Ranking by Loops: a new approach to categorization

Valery Van Kerrebroeck and Enzo Marinari
Dipartimento di Fisica, “Sapienza” Università di Roma, INFN-CNR and INFN,
P.le A. Moro 2, 00185 Roma, Italy.

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We introduce Loop Ranking, a new ranking measure based on the detection of closed paths, which can be computed in an efficient way. We analyze it with respect to several ranking measures which have been proposed in the past, and are widely used to capture the relative importance of the vertices in complex networks. We argue that Loop Ranking is a very appropriate measure to quantify the role of both vertices and edges in the network traffic.

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Finding the most important vertices is an important problem in complex network analysis [1]. In technological networks, such as the Internet, the main hubs (i.e., the vertices with many links to other vertices) play an important role in the stability of the network [2]. Instead, the removal of any kind of species in food webs may cause the disintegration of the corresponding network [3]. The order of importance of the vertices is referred to as a ranking. In general the importance of a vertex, and thus its ranking, depends very much on the type of network which is under consideration. The measures that are based on topological features are assumed to be more objective, and typically result in more adequate rankings.

The most simple topology based ranking measure is the degree, i.e., the number of neighboring vertices of a vertex. While the degree is easy to compute, it is not a very refined measure, as it solely depends on the local neighborhood around a vertex. Several more global measures [4,5,6,7,8] have been proposed which do take the overall structure of the network into account. Apart from finding a fast way to compute these measures, another challenge is usually to decide which of these measures are more appropriate for which type of network.

We start our reasoning from the observation that the link structure of complex networks describes the topology of interactions taking place in a dynamic complex system: the importance of a vertex (or edge) to the network traffic is related to the number of paths or walks it lies on [9].

The topology of most real-world networks is represented by a directed graph $G(V,E)$ which is completely characterized by its set $V$ of $N$ vertices $i$ and by the set $E$ of $M$ directed edges $i \rightarrow j$, where $i$ and $j$ are said to be the starting and ending vertex, respectively, of the directed edge $i \rightarrow j$. For undirected graphs either one of the ending vertices $i$ and $j$ of the edge $\{i,j\}$ can be the ending or starting vertices. Accordingly, information can travel in either direction along the edges of an undirected network. In case of weighted directed graphs, we associate a weight $r_{i \rightarrow j}$ to each one of the directed edges $i \rightarrow j$. For unweighted graphs all edge weights are uniformly equal to one. We denote the set of edges or the set of vertices of these edges distinct from $i$ (as it is always clear from the context) of which $i$ is an ending vertex or starting vertex as $\partial^+_{i}$ or $\partial^-_{i}$, respectively. Correspondingly, the in-degree $d^+_i$ and out-degree $d^-_i$ of a vertex $i$ are defined as the sum of the weights of the edges of which that vertex $i$ is an ending vertex, or starting vertex, respectively.

Walks are defined as sequences of vertices $(i_1, \ldots, i_L)$, where for each couple of subsequent vertices $i_{k-1}$ and $i_k$, for $k = 2, \ldots, L$, the directed edge $i_{k-1} \rightarrow i_k$ belongs to $E$. As such, they can cross the same edge or vertex infinitely many times. Instead, paths are defined as self-avoiding walks. In particular, a cycle or loop is a closed path. More formally, it is defined as a sequence $(i_1, i_2, \ldots, i_L, i_1)$ of vertices, where for all $k = 1, 2, \ldots, L$ these $i_k$ are distinct from each other, and, for all $k = 2, \ldots, L$, each couple of subsequent vertices $i_{k-1}$ and $i_k$ are connected by a directed edge $i_{k-1} \rightarrow i_k$ belonging to $E$, as does $i_L \rightarrow i_1$. The weight of any of these subgraphs is defined as the product of the weights $r_{i_{k-1} \rightarrow i_k}$ of the edges composing that subgraph. In case of a cycle defined by a sequence $(i_1, i_2, \ldots, i_L, i_1)$, its corresponding weight is given by $w[C] = r_{i_1 \rightarrow i_2} r_{i_2 \rightarrow i_3} \cdots r_{i_{L-1} \rightarrow i_1}$.

One measure which is widely used to find the most relevant vertices of a network is PageRank [6]. PageRank is an iteratively computed ranking measure where the PageRank of a given vertex depends on the PageRank of its neighboring vertices. More formally, the PageRank $P(i)$ of a vertex $i$ is defined as

\begin{equation}
P(i) = c \sum_{j \in \partial^+_{i}} \frac{P(j)}{d_j} + \frac{1-c}{N},
\end{equation}

where $c$ is a damping factor chosen in the interval $[0,1]$. In matrix form this becomes $P = c \frac{C^T}{d^-} P + \frac{1-c}{N} \delta$, where $P$ is a $N$-dimensional vector, $\delta$ is a $N$-dimensional vector with all elements equal to one, and the elements $C_{ij}$ of the $N \times N$ matrix $C$ are equal to $1/d^-_i$ if the edge $i \rightarrow j$ belongs to $E$, and zero otherwise. As the sum of the entries of a column of this matrix $C$ is equal to one, it can be interpreted as a Markov matrix. The resulting PageRank is then proportional to the probability with which a random walker will come across a given vertex. As such,
PageRank is an importance measure for vertices which, being based on random walks, takes the overall structure of the network into account. However, the question naturally arises whether it is not preferable to emulate the behavior of a more efficient self-avoiding random walker.

Motivated by the latter observation, we introduce a new ranking measure based on paths rather than walks. Several centrality measures based on either the number or length of shortest paths passing through or ending at a given vertex have already been proposed. In particular, the Betweenness Centrality \( B \) of a given vertex (or edge) is defined as the fraction of shortest paths on which that vertex (or edge) lies. Defining \( \sigma_{k,l} \) as the number of shortest paths between the vertices \( k \) and \( l \), and \( \sigma_{k,l}(i) \) and \( \sigma_{k,l}(i \rightarrow j) \) the number of these passing through vertex \( i \) or edge \( i \rightarrow j \), we have

\[
B(i) = \sum_{k,l \in V} \sigma_{k,l}(i) \quad \text{and} \quad B(i \rightarrow j) = \sum_{k,l \in V} \frac{\sigma_{k,l}(i \rightarrow j)}{\sigma_{k,l}},
\]

for the BC of vertex \( i \) and the edge \( i \rightarrow j \), respectively. One fundamental problem that prevents these measures from becoming widely used in real network analysis is that they cannot be computed as fast as, for example, PageRank. Moreover, a measure based on shortest paths only may not be adequate enough as also longer paths (with possibly higher weights) could add to the centrality of a given vertex, or edge.

We propose a ranking based on the presence of closed paths, i.e., cycles, through a given vertex. We consider the probability of presence of cycles, rather than all, i.e., also open, paths, for a specific reason. Namely, it allows us to compute the corresponding ranking by means of Belief Propagation, a distributed, message passing algorithm which converges in linear time in the system size to the marginal probabilities of presence of these cycles. This restriction to closed paths results in a ranking which reflects the geometric position of each one of the vertices, and gives a subjective view of how each vertex sees the overall network based on paths.

In particular, we propose a ranking based on the sums of the weights of these cycles. As such it represents the probability with which a self-avoiding walker returns to the same vertex while exploring the network, taking the weight of each path into account. We define the Loop Ranking \( L \) of a vertex \( i \), or edge \( i \rightarrow j \), as the sum of the weights \( w \) of all cycles \( C \) passing through that vertex \( i \), or edge \( i \rightarrow j \) respectively, i.e.,

\[
L(i) = \sum_{C \ni i} w[C] \quad \text{and} \quad L(i \rightarrow j) = \sum_{C \ni (i \rightarrow j)} w[C].
\]

In practice, we do not compute the actual Loop Ranking, but rather the marginal expressing the probability with which a cycle passes through a given vertex, i.e., \( L(i)/\sum_C w[C] \), which produces the same ordering. The latter can be obtained by reformulating the problem of identifying all cycles of a given graph as a constraint satisfaction problem.

We define an appropriate phase space in which all (simple) subgraphs, such as cycles, are represented by a unique configuration. To this purpose we associate with each edge \((i \rightarrow j)\) an Ising-like variable \( S_{i \rightarrow j} \), where \( S_{i \rightarrow j} \) takes on the value zero or one if the corresponding edge \((i \rightarrow j)\) belongs, or does not belong to the considered subgraph, respectively. In this way, we establish the desired one-to-one correspondence between any simple subgraph of the original graph \( G \) and all configurations defined by any of \( 2^M \) sequences \( \mathbf{S} = (S_1, \ldots, S_M) \). For simplicity, we also introduce the notation \( \mathbf{S} \) which denotes the set of all edge variables \( S_{i \rightarrow j} \) and \( S_{j \rightarrow i} \) of which \( i \) is a starting or ending vertex, respectively.

We can now define the probability law

\[
\text{Prob}(\mathbf{S}) = \frac{1}{Z} \prod_{(i-j) \in E} (r_{i \rightarrow j})^{S_{i \rightarrow j}} \prod_{i \in V} f_i(\mathbf{S}), \quad (4)
\]

where the local constraints \( f_i(\mathbf{S}) \) are equal to one if \( \sum_{\mathbf{S} \in \mathcal{S}} S_{i \rightarrow j} = \sum_{\mathbf{S} \in \mathcal{S}} S_{j \rightarrow i} \) is zero or one, while \( f_i(\mathbf{S}) \) are equal to zero otherwise, and \( Z \) is a normalization constant. The complete set of local constraints \( f_i \) ensures that only those configurations representing subgraphs composed of (possibly vertex disjoint) directed cycles have a non zero probability. The first product appearing in relation (4) makes the probability of the allowed configurations proportional to the weight of the subgraph they represent.

An approximation to the marginals of (4) can be obtained using a local Monte Carlo like algorithm as presented in [11]. However, for factorizable probability laws, such as (4), they can also easily be computed by means of message passing algorithms, such as Belief and Survey Propagation [13]. Belief Propagation (BP) is a distributed, iterative algorithm which is intrinsically linear in the system size. It requires the introduction of \( 2M \) real-valued message variables, \( M \) of type \( x_{i \rightarrow j} \) in the same direction of the edges \( S_{i \rightarrow j} \), and \( M \) of type \( y_{j \rightarrow i} \) going in the opposite direction. Initially, they all take on a random value in the interval \([0,1]\). Each BP iteration then consists in an update of these \( 2M \) variables.

Assuming (4), the update rules have the following form,

\[
x_{i \rightarrow j} = \frac{\sum_{k \in \partial^+} r_{k \rightarrow i} x_{k \rightarrow i}}{1 + \sum_{k \in \partial^+} r_{k \rightarrow i} x_{k \rightarrow i} \sum_{k' \in \partial^- \setminus j} r_{i \rightarrow k'} y_{k' \rightarrow i}}, \quad \text{and} \quad y_{j \rightarrow i} = \frac{\sum_{k \in \partial^-} r_{j \rightarrow k} y_{j \rightarrow k}}{1 + \sum_{k \in \partial^-} r_{j \rightarrow k} y_{j \rightarrow k} \sum_{k' \in \partial^+ \setminus i} r_{j \rightarrow k'} x_{k' \rightarrow j}}.
\]

On acyclic graphs, the successive repetition of these BP iteration steps always leads to a fixed point solution. For generic graphs containing cycles, BP does not necessarily converge [14]. However, at least for sparse graphs, which do not contain too many small loops and locally are tree-like, usually it does.
Once the fixed point has been reached, the corresponding value of the message variables can be used to obtain the desired marginal probabilities. In our particular case, we are interested in the vertex and edge marginals expressing the probability with which a cycle contains that particular vertex or edge. Upon convergence of the BP algorithm, these marginals can be obtained from the message variables at the fixed point as

$$p_i = \frac{\sum_{k \in \partial^+} r_{k\rightarrow i} x_{k \rightarrow i} \sum_{k' \in \partial^-} r_{i \rightarrow k'} y_{k' \rightarrow i}}{1 + \sum_{k \in \partial^+} r_{k\rightarrow i} x_{k \rightarrow i} \sum_{k' \in \partial^-} r_{i \rightarrow k'} y_{k' \rightarrow i}},$$

and

$$p_{i \rightarrow j} = \frac{r_{i \rightarrow j} x_{i \rightarrow j} y_{j \rightarrow i}}{1 + r_{i \rightarrow j} x_{i \rightarrow j} y_{j \rightarrow i}},$$

respectively. On a generic, cyclic graph, the above expressions are an approximation to the actual vertex and edge marginals. However, in general, these approximations are very reasonable to work with. The marginals of (1) actually express the probability with which a vertex, or edge, is part of a subgraph composed of possibly several vertex disjoint directed cycles. Thus, exact marginals of (1) are possibly an overestimation of the desired marginals expressing the probability of presence of a (single) closed path. However, for weighted graphs where the edge weights have been rescaled such that they all lie in the interval [0, 1], this effect is largely reduced, and has only a minor impact on the resulting ordering [12].

In order to get hints about which is a good ranking measure for dynamic networks, we have looked at a number of examples and particular cases. We discuss here explicitly the case of two directed small world networks that we consider very telling. We assume them to be unweighted for simplicity. We first consider the graph shown in figure 1. If we only take the outer ring of edges into account, all information can be exchanged between any two vertices in two ways, either in clockwise or counter-clockwise direction, in which case all vertices and edges are considered to be equally important.

The presence of the directed “short cut” edges (which are all out-bound from vertex 0) reduces the length of the shortest paths, a feature which is typical of most real world networks [13]. The resulting “smaller world” (from the point of view of a single vertex) has a large impact on the mobility inside a network. In particular, the vertex 0 will play a more crucial role than other vertices in dispatching packages along the network. Similarly, in a minor way, the ending vertices of the extra out-bound short cuts, i.e., 3, 5 and 8, should play a more important role in the traffic along this network. Also, we expect the presence of these edges to break the symmetry of the role of the single edges in the network flow.

The results according to the various ranking schemes and corresponding ordering for the vertices of graph $G_1$ are reported in table I. We have rescaled the PageRank, Loop Ranking and BC results such that they all lie in the interval [0, 1]. Clearly, the different ranking schemes attribute various degrees of importance to the vertex 0. As the PageRank of a vertex depends primarily on the number of edges directed towards that vertex and the rescaled PageRank they transmit (rescaled by the out-degree of their respective starting vertices), vertex 0 of graph $G_1$ has a relative low PageRank. Instead, as it does lie on most of the (closed) paths of graph $G_1$, its central role is acknowledged by both the Loop Ranking as the BC. Moreover, the latter two rankings recognize the increased role of the vertices 3, 5 and 8 with respect to the other vertices, while PageRank makes no clear-cut difference between them. For the other vertices, the ordering does differ depending on which path based ranking is considered, as Loop Ranking depends on all closed paths, while BC is only based on the number of shortest paths.

The importance ordering of both the vertices and the edges produced by Loop Ranking and BC is schematically presented by figure 1. As in case of the vertices, Loop Ranking and BC do not produce the exact same ordering of edges, but there are no essential huge shifts between the two corresponding rankings. Note that edges with high ranking usually connect one vertex with high and another with low ranking. The presence of these edges has been observed in case of protein networks [16], where it was argued that they play a crucial role in the

![FIG. 1: Directed small world network $G_1$. The various colors express the ranking of the vertices and edges based on Loop Ranking (on the left) and Betweenness Centrality (on the right).](image)
overall robustness of the network.

Graph $G_2$, shown in figure 2, represents a slightly different type of small world network than $G_1$. The extra short-cut edges are in this case pointing towards vertex 0, increasing its role in dispatching information along the network. We also expect the starting vertices 3, 5, 8 of the short-cut edges to play an increased role.

The various ranking results are also reported in table I. All rankings recognize the vertex 0 as the more important one. Loop Ranking and BC also capture the special status of the vertices 3, 5 and 8, even if in a different order. This is not the case for PageRank, due to the fact that it does not consider the out-degree of a given vertex to be very relevant. A comparison of the Loop Ranking of both types of graphs shows that the in- and out-bound edges of the vertices are treated in an identical way, resulting in the same set of Loop Ranking values for all vertices. This is not the case for BC (even though it does result in the same ordering for both graphs), as it does not rely on all, but only on the shortest paths.

Figure 2 also includes a schematic representation of the edge and vertex ranking according to Loop Ranking and BC of graph $G_2$. In the case of graph $G_2$, the edges leading away from vertex 0 play a more significant role, while in graph $G_1$ the edges going to vertex 0 are more important for obvious reasons.

In conclusion, Loop Ranking reflects the role of vertices and edges during the dissipation of information along the network. We have discussed unweighted small world networks to allow for an easier comparison between the various ranking methods. Note that Loop Ranking can naturally be extended to weighted networks, which is a clear advantage in the analysis of real world networks.

While PageRank is more sensitive to the in-degree of a given vertex, Loop Ranking treats all paths (passing in either direction through a given vertex or edge) in an equivalent way. It produces a slightly different ordering of importance with respect to BC as it takes all paths (with their relative weight) into account. Another advantage of the path based rankings we considered here is that they produce both results for the vertices as the edges. Moreover, Loop Ranking can be computed by means of Belief Propagation, which has a linear time complexity in the system size, and this is a remarkable practical advantage. This should also allow for an easier dynamical analysis of rankings, an aspect which has already been studied more carefully for BC.

A limitation of Loop Ranking is that it is only based on loops. As such, it can only produce results regarding the vertices and edges belonging to the 2-core of the graph, i.e., the subgraph for which all vertices have an in- and out-degree of at least one. It is reasonable to assume that the 2-core contains those vertices and edges which are important to the traffic flow: integration with different schemes could eventually allow to design ranking methods optimized for different applications.

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