BAREKENG: Journal of Mathematics and Its Applications
March 2026 Volume 20 Issue 1 Page 0829–0840
P-ISSN: 1978-7227 E-ISSN: 2615-3017
https://doi.org/10.30598/barekengvol20iss1pp0829-0840

ESTIMATING MODULARITY BOUNDS FOR HOMOPHILIC SCALE-FREE NETWORKS

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Article Info

Article History:

Received: 5th June 2025
Revised: 4th July 2025
Accepted: 4th August 2025
Available online: 24th November 2025

Keywords:

Communities;
Homophilic networks;
Modularity boundaries;
Network analysis;
Scale-free networks

ABSTRACT

The problem of estimating the modularity boundaries for networks that are both homophilic and scale-free is considered. The key property of homophilic networks is the tendency of nodes to link with similar nodes, i.e., belonging to the same community. Thus, homophily is a natural mechanism for community formation, i.e., network structuring. One of the measures of network structuring is modularity. In homophilic networks, not only can the distribution of node degrees be scale-free, but also the distribution of community sizes. In this case, communities can differ significantly in size, which leads to narrowing the achievable modularity boundaries. Estimates of the modularity boundaries of networks of the considered class are obtained. Mathematically strict estimates contain non-elementary functions, which complicates the practical application of such estimates. Approximate estimates with high (0.005) accuracy for the most characteristic values of network parameters are obtained.

How to cite this article:

V. Shergin, S. Udovenko, T. Miroshnychenko, L. Chala, and O. Dorokhov, "ESTIMATING MODULARITY BOUNDS FOR HOMOPHILIC SCALE-FREE NETWORKS", *BAREKENG: J. Math. & App.*, vol. 20, no. 1, pp. 0829-0840, Mar, 2026.

Journal homepage: *https://ojs3.unpatti.ac.id/index.php/barekeng/*
Journal e-mail: *barekeng.math@yahoo.com; barekeng.journal@mail.unpatti.ac.id*

Research Article · Open Access

1. INTRODUCTION

It is common knowledge that one of the characteristic properties of complex networks is their structured nature. Nodes of such networks are grouped into more or less distinct communities (clusters), so the density of connections within communities is significantly higher than the density of connections between nodes of different communities. The task of partitioning a network into communities is very relevant; there are many options for setting this problem, methods for solving it, and, accordingly, criteria for assessing the partition quality.

The most common criterion for the quality of partitioning a network into communities is modularity. This criterion, proposed by Girvan and Newman [1] is used not only as a maximized objective function of network partitioning algorithms, as in the Louvain algorithm [2], but also as an external criterion for the partition quality. That is, to assess the effectiveness of solving the problem of identifying communities using methods that are not based on modularity. Modularity is additive with respect to communities and even single nodes, and is easy to calculate, which explains its widespread use. An alternative to modularity can be such criteria as conductivity and entropy ratio [3]. According to experimental studies [4] if one of the three criteria indicates a high/low network structure, the other two also indicate the same.

The modularity criterion is based on comparing the actual number of connections within communities with the number predicted by the null model. A homogeneous unstructured graph with the same distribution of vertex degrees as for the network under consideration is treated as such a model. The modularity value is generally in the range [-1, 1]. Positive values correspond to homophilic networks [5]-[7], i.e., those in which nodes tend to connect with nodes of their communities. Negative modularity indicates a homophobic nature of network nodes, i.e., a preference for forming connections with nodes belonging to other communities. A network that does not contain distinct communities (i.e., homogeneous) has a modularity asymptotically equal to zero.

It is known [8] , [9] that many real-world networks are scale-free. The key property of such networks is the power law of node degree distribution [10], [11]. Models of scale-free networks are based on using the preferential attachment rule [12]. Some of such models are rather simple [13]-[15]. Others are more complex, based on multi-type branching processes [16], [17], but most of them generate homogeneous networks. The most important class of network models is generative ones, i.e., those that allow creating a network in step-by-step mode [18], [19].

In [20] a generative model of a homophilic scale-free network was proposed. It is based on a two-stage application of the preferential attachment rule: first, it is used to select a community to which a new node will belong, and then to select the nodes of this community to which the new node will be connected. This ensures the creation and maintenance of a natural community structure and, at the same time, scale-freeness is preserved. It is important to note that for homogeneous networks, the scale-free property refers to the distribution of node degrees (and means the discrete-power Yule-Simon law [21]-[24].

Then, in the case where the network consists of communities, the distribution of the sizes of these communities can also be scale-free. Obtaining analytical estimates of various characteristics of scale-free networks has been and remains [25] a relevant theoretical problem. Thus, in [26] an asymptotic estimate of the average path length in a hierarchical scale-free network was obtained. At the same time, the issue of asymptotic boundaries of the modularity of homophilic scale-free networks remains insufficiently studied.

Despite the simplicity of calculation and wide use, the practical application of modularity as a criterion for the degree of homophily/homophobia of a network faces serious problems. Thus, an undesirable property of the modularity criterion is that the null model underlying it assumes that communities have approximately the same density of connections. A significant difference in the density of connections of communities affects both the absolute value and even the sign of the network's modularity. To eliminate this drawback, a modified modularity criterion was proposed [27], which explicitly takes into account the number of nodes in communities.

An important problem is the limited resolution of the modularity criterion. It consists of the fact that for large network sizes, maximizing modularity leads to forced merging of small-sized communities. This problem was considered in detail by Lancichinetti and Fortunato [28]. To increase the resolution, it was proposed to introduce a resolution parameter $\gamma > 1$ into the modularity calculation formula. Its increase improves the resolution of community detection methods based on modularity maximization. At the same time, it was noted that the actually achievable upper limit of modularity is less than one, but its evaluation was not included in the scope of these works [29], [30].

Thus, the problem of quantitative assessment of network modularity boundaries under conditions of significant unevenness of community sizes remains open. This problem acquires particular relevance when assessing the degree of homophily of structured scale-free networks due to the unevenness of community sizes inherent in such networks.

The solution to the problem of finding quantitative estimates of the modularity boundaries for homophilic scale-free networks is implemented in two stages. Section 2 provides definitions of network modularity, analyzes the reasons for its significant dependence on the distribution of community volumes, and provides mathematical expressions for the distribution of community volumes for homophilic scale-free networks.

In Section 3, analytical estimates of the modularity boundaries for networks of the considered class are obtained in a strict form. Such estimates are expressed through non-elementary mathematical functions and, therefore, are of little practical use. So, the problem of numerical approximation of estimates of the modularity boundaries of homophilic scale-free networks for asymptotically large networks is posed and solved. For this purpose, the hypergeometric function included in the analytical estimate of modularity is approximated, then estimates of the sum of squares of the relative volumes of network communities are found, and then approximate estimates of the modularity boundaries of homophilic networks with a scale-free distribution of their community volumes are found.

2. RESEARCH METHODS

2.1 Criteria of Modularity

Let $G = \{V, E\}$ be a network with n nodes and m edges. Given a partition, the network modularity is defined [1] as:

$$\mu(G) = \frac{1}{2m}\sum_{i,j}(A_{ij} - P_{ij})\delta_{c_i,c_j}, \tag{1}$$

where the summation runs over all pairs of vertices, A is the adjacency matrix, P_{ij} is the expected number of edges between vertices i and j in a null graph, c_k is a community to which node k belongs, $\delta_{x,y}$ is the Kronecker delta.

Therefore, network modularity essentially depends on the null graph model, i.e., on P_{ij}. According to the conventional approach, $P_{ij} = deg_i \cdot deg_j/2m$, where deg_k is the degree of node k. In this case modularity of a particular community is:

$$\mu_k = e_k^{in} - (e_k^{tot})^2, \tag{2}$$

where e_k^{in} is the relative number of links between nodes within community k, $e_k^{tot} = vol(c_k)/vol(G)$ is the relative volume of the k-th community, i.e., the relative sum of degrees of nodes that belong to the k-th community. Relativity means normalizing the corresponding amounts by dividing by the network volume ($vol(G) = 2m$).

Network modularity is the sum of modularity of particular communities in Eq. (2):

$$\mu(G) = \sum_{k=1}^{K}\left(e_k^{in} - (e_k^{tot})^2\right). \tag{3}$$

In the case when the resolution parameter $\gamma > 1$ is used, the network modularity definition in Eq. (3) is modified [29] as:

$$\mu(G,\gamma) = \sum_{k=1}^{K}\left(e_k^{in} - \gamma(e_k^{tot})^2\right). \tag{4}$$

The modified modularity criterion [27], which explicitly takes into account the number of nodes in communities, has the form:

$$\mu^*(G) = \sum_{k=1}^{K} \left(e_k^{in} - p_k \cdot e_k^{tot}\right), \tag{5}$$

where $p_k = (n_k - 1)/(n - 1)$, n_k is the size of k-th community, i.e., the number of nodes in it.

It is easy to see that modularity, in all variants in Eqs. (3) – (5) of its definition, which depends on the share of connections within communities e_k^{in} compared to their volumes e_k^{tot}. This is quite natural and reflects the essence of this indicator as a measure of the clarity of the partition of the network into communities. Obviously, for any network and any community $0 \le e_k^{in} \le e_k^{tot}$. The upper limit ($e_k^{in} = e_k^{tot}$) is achieved only in the case when community k forms a separate component of network connectivity.

However, at the same time, modularity expressions in Eqs. (3) – (5) contain the sums of squares of relative volumes of communities, and this factor is determined by the distribution of communities by their volumes, i.e., it is a characteristic of the structural properties of the network, and not a measure of the quality of the community extraction algorithm. The specified sums of squares take a minimum value (1/*K*) in the case when communities have the same volume (also equal to 1/*K*).

2.2 Modularity Property of Homophilic Scale-Free Networks

As noted in [20], a natural property of homophilic scale-free networks is a scale-free (i.e., discrete-power) distribution of volumes (and sizes) of communities:

$$e_k^{tot} = g(K, \alpha, \delta) \cdot \frac{\Gamma(k + \delta)}{\Gamma(k + \delta + \alpha)}, \tag{6}$$

where factor $g(K, \alpha, \delta)$ depends on the total number of communities (K), scaling factor of community volumes ($\alpha > 0$) and delay factor ($\delta > -\min\{1, \alpha\}$):

$$g(K, \alpha, \delta) = (\alpha - 1) \cdot \frac{\Gamma(\delta + \alpha)}{\Gamma(\delta + 1)} \cdot \frac{\dfrac{\Gamma(K + \delta + \alpha)}{\Gamma(K + \delta)}}{\dfrac{\Gamma(K + \delta + \alpha)}{\Gamma(K + \delta)} - \dfrac{\Gamma(\delta + \alpha)}{\Gamma(\delta + 1)} \cdot (K + \delta)}. \tag{7}$$

Factor δ determines not only the delay in the power law in Eq. (6) but also the intensity of the appearance of new communities compared to the growth rate of the number of network nodes. An example [20] of the network of 500 nodes and 7 communities (*delta* is 0, *alpha* equals 3, having a scale-free distribution Eq. (6) of community volumes) is shown in Fig. 1.

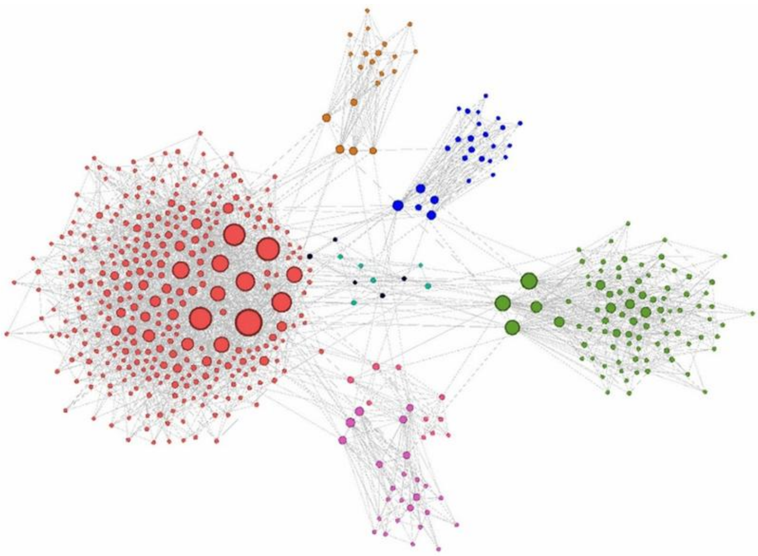

Figure 1. Example of a Homophilic Scale-Free Network

The rank distribution of the community sizes of the considered network is shown in Fig. 2. Markers' colors in Fig. 2 correspond to the colors of the communities in Fig. 1, while the solid line shows the community sizes predicted by the scale-free distribution law in Eq. (6). Therefore, the community sizes of the generated homophilic network are distributed in good accordance with the theoretically predicted law, and this distribution law is scale-free.

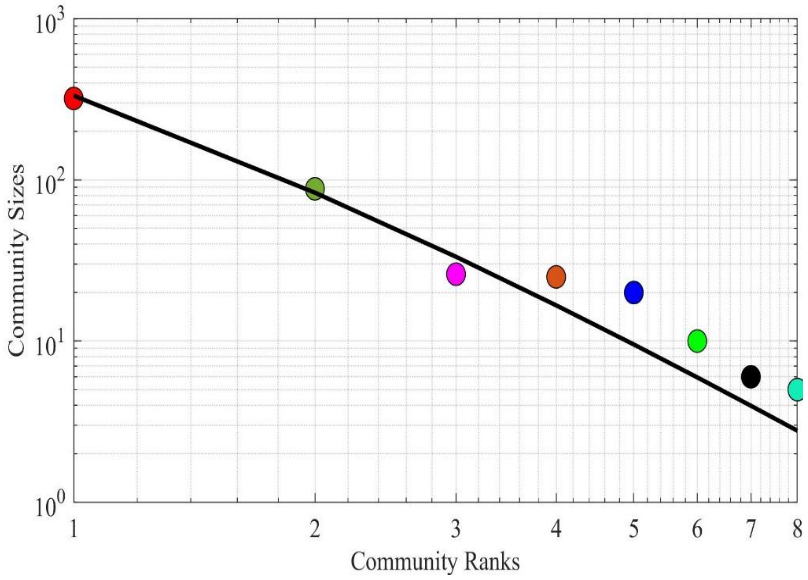

Figure 2. Rank Distribution of the Community Sizes of the Considered Example of a Homophilic Scale-Free Network

An example of the node degrees distribution for the homophilic scale-free network is shown in Fig. 3. The considered network is of $n = 10000$ nodes, alpha $= 4$, and the number of communities is 11. As one can see, not only do community sizes follow a scale-free distribution, but node degrees too.

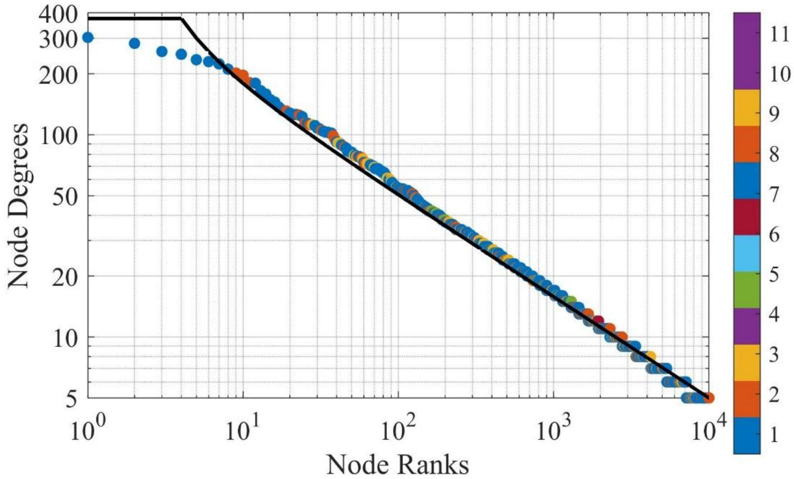

Figure 3. Example of the Rank Distribution of Degrees of Nodes of a Homophilic Network

Distribution in Eq. (6) follows from the ratio of the volumes of two consecutive communities (with numbers k and $k + 1$), which has the form:

$$e_{k+1}^{tot} = e_k^{tot} \cdot \frac{k + \delta}{k + \delta + \alpha}. \tag{8}$$

The model based on Eq. (8) is generative and is intended for step-by-step modeling of a growing network with the properties of homophily and scale-freeness, similar to the example shown in Fig. 1. At the same time, for real networks, the relation in Eq. (8) may not be fulfilled exactly, or may be fulfilled only asymptotically. The necessity of the community volumes corresponding to Eq. (8), and therefore distribution in Eq. (6), is a limitation of the considered model.

In the general case, estimating the dependence $K(n)$ of the number of communities on the network size is a non-trivial problem [31], [32]. According to the model [20], the number of communities depends functionally not only on the network size (n), but also on homophilicity factors α and δ, but this dependence is rather cumbersome. Asymptotic form of this dependence for large networks ($n \to \infty$) is

$$n \approx \begin{cases} const \cdot (K+\delta)^{\alpha}, & \alpha > 1, \\ const \cdot (K+\delta) \cdot \ln(K+\delta+1), & \alpha = 1, \\ const \cdot (K+\delta), & 0 < \alpha < 1. \end{cases} \quad (9)$$

Therefore, if $\alpha < 1$, then the number of communities grows asymptotically linearly with n, while this dependence is a power law for $\alpha > 1$:

$$K \approx \begin{cases} \theta\left(n^{\frac{1}{\alpha}}\right), & \alpha > 1, \\ \theta(n), & 0 < \alpha < 1. \end{cases} \quad (10)$$

In the general case (i.e., K is finite), the factor in Eq. (7) is very unwieldy, but this expression can be substantially simplified in the asymptotic case $K \to \infty,\ \alpha > 1$:

$$g^{as}(\alpha,\delta) = \lim_{K\to\infty} g(K,\alpha,\delta) = (\alpha-1)\cdot\frac{\Gamma(\delta+\alpha)}{\Gamma(\delta+1)}\ . \quad (11)$$

It should be noted that the asymptotic transition $K \to \infty, \alpha > 1$ limits the admissibility of replacing Eq. (7) with Eq. (11). The question of how large the network size (n), the number of communities (K), and the alpha factor should require further research.

Substituting Eq. (11) into Eq. (6), we get

$$(e_k^{tot})^{as} = g^{as}(\alpha,\delta)\cdot\frac{\Gamma(k+\delta)}{\Gamma(k+\delta+\alpha)} = (\alpha-1)\cdot\frac{\Gamma(\delta+\alpha)}{\Gamma(\delta+1)}\cdot\frac{\Gamma(k+\delta)}{\Gamma(k+\delta+\alpha)}\ . \quad (12)$$

The dependence in Eq. (12) for different values of α and δ is shown in Fig. 4.

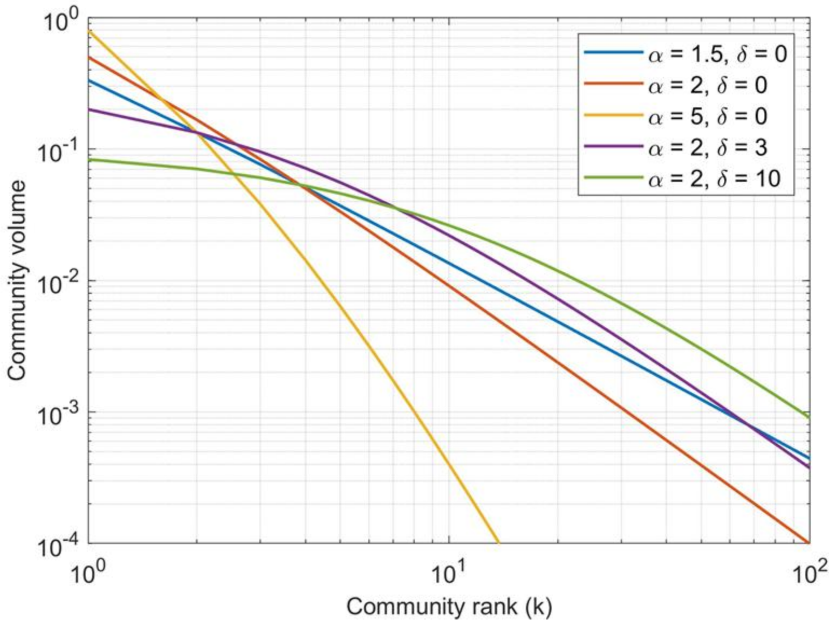

Figure 4. Dependence of Eq. (12) of the Asymptotical Volume of Communities on Community Rank for Homophilic Scale-Free Networks

As one can see, this dependence asymptotically follows a power law with a scaling factor α. At the same time, factor δ influences the rate of approximation of the dependence in Eq. (12) to the power law and the deviation from it for small values of the community number (k).

3. RESULTS AND DISCUSSION

3.1 Obtaining Strict Estimates of the Modularity Boundaries of Homophilic Scale-Free Networks

Considering that $\min\{\sum e_k^{in}\} = 0$ and $\max\{\sum e_k^{in}\} = \sum e_k^{tot} = 1$, the actual boundaries of the modularity criterion in Eq. (3) are determined by the sum of the squares of the relative volumes of the communities. Therefore, the asymptotic boundaries of modularity have the form:

$$-S(\alpha, \delta) \leq \mu(G) \leq 1 - S(\alpha, \delta), \tag{13}$$

where

$$S(\alpha, \delta) = \sum_{k=1}^{\infty} ((e_k^{tot})^{as})^2 = \left(g^{as}(\alpha, \delta)\right)^2 \cdot \sum_{k=1}^{\infty} \left(\frac{\Gamma(k+\delta)}{\Gamma(k+\delta+\alpha)}\right)^2. \tag{14}$$

The problem is to estimate this sum at least in the considered asymptotic case ($K \to \infty, \alpha > 1$).

The exact value of Eq. (14) is equal to

$$S(\alpha, \delta) = \left(\frac{\alpha - 1}{\alpha + \delta}\right)^2 \cdot {}_3F_2(1, \delta + 1, \delta + 1; \alpha + \delta + 1, \alpha + \delta + 1; 1), \tag{15}$$

where ${}_3F_2(a_1, a_2, a_3; b_1, b_2; z)$ is the hypergeometric function.

Thus, exact expressions in Eqs. (13) and (15) for boundaries of modularity of homophilic scale-free networks for the case of asymptotically large ones are obtained.

3.2 Approximation of the Hypergeometric Function ${}_3F_2$

The essence of the problem is that ${}_3F_2(\dots)$ is not an elementary mathematical function and cannot be expressed through them except in some special cases (α is a small positive integer or half-integer). Hence, one has difficulty in practically using the mathematically strict form, Eq. (15), of the modularity boundaries.

The dependence of Eq. (15) is shown in Fig. 5.

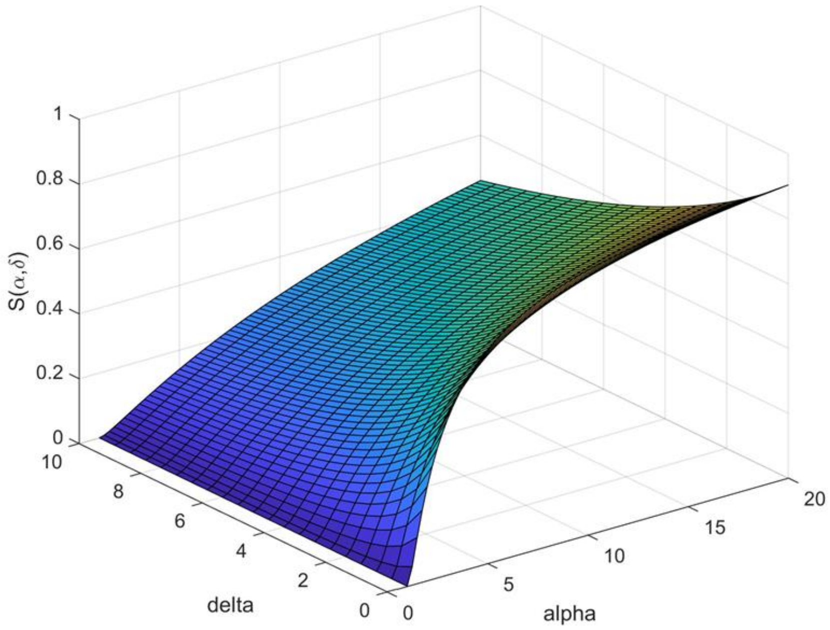

Figure 5. Dependence of Eq. (15) of the Asymptotic Sum of Squares of Relative Community Volumes on Scale and Delay Factors

Thus, for $\alpha = 2$, Eq. (15) takes the form

$$S(2, \delta) = 2(\delta + 1)^2 \cdot \psi^{(1)}(\delta + 1) - (2\delta + 3). \tag{16}$$

Here function $\psi^{(1)}(x)$ (that is first derivative of the digamma function) is also not elementary. However, the approximation of Eq. (16) is rather simple:

$$S(2,\delta) \approx \frac{1}{3(\delta+1)}. \tag{17}$$

Therefore, the problem of approximation the $_3F_2$ function arises. We first consider an important special case of Eq. (15): namely, $\delta = 0$. In this case, the function $_3F_2(1,1,1;\alpha+1,\alpha+1;1)$ can be approximated (Fig. 6) with very high accuracy using:

$$_3F_2(1,1,1;\alpha+1,\alpha+1;1) \approx 1 + \left(\frac{\pi^2}{6} - 1\right) \cdot \alpha^{-2}. \tag{18}$$

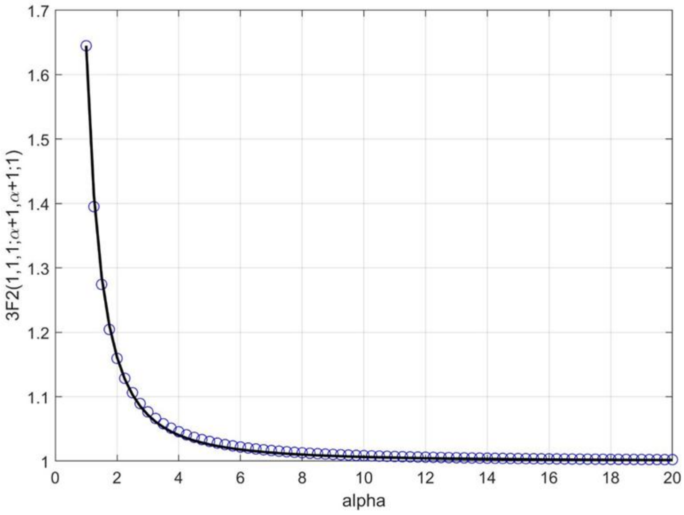

Figure 6. Dependence $_3F_2$(1, 1, 1; α+1, α+1; 1) on α

In the general case, function $_3F_2(1,1,1;\alpha+1,\alpha+1;1)$ was approximated as:

$$_3F_2(1,\delta+1,\delta+1;\alpha+\delta+1,\alpha+\delta+1;1) \approx 1 + (b\cdot\delta + d)\cdot\alpha^{-2} + c\cdot\delta\cdot\alpha^{-1}, \tag{19}$$

where $b = 0.6746,\ c = 0.308,\ d = 0.522$.

The surface plot of the approximation error of the function $_3F_2(\dots)$ by Eq. (19) is shown in Fig. 7.

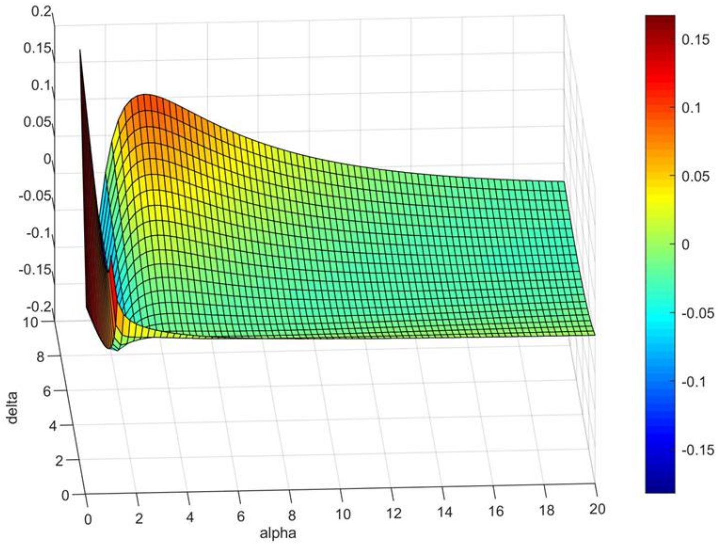

Figure 7. Approximation for the Error of the Function $_3F_2(\dots)$ by Eq. (19)

The R-squared approximation criterion is 0.9988, the maximum absolute value of the error does not exceed 0.2, and thus, this approximation can be considered as rather accurate.

Moreover, the approximation error is most significant for alpha values close to unity, but due to Eq. (15), it can be assumed that the approximation error of ${}_3F_2(\dots)$ with α close to one will not greatly affect the accuracy of approximation the desired dependence $S(\alpha,\delta)$.

3.3 Approximation of the Sum of Squares of Relative Community Volumes

By substituting Eq. (19) into Eq. (15), we get the desired approximation of the sum of squares of relative community volumes in the asymptotic case:

$$S^{app}(\alpha,\delta)=\left(\frac{\alpha-1}{\alpha+\delta}\right)^2\cdot\left(1+\frac{b\cdot\delta+d}{\alpha^2}+c\cdot\frac{\delta}{\alpha}\right). \tag{20}$$

A graphical representation of the error in approximating the asymptotic sum of squares of the relative volumes of communities, Eq. (15), by the obtained function in Eq. (20) is shown in Fig. 8.

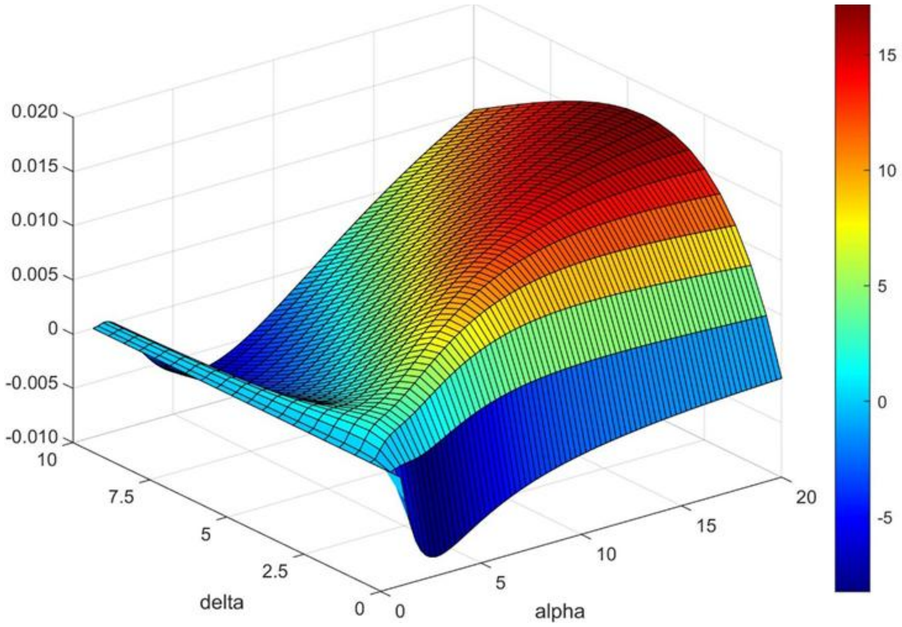

Figure 8. Approximation of the Error of the Asymptotic Sum of Squares of the Relative Volumes of Communities

It can be seen that the accuracy of the approximation provided by Eq. (20) is rather high.

Moreover, it should be taken into account that the characteristic range of variation of the scaling parameter is $\alpha\le 5$. In most of this range, the approximation error does not exceed ± 0.005, which further demonstrates the acceptability of the obtained approximation.

3.4 Estimation of Asymptotic Modularity Bounds for Homophilic Scale-Free Networks

According to the approximation in Eq. (20), the asymptotic boundaries, Eq. (13), of modularity have the form

$$-S^{app}(\alpha,\delta)\le\mu(G)\le 1-S^{app}(\alpha,\delta). \tag{21}$$

For the most important special cases, namely, $\delta=0$ and $\delta=1$, the asymptotic estimates of the modularity bounds are:

$$-\left(\frac{\alpha-1}{\alpha}\right)^2\cdot\left(1+\frac{0.522}{\alpha^2}\right)\le\mu(G)|_{\delta=0}\le 1-\left(\frac{\alpha-1}{\alpha}\right)^2\cdot\left(1+\frac{0.522}{\alpha^2}\right), \tag{22}$$

$$-\left(\frac{\alpha-1}{\alpha+1}\right)^2\left(1+\frac{1.1966}{\alpha^2}+\frac{0.308}{\alpha}\right)\le\mu(G)|_{\delta=1}\le 1-\left(\frac{\alpha-1}{\alpha+1}\right)^2\left(1+\frac{1.1966}{\alpha^2}+\frac{0.308}{\alpha}\right). \tag{23}$$

Graphs of the upper bounds of Eqs. (22) and (23) of modularity for networks with scale-free distribution of community volumes are shown in Fig. 9.

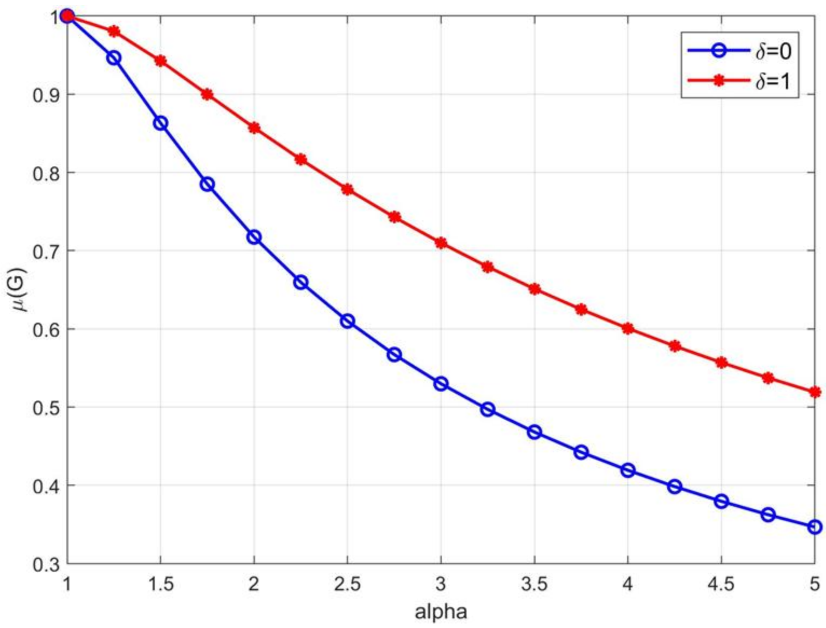

Figure 9. Upper Bounds of Modularity for Networks with Scale-Free Distribution of Community Volumes

As already mentioned, the characteristic range of the scaling parameter is $\alpha \le 5$, and in most cases of homophilic scale-free networks $\alpha \in [2; 3]$. Thus, the examples in Fig. 9 show that the modularity values of $0.5 \div 0.7$ in most cases should be considered as close to the achievable upper limit.

Returning to the discussion of figures in general, it should be borne in mind that most of them (Figs. 4, 5, 7, and 8) are based on an *alpha-delta* coordinate plane, which reflects the influence of the δ parameter on the displayed values. Graphs of the upper bounds of Eqs. (22) and (23) of modularity (Fig. 9) are really built only for special cases $\delta = 0$ and $\delta = 1$. And we treated that cases as the most important.

4. CONCLUSION

Our general comments on the possibility, necessity, and direction of further research are as follows:

1. The problem of estimating the boundaries for modularity of homophilic scale-free networks is solved. In conclusion, we consider it appropriate to note that conductivity and entropy ratio, as well as modularity, are determined by the ratios of community volumes (e_k^{tot} in the manuscript). At the same time, analytical evaluation of these metrics is significantly more complex and even more cumbersome than in the case of modularity. It should also be noted that these alternative metrics are used quite rarely. For this reason, the evaluation of conductivity and entropy ratio is considered a promising topic for our further work in this direction.
2. According to definitions of network modularity and mathematical expressions for the distribution of communities by their volumes, analytical estimates of the modularity boundaries for homophilic scale-free networks are found, Eqs. (13) and (15). The obtained estimates are shown in Fig. 5. However, the obtained estimates are expressed through a non-elementary mathematical function (hypergeometric function ${}_3F_2$), and therefore are of little use for practical application. Therefore, the problem of approximating the estimate Eq. (15) arises.
3. The hypergeometric function ${}_3F_2$ was approximated by a rather simple fractional-polynomial form, Eq. (19). Considering this, an approximation in Eq. (20) was obtained for the sum of the squares of the relative sizes of communities. The accuracy of this approximation is very high. In most of the characteristic range of varying network parameters, the approximation error does not exceed ± 0.005, which was illustrated in Fig. 8. As for the examples shown in Fig. 9, an achievable upper limit of modularity values for homophilic networks in most cases is close to $0.5 \div 0.7$.
4. Thus, estimates of the modularity boundaries of homophilic networks with a scale-free distribution of the volumes of their communities have been found, both in a mathematically exact form, Eq. (15), and in an approximate form, Eq. (20). Assessing other measures of network

homophilicity, such as conductance and entropy ratio, is considered a promising direction for future research.

Author Contributions

Vadim Shergin: Conceptualization, Methodology, Formal Analysis, Writing Draft, Software, Validation. Serhii Udovenko: Data Curation, Resources, Draft Preparation. Tetiana Miroshnychenko: Formal Analysis, Validation. Larysa Chala: Formal Analysis, Software. Oleksandr Dorokhov: Validation, Writing-Review and Editing. All authors discussed the results and contributed to the final manuscript.

Funding Statement

This research received no specific grant from any funding agency in the public, commercial, or not-for-profit sectors.

Acknowledgment

The author's team would like to thank the participants of the scientific seminar "Models and methods of artificial intelligence in scientific research" of the Kharkiv National University of Radio Electronics (Ukraine) for their support and useful advice.

Declarations

The authors declare no competing interests.

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