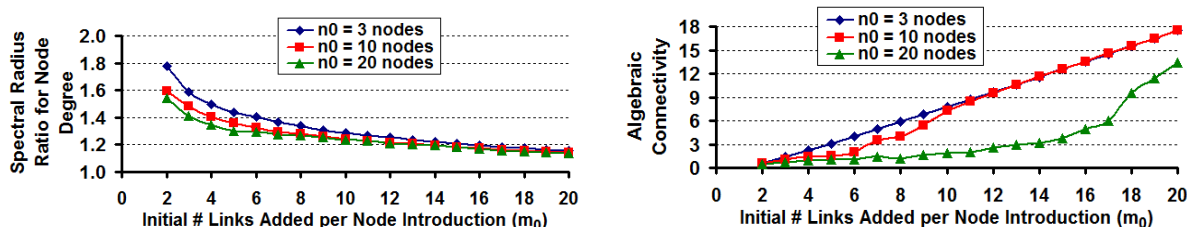


Figure 15. Spectral Radius and Algebraic Connectivity of Scale-Free Networks under the BA Model

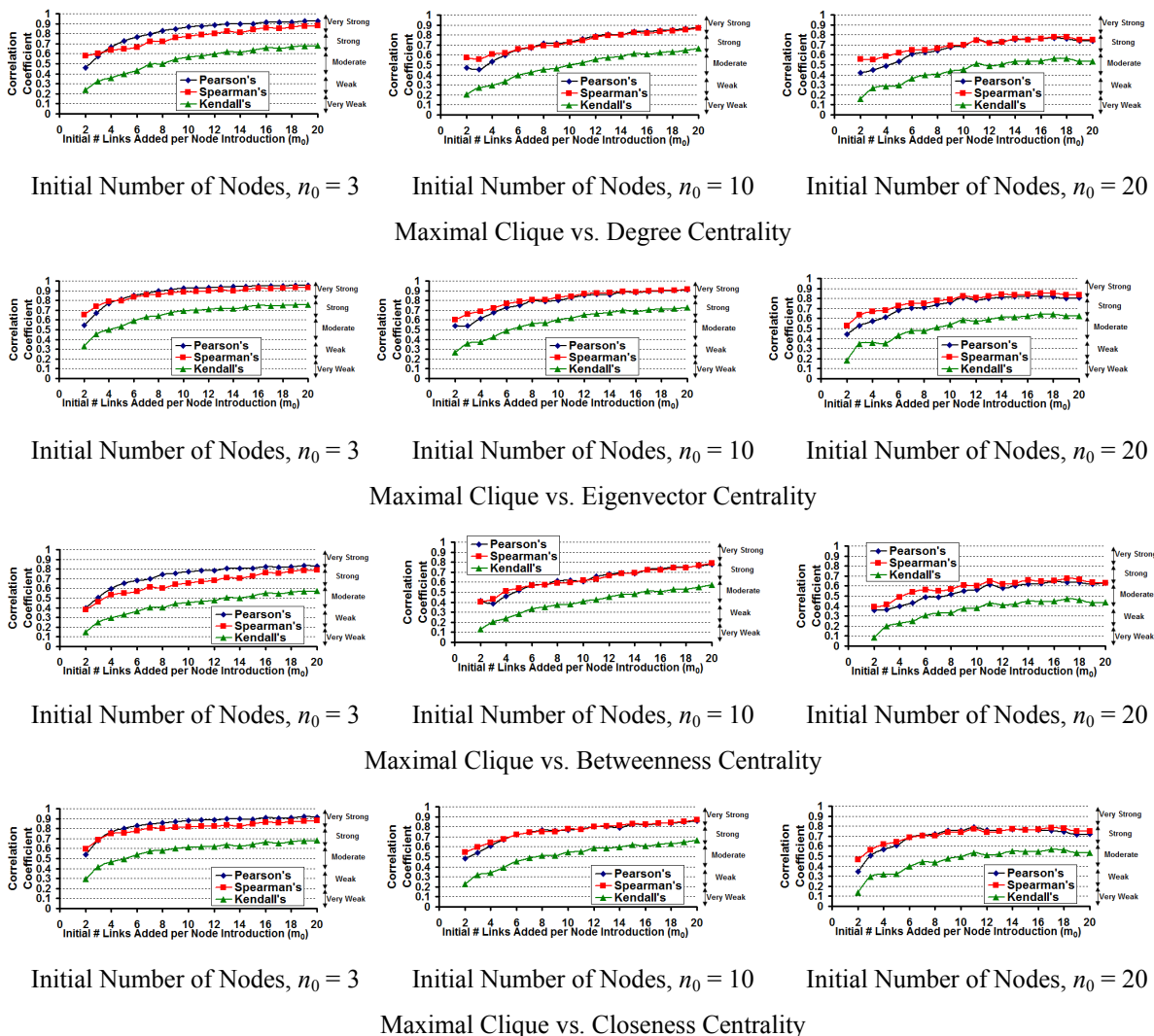


Figure 16. Distribution of the Correlation Coefficient Values for the BA Model based Scale-Free Networks (from the Correlation Measures Viewpoint)

For the simulations, we generated scale-free networks comprising of $n = 100$ nodes and varied the initial number of nodes and links respectively with values of $n_0 = 3, 10$ and 20 , and $m_0 = 2, 3, \dots, 20$ (in increments of 1). For a fixed n_0 and m_0 , we ran the simulations 100 times and averaged the results for the correlation coefficient values obtained for maximal clique size with each of the four centrality metrics under each of the three correlation measures. Figure 15 displays the impact of n_0 and m_0 on spectral radius ratio for node degree and algebraic connectivity for a scale-free network of 100 nodes (the results are the average of the 100 simulation runs for each combination n_0 and m_0). We observe the networks to be relatively more scale-free for lower values of n_0 and m_0 , and as either of them or both increases, we observe the variation in node degree to decrease. For a fixed m_0 , we observe both the spectral radius ratio for node degree and algebraic connectivity to decrease with increase in n_0 ; the decrease in the algebraic connectivity is more prominent for larger values of n_0 (especially, with increase in m_0). For a fixed n_0 , we observe the spectral radius ratio for node degree (λ_{sp}) to decrease at a much faster rate and the algebraic connectivity to increase (sub linearly for $m_0 < n_0$ and linearly for $m_0 \geq n_0$) with increase in m_0 . We could thus characterize the scale-free networks (under evolution with the BA model) to fall into two regimes: the sub-linear connectivity regime (where $m_0 < n_0$) and the linear connectivity regime (where $m_0 \geq n_0$).

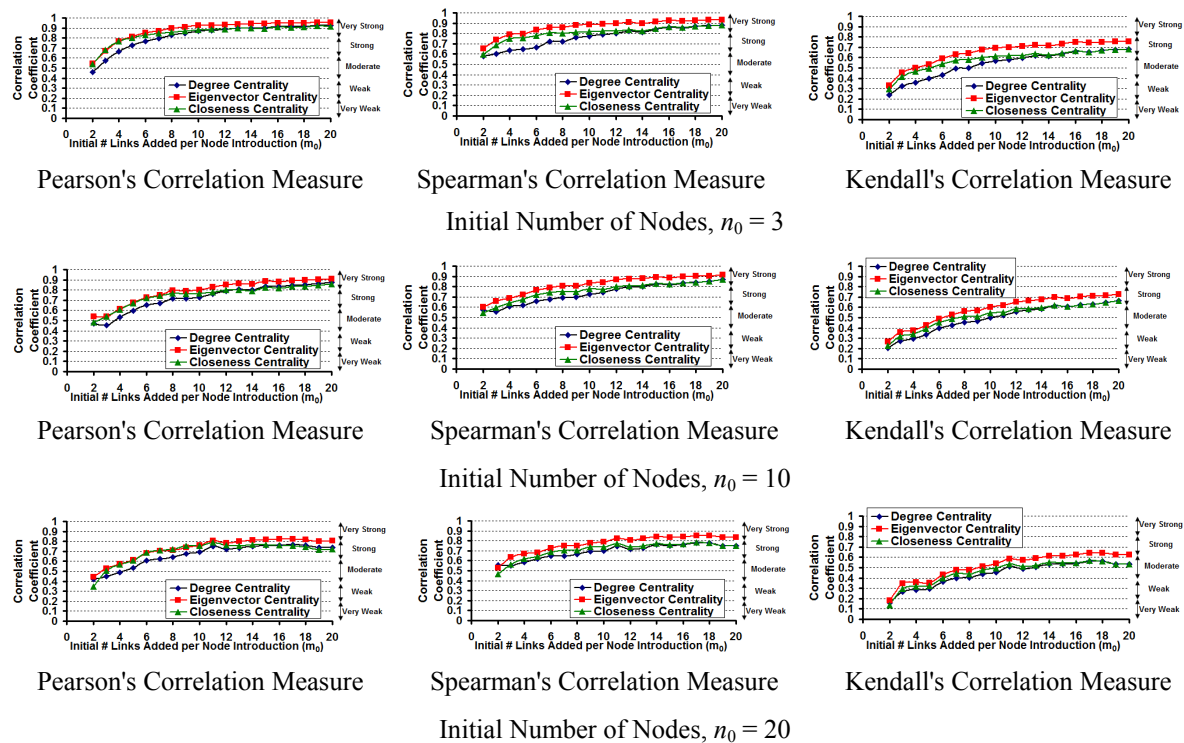


Figure 17. Distribution of the Correlation Coefficient Values for the BA Model-based Scale-Free Networks (from the Centrality Metrics Viewpoint)

The overall trend of the results (see Figure 16) with respect to the correlation measures is that when operated in the linear connectivity regime ($m_0 \geq n_0$), the Pearson's product moment-based correlation measure is likely to determine higher level of correlation compared to that of the Spearman's rank-based correlation measure; on the other hand, when operated in the sub-linear connectivity regime ($m_0 < n_0$), both the Pearson's and Spearman's correlation measures return almost the same level of correlation (the Spearman's correlation coefficient values are just marginally larger and the difference is almost negligible for most of the scenarios). The Kendall's correlation measure returns the lowest levels of correlation for both the linear and sub-linear connectivity regimes for all the centrality metrics.

For any given centrality metric, we observe the level of correlation with the maximal clique size to increase as we transition from a sub-linear connectivity regime to a linear connectivity regime (especially when the number of new links added per node introduction gets significantly larger than the initial number of nodes in the network). For a given value of n_0 and m_0 , we observe the neighbor-based centrality metrics to exhibit a relatively higher level of correlation compared to the shortest path-based centrality metrics, with the betweenness centrality

exhibiting the lowest level of correlation in all the cases. For a given m_0 , as we increase the initial number of nodes, the level of correlation for each centrality metric is likely to drop by one level (from very strong to strong or from strong to moderate, etc).

From Figure 17, it is evident that given a particular value of m_0 and n_0 , for both the linear and sub-linear connected regimes, the eigenvector centrality (EVC) is more likely to exhibit the largest value for the correlation coefficient (under all the three correlation measures), followed by the closeness centrality (CIC) and degree centrality (DegC) metrics. Under the Pearson's and Spearman's correlation measures, the three centrality metrics (EVC, CIC and DegC) are likely to exhibit a moderate-strong positive correlation in the sub-linear connectivity regime and strong-very strong correlation in the linear connectivity regime; on the other hand, the betweenness centrality metric is likely to exhibit a weak-moderate positive correlation in the sub-linear connectivity regime and moderate-strong correlation in the linear connectivity regime. Under the Kendall's correlation measure, for any given n_0 and m_0 , the level of correlation appears to drop by one or two levels (the drop is just by one-level for most of the scenarios) for any centrality metric compared to that incurred with the Pearson's and Spearman's measures.

7. Related Work

Recently, we published two articles (Meghanathan, 2015a; Meghanathan, 2016) analyzing the correlation between the maximal clique size and the centrality metrics for complex real-world network graphs (DuBois & Smyth, 2008; Newman, 2013; Leskovec & Krevl, 2014). The two articles are restricted to just using the Pearson's product moment-based correlation measure and analyzed only the real-world network graphs. In this paper, in addition to the Pearson's measure, we have also used two other correlation measures (Spearman's rank-based and Kendall's concordance-based measures) so that we are able to identify the best-case and worst-case levels of correlation between maximal clique size and the centrality metrics. Instead of analyzing the real-world network graphs, we have analyzed theoretical networks generated from the Erdos-Renyi (ER) model (for random networks) and the Barabasi-Albert (BA) model (for scale-free networks). We observe that it is possible to directly associate the correlation levels with the state of the random networks in the supercritical and fully connected regimes of evolution under the ER model as well as with the state of the scale-free networks in the sub-linear and linear connectivity regimes of evolution under the BA model. To the best of our knowledge, there is no other work that has reported the correlation between maximal clique size and the centrality metrics for random networks and scale-free networks.

Prior to (Meghanathan, 2015a; Meghanathan, 2016) and this paper, researchers have analyzed the centrality metrics and maximal clique size only in isolation. Li et al (2015) and Meghanathan (2015b) conducted correlation analysis study among the centrality metrics for real-world network graphs using the Pearson's product moment-based correlation measure. In addition, centrality metrics have also been widely studied for the analysis and visualization of complex networks in several domains, ranging from biological networks to social networks (Koschutski, 2008; Opsahl et al., 2010). With regards to the maximal clique size of the individual vertices (the largest size clique that a vertex is part of), Meghanathan (2015c) observed the distribution of the maximal clique size values for the vertices in several real-world network graphs as well as those of the small-world networks under the evolution of the Watts-Strogatz model (Watts & Strogatz, 1998) to follow a Poisson-style distribution. Most of the other works in the literature focused on developing efficient approximation heuristics as well as exact algorithms to determine the maximum clique size (an NP-hard problem) for the entire network graphs. Though branch-and-bound has been the common theme among the exact algorithms to determine the maximum clique size, the difference lies in the approach used to prune the search space: node degree (Pattabiraman et al., 2013), vertex coloring (Ostergard, 2002) and vertex ordering (Carraghan & Pardalos, 1990). As is observed in this paper, the savings in time (due to pruning) incurred by the branch-and-bound based exact algorithms for maximum clique size of an entire graph is lost to a certain extent when these algorithms are adapted to determine the maximal clique size of the individual vertices of the graph. Owing to the time-consuming nature of the exact algorithms to determine maximal clique size of the vertices in a graph, it becomes imperative to identify one or more computationally light-weight metrics (like the degree centrality) that can be used to rank the vertices in a complex network graph in almost the same order (if not exact) that would be obtained using the maximal clique size.

8. Conclusions

Overall, the work presented in this paper could serve as a framework for evaluating the various levels of correlation (inclusive of identifying the best-case and worst-case scenarios) between any two metrics for complex network graphs. We qualitatively categorize the levels of correlation based on the quantitative values of

the correlation coefficient observed. We also show that the computationally light-weight centrality metrics (especially the neighbor-based degree and eigenvector centrality metrics) could serve as alternate metrics to rank the vertices of a network graph in lieu of the maximal clique size, a computationally hard metric. The above assertion holds very much true for scale-free networks and random networks in the supercritical regime; but, only to a certain extent for random network graphs in the fully connected regime (for which we observe only a moderately positive correlation).

The more specific results are as follows: For random networks generated under the ER model, the degree centrality and closeness centrality metrics exhibit strong-very strong positive correlation when the network is under the supercritical regime of evolution; whereas we observe all the centrality metrics to at best exhibit a moderately positive correlation when the network is under the fully connected regime of evolution (with a single giant component encompassing all the nodes). For scale-free networks generated under the BA model, we observe the eigenvector centrality to exhibit the largest levels of correlation (under all the three correlation measures) in both the sub-linear and linear connectivity regimes of the network. For all the four centrality metrics, we observe the correlation level to increase as we transition from the sub-linear connectivity regime to the linear connectivity regime of a scale-free network under evolution. The betweenness centrality metric incurs the lowest levels of correlation with the maximal clique size for both the theoretical networks. With respect to the correlation measures used, we observe the following: There is negligible difference in the correlation levels identified with the Spearman's and Pearson's correlation measures for both the random and scale-free networks generated from the theoretical models. The Kendall's concordance-based correlation measure provides the lowest possible levels of correlation that could be observed between a centrality metric and the maximal clique size.

Acknowledgments

The research is financed by the NASA EPSCoR sub award (#: NNX14AN38A) from University of Mississippi.

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