1 Introduction

The interest in real world systems such as particular types of social (the network of acquaintances between individuals, collaboration of scientists, collaboration between actors in who acted in same movies, ...), biological (the network of metabolic pathways, genetic regulatory network, food web, protein interaction network, ...), technological (Internet, Power Grid, the telephone network, ...), informational (the network of citations between academic papers, World Wide Web, ...), etc. systems was in recent years remarkable [1], [2]. The above mentioned systems are characterized by two sets - a set of items and a set of connections or relationships between them. This kind of system we call network. The overall connectivity of the whole system is not simple, regardless of pairwise connections of items, and far from regularity. Hence, we call these physical systems complex networks, and they induced the development of complex networks theory. In the essence of this theory was the attempt to make classification of such systems with respect to the underlying structure, as well as to understand organizational principles which lead to formation of characteristic structures. Different kinds of dynamical processes on real world systems (such as deletion/addition of elements, and/or connections; information flow, etc.) takes place, and properties of these dynamical processes are influenced by the underlying structure. Hence, the notion of structure is certainly one of central concepts of complex networks theory. The most usual property for characterizing a structure is the distribution of number of connections which items have.

Since the beginning of its development, the complex networks theory relied on the concepts of graph theory. This reliance is understandable since the treatment of real world networks as sets of entities and their pairwise connections was natural and easiest to represent mathematically as a graph. On the other hand, the branch of mathematics called combinatorial algebraic topology [3], [4] introduced us the concepts of simplices and simplicial complexes, as objects which have local connectivity properties not so simple as those in graph theory. Let us in short make some parallels between graphs and simplicial complexes. While the main entity in graph is a node, in simplicial complex main entity is simplex, which is defined as a set of vertices. A pair of nodes in graph are connected by link, while in simplicial complex two simplices are connected if sets which define them have some vertices in common (these shared common vertices we call face). From this short comparison we can anticipate that simplices form connectivity structure which is more complex than graph. Furthermore, connectivity, as well as structural properties, can be considered from three aspects: combinatorial, algebraic, and topological. Hence, at this point we came to the main
idea of this paper, which is the following: can we represent physical complex network as simplicial complex, and if we can, what are the statistical mechanics properties of measures which emerge from combinatorial, algebraic, and topological aspect, analogously to the statistical mechanics approach to graph representation of complex network? Furthermore, if we can do all this, another problem arises: can we make some relationship between properties of complex networks which emerges from two representation - graph and simplicial complex representation?

2 Simplicial complexes

2.1 Definition and topological features of simplicial complexes

Consider two sets \( A = \{a_1, a_2, \ldots, a_n\} \) and \( B = \{b_1, b_2, \ldots, b_m\} \). We can define binary relation \( \lambda \) which, by some rule, assigns for every element in \( A \), one or more elements in \( B \), i.e. for every \( a_i \in A \) exists \( b_j \in B \), such that \( a_i \lambda b_j \). In this way the relation \( \lambda \) defines the unique set of pairs \( (a_i, b_j) \in A \times B \). Also, every subset of \( A \times B \) can be taken as the set that defines relation. Furthermore, the set \( A \) and relation \( \lambda \) determine the subset \( K \) of the power set of \( B \), and the union of all elements of \( K \) is the set \( B \). The elements of the set \( B \) we call vertices, the elements of the set \( K \) we call simplices, and the set \( K \) we call the simplicial family \([5]\). If two elements of set \( K \) have nonempty intersection, we say that they share face. The set of simplices and their faces is called simplicial complex, which is denoted like \( K_A(B, \lambda) \). The notation \( \sigma_q(a_i) = \langle b_{\alpha_0}, b_{\alpha_1}, b_{\alpha_2}, \ldots, b_{\alpha_q} \rangle \) means that the element \( a_i \) of the set \( A \) is \( \lambda \)-related to \( q+1 \) elements \( \{b_{\alpha_0}, b_{\alpha_1}, b_{\alpha_2}, \ldots, b_{\alpha_q}\} \) of the set \( B \). This property implies the definition of the sigma-mapping \( \sigma : A \to K_A(B, \lambda) \), defined as \( \sigma : a_i \to \sigma(a_i) \), and has the meaning of assigning the name of the element from the set \( A \) to the set of elements to which it is related. This makes it clear that the elements of \( A \) and the simplices of \( K_A(B, \lambda) \) are different entities \([6]\). It is important to point out that the construction of simplicial complex can also be made on only one set. Hence, we can equivalently define simplicial complex taking the relation \( \lambda \) as relation between elements of only one set, for example \( A \). Then, the obtained simplicial complex is \( K_A(A, \lambda) \), and \( \lambda \subseteq A \times A \).

Formally, starting from the previously defined set of simplices \( K \), every element \( \sigma_q \) of that set is called \( q \)-dimensional simplex or \( q \)-simplex, if it has \( q+1 \) elements, and the largest dimension represents the dimension of \( K \). Every \( q \)-simplex can be represented as a polyhedron in \( q \)-dimensional space, i.e. a \( q \)-simplex is graphically represented as complete graph with \( q+1 \) vertices, hence, a 0-simplex is being a point, 1-simplex being a line, a 2-simplex being a triangle, and so on (Figure 1).
If we take two simplices $\sigma_p$ and $\sigma_q$ ($p \leq q$), we say that simplex $\sigma_p$ is $p$-dimensional face of $\sigma_q$ or $p$-face of $\sigma_q$, if and only if every vertex of $\sigma_p$ is also vertex of $\sigma_q$. Notation $\sigma_p \leq \sigma_q$, means $\sigma_p$ is face of $\sigma_q$. Now, $K$ is called the simplicial complex if and only if $\sigma_q \in K$ and $\sigma_p \leq \sigma_q$ imply $\sigma_p \in K$. Figure 2 illustrates an example of the simplicial complex constructed from the sets $A = \{a, b, c, d, e, f\}$ and $B = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12\}$. The elements from the set $A$ are related to the elements of the set $B$ in a way that for example the element $a$ is related to the elements $\{1, 2, 3, 4\}$ and obtained simplex is $\sigma_3(a) = (1, 2, 3, 4)$. The other simplices are: $\sigma_2(b) = (3, 4, 5)$, $\sigma_1(c) = (5, 8)$, $\sigma_2(d) = (3, 6, 7)$, $\sigma_4(e) = (7, 8, 9, 10, 11)$ and $\sigma_3(f) = (9, 10, 11, 12)$. Also, as can be seen, for example, simplices $\sigma_3(a)$ and $\sigma_2(b)$ share 1-dimensional face $(3, 4)$, simplices $\sigma_4(e)$ and $\sigma_3(f)$ share 2-dimensional face $(9, 10, 11)$, and so on. By convention, if two simplices does not share face, we say that they share $(-1)$-dimensional face.
Figure 2. Simplicial complex $K_A(B, \lambda)$ constructed from the sets $A = \{a, b, c, d, e, f\}$ and $B = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12\}$. Simplices are $\sigma_3(a) = \langle 1, 2, 3, 4 \rangle$, $\sigma_2(b) = \langle 3, 4, 5 \rangle$, $\sigma_1(c) = \langle 5, 8 \rangle$, $\sigma_2(d) = \langle 3, 6, 7 \rangle$, $\sigma_4(e) = \langle 7, 8, 9, 10, 11 \rangle$ and $\sigma_3(f) = \langle 9, 10, 11, 12 \rangle$.

The inverse relation of $\lambda$ is denoted $\lambda^{-1}$. It is defined as $\lambda^{-1} \subseteq B \times A$ with $(b_j, a_i) \in \lambda^{-1}$ if and only if $(a_i, b_j) \in \lambda$. The simplicial complex obtained in that way is called the conjugate complex $K_B(A, \lambda^{-1})$ (Figure 3). In the special case where $\lambda$ is a 1–1 mapping, $\lambda^{-1}$ is the usual inverse mapping.

Figure 3. The conjugate complex $K_B(A, \lambda^{-1})$ of simplicial complex $K_A(B, \lambda)$ from Figure 4.

The definition of the simplicial complex through simplices and faces which they share, indicate certain relationship between simplices. Hence, we can introduce the concept of $q$-nearness in the following way: two simplices are said to be $q$-near in $K$ if and only if they share a $q$-dimensional face in $K$ (Figure 4).

Figure 4. Examples of $q$-nearness. 4-simplex and 3-simplex are (a) 0-near (share one vertex), (b) 1-near (share two vertices), and (c) 2-near (share three vertices).
Furthermore, two simplices are \( q \)-connected if there is a chain of pairwise \( q \)-near simplices between them (Figure 5). Formally, two simplices \( \sigma \) and \( \sigma' \) are \( q \)-connected if there is a chain of simplices \( \sigma(1), \sigma(2), \ldots, \sigma(n) \) with \( \sigma = \sigma(1), \sigma(n) = \sigma' \) and \( \sigma(i) \) \( q \)-near \( \sigma(i + 1) \) for \( i = 1, \ldots, n - 1 \).

\[ \text{(a) 0-connected} \quad \text{(b) 1-connected} \]

Figure 5. First and last (from the left) simplices are (a) 0-connected since there is a chain of 0-near simplices, and (b) 1-connected since there is a chain of 1-near simplices

An important feature of a simplicial complex, as defined here, is that it not only defines a topological space, but it also represents a combinatorial object which has a geometrical representation. This multifaceted property of simplicial complexes makes them particularly convenient for modeling complex structures and connectedness between different substructures.

2.2 Invariants of simplicial complexes

Simplicial complexes may be considered from three different aspects:
1. a combinatorial model of a topological space,
2. a combinatorial object and
3. an algebraic model.

Consequently, the invariants of simplicial complexes may be defined based on their different aspects, and each aspect provides completely different measures of the complex. In the case when they are considered as a combinatorial model of a topological space, various algebraic topological measures may be associated such as homotopy and homology groups [7]. In the case when a simplicial complex is considered as a combinatorial object, several invariants may be defined and numerically evaluated. The first is the dimension of the complex. The next one is so called an \( f' \)-vector (also known as the second structure vector) [8], [9], [10], [11], which is an integer vector with \( \text{dim}(K) + 1 \) components, the \( q \)-th one being equal to the number of \( q \)-dimensional simplices in \( K \). A measure similar to \( f' \)-vector is the \( f \)-vector, which has the equal length as \( f' \)-vector, but \( q \)-th entry is equal to the number of \( q \)-dimensional simplices including \( q \)-faces.

The \( q \)-connectivity relation between simplices of the complex \( K \) is an equivalence relation which will be denoted by \( \gamma_q \). Let \( K_q \) be the set of simplices in \( K \) with dimension greater than or equal to \( q \). Then \( \gamma_q \) partitions \( K_q \) into equivalence classes of \( q \)-connected simplices. These equivalence classes are members of the quotient set \( K_q/\gamma_q \) and they are called the \( q \)-connected components of \( K \). Every simplex in a \( q \)-component is \( q \)-connected to every other simplex in that component, but no simplex in one \( q \)-component is \( q \)-connected to any simplex on a distinct \( q \)-connected component. The cardinality of \( K_q/\gamma_q \) is denoted \( Q_q \) and is the number of distinct \( q \)-connected components in \( K \). In this way, we came to the third important invariant - a \( Q \)-vector (first structure vector), an integer vector of the same length
as the $f'$-vector, whose $q$-th component is equal to the number of $q$-connectivity classes. The structure vectors, illustrated in Figure 6, represent global topological feature of the complex, and provides information about connected components at each level of connectivity with initial level equal to the dimension of the complex.

<table>
<thead>
<tr>
<th>levels</th>
<th>$Q$-vector (first structure vector)</th>
<th>$f$-vector (second structure vector)</th>
<th>geometric representation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$q=4$</td>
<td>$Q_4=1$</td>
<td>$f_4=1$</td>
<td></td>
</tr>
<tr>
<td>$q=3$</td>
<td>$Q_3=3$</td>
<td>$f_3=3$</td>
<td></td>
</tr>
<tr>
<td>$q=2$</td>
<td>$Q_2=4$</td>
<td>$f_2=5$</td>
<td></td>
</tr>
<tr>
<td>$q=1$</td>
<td>$Q_1=4$</td>
<td>$f_1=6$</td>
<td></td>
</tr>
<tr>
<td>$q=0$</td>
<td>$Q_0=1$</td>
<td>$f_0=6$</td>
<td></td>
</tr>
</tbody>
</table>

Figure 6. Values and geometric representation of first, and second structure vector at different levels of connectivity for simplicial complex from Figure 2.

Another important topological invariant is the sequence of Betti numbers. They can be associated to the simplicial complex when the abstract algebra is applied. In simple terms, the Betti numbers are a topological invariant allowing to measure either the number of holes (simplices representing holes) of various dimensions present in a simplicial complex, or equivalently, the number of times the simplex loops back upon itself. Hence, Betti numbers form an integer vector where each component corresponds to a distinct dimension.

3 Simplicial complexes of complex networks

3.1 Matrix representation(s)

3.1.1 Simplicial complex

The geometrical representation of simplicial complex is one way, computationally not so practical, to represent the relation between two sets. Recalling the example of the previous section
illustrated on Figure 2, we can introduce another simplicial complex representation. Therefore, starting from two sets $A = \{a, b, c, d, e, f\}$ and $B = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12\}$ and introducing the relation $\lambda$, we obtain the simplicial complex $K_A(B, \lambda)$ with simplices $\sigma_3(a) = \{1, 2, 3, 4\}$, $\sigma_2(b) = \{3, 4, 5\}$, $\sigma_1(c) = \{5, 8\}$, $\sigma_2(d) = \{3, 6, 7\}$, $\sigma_1(e) = \{7, 8, 9, 10, 11\}$ and $\sigma_3(f) = \{9, 10, 11, 12\}$. We can, now, define the matrix $\Lambda$ of the relation $\lambda$, such that rows represent simplices, and columns represent vertices, and the element $[\Lambda]_{ij}$ is equal to 1 if $a_i \in A$ is $\lambda$-related to $b_j \in B$, or equivalently if simplex $\sigma(a_i)$ contains vertex $b_j$, and otherwise is 0. This matrix is called incidence matrix [6]. The geometrical and matrix representations of the above example are illustrated on the Figure 7.

$$
\begin{bmatrix}
\lambda & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \\
A & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
B & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
C & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
D & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\
E & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\
F & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\
\end{bmatrix}
$$

Figure 7. Relationship between geometrical and incidence matrix representations of simplicial complex from Figure 2. An example of this relationship is illustrated on the simplex $\sigma_4(e) = \{7, 8, 9, 10, 11\}$.

The matrix representation of the conjugate complex $K_B(A, \lambda^{-1})$ of the simplicial complex $K_A(B, \lambda)$ is the transpose matrix of $\Lambda$ ($\Lambda^T$), as illustrated on the Figure 8.

$$
\begin{bmatrix}
\lambda^T & a & b & c & d & e & f \\
1 & 1 & 0 & 0 & 0 & 0 & 0 \\
2 & 1 & 1 & 0 & 0 & 0 & 0 \\
3 & 1 & 1 & 0 & 1 & 0 & 0 \\
4 & 1 & 1 & 1 & 0 & 0 & 0 \\
5 & 0 & 1 & 1 & 0 & 0 & 0 \\
6 & 0 & 0 & 0 & 1 & 0 & 0 \\
7 & 0 & 0 & 0 & 1 & 0 & 0 \\
8 & 0 & 0 & 1 & 0 & 1 & 0 \\
9 & 0 & 0 & 0 & 1 & 1 & 0 \\
10 & 0 & 0 & 0 & 1 & 1 & 0 \\
11 & 0 & 0 & 0 & 1 & 1 & 0 \\
12 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
$$

Figure 8. Relationship between geometrical and incidence matrix representations of conjugate simplicial complex of complex from Figure 7. An example of this relationship is illustrated on the simplex $\sigma_1(5) = \{b, c\}$.
The matrix that captures main properties of simplices and simplicial complex is called $q$-connectivity matrix ($\Pi$), and is defined like [12]:

$$\Pi = \Lambda \cdot \Lambda^T - \Omega,$$

where $\Lambda$ is incidence matrix, and $\Omega$ is matrix with all entries equal to 1. Rows and columns of the matrix $\Pi$ represent simplices, the diagonal elements represent dimension of simplices, and the non-diagonal elements represent the dimensionality of faces which simplices share. At Figure 9 the relation between geometrical and matrix representations is illustrated for the above example. Analogously we can define $q$-connectivity matrix of the conjugate complex.

![Diagram of a simplicial complex with labels and dimensions for simplices and faces.

Figure 9. Relationship between geometrical and $q$-connectivity matrix representation of connectivity of simplicial complex from Figure 7. The diagonal elements of $q$-connectivity matrix are equal to dimensions of simplices (for example, dimension of simplex $\sigma(a)$ is equal to 3), while off-diagonal elements are equal to dimensions of faces which simplices share (for example, simplices $\sigma(e)$ and $\sigma(f)$ share 2-dimensional face).

3.1.2 Complex network

Defining a graph of complex network as set of nodes and set of links, we can represent it as the matrix in the following way. Let $V$ be a set of nodes, and let rows and columns of the matrix $A$ represent those nodes. The element $[A]_{ij}$ is equal to 1 if nodes $v_i \in V$ and $v_j \in V$ are connected by the link, and otherwise is 0 [2]. The matrix $A$ defined in this way is called adjacency matrix. The example in Figure 10 illustrates the matrix representation of the undirected network without selfloops, and defined by the set of nodes $V = \{1, 2, 3, 4, 5, 6, 7, 8, 9\}$ and set of links $E = \{(1, 2), (1, 3), (1, 4), (1, 5), (4, 5), (5, 6), (5, 7), (7, 8), (7, 9), (8, 9)\}$.
Figure 10. Geometrical and adjacency matrix representation of network defined by set of nodes $V = \{1, 2, 3, 4, 5, 6, 7, 8, 9\}$ and set of links $E = \{(1, 2), (1, 3), (1, 4), (1, 5), (4, 5), (5, 6), (5, 7), (7, 8), (7, 9), (8, 9)\}$.

The adjacency matrix completely captures main properties of network, and represents the main starting object for computation network characteristics. For example, the degree $k_i$ of a node $v_i$ is defined in terms of the adjacency matrix as [2]:

$$k_i = \sum_{j \in V} [A]_{ij},$$

the length $l$ of the shortest path between vertices $v_i$ and $v_j$ is equal to the minimal power of the adjacency matrix with a non-zero $\{ij\}$ element [13]:

$$[A^{l-1}]_{ij} = 0, \quad [A^l]_{ij} \neq 0,$$

the local clustering coefficient $c_i$, i.e. the clustering coefficient of a node $v_i$ is defined in terms of the adjacency matrix elements as [2]:

$$c_i = \frac{\sum_{j,m} [A]_{ij} [A]_{jm} [A]_{mi}}{k_i(k_i - 1)}.$$

### 3.2 Simplicial complexes from graphs

Complex network defined by the sets of nodes and links, can be constructed either by the graph or by the simplicial complex, depending on the properties that we want to capture. Actually, any property of the network that is preserved under deletion of nodes or links may be used for construction purposes. The natural and simplest way to represent network is by constructing a graph, which is defined by the binary relation between pairs of network elements. On the other hand, the simplicial complex represent n-ary relation, in the sense that it is the mapping one to many of the binary relation [14]. Furthermore, it is multilevel and multidimensional representation of complex network. This lead us to the problem of representing complex network as graph and as simplicial complex, and exploring relationship between these two representations as well as exploring properties of obtained structures.
Let start with the network whose set of nodes is $V$ and set of links is $E$. This network defines graph with the same sets of nodes and links, in terms of graphical and matrical representation as illustrated in Figure 10. Therefore, we can say that there is 2-ary (binary) relation between each pair of nodes. Now, we can define binary relation that relates each node with its neighboring nodes, and we will call it neighboring relation - $\nu$. This kind of definition can have two versions: (1) relation includes the referent node, since the node can also be the neighbor of itself, and (2) relation does not include referent node. The first version we will assign $NC_1$ and the second $NC_0$. In the version $NC_0$ every node $v_i \in V$ is in neighboring relation with nodes to which it is linked in the original network. Hence, every node is defined by its neighboring nodes, i.e. for example, in Figure 10 the node 1 is defined by the set $\{2, 3, 4, 5\}$. If we apply sigma-mapping to the node 1, i.e. if we assign name of the node 1 to the set of its neighbors $\{2, 3, 4, 5\}$, we obtain new entity - simplex $\sigma_3(1) = \langle 2, 3, 4, 5 \rangle$. By continuing this procedure we obtain the whole simplicial complex with incidence matrix identical to the adjacency matrix of graph, but different geometrical representations. The last property comes from the definitions of incidence and adjacency matrices, i.e. while in the matrix representation of graph (adjacency matrix) rows and columns represent nodes of complex network, in the matrix representation of simplicial complex (incidence matrix) rows represent simplices and columns represent vertices. The relationship between these two representations can be seen in Figure 11, which is illustration of $NC_0$ complex of the example of Figure 10. There is simple relationship between these two representations of the basic connectivity properties. Dimension $q_i$ of simplex $\sigma(i)$ defined by node $v_i$ is equal to the node degree $k_i$ minus 1, and two simplices $\sigma(i)$ and $\sigma(j)$ defined by nodes $v_i$ and $v_j$ share $q$-dimensional face if nodes $v_i$ and $v_j$ have $q + 1$ common neighbors.
In the version $NC_1$, since we include property of the node to be the neighbor of itself, the simplex contains an additional vertex, that is the referent node. In this sense the incidence matrix of simplicial complex is obtained from adjacency matrix of graph by adding 1 in diagonal entries. For example, the node 1 is now represented as simplicial complex $\sigma_4 = \langle 1, 2, 3, 4, 5 \rangle$ (see Figure 11). Unlike for the $NC_0$ complex, the dimension $q_i$ of simplex $\sigma(i)$ defined by node $v_i$ is equal to the node degree $k_i$. If nodes $v_i$ and $v_j$ are neighbors of each other and share $q$ other neighbors, the simplices defined by these nodes share $q$-dimensional face, and if they are not neighbors of each other, the associated simplices share $(q-1)$-dimensional face. The construction of simplicial complex $NC_1$, and name (neighborhood complex), is introduced in [15]. On the other hand, in [16] the complex $NC_0$ is introduced as neighborhood complex.

In the above construction procedures we assumed that the observed complex network is undirected. If we now take into consideration a directed network, the procedure is the same, but with a significant difference. The simplex of node is defined by its neighbors to which the node is neighbor by outgoing links of referent node. Analogously, we can define simplex of node by its neighbors to which the node is neighbor by its incoming links.

There is another direct construction of simplicial complex from complex network, and again we can start from network introduced in the example illustrated at Figure 10. Having set of nodes $V = \{1, 2, 3, 4, 5, 6, 7, 8, 9\}$ and set of links $E = \{(1, 2), (1, 3), (1, 4), (1, 5), (4, 5), \ldots\}$,
we can introduce the relation $\lambda$ between set of nodes and set of links by the following definition: the element of set $V$ is $\lambda$-related to the element of set $E$ if it is contained in the pair from $E$. In other words, the node $v_i \in V$ is $\lambda$-related to all links that outgoes from that node, and for example, node 1 is $\lambda$-related to links $\{(1,2), (1,3), (1,4), (1,5)\}$. Applying sigma-mapping to node 1 and assigning name to it $\sigma_3(1)$, we can obtain simplex defined by the node representing the name of simplex, and all its links representing vertices, i.e. $\sigma_3(1) = ((1,2), (1,3), (1,4), (1,5))$. Continuing this procedure, we can construct simplicial complex, which is represented by incidence matrix with rows representing simplices obtained from nodes, and columns representing vertices obtained from links. Simplicial complex constructed in this way from complex network we will call links-nodes simplicial complex and denote it like $LN$. Transition between graph and $LN$ representations of complex network, as well as matrix representation of the constructed simplicial complex of the above example is illustrated in Figure 12.

![Figure 12](image.png)

The dimension $q_i$ of simplex $\sigma(i)$ in complex $LN$ which represent node $v_i$ of initial graph is equal to degree of that node $k_i$ minus 1, and simplices share 0-dimensional faces, since there is only one link between vertices. This kind of relationship between graph and associated simplicial complex is introduced in [5], but it is defined in different way. Nevertheless, the obtained structure is the same. As illustration of this transition we can observe the network of streets and their intersections, as well as network of roads and their intersections. From graph point of view, the streets (roads) represent nodes, and two nodes are connected if they share intersection (see for example [17]). On the other hand, from simplicial point of view, streets (roads) represent simplices, defined by vertices which are intersection which they have, and two simplices share face if two streets (roads) share intersection (see for example [18]).
There are other ways to construct simplicial complex from complex network [19]. One such way is from bipartite network. This kind of network is defined by two disjoint sets, and links are defined between the elements of these sets, but not between the elements of the same set. Hence, we can construct simplicial complex following the procedure of construction of simplicial complexes. Furthermore, representing all complex networks as bipartite structures, as proposed by Guillaume et al. [20], we can construct simplicial complex of complex network in the way in which we construct simplicial complex of bipartite network. In other words, since simplices are geometrically represented like complete graphs, we can find maximal complete subgraphs (cliques) of the network and assign to each of them a name, and construct simplicial complex. Such simplicial complex is called clique complex (CC) (or flag complex) [3], and an example of clique complex can be seen at the Figure 13a. More formally, given an arbitrary graph $G$, the clique complex $CC(G)$ is a simplicial complex whose set of vertices is set of vertices $V(G)$ of $G$, and whose simplices are all subsets $S$ of $V(G)$, such that each subset complete subgraph in $G$ [3]. The number of elements $n_i$ of each subset $S_i$ of $S$ defines the simplex dimension $q_i$ which is equal to $n_i - 1$.

![Figure 13a. Transition from graph (left) to clique complex (right) representation of complex network. The colors indicate different simplices obtained from graph.](image)

### 4 The choice of simplicial complex representation

The natural and simplest way to represent complex networks is by constructing a graph. The main constitutive entities of graph are nodes, i.e. in geometrical representation - points, and they are connected by links, i.e. in geometrical representation - lines. On the other hand, complex network can be represented as simplicial complex. In contrast to complex network $\rightarrow$ graph representation, which is usually unique, complex network $\rightarrow$ simplicial complex representation is not unique. Furthermore, the main entities that constitute simplicial complex are simplices, which has polyhedral geometrical representation, and they have more complex connectivity, since they are connected by sharing faces. Hence, the question about transition between these two representations immediately emerges. The answer is that there exists transition from graph representation of complex network to simplicial complex representation of complex network, and in some cases (such are neighborhood complexes, or links-node complex) important features of graph are preserved in simplicial complex representation.

The first problem which emerges is the choice of simplicial complex representation of complex network. Naturally, the choice depends on the concrete problem which we want to explore. On the other hand, this paper concentrates on general properties about simplicial complexes obtained from complex networks, hence the choice can be quite arbitrary.
The leading idea in choice of the representation is the following: we want to construct simplicial complex of complex network which preserves properties of the node connectivity as well as some kind of community structure. It is pointed out some kind of community structure, since there is not strict definition of community. Hence, we are looking for simplicial complex representation of complex network which captures these properties, and the choice has fallen on neighborhood complex $NC_1$. It captures node connectivity (the dimension of simplex obtained from node is equal to the node degree), and if two nodes are connected, the corresponding simplices are also connected. Furthermore, two nodes are also connected through the common neighbors (i.e. in terms of simplicial complex they share face). These properties of the relationship between two representations are illustrated at the Figure 13.

Figure 13. Relation between connectivity properties of two complex network representations, graph (left) and simplicial complex (right): (a) equality between node degree and dimension; (b) preservation of connectivity between neighboring nodes in their corresponding simplex representation; (c) additional information about connectivity obtained from simplicial complex.

The simplest community structure (neighborhood community) in this representation is the node itself (in context of complex network), and all its neighbors, that is, the node corresponding simplex. The advantage of this definition of community is in its strict mathematical
definition, since the simplices are well defined objects. More complex communities emerge from connectivity of simplices through shared multidimensional faces, that is in terms of complex networks, the communities defined by two nodes are connected if they share common neighbors, but also these nodes are connected through their common neighbors regardless of their mutual connection.

Beside NC1 representation we are dealing also with clique complex (CC) representation. Namely, the research interest in recent years in the complex networks structure [2] shifted from the global properties emerging from simple local node-node connectivity to the exploration of structural, as well as functional, properties emerging from meso-scale, subnetwork, structures and their relationships. There are numerous definitions and detection algorithms of these subnetworks (called communities, modules, or motifs) [21], mostly depending on some basic requirements, such as locality, high node density, and overlapping property. Another simple community definition (beside neighborhood community) satisfying these requirements is treating community as a clique, i.e. completely connected graph in each node is connected to each other [22]. In [22] the $k$-clique is defined as clique formed by $k$ nodes, and two $k$-cliques overlap if they share $k - 1$ nodes. We have extended the definition of community as a clique in a stronger sense defining a community as maximal clique, i.e. the clique that cannot be contained inside any larger clique. Furthermore, two maximal cliques overlap, regardless of the number of nodes which form them, as long as they share some vertices. This approach give us an adequate framework for dealing with clique complex representation of complex network.

5 Simplicial complex measures

At this point the measures which capture the main topological properties will be defined. They are introduced in Q-analysis [8], [9], [10], [11]. Some of them are already defined in section about simplicial complexes, such as simplex dimension, first structure vector, or second structure vector.

5.1 Third structure vector

The entries of the third structure vector $Q_q$ are defined in the following way [23]:

$$Q_q = 1 - \frac{Q_q}{j'_q},$$

(2)

where $Q_q$ is $q$-th entry of the first structure vector, and $j'_q$ is $q$-th entry of the second structure vector. The third structure vector measures the degree of connectedness on each $q$-level, or in other words, it measures the number $q$-connected components per number of simplices.

5.2 Obstruction vector

The obstruction vector [6] $Q^*_q$ is defined as the first structure vector minus vector with all entries equal to 1. It measures the number of structural restrictions at $q$-levels, or in other words it measures the number of gaps on $q$-levels. The larger values indicate that the structure is fragmented.
5.3 Eccentricity

The simplex in simplicial complex is defined by its vertices. If all its vertices are part of some other simplex, the starting simplex is completely integrated in another simplex. In terms of simplicial complexes, the simplex is face of some other simplex, which can have equal or larger dimension. Hence, it does not have integrity or individuality in complex as a whole. On the other hand, if simplex does not share vertices with any other simplex, we can say that it is not well integrated or it does have individuality in simplicial complex.

We can define $\hat{q}$ (called bottom $q$) of simplex $\sigma$ as the largest dimension of faces which $\sigma$ share with other simplices, i.e. the largest $q$-nearness value. This is equivalent to the value of the $q$-level on which the simplex firstly connects to some other simplex. We can, also define $\hat{q}$ (called top $q$) which is equal to the dimension of the simplex. Than the eccentricity of simplex $\sigma$ is defined like [12]:

\[
\text{ecc}(\sigma) = \frac{\hat{q} - \hat{q}}{\hat{q} + 1}.
\]

From the definition one sees that $\hat{q} + 1$ is the total number of vertices that define simplex $\sigma$, and $\hat{q} - \hat{q}$ is the minimal number of vertices which make simplex $\sigma$ different from the other simplex. Hence, $\text{ecc}(\sigma)$ measures the individuality or differentness of simplex, and indicates the degree of integrity of simplex $\sigma$ in simplicial complex. The simplex which has $\text{ecc} = 0$ is completely integrated into the structure, i.e. the simplex is face of another simplex. The simplex which has $\text{ecc} = 1$ does not share vertices (faces) with any other simplex, i.e. it is completely disintegrated. The example of these properties is illustrated on Figure 14.
Figure 14. Examples of properties obtained from eccentricity values: (a) arbitrary simplicial complex: well integrated (σ(e)) and disintegrated (σ(g)) simplices, and (b) neighborhood complex: well integrated (σ(9), σ(10), σ(4)) and bad integrated (σ(6)) simplices.

The eccentricity, defined in this way, have a following weakness: two (or more) simplices which are situated on different places in the structure, can have the same value of eccentricity. In other words, simplices can have the same value of eccentricity, regardless of their different neighborhoods. Hence, let simplex σ(1) have dimension \( \hat{q} \), and σ(1) firstly connects into the structure at the level \( \check{q} \) (\( \check{q} \leq \hat{q} \)). As we already said, that means that the largest dimension of the face which σ(1) shares with another simplex is \( \check{q} \). Then its eccentricity can be calculated from the equation (3), and is equal to ecc(1). Any simplex with the same dimension and the same value of eccentricity must have the same \( \check{q} \), regardless of its neighborhood.

It is important to mention that (3) is not the only definition of eccentricity [12], [23]. All of them measure the same properties, and have the mentioned weakness, but the range of values is different. Since the range of eccentricity defined by (3) is \([0, 1]\), it was chosen because of practical reasons.
5.4 Vertex significance

One vertex can be part of many simplices, and we can define a vertex weight $\theta$ as the number of simplices which are created by that vertex. Hence, the vertex weight is the measure that characterizes a vertex. On the other hand, since the simplex is defined by vertices, we can introduce a measure that characterizes a simplex with respect to the vertices that create it. Summing weights of all vertices which create simplex $\sigma_q(i)$, we obtain a variable $\Delta(\sigma_q(i))$.

Now we can define vertex significance of the simplex with respect to the simplices which create it like [23]:

$$vs(\sigma_q(i)) = \frac{\Delta(\sigma_q(i))}{\max_k \Delta(\sigma_q(k))},$$

where $\max_k \Delta(\sigma_q(k))$ is the maximal value of all $\Delta(\sigma_q(i))$. The larger values of $vs$ indicate larger importance of the simplex with respect to the vertices which create it. The example of this property is illustrated at the Figure 15.

Figure 15. Examples of properties obtained from vertex significance values: (a) arbitrary simplicial complex: most significant ($\sigma(e)$) and least significant ($\sigma(g)$) simplices, and (b) neighborhood complex: most significant ($\sigma(5)$) and least significant ($\sigma(9), \sigma(10)$).
In context of the neighborhood complex $NC_1$ created from the complex network, the relationship can be made between vertex significance and nearest-neighbor degree-degree correlation function $k_{nn,i}$ which is defined in the following way [2]:

$$k_{nn,i} = \frac{D_i}{k_i},$$

where $D_i$ is the sum of the degrees of nearest neighbors of the node $i$, and $k_i$ is the degree of the node $i$. Having in mind the relationship of the degree of node $i$, and the dimension of its simplex representation $\sigma_q(i)$, ($q_i = k_i$), it is easy to see that $\Delta(\sigma_q(i)) = D_i + q_i$. Therefore, the relationship between vertex significance of the simplex $\sigma_q(i)$ in simplicial complex representation of complex network, and degree-degree correlation function of node $i$ in graph representation of complex network is:

$$vs(\sigma_q(i)) = \frac{k_i + 1}{\max_j(D_j + k_j)}k_{nn,i}.$$

### 5.5 Simplex clustering

In analogy to networks [1], one may define the clustering coefficient of simplices. We can define this variable between the reference simplex and its neighbors in the following way. Suppose we have two simplices $\sigma(i)$ and $\sigma(j)$ which share face of dimension $f_{ij}$. The dimensions of the simplices $\sigma(i)$ and $\sigma(j)$ are $q_i$ and $q_j$, respectively. Since they share face whose dimension is $f_{ij}$, they also share faces with dimensions $f_{ij} - 1$, $f_{ij} - 2$, ..., 0. We can define quantity which characterizes the neighborhood of the simplex $\sigma(i)$ with respect to the faces that neighbor-simplices share between themselves. We can define it in the following way:

$$C''_i = \frac{\text{Number of faces that neighbor-simplices share between themselves}}{\frac{z_i - 1}{2}}\left(\frac{\text{Total number of faces that neighbor-simplices can share between themselves}}{}ight),$$

where $z_i$ is number of neighbor-simplices of simplex $\sigma(i)$. Hence, the following equation emerges:

$$C''_i = \frac{\frac{1}{2} \sum_{j,k \in \{nn\}_i} \left( \sum_{f=0}^{f_{jk}} \alpha_{q_f} \right)}{(z_i - 1)\left(\sum_{f=0}^{q_i} \alpha_{q_f} + \sum_{f=0}^{q_j} \alpha_{q_f} + \cdots + \sum_{f=0}^{q_z} \alpha_{q_f}\right)},$$

where

$$\alpha_{x,f} = \frac{(x + 1)!}{(f + 1)!(x - f)!},$$

and $x = f_{ij}, q_i, q_j$. Simplifying equation (7) we get

$$C''_i = \frac{\frac{1}{2} \sum_{j,k \in \{nn\}_i} \left( -1 + 2^{1+f_{jk}} \right)}{(z_i - 1)^2} \left( z_i + \sum_{r=1}^{z_i} 2^{1+q_r} \right).$$

We can, now, examine two boundary cases for the values of clustering coefficient defined by the equation (9). Suppose that we have the reference simplex $\sigma(i)$ whose neighbors does not share face of any dimension, i.e. $f_{jk} = -1$, for all pairs $j, k \in \{nn\}_i$. Than the summation in the numerator is zero, and $C''_i = 0$. Now suppose that we have the reference
simplex $\sigma(i)$ with $z_i$ neighbors, and all neighbor-simplices have dimension $q$, and every pair of neighbors share face of dimension $f$. Then

$$C''_i = \frac{-1 + 2^{1+f}}{-1 + 2^{1+q}},$$

and, if $f = q$, follows $C''_i = 1$.

6 Results for neighborhood complexes

6.1 Random network

The simplest type (and model) of network, despite of its inadequacy for explaining the real world networks, is examined from the aspect of the simplicial complex representation, more concretely, from the aspect of the associated neighborhood complex $NC_1$. This is done for the comparison as well as an illustration of the concepts and measures defined in previous sections. Hence, the examined random network consists of 2000 nodes, and with the probability $p = 0.005$ that two nodes have a link. As it is mentioned before there is straightforward relationship between the degree of the node and the dimension of the corresponding simplex. That implicates the equivalence between degree distribution and dimension distribution. Furthermore, we expect that dimension distribution follows the well known bell-shaped form, which is characteristic of random networks. This property is presented at the Figure 16.

![Figure 16. Distribution of dimensions of random network with $N = 2000$ nodes and probability $p = 0.005$ that two nodes have a link.](image)

A random network has a characteristic scale in its node connectivity reflected by the peak of the distribution which corresponds to the number of nodes with the average number of links. Because of the equivalence of the distributions of degrees and dimensions, this property holds also for the corresponding simplicial complex representation.
The distribution of vector valued measures is illustrated by distributions of the first and second structure vector (Figure 17), as well as third structure vector (Figure 18).

Figure 17. Values of first and second structure vectors for random network with \( N = 2000 \) nodes and linkage probability \( p = 0.005 \).

![Figure 17](image17.png)

Figure 18. Values of third structure vector for random network with \( N = 2000 \) nodes and linkage probability \( p = 0.005 \).

![Figure 18](image18.png)

The graphics of structure vectors indicate an interesting property of the structure of simplicial complex representation of random networks. From the highest up to the third level the structure is not connected, and then there is a jump in the connectivity of structure. The structure, observing it globally, is homogenous and there is not any preferential pattern of formation of connectivity classes.
The distribution of the eccentricity for random network simplicial complex representation is illustrated at the Figure 19.

![Eccentricity Distribution](image)

Figure 19. Eccentricity distribution of random network with $N = 2000$ nodes and linkage probability $p = 0.005$.

As can be seen from the graph of eccentricity distribution at the Figure 19, almost all simplices have eccentricity approximately in the region $ecc \in [0.7, 0.9]$, with the peak at the value $ecc = 0.8$. This indicates certain homogenous behavior of simplices’ individuality, which is expected for the random network.

The vertex significance distribution is presented at the Figure 20. From this figure one sees bell-shaped behavior of vertex significance distribution, hence one notion immediately arises - the behavior of vertex significance distribution follows the behavior of dimension distribution. Therefore we can make a hypothesis that the vertex significance is another topological invariant, or just a measure with strong dependance on dimension.

![Vertex Significance Distribution](image)

Figure 20. Vertex significance distribution of random network with $N = 2000$ nodes and linkage probability $p = 0.005$. 

22
6.2 Barabási-Albert model of scale-free networks

Following the algorithm introduced in [24], the scale-free network is generated. At this moment we will repeat just important features of this algorithm. Starting with $m_0$ randomly connected nodes, at each time step we add one new node which can be linked to $m$ nodes already present in the network. The probability of connection to some old node $i$ depends on its number of links $k_i$ like

$$\Pi(k_i) = \frac{k_i}{\sum_j k_j}.$$

In this way two properties of real world network are captured: growth and preferential attachment. In this paper we have chosen $m_0 = 5$ and $m = 3$ values of parameters, and following the above procedure the network with $N = 5000$ nodes was generated. As it is already mentioned there is equivalence between degree distribution of complex network and dimension distribution of its corresponding neighborhood complex $NC_1$. Hence, at the Figure 21 the dimension distribution is presented.

![Figure 21. Dimension distribution of Barabási-Albert scale-free network type with $N = 5000$ nodes and parameters $m_0 = 5$ and $m = 3$.](image)

The vector valued distributions of first, second, and third structure vectors are presented at the Figure 22 left, Figure 22 right, and Figure 23, respectively.
Observing Figure 22 we can notice that first and second structure vectors follow power-law behavior, at least over large number of decades. The discrepancy from the power-law behavior for dimension distribution over the whole range comes from the smallness of the network, i.e. from its finiteness, as well as because of the degree randomness of the linking process. Hence, we can assume that this features have influence on the behavior of the first and second structure vectors.

By definition the length of the third structure vector is equal to the length of first and second, hence, from the Figure 23 we can make conclusion that from the largest up to the 14th level the structure is disconnected.

The eccentricity distribution presented at the Figure 24 indicate that simplices have well defined specific individualities. This further implicates on the heterogenous property of this type of network, but from the aspect of the simplex individuality.
The vertex significance distribution is presented at the Figure 25, and overall behavior is power-law, that is the vertex significance distribution follows the behavior of dimension distribution.

6.3 Exponential network

It is already mentioned that the majority of the real world networks as its main characteristic has power-law degree distribution. Nevertheless, there are some networks which has as the
The main topological characteristic exponential degree distribution. As an illustrative example of this type of network the US Power Grid, as the representative of the technological network, have been chosen [25]. The nodes of this network are generators, transformers, and substations, and links are high-voltage transmission lines. In this paper we analyzed a US power grid network of the western United States which consists 4941 nodes [26]. The dimension distribution, as well as vector valued measures (normalized values of 1st- and 2nd-structure vectors) are illustrated at the Figure 26 left, and third structure vector is presented at the Figure 26 right. As can be seen from these figures, all four measures are well fitted to the exponential function. Furthermore, the vertex significance distribution is also well fitted to the exponential function (Figure 27).

![Figure 26](image1.png)

Figure 26. Degree (dimension) distribution, first, and second structure vectors (left) and third structure vector (right) for exponential US Power grid network. The exponential fit is indicated.

![Figure 27](image2.png)

Figure 27. Vertex significance distribution of exponential US Power grid network. The exponential fit is indicated.

The distribution of eccentricity is presented at the Figure 28. Two characteristic peaks at $ecc = 0$ and $ecc = 0.5$ indicate the presence of significant number of simplices (i.e. nodes
in complex network) without individuality and simplices whose largest face is half of its dimension, respectively.

![Figure 28. Eccentricity distribution of exponential US Power grid network.](image)

### 6.4 Scale-free networks

As an example of network with power-law degree (i.e. dimension) distribution as an information type of network will be considered. This network we will call *epa*, and it represents pages linking to www.epa.gov, and consists $N = 4772$ nodes [26]. “This graph was constructed by expanding a 200-page response set to a search engine query, as in the hub/authority algorithm.” [26]

The distribution of dimensions of *epa* network is presented at the Figure 29.

![Figure 29. Dimension distribution of scale-free *epa* network.](image)
Vector valued measures of 1st and 2nd structure vectors are illustrated at Figure 30, and 3rd structure vector is presented at the Figure 31. The connectivity levels are filled with simplices but they are not $q$-connected up to some value of $q$-level. This level is rather high comparing with other types of simplicial complex representations of complex networks studied in previous sections.

Figure 30. Values of first and second structure vectors for scale-free $epa$ network.

Figure 31. Values of third structure vector for scale-free $epa$ network.

The eccentricity distribution is presented at the Figure 32, and vertex significance distribution is presented at the Figure 33. From Figure 32 we can see that majority of simplices (about 75%) have eccentricity equal to $ecc = 0$, and that they are completely integrated into the structure, i.e. they does not have individuality. The characteristic is presence
of small number of simplices with eccentricity values $ecc = 0.33, 0.5, 0.66$. The behavior of vertex significance distribution from Figure 33 has very small discrepancy from power-law behavior.

![Eccentricity distribution of scale-free EPA network.](image)

**Figure 32.** Eccentricity distribution of scale-free EPA network.

![Vertex significance distribution of scale-free EPA network.](image)

**Figure 33.** Vertex significance distribution of scale-free EPA network.

### 6.5 Q-exponential networks

As example of q-exponential network, i.e. networks whose degree (dimension) distribution fits well with q-exponential function, a biological network will be considered. It represents protein-protein interaction network in yeast and consists 2361 nodes (we will call it PPI). The dataset of this network is downloaded from [26], and this particular dataset is analyzed
in [27]. Nevertheless, this type of network was analyzed in many other papers, but it will not be cited here.

In this example the degree (i.e. dimension) distribution follows q-exponential function [28]

\[ P(k) = e_q^{\frac{k-1}{\kappa_0}} = \left[1 - (1 - q)\frac{k - 1}{\kappa_0}\right]^{\frac{1}{1-q}}, \]

where \( k \) is node degree, \( q \geq 1 \), and \( \kappa_0 \) is some characteristic number of links. The fitting of dimension distribution, as well as fitting other variables, is done following the algorithm introduced in [28].

The distribution of dimensions is presented at the Figure 34. The parameters obtained from fitting for PPI network are \( q = 1.28 \), and \( \kappa_0 = 0.3026 \). Since asymptotically q-exponential function follows power-law, the exponent \( \gamma = \frac{1}{1-q} \) for PPI network is \( \gamma = 3.57 \).

![Figure 34. Dimension distribution of q-exponential PPI network. The q-exponential fit is indicated.](image)

The values of 1st, and 2nd structure vectors are presented at the Figure 35, and 3rd structure vector is presented at the Figure 36.
Figure 35. Values of first and second structure vectors for \( q \)-exponential PPI network.

Figure 36. Values of third structure vector for \( q \)-exponential PPI network.

The eccentricity distribution is illustrated at the Figure 37, whereas vertex significance distribution is illustrated at the Figure 38. The presence of large number of simplices, from Figure 37, (approximately 45%) are well integrated into the structure and does not have individuality \( (ecc = 0) \), is followed by simplices with other values of \( ecc \), particularly \( ecc = 0.33 \) and \( ecc = 0.5 \). As can be seen from Figure 38 vertex significance distribution is well fitted to \( q \)-exponential function with parameters \( q = 1.32 \), and \( \kappa_0 = 0.253 \).
7 Results for clique complex

Using Bron-Kerbosch algorithm (BK) [29], we have determined all maximal cliques of several characteristic types of complex networks. After that we have constructed clique complex, and computed simplicial complex measures as well as topological invariant known as Betti numbers.

7.1 Random network

The examined random network is formed by \( N_n = 2000 \) nodes, connected with probability \( p = 0.005 \). After application of the BK algorithm we obtained a clique complex formed by \( N_s = 9688 \) simplices, and \( N_v = N_n = 2000 \) vertices. The dimension of this clique complex

\[32\]
is equal to 2, meaning that it is formed only by the triangles. This result was expected since the connectivity probability is small, that is, the network is sparse. From eccentricity distribution Figure 39 we can see that almost all simplices have $ecc = 0.5$. This means that almost all cliques have individuality characterized by sharing half of their vertices with some other clique.

The vertex significance distribution follows bell-shaped behavior, as can be seen from the Figure 40, well known property of random networks, hence, there is some characteristic value of significance of cliques due to the vertices which form them.
7.2 Barabási-Albert model of scale-free network

Following the algorithm introduced in [24] we have generated complex network formed by \( N_n = 2000 \) nodes. After application of the BK algorithm we obtained a clique complex formed by \( N_s = 5576 \) simplices, and \( N_v = N_n = 2000 \) vertices. At the Figure 41 vector-valued quantities, that is Q-vector (first structure vector), f’-vector (second structure vector, at Figure 41 marked by \( f_1 \)), and f-vector are presented. As can be seen the clique complex dimension is equal to 4, and the behaviors of all vectors are the same.

![Graph showing vector-valued quantities](image)

Figure 41.

At Figure 42 the eccentricity distribution is presented, and like for clique complex of random network, almost all simplices have eccentricity equal to 0.5, but unlike the random network case there is a small number (about 4%) of cliques with \( ecc = 0.33 \).

![Graph showing eccentricity distribution](image)

Figure 42.

34
At Figure 43 the vertex significance distribution is presented. In analogy to the results for clique complex of random network we would assume that vertex significance distribution follows power-law. Nevertheless, this is not the case, but we should have in mind that we have calculated vertex significance distribution of cliques of scale-free network from one sample of the model, but not from an ensemble.

7.3 Exponential network

In order to analyze clique complex of an exponential network, we have chosen an email network [30] whose dataset was downloaded from [31]. Each e-mail address in this network represents a node and links between nodes indicate e-mail communication between them. After application of the BK algorithm we obtained a clique complex formed by $N_s = 3267$ simplices and $N_v = N_n = 1133$ vertices. At the Figure 44 vector-valued quantities, that is $Q$-vector (first structure vector), $f'$-vector (second structure vector), and $f$-vector are presented, and the dimension of clique complex is equal to 11, and can be fitted well to the exponential function.
At Figure 45 the eccentricity distribution is presented, and unlike the model networks the majority of cliques have eccentricity between 0.25 and 0.5, with picks at $ecc = 0.25, 0.33, 0.5$.

At Figure 46 the vertex significance distribution is presented, and follows the behavior of degree distribution, i.e. in the best approximation it is exponential.
7.4 Q-exponential network

As an example of q-exponential network we have chosen the protein-protein interaction network in yeast, the same as the one considered for the neighborhood complex. After application of the BK algorithm we obtained a clique complex formed by $N_s = 5012$ simplices and $N_v = N_n = 2361$ vertices. At the Figure 47 vector-valued quantities, that is Q-vector (first structure vector), f'-vector (second structure vector), and f-vector are presented, and the dimension of clique complex is equal to 8.

At Figure 48 the eccentricity distribution is presented, and as for email network almost all cliques have $ecc \in [0.25, 0.5]$, but with a difference in the leading pick, which is much
larger than other picks for PPI network.

Figure 48.

At Figure 49 the vertex significance distribution is presented.

Figure 49.

7.5 Betti numbers

We have calculated Betti numbers of clique complexes of four networks: Barabási-Albert scale-free network model, random network model, email network, and protein-protein interaction network in yeast. The results are presented at the Table 1. Recalling that $q^{th}$ Betti number enumerates the number of $q$-dimensional holes in simplicial complex, we can notice
that two model networks does not contain 3-dimensional holes, but two real-world networks does.

<table>
<thead>
<tr>
<th>network</th>
<th>$q = 0$</th>
<th>$q = 1$</th>
<th>$q = 2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>basf</td>
<td>1</td>
<td>3634</td>
<td>0</td>
</tr>
<tr>
<td>email</td>
<td>1</td>
<td>1186</td>
<td>53</td>
</tr>
<tr>
<td>yeast</td>
<td>101</td>
<td>2357</td>
<td>14</td>
</tr>
<tr>
<td>random</td>
<td>2</td>
<td>1484</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 1

At Figures 50 and 51 are presented the values of Betti numbers for email network, and protein-protein interaction network in yeast, respectively.

![Figure 50.](image1.png)

![Figure 51.](image2.png)
7.6 Betti numbers of generalized random network clique complex

Using the method introduced in [32] we have generated random networks with arbitrary power-law degree distribution. Tuning power-law exponent $\gamma$ of degree distribution we have generated scale-free networks formed by $N_n = 2000$ nodes. From every obtained network we formed clique complex and computed Betti numbers. It turns out that the dependence of $\beta_1$ on the exponent $\gamma$ follows power-laws for different exponent ranges with different exponent value (Figure 52). Namely in the range $\gamma \in [2, 3.5]$ the exponent is equal to $-0.9$, and in the range $\gamma \in [3.5, 5.1]$ the exponent is equal to $-0.4$. At the Figure 53 the dependence of $\beta_2$ on the exponent $\gamma$ is presented. The results are obtained for over 100 samples.
8 Barabási-Albert scale-free network with implicitly introduced fitness

Having simplicial complex, let us introduce a local property related to a simplex and its close neighborhood, which we will call generalized connectivity degree. The reason for using this name will be more clear in the following. Take two simplices $\sigma(i)$ and $\sigma(j)$ which share face of dimension $f_{ij}$. The dimensions of the simplices $\sigma(i)$ and $\sigma(j)$ are $q_i$ and $q_j$, respectively. Since they share face whose dimension is $f_{ij}$, they also share faces with dimensions $f_{ij} - 1$, $f_{ij} - 2$, $\ldots$, $0$. The generalized connectivity degree is defined as

$$C'_{ij} = \frac{\text{Number of shared faces}}{\frac{1}{2}(\text{Overall number of faces that each of simplices can have})},$$

or

$$C'_{ij} = \frac{\sum_{f=0}^{f_{ij}} \alpha_{f_{ij}, f}}{\frac{1}{2} \left( \sum_{f=q_i}^{q_i} \alpha_{q_i, f} + \sum_{f=q_j}^{q_j} \alpha_{q_j, f} \right)},$$

where

$$\alpha_{x, f} = \frac{(x + 1)!}{(f + 1)!(x - f)!},$$

and $x = f_{ij}, q_i, q_j$. If we sum over all neighbors of the simplex, we get the variable which characterizes the simplex, i.e.

$$C'_i = \sum_{j \in \{nn\}_i} C'_{ij},$$

where $\{nn\}_i$ stands for nearest-neighbors of the simplex $\sigma(i)$.

Simplifying equation (10) one gets

$$C'_{ij} = \frac{2(-1 + 2^{1+f_{ij}})(1 + f_{ij})!}{\Gamma(2 + f_{ij}) \left( \frac{(-1+2^{1+q_i})(1+q_i)!}{\Gamma(2+q_i)} + \frac{(-1+2^{1+q_j})(1+q_j)!}{\Gamma(2+q_j)} \right)},$$

where $\Gamma(z)$ is gamma-function. We can further simplify equation (13) and get

$$C'_{ij} = \frac{2^{1+f_{ij}} - 1}{2^{q_i} + 2^{q_j} - 1},$$

and for the simplex $\sigma(i)$

$$C'_i = \sum_{j \in \{nn\}_i} 2^{1+f_{ij}} - 1.$$

Simplices $\sigma(i)$ and $\sigma(j)$ are connected if they share face, and in the limit $f_{ij} \to 0$ and $q_i, q_j \to 0$ the value of $C'_{ij}$ defined by (14) equals 1. This result can be understood as the transition from simplicial complex to graph in the sense that simplices $\sigma(i)$ and $\sigma(j)$ become nodes $i$ and $j$ and the face $f_{ij}$ which they share become a link $(i, j)$. This transition is even more clear if we consider equation (15) in the limit $f_{ij} \to 0$ and $q_i, q_j \to 0$. In this case we have

$$C'_i = \sum_{j \in \{nn\}_i} \frac{2^{1+f_{ij}} - 1}{2^{q_i} + 2^{q_j} - 1} \to \sum_{j \in \{nn\}_i} 1 = z_i = k_i,$$

where $z_i = k_i$.  

41
where \( z_i \) is the number of its nearest neighbors, and \( k_i \) is the corresponding degree of the complex network obtained from the simplicial complex when simplices become nodes, and faces become links. In this sense, the variable \( C' \) corresponds to generalized node degree, or, as we mentioned at the beginning, the generalized connectivity degree.

The main idea is to create the model of the evolution of the simplicial complex in analogy to the Barabási-Albert scale-free model [24], as long as in the limit \( f_{ij} \to 0 \) and \( q_i, q_j \to 0 \) we get BA scale-free network, i.e.

\[
P(C') \sim C'^{-\gamma} \to P(k) \sim k^{-\gamma}.
\]

Start with the arbitrary number of simplices, for example \( N_0 \). At equal time intervals we add new simplex in the simplicial complex which has the value of connectivity degree of the simplex equal to \( K' \). Since \( K' \) depends on \( f_{ij}, q_i \) and \( q_j \), in the limit \( f_{ij} \to 0 \) and \( q_i, q_j \to 0 \), it becomes \( m \), i.e. the number of nodes to which the new node will connect in the corresponding complex network. The new simplex will share face with simplex \( \sigma(i) \) already present in the complex preferentially with probability

\[
\Pi(C'_i) = \frac{C'_i}{\sum_j C'_j}.
\] (17)

In the limit \( f_{ij} \to 0 \) and \( q_i, q_j \to 0 \) the preferential attachment (17) becomes

\[
\Pi(k_i) = \frac{k_i}{\sum_j k_j}.
\]

The rate at which the simplex acquires new connections is

\[
\frac{\partial C'_i}{\partial t} = K' \frac{C'_i}{\sum_j C'_j}.
\] (18)

We can denote the sum in the denominator by \( \beta \), i.e.

\[
\beta = \sum_j \sum_k \frac{2^{1+f_{jk}} - 1}{2^{q_j} + 2^{q_k} - 1},
\]

and since it is symmetric under change of indexes we can write

\[
\beta = 2 \sum_{j<k} \frac{2^{1+f_{jk}} - 1}{2^{q_j} + 2^{q_k} - 1}.
\]

The sum \( \beta \) changes over time, since new simplices are added. If we assume that \( \beta \) depends on time in the simplest way, i.e. depends linearly on time

\[
\beta \approx 2h(f, g)t,
\]

where \( h(f, g) \) is some function that depends on the dimension of faces and dimension of simplices and \( h(f, g) \to 1 \), as \( f, g \to 0 \), the rate equation has the form

\[
\frac{\partial C'_i}{\partial t} \approx \frac{C'_i}{2h(f, g)t}.
\] (19)
Solving equation (19) one gets

\[ C'_i(t) \approx K' \left( \frac{t}{t_i} \right)^{\frac{1}{2h(f,g)}}. \]  

The connectivity degree probability density asymptotically has the form:

\[ P(C') \sim \frac{2h(f,g)K'^{2h(f,g)}}{C'^{2h(f,g)+1}}, \]

with exponent \( \eta = 2h(f,g)+1 \). In the limit when \( f, g \to 0 \), \( C' = k \), \( K' = m \) and \( h(f,g) \to 1 \), one gets

\[ P(k) \sim \frac{2m^2}{k^3}. \]

Comments

The formation of simplicial complex defined in this way can be understood as the formation of complex network with fitness, in which a simplex corresponds to fitness associated to a node. Nevertheless, unlike the other complex network models with fitness like [33], [34], or [35], we have not introduced fitness as a sort of external property drawn from some distribution and associated to nodes, but the concept of fitness may naturally arise as implicit property related to simplices. Another discrepancy comes from the fact that if we consider fitness as simplex we are dealing with a discrete quantity, whereas in the models [33], [34], or [35] fitness is treated as continuous quantity. This discrepancy can be a shortcoming since in some systems we can not treat fitness as a discrete quantity. Nevertheless, if we assume that fitness of a single node is \( q \)-dimensional ball, than simplex can be understood as \( q \)-dimensinal polyhedron obtained by triangulation of a ball. In this context fitness defined in [33], [34], or [35] can be understood as a 0-dimensional simplex. The model that we introduced have some similarities with the model [33] primarily in computational method that we have used and the concept of preferential attachment. The major difference is clearly in the generalized connectivity due to the overlapping property of simplices through the faces.

The result that we have obtained (power-law exponent equals 3) is the same as the one for Barabási-Albert scale-free networks [24], but the crucial reason for obtaining such a result is in the assumption that the sum \( \beta \) grows linearly in time, and that the function \( h(f,g) \) is equal to 1 when \( f, g \to 0 \). Changing these assumptions, primarily the behavior of the function \( h(f,g) \) can lead us to the other exponent values, and even multiscaling.

On the other hand, having in mind that the simplicial complex is a topological space, the model that we have introduced can be understood as the formation of topological space. Furthermore, such a topological space shapes the behavior of degree distribution of the underling complex network.

References


44


