Comment on “Subgraph centrality in complex networks”

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We disprove a conjecture of Estrada and Rodríguez-Velázquez [Phys. Rev. E 71, 056103 (2005)]
that if a graph has identical subgraph centrality for all nodes, then the closeness and betweenness
centralities are also identical for all nodes.

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Estrada and Rodríguez-Velázquez [1] introduced the subgraph centrality measure of a node in a network as the
weighted sum of the numbers of closed walks of different lengths that start and end at that node. Specifically, if
$A$ is the adjacency matrix of a network, the numbers of closed walks of length $k$ are the diagonal entries of the
matrix $A^k$ [2], and the subgraph centrality of a node $u$ is defined in [1] as

$$C_S(u) = \sum_{k \geq 0} \frac{(A^k)_{uu}}{k!}. \tag{1}$$

They compared the subgraph centrality to standard centrality measures:

$C_D = $ the degree centrality, defined as the number of links incident to a node;

$C_B = $ the betweenness centrality, defined for the measured node $u$ as $\sum_{v,w\neq u} \frac{g(v,u,w)}{g(v,w)}$, where $g(v,w)$ is the number of shortest paths between $v$ and $w$, and $g(v,u,w)$ is the number of shortest paths between $v$ and $w$ that pass through $u$;

$C_C = $ the closeness centrality, defined as the reciprocal of the sum of distances from the measured node to all other nodes;

$C_E = $ the eigenvector centrality, defined as the component of the principal eigenvector of the adjacency matrix of a network.

The comparison of these measures was performed for the set of 210 regular graphs, whose number of nodes
ranges from 6 to 10 and the node degree ranges from 3 to 7, as well as for eight real-world networks. They observed
that for this particular set of regular graphs holds:

(i) if all nodes in a graph have identical subgraph centrality, then all nodes also have identical values of $C_D$, $C_B$, $C_C$ and $C_E$, and

(ii) there exist examples of graphs in which all nodes have identical values of $C_D$, $C_B$, $C_C$ and $C_E$, while not all nodes have identical values of subgraph centrality,
or, in other words, that the subgraph centrality has the greatest discriminative power in this set of graphs. So,
they conjectured that this will always be the case:

**Conjecture [1]:** Let $G$ be a graph having identical subgraph centrality for all nodes. Then the degree, eigenvector, closeness and betweenness centralities are also identical for all nodes.

The purpose of this comment is to elaborate further on this conjecture, by providing counterexamples for the
second part of the conjecture that if a graph has identical subgraph centrality for all nodes, then the closeness and
betweenness centralities are also identical for all nodes.

For this, we first need to recall the notion of graph angles from [3, Chapter 4]. Denote the nodes of the graph $G$
by $1, \ldots, n$. Let $\mu_1, \ldots, \mu_m$ be the distinct eigenvalues of its adjacency matrix $A$, with multiplicites $k_1, \ldots, k_m$, respectively, and let $x_{i,1}, \ldots, x_{i,k_i}$ be the basis of
the eigenspace $\varepsilon_i$, corresponding to the eigenvalue $\mu_i$, $i = 1, \ldots, m$. The angle $\alpha_{u,i}$, corresponding to the node
$u$ of $G$ and the eigenspace $\varepsilon_i$, is defined as

$$\alpha_{u,i} = \sqrt{\sum_{j=1}^{k_i} (x_{i,j})^2 u}. \tag{2}$$

The value $\alpha_{u,i}$ is actually the cosine of the angle between the vector $e_u$ of the standard orthonormal basis of $\mathbb{R}^n$ and the eigenspace $\varepsilon_i$, thus providing an explanation for its name. The most basic properties of graph angles are as follows [3, Chapter 4]:

(i) $\sum_{u=1}^{n} \alpha_{u,i}^2 = k_i$, $i = 1, \ldots, m$,

(ii) $\sum_{i=1}^{m} \alpha_{u,i}^2 = 1$, $u = 1, \ldots, n$,

(iii) $(A^k)_{uu} = \sum_{i=1}^{m} \alpha_{u,i}^2 \mu_i^k$, $u = 1, \ldots, n$, $k \geq 0$.

A graph $G$ is walk-regular if the number of closed walks of an arbitrary length $k \geq 0$ that start and end at a node $u$ does not depend on $u$. Due to (iii) above, this is equivalent to stating that a graph is walk-regular if all nodes have identical angle sequences $\alpha_{u,1}, \ldots, \alpha_{u,m}$. A walk-regular graph is necessarily degree regular, since the degree of a node is equal to the number of closed walks of length two starting and ending at that node. For a connected graph, the degree regularity further implies that the principal eigenvector of $A$ has equal components for all nodes [2, Theorem 3.8].
The subgraph centrality is easily represented via graph angles, as noticed already by Estrada and Rodríguez-Velázquez [1]:

\[ C_S(u) = \sum_{k \geq 0} \frac{(A^k)_{uu}}{k!} = \sum_{k \geq 0} \frac{1}{k!} \sum_{i=1}^{m} \alpha_{u,i}^2 \mu_i^k \]

\[ = \sum_{i=1}^{m} \alpha_{u,i}^2 \sum_{k \geq 0} \frac{\mu_i^k}{k!} = \sum_{i=1}^{m} \alpha_{u,i}^2 e^{\mu_i}. \]

Hence, if a graph is walk-regular, then every node has identical subgraph centrality.

Before we delve deeper into the subject of walk-regular graphs, let us note that, should the conjecture, slightly more expectedly, stated that if two nodes have identical subgraph centralities, then the other four centralities are also identical for these two nodes, then the tree at Fig. 1 would immediately provide a counterexample.

![FIG. 1. (Color online) Two blue diamond nodes have identical angle sequences, but different closeness and betweenness centralities.](image)

The fact that the two blue nodes in this tree have identical angle sequences, has been famously used by Schwenk [4] to prove that almost all trees have a cospectral mate.

However, Estrada and Rodríguez-Velázquez asked in their conjecture that all nodes have identical subgraph centralities. We will, therefore, shift our focus to walk-regular graphs as the examples of graphs in which all nodes have identical subgraph centralities.

There is one particular class of walk-regular graphs for which Conjecture 1 holds: vertex-transitive graphs. Let \( V(G) \) denote the set of nodes of \( G \). A graph \( G \) is vertex-transitive if, given any two nodes \( u, v \in V(G) \), there exists an automorphism \( f_{u,v} : V(G) \rightarrow V(G) \) such that \( f_{u,v}(u) = v \). Recall that a graph automorphism preserves node adjacencies, so that for any two nodes \( s, t \in V(G) \), \( s \) is adjacent to \( t \) if and only if \( f_{u,v}(s) \) is adjacent to \( f_{u,v}(t) \). As a consequence, a graph automorphism also preserves node distances. Actually, any node-based graph invariant necessarily has identical values for all nodes in a vertex-transitive graph. For example,

\[ \frac{1}{C_C(u)} = \sum_{w \in V(G)} d(u, w) = \sum_{f(w) \in V(G)} d(f(u), f(w)) \]

\[ = \sum_{w \in V(G)} d(v, w') = 1/C_C(v), \]

where \( d(u, w) \) denotes the distance between nodes \( u \) and \( w \) in \( G \).

Hence, the counterexamples to Conjecture 1 should be sought among the walk-regular graphs that are not vertex-transitive. These graphs did not receive much attention—up to now, there seems to be a unique example of a walk-regular, non-vertex-transitive graph published in [5], which is shown in Fig. 2(i). This graph is also the first counterexample to Conjecture 1, as all of its nodes have identical subgraph centrality, yet the blue nodes have closeness centrality of \( 1/19 \) and betweenness centrality of \( 8 \), while the orange nodes have closeness centrality of \( 1/18 \) and betweenness centrality of \( 7 \).

To find further counterexamples, we used the \textit{geng} program from the \textit{nauty} package, which is available from \url{http://pallini.di.uniroma1.it/} and described in [6, 7]. Advised by Brendan McKay, we implemented the pruning function in \textit{geng} which, during the construction of regular graphs, filters out non-walk-regular graphs by checking whether the diagonal of each power of the adjacency matrix \( A \) up to \( A^n \) has constant entries (i.e., whether the numbers of closed walks of lengths up to \( n \) are identical for all nodes). We used such a modification of \textit{geng} to search for walk-regular graphs among regular graphs whose node degree ranges from three to seven, and the search results are presented in Table I. Note that the pruning function tests for walk-regularity only—the graphs found may still be (and most of them are) vertex-transitive. There are 174 walk-regular graphs found, which are provided as supplemental material [8]. Among these 174 walk-regular graphs there is a total of eight non-vertex-transitive graphs, which all present counterexamples to Conjecture 1. These graphs are shown in Fig. 2, with the closeness and betweenness centralities given in the caption.

<table>
<thead>
<tr>
<th>Degree</th>
<th>Nodes ( n )</th>
<th>Regular graphs</th>
<th>Walk-regular graphs</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>( 6 \leq n \leq 22 )</td>
<td>7,875,917</td>
<td>34</td>
</tr>
<tr>
<td>4</td>
<td>( 6 \leq n \leq 16 )</td>
<td>8,943,748</td>
<td>55</td>
</tr>
<tr>
<td>5</td>
<td>( 6 \leq n \leq 14 )</td>
<td>3,467,295</td>
<td>26</td>
</tr>
<tr>
<td>6</td>
<td>( 7 \leq n \leq 14 )</td>
<td>21,985,302</td>
<td>35</td>
</tr>
<tr>
<td>7</td>
<td>( 8 \leq n \leq 14 )</td>
<td>21,610,854</td>
<td>24</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>63,883,116</td>
<td>174</td>
</tr>
</tbody>
</table>

TABLE I.

To conclude, if a graph has identical subgraph centrality for all nodes, then the closeness and betweenness centralities need not be identical for all nodes. It was hard to find the counterexamples simply because the premise narrows the conjecture to a rather small set of graphs, examples of which are walk-regular graphs. Nevertheless, as observed by Estrada and Rodríguez-Velázquez in [1] on the examples of real-world complex networks, the subgraph centrality measure may give a distinctly different ranking of nodes than the closeness and betweenness centrality measures, and provide additional insight into the importance of network nodes, making the subgraph centrality measure and the underlying graph angles, a welcome addition to the study of complex networks.
FIG. 2. (Color online) Counterexamples to the conjecture of Estrada and Rodríguez-Velázquez. (i) Blue diamond nodes have closeness $1/19$ and betweenness $8$, while orange circular nodes have closeness $1/18$ and betweenness $7$. (ii) All nodes have closeness $1/17$. Blue diamond nodes have betweenness $22/3$, while orange circular nodes have betweenness $16/3$. (iii) All nodes have closeness $1/16$. Blue diamond nodes have betweenness $73/15$, while orange circular nodes have betweenness $76/15$. This graph is the complement of graph (ii). (iv) All nodes have closeness $1/15$. Blue diamond nodes have betweenness $58/15$, while orange circular nodes have betweenness $61/15$. This graph is the complement of graph (i). (v) Blue diamond nodes have closeness $1/26$ and betweenness $32/3$, while orange circular nodes have betweenness $34/3$. (vi) Red triangle nodes have closeness $1/32$ and betweenness $15$, blue diamond nodes have closeness $1/32$ and betweenness $49/3$, while orange circular nodes have closeness $1/30$ and betweenness $16$. (vii) All nodes have closeness $1/28$. Blue diamond nodes have betweenness $14$, while orange circular nodes have betweenness $38/3$. (viii) Blue diamond nodes have closeness $1/48$ and betweenness $30$, while orange circular nodes have closeness $1/50$ and betweenness $91/3$.
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