The construction and use of distance matrix to study the topological properties of complex networks

Self-presentation to conduct habilitation

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Contents

1 Presentation of scientific achievements forming the basis for habilitation proceeding

As a scientific achievement within the meaning of Art. 16, par. 2 of the Act of 14 March 2003 "On Academic Degrees and Academic Title and on Degrees and Title in Art" (Journal of Laws No. 65, item 595, as amended) I present a series of six related publications

[H1] K. Malarz, J. Czaplicki, B. Kawecka-Magiera, and K. Kułakowski. "Average distance in growing trees". *International Journal of Modern Physics C* **14**.9 (2003), 1201–1206.

[H2] K. Malarz, J. Karpińska, A. Kardas, and K. Kułakowski. "Node-node distance distribution for growing networks". *TASK Quarterly* **8**.1 (2004), 115–119.

[H3] K. Malarz and K. Kułakowski. "Dependence of the average to-node distance on the node degree for random graphs and growing networks". *European Physical Journal B* **41**.3 (2004), 333–336.

[H4] K. Malarz and K. Kułakowski. "Matrix representation of evolving networks". *Acta Physica Polonica B* **36**.8 (2005), 2523–2536.

[H5] K. Malarz and K. Kułakowski. "Memory effect in growing trees". *Physica A* **345**.1-2 (2005), 326–334.

[H6] K. Malarz. "Numbers of n-th neighbors and node-to-node distances in growing networks". *Acta Physica Polonica B* **37**.2 (2006), 309–318.

under a common title: "**The construction and use of distance matrix to study the topological properties of complex networks**".

1.1 Introduction

1.1.1 The growing networks

The intensity of complex networks [2, 9, 11, 12] studies by physicists definitely intensified after the publication in 1999 in Science the paper by Albert and Barabási entitled "The emergence of scaling in random networks" [19]. Search for "complex networks" in the Web of Science database now returns 11 433 papers of which only 196 published before the year of Ref. [19] publication. The paper [19] has today more than nine thousand citations. What was the phenomenon of the discovery of Albert and Barabási?

To answer this question we have to return to the works of the Hungarian mathematicians published in the sixties of the twentieth century... In Refs. [27, 29] Erdős and Rényi studied classical random graphs (now also often referred to as Erdős–Rényi networks). These graphs are created by a random connection of N nodes with L edges. The nodes degree distribution of such graphs proved to be Poissonian

$$\mathcal{P}_k(k) = \frac{\bar{k}^k}{k!}\exp(-\bar{k}), \qquad \bar{k} = \frac{1}{N}\sum_{i=1}^{N} k_i, \tag{1}$$

where $\bar{k}$ is the average degree of vertex. This means that in classical random graph there is a "typical" node having "typical" number of the nearest neighbours. Meanwhile, the real networks either technology ones (such as networks of plane connections between the cities,

power grids, a network of websites or the Internet lying in a layer of its infrastructure) or social networks (networks of friends and their virtual counterparts in social networks, networks of movie actors linked by an edge if they performed in the same movie or networks of scientists linked by an edge if they are co-authors of the same publication, etc.) do not possess such "typical" node. The above-mentioned networks have mostly the power-law distribution of degrees of vertices

$$\mathcal{P}_k(k) \propto k^{-\gamma}, \tag{2}$$

with an exponent $\gamma \in [1, 3]$.

Reason for the popularity of Ref. [19] was identification, by Barabási and Albert, of the mechanism of a random complex networks creation, which leads to scale-free distribution of nodes degrees (2). This mechanism is based on the snowball effect (or evangelical Mathew effect[1]): Barabási and Albert network is a growing network, i.e. new network nodes are attached to the pre-existing structure using m links and the probability of the creation of links to existing nodes is proportional to their current degree k. The Albert and Barabási algorithm leads to the creation of hubs in a network: a small privileged "caste" of nodes with an above-average amount of its nearest-neighbours.

Another example of growing networks are exponential networks. The name of the network—as in the case of scale-free networks—mirrors the shape of the probability distribution of node-degrees of the network

$$\mathcal{P}_k(k) \propto a^{-k}, \qquad a > 0. \tag{3}$$

An example of a real-world network with exponential nodes degrees distribution is, for example, power grid of western United States [35]. In contrast to the scale-free network in exponential growing network new nodes are attached with m bonds to an existing network in a totally random manner and not in a preferential one. The i-th node added to the exponential network is attached by m edges to m among $i-1$ pre-existing nodes. The probability of selecting a node to which the connection will take place is given as [6]

$$p(k, i) = \frac{1}{i-1}, \tag{4}$$

while for growing scale-free networks this probability is [6, 15, 18]

$$p(k, i) = \frac{1 + k_i/m}{2i}. \tag{5}$$

In both cases (i.e. for exponential and scale-free) of growing networks the starting point for the growth process of the network is fully connected graph with m vertices, where m is the number of bonds used to attach a new node to the existing network.

In Refs. [H1, H2, H5, H6] the topological properties of the growing network were discussed.

1.1.2 Small worlds

A distinct feature many growing network is the presence in them of the "small world" effect. This effect manifests itself as not faster than logarithmic increase of the average

[1] For whoever has will be given more, and they will have an abundance. Whoever does not have, even what they have will be taken from them. [Matthew 25:29]

distance d_N between network nodes[2] with the network size N. For example, a network in which nodes are $N = 450000$ actors linked together with edges if they starred in the same movie, the average distance between nodes is only 3.5 [9].

"Small world" effect was detected nearly fifty years ago by Milgram in a brilliant sociometric experiment [24]. In this experiment, a group of people was asked to send a letter through intermediaries to a broker in Boston. The selection of intermediaries had to be made among senders' friends, who (in the senders' assessing) might know the broker or at least might know broker's friends. Although many of letters on their way to Boston were lost and never arrived there, the ones that reached a broker needed on average less than seven intermediaries. This is way the "small world" effect is often referred as "six degrees of separation" hypothesis.

This effect occurs not only in the growing networks discussed above but also in classical random networks or a Watts–Strogatz networks constructed on the basis of the regular network [35]. In the latter a fraction f edges of regular lattice is randomly rewired to another nodes in a network. Finding the proper candidate for an intermediary in the contact processes is not a trivial task, and there are several strategies for its selection. In Ref. [H3] a measure the effectiveness of the search process for ideal intermediary were discussed.

1.1.3 Purpose of works [H1–H6]

In Refs. [H1–H3, H5, H6] the algorithms for finding the shortest paths between all pairs of vertices were presented. In contrast to the conventional algorithms [3] the newly proposed schemes *do not* require prior encoding of the graph structure in an adjacency matrix or an adjacency list. For evolving (growing) networks the newly designed algorithms allow for distance matrix creation *simultaneously* with the growth of the network itself. Then, the obtained distance matrices were used to study the structural and transport properties of complex networks. Ref. [H4] is devoted to a compact review of the results of the works [H1–H3].

1.2 Discussion of the works that make up the series of publications which have been the basis for the request for a habilitation

1.2.1 K. Malarz, J. Czaplicki, B. Kawecka-Magiera, and K. Kułakowski. "Average distance in growing trees". *International Journal of Modern Physics C* 14.9 (2003), 1201–1206

In Ref. [H1] node-to-node average distance relationship d_N on the number of nodes N in the growing trees was studied. The term tree means simple undirected connected graph which does not contain cyclic paths. A characteristic feature of trees is unique path that one has to travel between two arbitrarily selected nodes—such a travel can be made only in a unique way. We analyzed two types of growing trees: the so-called exponential trees and scale-free ones. The exponential tree arises from the process of adding new nodes and appending them by a single bond ($m = 1$) to a randomly selected node from an already existing structure. The growth of scale-free trees is carried out in a similar manner except

[2] The average node-to-node distance is also often termed as the diameter of the graph and its formal definition is given by Eq. (6).

that the selection of the node to which new node is connected takes place according to the algorithm proposed by Albert and Barabási [19]. In this scheme, the probability of selection of a node i to which the connection takes place is proportional to the current node degree $k(i)$.

The traditional approach to determine the average distance between the vertices of the graph bases on search algorithms, including breadth-first search [26, 31] and depth-first search [23] and the algorithms for calculating shortest paths between all pairs of nodes [22, 25, 28, 32].

However, in all these cases, the prior knowledge of the adjacency matrix (or list) representing the graph topology is required. In Ref. [H1] an alternative approach to this problem was proposed. Determination of the average distance d_N between the nodes of *a typical* tree t_N with N nodes requires determination the distance $s_N(i,j)$ between each pair of nodes $i-j$ among N vertices of the graph. Then

$$d_N \equiv \left\langle \frac{1}{N(N-1)} \sum_{i,j\neq i}^{N} s_N(i,j) \right\rangle, \tag{6a}$$

where $\langle \cdots \rangle$ stands for the average over the topologically different trees of size N.

A way of selecting a "typical" tree of size N for a family of trees (whether scale-free or exponential) also requires explanation. Note, that extreme cases of trees, i.e. a star and a linear chain of nodes have radically different diameters. Therefore, the choice of a typical tree must be replaced by *the averaging procedure* over M randomly selected trees of size N:

$$d_N = \frac{1}{N(N-1)} \sum_{t_N} P(t_N) \sum_{i,j\neq i}^{N} s_N(i,j), \tag{6b}$$

where $P(t_N)$ stands for the probability of tree t_N selection and $\sum_{t_N} P(t_N) = 1$.

The algorithms [3, 22, 23, 25, 26, 28, 31, 32] allow to construct a matrix of distances $\mathbf{S}_N$ if we have a network topology encoded as an adjacency list or an adjacency matrix $\mathbf{A}_N$. The adjacency matrix is a binary matrix whose elements

$$a_N(i,j) = \begin{cases} 1, & \text{when nodes } i \text{ and } j \text{ are directly connected,} \\ 0, & \text{otherwise.} \end{cases}$$

The novelty of the approach proposed in Ref. [H1] is based on the distance matrix construction simultaneously with the growth of the tree, i.e. before the construction of a complete graph adjacency matrix $\mathbf{A}_N$. Moreover, the proposed algorithm *does not* require prior knowledge of an adjacency matrix or an adjacency list [3, 22, 23, 25, 26, 28, 31, 32].

Having a distance matrix for the tree of size N and adding to that tree $(N+1)$-th vertex we need to add to the distance matrix a new row and a new column which represent the distances that come with the new node to all other nodes. The elements of this new $(N+1)$-th column (row) are created basing on the elements of the q-th column (row) of distance matrix, where q corresponds to the label of the node to which the new node is attached. Distance of the newly added $(N+1)$-th node to any other node will be greater by one than the distance of these nodes to the node labeled as q:

$$s_{N+1}(N+1,i) = s_N(q,i) + 1, \text{ for } i = 1,2,...,N. \tag{7a}$$

Of course, distance matrix is symmetric and on its diagonal has only zero elements:

$$s_{N+1}(i,N+1)=s_{N+1}(N+1,i) \text{ and } s_{N+1}(N+1,N+1)=0, \text{ for } i=1,2,...,N. \quad (7b)$$

Assuming that the distances matrix for $N=4$ is given by

$$\mathbf{S}_4=\begin{bmatrix} 0 & 1 & \mathbf{2} & 2 \\ 1 & 0 & \mathbf{1} & 1 \\ 2 & 1 & \mathbf{0} & 2 \\ 2 & 1 & \mathbf{2} & 0 \end{bmatrix}$$

and the fifth node is attached to the node labeled as three yields

$$\mathbf{S}_5=\begin{bmatrix} 0 & 1 & 2 & 2 & \mathbf{3} \\ 1 & 0 & 1 & 1 & \mathbf{2} \\ 2 & 1 & 0 & 2 & \mathbf{1} \\ 2 & 1 & 2 & 0 & \mathbf{3} \\ 3 & 2 & 1 & 3 & \mathbf{0} \end{bmatrix}.$$

Applying successively Eqs. (7) and (6) we were able to determine numerically dependencies d_N for the exponential and scale-free trees. The average $\langle\cdots\rangle$ were made over a thousand of different trees. These relationships are shown in Ref. [H1] in Figure 2. In both cases, the relationship is logarithmic for large values of N: $d_N \asymp 2\ln N + c_1$ for exponential trees and $d_N \asymp \ln N + c_2$ for scale-free trees.

Note, that zero elements on the diagonal distance matrix $\mathbf{S}_N$ allows you to pair the average node-to-node distance d_N with an average distance matrix element ℓ_N

$$\ell_N \equiv \frac{1}{N^2}\sum_{t_N} P(t_N)\sum_{i,j}^{N} s_N(i,j) = \left\langle \frac{1}{N^2}\sum_{i,j=1}^{N} s_N(i,j)\right\rangle \quad (8)$$

as

$$(N-1)d_N = N\ell_N. \quad (9)$$

Eq. (4) displayed in Ref. [H1] shows an iterative formula for average element ℓ_N of the matrix $\mathbf{S}_N$. For exponential trees the conditional probability $P(q|t_N)$ for attaching a new vertex to a node labeled as q is $1/N$. Taking this fact and Eq. (9) into account, formula (4) from Ref. [H1] allows deduce an iterative formula for analytical determination of d_{N+1} if we know d_N:

$$d_{N+1} = \frac{(N+2)(N-1)}{N(N+1)}d_N + \frac{2}{N+1}. \quad (10)$$

Similarly, the average square element of the distance matrix

$$\ell_N^2 = \left\langle \frac{1}{N^2}\sum_{i,j}^{N}[s_N(i,j)]^2\right\rangle \quad (11)$$

allows for derivation of the iterative formula for the mean square node-to-node distance

$$d_{N+1}^2 = \frac{(N+2)(N-1)}{N(N-1)}d_N^2 + \frac{4(N-1)}{N(N+1)}d_N + \frac{2}{N+1}. \quad (12)$$

The combination of formulas (4) and (8) from Ref. [H1] allows to construct an iterative formula for the node-to-node distance variance $\sigma_N^2 = d_N^2 - (d_N)^2$ for the exponential

growing trees. Figure 3 in Ref. [H1] presents the dependence d_N and σ_N^2 derived from iterative formulas for trees with $N \leq 10^9$ vertices. A comparison of these results with the results of direct simulations for exponential trees of less than a thousand nodes are presented as well. The results of simulations were averaged over $M = 10^3$ realizations of the growth process. In both cases, i.e. for d_N and σ_N^2 these relationships are linear with $\ln(N^2)$. Excellent agreement of the results of direct simulation and iterative formulas for $N \leq 10^3$ allows apply derived iterative formulas also for $N \gg 10^3$. In these areas of graph sizes the direct simulations of trees growth is cumbersome, both in terms of time- and memory-consuming. Additionally, the reliability of the results strongly depends on good enough statistics, i.e. the number M of trees used in the averaging procedure $\langle \cdots \rangle$. Let us recall, that for sufficiently large values of N the number of trees with N vertices is given by the approximate Otter's formula [33]:

$$T_O(N) = \beta \cdot \alpha^N \cdot N^{-5/2}, \quad \alpha \approx 2.9557652856, \quad \beta \approx 0.5349496061.$$

So even for $N = 10^3$ we have to check a set of $M = 7.73 \times 10^{462}$ trees. On the other hand predictability of these formulas is limited only to the growing exponential trees and hence the results differ, for example, from those obtained in Ref. [8].

1.2.2 K. Malarz, J. Karpińska, A. Kardas, and K. Kułakowski. "Node-node distance distribution for growing networks". *TASK Quarterly* 8.1 (2004), 115–119

The concept of construction of a distance matrix $\mathbf{S}_N$ simultaneously with the increase of the graph presented in Ref. [H1] has been extended in Ref. [H2] for growing simple graphs where the newly attached $(N+1)$-th node is simultaneously attached to $m = 2$ so far existing nodes of the graph with N vertices. In this case, the new $(N+1)$-th column (row) added to matrix $\mathbf{S}_N$ is generated according to the formula:

$$s_{N+1}(N+1, i) = s_{N+1}(i, N+1) = \min\big(s_N(p, i), s_N(q, i)\big) + 1, \tag{13a}$$

where the indices p and q correspond to two selected vertices which will join the new node.

This means that the distance $s_{N+1}(N+1, i)$ of the newly added node to all the other vertices $1 \leq i \leq N$ in the network is larger by one than the distance between them and vertices p or q, and to determine this distance we selected this node of the (p, q)-pair which gives the shorter path. Since joining the vertex of the graph using the two bonds can introduce into the network shortcuts between existing vertices, it is necessary to reevaluate all distances between nodes:

$$s_{N+1}(i, j) = \min\big(s_N(i, j), s_N(i, p) + 2 + s_N(q, j)\big), \qquad 1 \leq i, j \leq N. \tag{13b}$$

The distance matrix diagonal elements are zero like for the trees

$$s_{N+1}(N+1, N+1) = 0. \tag{13c}$$

Similarly as in Ref. [H1], the selection of the nodes p and q to which the connection will take place can be random or preferential. In the first case, the distribution of the graph nodes degree will be exponential $\mathcal{P}_k(k) \propto \exp(-k)$ while for the latter case it will be scale-free $\mathcal{P}_k(k) \propto k^{-\gamma}$.

Basing again on zero diagonal elements of the matrix $\mathbf{S}_N$ also for non-tree-like networks we can formulate an analogy to Eq. (9). Namely, we can propose a relation between average n-th power of the matrix elements $s_N^n(i,j)$ calculated with the diagonal elements of the matrix $\mathbf{S}_N$

$$\ell_N^n = \left\langle \frac{1}{N^2} \sum_{i,j=1}^{N} [s(i,j)]^n \right\rangle , \tag{14}$$

or without them

$$d_N^n = \left\langle \frac{1}{N(N-1)} \sum_{i=1, j\neq i}^{N} [s(i,j)]^n \right\rangle \tag{15}$$

and averaging procedure $\langle \cdots \rangle$ takes place over M independent realizations of the network growth process. Zeros on the diagonal $s_N(i,i) = 0$ make the sum in formulas (14) and (15) equal each to other, and hence

$$N\ell_N^n = (N-1)d_N^n. \tag{16}$$

For exponential trees—where adding a new node takes place to randomly selected existing node p—one can build iterative formula

$$(N+1)^2 \ell_{N+1}^n = \left\langle \sum_{i,j=1}^{N+1} s_{N+1}^n(i,j) \right\rangle = N^2 \ell_N^2 + 2 \left\langle \sum_{i=1}^{N} [1 + s(i,p)]^n \right\rangle , \tag{17}$$

correlating average matrix element ℓ_{N+1}^n with the corresponding average matrix element ℓ_N^n of the network existing before attaching the $(N+1)$-th node to the vertex p.

A number "one" appearing on the right hand side of Eq. (17) comes from the freshly added edge connecting the new node with a node p of the network of size N, while number "two" appearing before the last sum of the mentioned equation reflects the symmetry of the matrix $\mathbf{S}$ (adding a new $(N+1)$-th column to matrix $\mathbf{S}$ is accompanied by the addition of this column transposition as the $(N+1)$-th row of the matrix). Substituting dependence (16) into the equation (17), we obtain an iterative formula

$$d_{N+1}^n = \frac{(N+2)(N-1)}{(N+1)N} d_N^n + \frac{2}{N+1} + \frac{2(N-1)}{(N-1)N} \sum_{k=1}^{n-1} \binom{n}{k} d_N^k. \tag{18}$$

Similarly as in Ref. [H1] the correctness of derived iterative formula (18) has been tested by comparing its predictions with the results of the direct simulation (see Figure 2 in Ref. [H2]).

For this purpose the matrices $\mathbf{S}_N$ were generated for the exponential trees with $2 \leq N \leq 10^3$ nodes and the average first, second, third and fourth powers of the matrix elements were calculated. These results were averaged over $M = 10^3$ various random trees and compared with dependencies of ℓ_N^i for $i = 1, 2, 3, 4$.

Knowing the average value of n-th power d_N^n of the off-diagonal matrix elements for matrix $\mathbf{S}_N$ allows for checking the node-to-node distance distribution characteristics dependence on the network size. The dependencies of average, variance, skewness and kurtosis of the above mentioned distribution were shown in Ref. [H2] in Figure 3. The node-to-node distance distributions accompanied with Poisson distributions were presented in Figure 1. The Poisson distributions approximate these node-to-node distance distributions quite fairly.

For trees ($m = 1$) and for simple graphs ($m = 2$) obtained dependencies d_N increase logarithmically with N

$$d_N = a_1 \ln N + b_1,$$

what indicate that these networks posses the "small world" property. For both, exponential and scale-free, trees ($m = 1$) also the variance of the node-to-node distribution $\sigma_N^2 = (d_N)^2 - d_N^2$ increases logarithmically with N

$$\sigma_N^2 = a_2 \ln N + b_2.$$

The least squares method best fit values of the parameters a_1, b_2, a_2 and b_2 for exponential and scale-free trees ($m = 1$) and simple graphs ($m = 2$) are presented in Ref. [H2] in Tables 1 and 2.

1.2.3 K. Malarz and K. Kułakowski. "Dependence of the average to-node distance on the node degree for random graphs and growing networks". *European Physical Journal B* 41.3 (2004), 333–336

In Ref. [H3] the concept of the distance matrix construction during the network growth was extended to the case of the Erdős–Rényi classical random graphs. As mentioned in the Introduction (Sec. 1.1.1) the classical random graphs can be formed either by a random combination of N nodes with L edges (the Erdős–Rényi construction [27, 29]), or through the implementation each of the possible $N(N-1)/2$ connections between nodes with a specified probability p (the Gilbert construction [30]). In the thermodynamic limit ($N \to \infty$) both, the Gilbert and Erdős–Rényi constructions lead to the same result ($p = 2L/[N(N-1)]$). In Ref. [H3] the Gilbert approach was applied to construct the classical random graph distance matrix. The starting point for constructing matrix $\mathbf{S}_N$ for graph with N nodes is a matrix consisting zeros at the diagonal and the off-diagonal elements equal to or greater than N. Scanning sequentially the off-diagonal elements of the matrix $s_N(i, j < i) \geq N$ and replacing them by unity, e.g. $s_N(i, j) = 1$ with probability p we create an edge between elements i and j. The distance matrix $\mathbf{S}_N$ is symmetric, so $s(j, i) = s(i, j)$. The creation of new edge can introduce shortcuts between so far connected nodes and therefore each link creation must be accompanied by reevaluation of all elements of a matrix $\mathbf{S}_N$:

$$s(m, n) = \min\big(s(m, n), s(m, i) + 1 + s(j, n), s(m, j) + 1 + s(i, n)\big). \tag{19}$$

The distance matrix formed in this way corresponds to a connected graph if none of its elements is greater than $N - 1$.

The main research task posed in Ref. [H3] has been defined as searching for quantitative characteristics of the complex networks allowing for estimating the efficiency of the contact processes on the networks. The complex networks studied in Refs. [H1–H6] are characterized by the "small world" effect. As mentioned in the Introduction (Sec. 1.1.2), the "small world" effect was detected in the experiment proposed by Milgram [24]. In this type of contact process to find the most appropriate contact person (the network node) appears to be a non-trivial task [13, 16]. One of the most obvious methods of the consecutive nodes selection seems to be selecting nodes being statistically closer to all other nodes in the network, i.e. the choice of the neighbor, which has the largest number of its own neighbors. Such strategy proved to be effective in the case of scale-free graphs but it fails for the classical random graphs [16]. In Ref. [H3] we show that this strategy works nicely for exponential graphs and especially for exponential trees.

In order to determine qualitatively the effectiveness of the strategy of finding subsequent nodes through which transportation in the contact process is the most efficient the distance matrices $\mathbf{S}_N$ for scale-free, exponential and the Erdős–Rényi networks were created. Then, for each vertex of the graph its degree $k(i)$ and its average distance $\xi(i)$ to all other nodes in the network

$$\xi(i) = \frac{1}{N-1} \sum_{j \neq i}^{N} s_N(i,j)$$

were determined.

With distance matrix $\mathbf{S}_N$, the degree of the i-th vertex of the graph may be calculated by counting the occurrence of unities in the i-th row (or the i-th column) of the matrix $\mathbf{S}_N$. Now, averaging obtained values $\xi(i)$ over all nodes of degree $k(i)$ one may obtain the relationship of the mean distance $\xi(k)$ to the node in the network as a function of the degree of vertex $k(i)$. We expect that the relationship $\xi(k)$ decreases with k as better connected nodes have a statistically greater chance of short paths to other nodes in the network. If decreasing ξ with increasing k is evident, the discussed above strategy of searching for nodes that are good candidates for middleman in the contact process will be an efficient one. Dependencies $\xi(k)$ for the exponential and scale-free simple graphs ($m = 2$) and trees ($m = 1$) and for the classical random graphs ($p = 0.02$, 0.05, 0.4) are shown in Ref. [H3] in Figure 1. Results for graphs with $N = 10^3$ nodes are averaged over the M simulations with $M = 10^7$, 10^3 and 10^2 for the trees, simple graphs and classical random graphs, respectively. Also the shapes of the curves $\xi(k)$ for ten times larger trees ($N = 10^4$) but averaged only over $M = 10$ trees realization are presented there. The slope of these curves

$$\eta(k) = -\frac{\partial \xi(k)}{\partial \ln(k)} \tag{20}$$

gives just a quantitative measure of the efficiency of the contact process.

Yet another averaging (this time over the vertices degrees k) would allow for each of the considered network for calculation of a single value η characterizing the "goodness" of the discussed strategy. As in such average procedure the contribution from the nodes of the small degree is dominant, the initial shape of the $\xi(k)$ dependence may be crucial. Instead of such averaging Figures 2(a) and 2(b) [H3] show the full dependence $\eta(k)$ for various kinds of networks. Presented results confirm the conclusions given in Ref. [16] that in the contact processes the nodes search strategy based on searching for the nodes with highest degree is not suitable for classical random graphs (the factor η practically does not depend on k and it is close to zero) while this strategy is effective for scale-free networks. Figures 2(a) and 2(b) in Ref. [H3] show clearly that this strategy works fine not only for scale-free networks but also for exponential simple graphs ($m = 2$) and even better for exponential trees ($m = 1$).

Enhanced effectiveness of the mentioned searching strategy for exponential trees as compared to the scale-free networks seems to be directly linked with the hierarchy of scale-free networks. As a result of the preferential attachment mechanism the fluctuations of node-degrees appearing in the scale-free networks in the direction of their higher value are naturally enhanced and network growth takes place in the vicinity of the nodes with more than the average number of neighbors. Then the discussed nodes search mechanism for conducting the contact process can lead us only to the local network center. For exponential trees the effect of local hubs formation is absent and therefore the factor η for these networks (especially for trees, where the paths between nodes are unique) is high.

Regardless of the network topology, the discussed strategy of nodes selection has its natural limits. One may expect, that it ceases to be efficient after reaching the true center of the network. Once such a center has been found, the method will be unable to indicate a new, more attractive candidate to navigate through the network. This limitation is shown in Figures 2(a) and 2(b) in Ref. [H3] as a clear maximum of $\eta(k)$ dependencies. On the other hand, Figure 1 in Ref. [H3] shows, that increasing the size of the network does not affect the shape of dependence $\xi(k)$—with the exception of shift of the curves for $N = 10^4$ as compared to the curves for $N = 10^3$ towards the higher values of ξ and logarithmically slow flow in the direction of higher values of k. As a consequence, dependencies $\eta(k)$ for various network sizes do not differ too much but they change—both, qualitatively and quantitatively—with the change of network generation mechanism.

1.2.4 K. Malarz and K. Kułakowski. "Matrix representation of evolving networks". *Acta Physica Polonica B* 36.8 (2005), 2523–2536

The results published in Refs. [H1–H3] were presented during the "1st Polish Symposium on Econo- and Sociophysics" [C1.17]. Ref. [H4] included in conference materials contains a presentation and a summary of the most important results of the above works. In particular, Ref. [H4] shows the methods of distance matrix $\mathbf{S}_N$ construction for scale-free and exponential trees ($m = 1$) and simple graphs ($m = 2$) and for classical random graphs. Also description of the design of iterative rules (18) for the average n-th power of the node-to-node distance d^n_{N+1} for exponential trees were repeated there. In Figure 7 in Ref. [H4] the values of d^n_{N+1} for $n = 1, \cdots, 10$ and $3 \leq N \leq 10^3$ obtained using (18) dependence were compared with the results of direct computer simulation. In Ref. [H4] we show methodology of teasing out from distance matrix numerical characteristics of each node (node-degrees and the average distance to any node in the graph), the global characteristics of the networks (such as the diameter of the network), and how to examine in these networks the effectiveness of the contact processes. In addition to presenting the aforementioned networks topology in Figure 1 (Ref. [H4]), Figure 5 shows also shapes of node-degrees distributions $\mathcal{P}_k(k)$ obtained from the computer simulations as compared with the theoretical distributions. In Figure 6 (Ref. [H4]) the node-to-node distance distributions were presented as well.

1.2.5 K. Malarz and K. Kułakowski. "Memory effect in growing trees". *Physica A* 345.1-2 (2005), 326–334

In Ref. [H5] the distance matrix $\mathbf{S}_N$ construction schemes presented in Refs. [H1, H2] and iterative rules (18) were applied to study the shape memory effect for growing scale-free and exponential networks. Both, trees ($m = 1$) and simple graphs—in which new nodes added to the growing networks are attached to two of the existing nodes ($m = 2$)—were studied. Since there is only single tree with three vertices[3] to study the effect of the shape of the embryo of growing network for network shape evolution as a starting point one must accept the tree consisting of at least $N = 4$ nodes. The shapes of these two trees were marked in Ref. [H5] as Z (for four-nodes chain) and Y (for the star-shaped tree).

[3]Here, we are talking only about topologically distinguishable trees, i.e. without taking into account possible graph nodes labelling. In the latter case, the amount of trees t_N with N vertices varies according to the Cayley's formula $t_N = N^{N-2}$ [34].

For both of these configurations the distance matrices were constructed:

$$\mathbf{S}_4^{\mathrm{Z}} = \begin{bmatrix} 0 & 1 & 2 & 3 \\ 1 & 0 & 1 & 2 \\ 2 & 1 & 0 & 1 \\ 3 & 2 & 1 & 0 \end{bmatrix} \text{ and } \mathbf{S}_4^{\mathrm{Y}} = \begin{bmatrix} 0 & 1 & 2 & 2 \\ 1 & 0 & 1 & 1 \\ 2 & 1 & 0 & 2 \\ 2 & 1 & 2 & 0 \end{bmatrix}.$$

The initial network structure shape memory effect was studied by observing the difference between the diameters d_N of growing networks

$$\Delta_N^1 \equiv d_N(\mathrm{Z}) - d_N(\mathrm{Y}) \tag{21}$$

and the difference between the mean squares off-diagonal matrix elements d_N^2 of the distance matrix $\mathbf{S}_N$

$$\Delta_N^2 \equiv d_N^2(\mathrm{Z}) - d_N^2(\mathrm{Y}), \tag{22}$$

where the labels Z and Y refer to the network growing from four-nodes chains and four-nodes star, respectively.

The dependencies Δ_N^1 and Δ_N^2 obtained by direct simulations (i.e. using distance matrix $\mathbf{S}_N$ construction scheme given in Eqs. (7) and (13)) and for both types of concerned trees and for $N \leq 10^3$ are presented in Figures 2 and 3 in Ref. [H5]. The simulation results were averaged over $M = 10^5$ realizations of the network growth process. In Figure 2 in Ref. [H5] these dependencies given by iterative formula (18) for the exponential trees and $4 \leq N \leq 10^9$ are presented as well. In this case, the information about the initial shape of a tree is encoded in values $d_4(\mathrm{Z}) = 5/3$, $d_4^2(\mathrm{Z}) = 10/3$ and $d_4(\mathrm{Y}) = 3/2$ and $d_4^2(\mathrm{Y}) = 5/2$. For both kinds of studied trees values Δ_N^1 tend to a constant value for $N \approx 100$, while Δ_N^2 is an increasing function of N. This means that studied trees remember the shape of their "embryo".

The dependencies Δ_N^1 and Δ_N^2 for scale-free and exponential simple graphs are presented in Figure 6 in Ref. [H5]. The presented results are averaged over $M = 10^3$ the network growth processes. For exponential graphs both of differences $\Delta_N^{1,2}$ are equal zero as soon as the network sizes reaches $N \approx 100$ nodes. From that moment network forgets its original form. For scale-free graphs values $\Delta_N^1 < 0.02$, while $\Delta_N^2 < 0.1$ and slowly decrease with N. For the latter network it is rather difficult to state clearly whether initial shape memory effect is present or absent in these graphs basing solely on the observation of behavior $\Delta_N^{1,2}$ for $N \leq 10^3$. Certainly, the initial shape memory effect is for these kind of networks qualitatively and quantitatively weaker than for three other studied network types. As the scale-free simple graphs were studied only through direct simulation—which is naturally limited by the maximum size of the distance matrix $\mathbf{S}_N$—and taking into account the slope of $\Delta_N^{1,2}$ dependence, one cannot rule out that for sufficiently large networks $N \gg 10^3$ the initial shape memory effect will disappear also for this kind of networks. In the case of the simple graphs—when the newly added node is attached to the existing network with $m = 2$ bonds—the "shortcuts" between existing vertices may appear. The appearance of a shortcut induces a permanent rewriting the distance matrix $\mathbf{S}_N$ according to Eq. (13b). Consequently, information about the initial shape of the network encoded in the 4×4 upper-left part of the matrix $\mathbf{S}_N$ is gradually erased. The effect of changes in these sixteen matrix $\mathbf{S}_N$ elements is absent in the case of trees and hence the investigated trees remember their initial shape during network growth.

1.2.6 K. Malarz. "Numbers of n-th neighbors and node-to-node distances in growing networks". *Acta Physica Polonica B* 37.2 (2006), 309–318

In Ref. [H6] the algorithms for distance matrix $\mathbf{S}_N$ creation presented in Refs. [H1, H2] were used to verify by means of direct computer simulations the theoretical predictions regarding the average number z_L of nodes in L-th coordination sphere of a randomly selected vertex of the complex network. Also the dependence of average node-to-node distance

$$\lambda(\pi) = \left\langle \frac{1}{N_\pi} \sum_{\substack{i,j>i,\\ k_i k_j = \pi}} s(i,j) \right\rangle \tag{23}$$

on the product π of the nodes i and j degrees were studied in Ref. [H6]. In Eq. (23) N_π stands for the number of nodes pairs, whose product of degrees $k_i k_j$ is equal to π.

The formula allowing for estimating the amount of neighbors z_L in the L-th coordination sphere of randomly selected node

$$z_L = z_1^{2-L} z_2^{L-1}, \tag{24}$$

was derived using the generating functions formalism [20] and predicted theoretically in Ref. [17]. In Eq. (24) symbols z_1 and z_2 stand for the amounts of the nearest neighbours and the next-nearest neighbours of a randomly selected node, respectively. Of course, the value of z_1 is an average node degree in the network

$$z_1 = \left\langle \frac{1}{N} \sum_{i=1}^{N} k_i \right\rangle, \tag{25}$$

while the number of the next-nearest neighbors (z_2) is given by the Shargel's formula [10]

$$z_2 = \left\langle \frac{1}{N} \left(\sum_{i=1}^{N} k_i^2 - \sum_{i=1}^{N} k_i \right) \right\rangle. \tag{26}$$

Using again the generating functions technique the theoretical dependence $\lambda(\pi)$ (defined in Eq. (23))

$$\lambda(\pi) = A + B \ln(k_i k_j), \tag{27a}$$

where

$$A = 1 + \frac{\ln(N z_1)}{\ln(z_2/z_1)} \quad \text{i} \quad B = -\frac{1}{\ln(z_2/z_1)} \tag{27b}$$

was derived in Ref. [14] and confirmed experimentally in the analysis of the real-world communication networks as well as in analyses of the simulated classical random graphs and scale-free networks [4, 5].

Since the generating function formalism has a mean-field character it should work properly only for homogeneous trees. The mean-field nature of this formalism is associated with its underlying principle—namely, an assumption of the lack of any correlation between nodes degrees. However, in the growing trees this assumption is not valid, as the oldest (and consequently with above-average degree) nodes of such network will be geometrically closer than nodes added to the network at the end of the growth process (and which are leafs of the tree).

The purpose of studies described in Ref. [H6] was to determine whether the prediction of formulas (24), (26) and (27) are suited for exponential trees.

In order to validate the predictions of Eq. (24) the dependence of difference

$$\delta_L(N) = z_1^{2-L} z_2^{L-1} - z_L \tag{28}$$

on the network size N for $L = 3, 4, 5$ and $N \leq 10^3$ was tested. The results were averaged over $M = 10^4$ independent network growth processes. The dependence (28) for exponential and scale-free trees ($m = 1$) and simple graphs ($m = 2$) are presented in Figure 1 in Ref. [H6].

While the size of simulated Albert–Barabasi networks are too small to observe agreement of z_L and $z_1^{2-L} z_2^{L-1}$ for $L = 3, 4, 5$ (or such agreement for these networks does not exist) then for exponential networks—and not just for trees but also for the simple graphs ($m = 2$)—$\delta_L(N)$ decreases monotonically with N for $N \approx 100$ and larger.

The expected values of the numbers of the nearest neighbours (z_1) and the next-nearest neighbors (z_2)—instead of performing direct simulations—can also be determined basing on nodes' degrees probability distribution $\mathcal{P}_k(k)$. This yields

$$z_1 = \sum_{i=m}^{\infty} k \mathcal{P}_k(k) \tag{29}$$

and basing on (26) also

$$z_2 = \sum_{i=m}^{\infty} k(k-1) \mathcal{P}_k(k). \tag{30}$$

The nodes degrees probability distributions for discussed networks are given by

$$\mathcal{P}_k(k \geq m) = \begin{cases} 2^{-k} & \text{for } m = 1, \\ \frac{3}{4}\left(\frac{3}{2}\right)^{-k} & \text{for } m = 2, \end{cases} \tag{31}$$

and

$$\mathcal{P}_k(k \geq m) = \frac{2m(m+1)}{(k+2)(k+2)k} \tag{32}$$

for exponential [H4, 12] and scale-free networks [6, 7], respectively.

In the thermodynamic limit ($N \to \infty$) the sum (30) diverges for scale-free networks (i.e. when the nodes degrees probability distribution $\mathcal{P}_k(k)$ is given by (32)). For a finite but large scale-free networks the sum in Eq. (30) may be fairly approximated as

$$z_2 \approx \hat{z}_2 = \sum_{k=m}^{N-1} k(k-1) \mathcal{P}_k(k) = 2m(m+1) \sum_{k=m}^{N-1} \frac{k-1}{(k+2)(k+1)}. \tag{33}$$

The dependencies $\hat{z}_2(N)$ for $m \leq N \leq 10^6$ are shown in Ref. [H6] in Figure 2. This sum grows logarithmically with $N \gg m$

$$\hat{z}_2(N) \asymp a_m \ln(N) + b_m \tag{34}$$

with the least squares method best fits coefficients $a_m = 3.99$, $b_m = -7.55$ (for $m = 1$) and $a_m = 11.96$, $b_m = -2.66$ (for $m = 2$).

The values of z_1 and z_2 for the trees ($m = 1$) and the simple graphs ($m = 2$) and for both considered kinds of networks (exponential and scale-free ones) obtained in direct simulation or calculated from formulas (29) and (30) were collected in Ref. [H6] in Table 1. The values z_1 [Eq. (25)] and z_2 [Eq. (26)] obtained in computer simulation agree with the

values calculated based on the probability distribution (29) and (30) for exponential trees ($m = 1$) and exponential simple graphs ($m = 2$). For scale-free networks this compatibility concerns only the values of z_1 while approximated values of sums $\hat{z}_2$ (33) differ significantly from values z_2 obtained in direct computer simulation [Eq. (26)]. In Table 1 in Ref. [H6] the average number z_3 of the next-next-nearest neighbours and the values of $z_3 = z_2^2/z_1$ calculated basing on Eq. (24) are presented as well. The values of z_1 and z_2 were obtained in the direct computer simulation. Similarly as for the numbers of the nearest and the next-nearest neighbours, the numbers z_3 of the next-next-nearest neighbours agree with theoretical predictions given by Eq. (24) only for exponential networks and this agreement is slightly better for tress ($m = 1$) than for simple graphs ($m = 2$).

In the second part of Ref. [H6] the utility of the Motter et al. formula (27) for the same set of networks was investigated. The dependencies $\lambda(\pi)$ together with the least squares method fits and theoretical predictions given by Eq. (27) are presented. The values of the coefficients A and B—which appear in Eq. (27a) and which are provided by Eq. (27b)—are collected in the lower part of Table 1 [H6] together with the same coefficients determined by the least squares fit of logarithmic function to the experimental data. Similarly as for the formula allowing for calculation of the number of successive L-th neighbors [Eq. (24)], the accuracy of theoretical predictions of Eq. (27) tested by means of computer simulations is satisfactory for the exponential network but only qualitative for scale-free networks.

As mentioned earlier on page 16, the predictions based on formulas (24) and (27)—derived in generating functions formalism—should be valid only for homogeneous trees. Meanwhile, Eqs. (24) and (27) work fine also for the exponential networks and not just for those having tree-like structure. The conclusions of Ref. [H6] contain suggestion, that the above-mentioned formulas may be useful for the network having—in the thermodynamic limit—the finite values of $\sum_{k=m}^{\infty} k^2 \mathcal{P}_k(k)$.

1.3 Summary

The common topic of Refs. [H1–H6] are computer simulations of the topological properties of complex networks examined on the basis of the distance matrix $\mathbf{S}_N$ properties. These matrices are built according to algorithms presented in Refs. [H1–H3]. These algorithms allow for the distance matrices $\mathbf{S}_N$ construction dismissing any necessity of constructing adjacency lists or adjacency matrix $\mathbf{A}_N$.

In summary, the most important achievements published in Refs. [H1–H6] are:

- proposing new algorithms [Eqs. (7), (13) and (19)] for constructing distance matrices $\mathbf{S}_N$, which do not require knowledge of the adjacency list or the adjacency matrix and, on the other hand, permitting for formation of distance matrices $\mathbf{S}_N$ simultaneously with the formation of the growing networks [H1, H2, H4] and for classical random graphs [H3, H4],

- derivation of the iterative formulas [Eqs. (10), (12) and (18)] for the node-to-node distance distribution moments d_N^n for the exponential trees [H1, H2, H4],

- introducing the new functional characteristics (20) allowing for examination of the effectiveness of contact processes on complex networks [H3, H4],

- indicating the existence of the initial shape memory effect in case of growing trees and the absence of such an effect for simple graphs which do not have a tree structure [H5]

- and showing that the formulas (24) and (27)—describing the number of L-th next-neighbors of the node ($L \geq 3$) and the average node-to-node distance in function of the products of the degrees of vertices, respectively—can be successfully applied also to the exponential graphs (which not necessarily have to possess a tree-like structure) [H6].

Most of the algorithms and ideas presented in Refs. [H1–H6] can be successfully applied to study the networks/graphs constructed as statistical ensembles rather as results of a growth process. This type of models find application in studies of many real-world networks (including those in molecular biology, genetics, transportation or sociology) where equilibration plays an important role. Examples of such systems may be protein interaction networks or genetic regulatory networks describing biological systems adapting for a long time to external conditions. For such systems one can define a partition function and assign a statistical weight to each individual network in the ensemble.

Once the partition function is defined one can ask if there are different phases depending on parameters of the model and if the system undergoes a phase transition [7]. For example one can examine how the nature of the phase transition is reflected in geometrical and topological properties of underling network or how the node-to-node distance is changing or what are the correlations at the transition point.

One can ask if the system self-averages, i.e. if there are typical graphs in the ensemble, how many loops there are in typical graphs, etc. Erdős–Rényi graphs—which are the simplest example of a statistical ensemble of graphs—are known to have very few loops. This turns out to be a generic situation for statistical ensembles of sparse graphs. Many real-world networks have much more loops than the corresponding Erdős–Rényi graphs, so an open question is how to generate statistical ensembles of sparse graphs with many loops.

It turns out that it is not that easy to define such models in a statistical way. The simplest attempt which relies on introducing a linear coupling for the number of loops is known to lead to an instability, called Strauss instability [21], which is a sort of phase transition to a phase, where graphs have a clique maximizing the number of short triangular cycles. These type of graphs, again, are not encountered in real-world networks. We believe it would be extremely interesting to search for a statistical ensemble of graphs with many cyclic paths with their density compared to those observed in nature [1].

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