Detecting Nestedness in Graphs

Alexander Grimm and Claudio J. Tessone

Abstract Many real-world networks have a nested structure. Examples range from biological ecosystems (e.g. mutualistic networks), industry systems (e.g. New York garment industry) to inter-bank networks (e.g. Fedwire bank network). A nested network has a graph topology such that a vertex's neighborhood contains the neighborhood of vertices of lower degree. Thus –upon node reordering– the adjacency matrix is stepwise, and it can be found in both bipartite and non-bipartite networks. Despite the strict mathematical characterization and their common occurrence, it is not easy to detect nested graphs unequivocally. Among others, there exist three methods for detection and quantification of nestedness that are widely used: BINMATNEST, NODF, and FCM. However, these methods fail in detecting nestedness for graphs with low (NODF) and high (NODF, BINMATNEST) density or are developed for bipartite networks (FCM). Another common shortcoming of these approaches is the underlying asumption that all vertices belong to a nested component. However, many real-world networks have solely a sub-component (i.e. not all vertices) that is nested. Thus,unveiling which vertices pertain to the nested component is an important research question, unaddressed by the methods available so far. In this contribution, we study in detail the algorithm *Nestedness detection based on Local Neighborhood* (NESTLON) [7]. This algorithm detects nestedness on a broad range of nested graphs independently of their density and resorts solely on local information. Further, by means of a benchmarking model we are able to tune the degree of nestedness in a controlled manner and study its efficiency. Our results show that NESTLON outperforms both BINMATNEST and NODF.

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1 Introduction

Two vertices are nested if the neighborhood of the one with larger degree contains the neighborhood of the lower degree one. We call *nested component* of a graph the maximum set of vertices that are nested. Following, a graph is nested if the extent of the nested component is such that it embraces all vertices. This definition applies in both bipartite and non-bipartite networks. Nested graphs include some common topologies like fully-connected ones or stars. In real-world networks, some edges violate the definition of pairwise nestedness given above; in this case, the lower the number of these violations, the larger the degree of nestedness of the network.

In Ecology, as it was discovered in the last decade, mutualistic networks show a pronounced degree of nestedness [4]. In Economics, e.g. the New York garment industry including 10'000 manufacturers over a period of 18 years was found to exhibit this property as well [15]. Among non-bipartite networks there are several examples of networks that show large degrees of nestedness: like inter-bank networks [13], and trade relations between countries [9].

Four methods have gained particular attention for detecting and quantifying Nestedness in the last decade: *Binary matrix nestedness temperature calculator* (BINMATNEST) [11], based on *Nestedness Temperature Calculator* (NTC) [2], *Nestedness metric based on overlap and decreasing filling* (NODF) [1], and *Fitness-Complexity Metric* (FCM) [14]. Nonetheless, these methods detect nestedness for only a specific density range (BINMATNEST, NTC and NODF fail in detecting nestedness for high density networks) or a specific class of graphs (FCM was developed for only bipartite ones).

All four methods assume that all vertices belong to a single nested component but, in general, this is not necessarily true. Such component might include solely a subset of vertices while the others lay outside it. Therefore, it is an important research question to devise a method that identifies the individual vertices that belong to a nested component. This question remains unaddressed by the methods available so far.

The widely used BINMATNEST is based on NTC, which compares the focal adjacency matrix with a "perfect ordered" matrix. The less these two matrices deviate from each other, the more the graph is judged as nested. However, the matrix of "perfect order" is a normative concept characterized by a static isocline [2] (i.e. matrix is filled up to the secondary diagonal). Both methods judge graphs only as nested if they have this particular "perfect order". They fail in detecting graphs that have locally nested components. This static and normative concept of nestedness relies only on global information (i.e. irrespective of local neighborhoods in the nested components). For large datasets it is important to develop methods for detecting nestedness that rely solely on local information, because they scale better [7].

In this contribution we review the method *Nestedness detection based on Local Neighborhood* (NESTLON) that reliably detects nestedness irrespective of graph density and network type (i.e. bipartite and non-bipartite networks) [7]. Although in this contribution we focus on non-bipartite graphs (for the sake of simplicity), all the results are easily extensible to bipartite ones.

The remainder of the paper is organized as follows. In the next section section we provide an overview about nestedness in graphs and the current methods for detecting it. In "Algorithm" section we review the alternative method NESTLON for detecting nestedness. In "Robustness Analysis" section we compare commonly used algorithms with NESTLON on a benchmarking graph. The final section concludes and discussed the main contributions of this Paper.

2 The Notion of Nestedness

2.1 Definition of Nestedness

We first give a colloquial definition of nestedness and later a proper mathematical definition. In a nested graph the neighborhood of a vertex includes the neighborhoods of vertices which have lower degrees [1]. Therefore, by sorting the adjacency matrix of a nested graph by degree (i.e. the number of direct neighbors) we obtain a stepwise matrix. For example, a star is nested and has a stepwise matrix. A star's central vertex has the highest degree (i.e. this vertex is connected every other vertex) and all other vertices have degree one (i.e. they are all connected only to the central high degree vertex) while the neighborhoods of all lower degree vertices are included in the neighborhood of the high degree vertex. Therefore, the adjacency matrix of a star has just one large step (i.e. from maximum degree to one-degree).

For a proper mathematical characterization we briefly recapture the nomenclature for graphs. The adjacency matrix, A, characterizes the topology of a graph object G. An non-zero entry in the adjacency matrix, $a_{ij} \neq 0$, indicates an edge between the two vertices i and j. Each vertex has a degree, k_i, which is the number of neighbors it is connected to. The total number of edges is e and the total number of vertices is n. N is the set of all vertices and E is the set of all edges. A graph can be decomposed by the concept of degree partition [10]:

Definition 2.1. Let $G = (N,E)$ be a graph whose distinct positive degrees are $k_{(1)} < k_{(2)} < \ldots < k_{(m)}$ and let $k_{(0)} = 0$ (even if no vertex with degree 0 exists in G). Further, define $\mathcal{D}_i = \{v \in N : k_v = k_{(i)}\}$ for $i = 0,\ldots,m$. Then the set-valued vector $\mathcal{D} = (\mathcal{D}_0, \mathcal{D}_1, \ldots, \mathcal{D}_m)$ is called the degree partition of G.

With this concept of degree partition a nested graph can be expressed as follows [10]:

Definition 2.2. Consider a nested graph $G = (N,E)$ and let $\mathcal{D} = (\mathcal{D}_0, \mathcal{D}_1, \ldots, \mathcal{D}_m)$ be its degree partition. Then the vertices N can be partitioned in independent sets $\mathcal{D}_i$, $i = 1,\ldots,\lfloor m/2 \rfloor$, and a dominating set $\bigcup_{i=\lfloor m/2 \rfloor+1}^{m} \mathcal{D}_i$ in the graph $G' = (N \setminus \mathcal{D}_0, E)$. Moreover, the neighborhoods of the vertices are nested. In particular, for each vertex $v \in \mathcal{D}_i, i = 1,\ldots,m$, we obtain the sets of vertices as

$$N_v = \begin{cases} \bigcup_{j=1}^{i} \mathcal{D}_{m+1-j} & \text{if } i = 1,\ldots,\lfloor m/2 \rfloor; \\ \bigcup_{j=1}^{i} \mathcal{D}_{m+1-j} \setminus \{v\} & \text{if } i = \lfloor m/2 \rfloor + 1,\ldots,m. \end{cases} \quad (1)$$

[1] This definition is for non-bipartite graphs, for bipartite graphs a similar definition holds [4].

An adjacency matrix is stepwise if the following definition holds [5]:

Definition 2.3. A stepwise matrix A is a symmetric, binary $(n \times n)$ matrix with elements a_{ij} satisfying the following condition: if $i < j$ and $a_{ij} = 1$, then $a_{hk} = 1$ whenever $h < k \leq j$ and $h \leq i$.

Thus, a nested graph has a stepwise adjacency matrix and its degree partition can be separated into an independent and a dominating sets.

A measure for determining the filling of an undirected graph is the density.

Definition 2.4. The density of an undirected graph is given by

$$\gamma_d = \frac{2 \cdot e}{n \cdot (n-1)} \tag{2}$$

In the following we propose a measure for counting the number of holes in a graph. We compare the neighborhoods of two vertices i and j. If the lower degree vertex j has a neighbor l, which is not neighbor of i, we will count a hole (because it appears as such in the sorted adjacency matrix). From there, the density of holes can be computed [7]

Definition 2.5. The total number of holes in an unweighted graph is given by

$$\gamma_h = \frac{\sum_{i,j \in N} \Theta(k_i - k_j) \sum_{l \in N} (1 - a_{li}) \cdot a_{lj}}{\sum_{i,j \in N} \Theta(k_i - k_j) \min(n - k_i, k_j)} \tag{3}$$

with $\Theta(x)$ the Heaviside function:

$$\Theta(x) = \begin{cases} 0 \text{ if } x < 0; \\ \frac{1}{2} \text{ if } x = 0; \\ 1 \text{ if } x > 0. \end{cases}$$

2.2 Detecting and Measuring Nestedness

In this section we briefly discuss three commonly used methods for quantifying nestedness in graphs. These measures are BINMATNEST (based on the NTC), NODF, and FCM.

Binary matrix nestedness temperature calculator (BINMATNEST)
NTC performs insufficiently if the number of holes in a graph is high. Therefore, BINMATNEST uses a genetic algorithm that reorders rows and columns so that the packing of the matrix increases. The matrix temperature T is a measure of how equally the edges are distributed across the matrix. If all edges are in the upper left corner the temperature is minimal ($T \to 0$). If all edges are equally distributed in the matrix the temperature is maximal ($T \to 100$). The normalized temperature of the adjacency matrix is given by the following expression [6]:

$$\mu_{BIN} = \frac{100 - T}{100} \tag{4}$$

If $\mu_{BIN} = 1$ (0) the matrix temperature will be minimal $T = 0$ (resp. maximal $T = 100$).

Nestedness metric based on overlap and decreasing filling (NODF)
NODF was developed for bipartite networks of ecological systems [1] but it is applicable to square matrices, too. This method is independent of row and column order since it computes the paired nested degree for each pair of both columns and rows. However, in contrast to BINMATNEST this method does not reshuffle the matrix. For the whole matrix the sum of nestedness degrees of all paired rows and columns is the total nestedness normalized by the number of all pairs. The NODF metric assigns a value M_{ij}^{H} to each neighboring pair of vertices ij:

$$M_{ij}^{H} = \begin{cases} 0, & \text{if } k_i = k_j \\ \frac{n_{ij}}{min(k_i,k_j)}, & \text{otherwise} \end{cases} \tag{5}$$

The total number of common edges among the two vertices i and j is given by n_{ij}. The procedure is carried out for rows (M_{ij}^{P}) and columns (M_{ij}^{A}) analogously. Finally, the total nestedness for square matrices is then given by [12]:

$$\mu_{NODF} = \frac{\sum_{i<j}^{P} M_{ij} + \sum_{i<j}^{A} M_{ij}}{\frac{2 \cdot n(n-1)}{n}} \tag{6}$$

An advantage of NODF is its independence of matrix shape because it goes through both rows and columns [12]. However, this method fails in detecting nestedness for nested graphs of low and high density because it cancels out all terms for vertices of same degree.

Fitness-Complexity Metric (FCM)
FCM ranks vertices in an iterative and non-linear process [14]. The iteration process couples a fitness term to a complexity term. Since FCM was solely developed for bipartite networks, we will not use it as a benchmark in this contribution.

2.3 Benchmark Graphs

We require a solid benchmarking framework for comparing robustness and reliability among different nestedness detection methods. A benchmark graph needs to differ in its network characteristics (i.e. degree distribution, graph density, vertex centrality, etc.) but keep a certain level of nestedness. The authors of [8, 9] propose a coherent formation process for generating nested graphs with a single exogenous parameter α that influences the topology of the generated graphs fundamentally. This network formation process has two contrasting dynamics, edge creation and severance. First, the edge creating dynamics allows each vertex to create an edge to the most central vertex in its second-order neighborhood (i.e. the neighbors of its own neighbors) with a probability α. Second, each vertex may severe the edge to the least central neighbor in its first-order neighborhood with the complementary probability $1-\alpha$. By changing α we can tune a nested graph between two limiting cases. On the one hand, we obtain a star topology for $\alpha \to 0$ and, on the other hand, we obtain a

fully-connected graph for $\alpha \to 1$. A first-order phase transition exists at the critical value $\alpha = 1/2$ [8].

The degree partition for the independent set of the nested graph is given by the following definition [9]:

Definition 2.6. For $0 < \alpha \leq 1/2$ and $n \to \infty$ the asymptotic expected proportion of vertices n_k in the independent set with degrees $k = 0, 1, ..., k^*$ if given by

$$n_k = \frac{1-2\alpha}{1-\alpha} \left(\frac{\alpha}{1-\alpha} \right)^k \tag{7}$$

where

$$k^*(n, \alpha) = \frac{\ln\left(\frac{(1-2\alpha)n}{2(1-\alpha)}\right)}{\ln\left(\frac{1-\alpha}{\alpha}\right)} \tag{8}$$

In this contribution we utilize this network topology to create benchmark graphs. In addition, it is possible to weaken the perfectly nested topology by an incremental increase of random rewiring of edges. This process works as follows. First, for a randomly chosen vertex we determine all of its next neighbors. Second, a connection to a randomly chosen neighbor is cut and the focal vertex is connected to another vertex to which it previously was not connected to. If a vertex is isolated or is connected to all nodes in the network, nothing happens. The total number of rewired edges e_{new} is given by the parameter ρ_{rew}. These two quantities are linked in the following way: $e_{new} = \rho_{rew} \cdot n$. The higher ρ_{rew} the more edges get randomly rewired. This process can be seen as a simplification of other rewiring mechanisms in nested networks [3].

3 Algorithm

In this section we briefly review the algorithm NESTLON as a method for detecting a nested component in graphs and its constituents [7]. The simple main concept behind the algorithm is to follow the definition of nestedness closely. NESTLON judges whether the neighborhood of a vertex includes the neighborhood of lower degree vertices in an iterative manner. A vertex belongs to the nested component if it respects the local definition of nestedness to an acceptable degree.

The method iterates through the connected component of a graph starting with the highest degree vertex and, therefore, is applicable on both bipartite and non-bipartite graphs. The procedure is analogous for either in-degree or out-degree (for simplicity we refer to the term degree in the following). We use the algorithm on a graph that is sorted by degree centrality. The algorithm performs the following steps subsequently:

Algorithm: *Nestedness detection based on Local Neighborhood* (NESTLON)

Conventions:

n	Number of vertices in the graph.
k_i	Degree of vertex i.
$\mathcal{N}_i^{(1)}$	First-order neighborhood of vertex i.
$\mathcal{N}_i^{(1^+)}$	Extended first-order neighborhood of vertex i $\left(\mathcal{N}_i^{(1)} \cup \{i\}\right)$.
ζ_i	Number of positive confirmations that the neighborhood of vertex i includes the neighborhoods of its first-order neighbors.
Λ	List of candidates (i.e. vertices that might belong to nested component).
$\lvert\cdot\rvert$	Number of elements in a set.

Input:

$\mathbf{A}$	Adjacency matrix of the graph object.
θ_{con}	Confirmation parameter of neighborhood similarity-
θ_{nest}	Parameter for counting focal vertex to nested component.

Output:

V_{nest}	Elements of nested component (i.e. vertices that belong to nested component).

Algorithm NESTLON

$V_{nest} \leftarrow \{\}$
$\Lambda \leftarrow \{i^*\}; i^*/k_{i^*} = max(k_i)$
while $\Lambda \neq 0$ **do**
  for $i \in \Lambda$ **do**
    $\zeta_i \leftarrow 0$
    for $j \in \mathcal{N}_i^{(1)}$ **do**
      if $\frac{\left|\mathcal{N}_j^{(1^+)} \cap \mathcal{N}_i^{(1^+)}\right|}{\min\left(\left|\mathcal{N}_j^{(1^+)}\right|, \left|\mathcal{N}_i^{(1^+)}\right|\right)} > \theta_{con}$ **then**
        $\zeta_i \leftarrow \zeta_i + 1$
        $\Lambda \leftarrow \Lambda \cup \{j\}$
      end if
    end for
    if $\frac{\zeta_i}{\left|\mathcal{N}_i^{(2)}\right|} > \theta_{nest}$ **then**
      $V_{nest} \leftarrow V_{nest} \cup \{i\}$
    end if
  end for
end while

The outcome of the algorithm is a set of vertices that belong to the nested component V_{nest}. Dividing the number of nested vertices by the highest degree of the graph is then a measure of the size of the component:

$$\mu_{NEST} = \frac{|V_{nest}|}{max(k_i)} \text{ , with } i \in N \tag{9}$$

This method has several important features. It is independent on the adjacency matrix shape and size. In contrast to NODF it calculates nestedness for rows and columns independently. Compared to NODF and BINMATNEST it can detect nested graphs irrespective of their density. We will investigate the robustness of the algorithm in the next section.

4 Robustness Analysis

A robust algorithm can detect the nested component independently of degree distribution, graph density, matrix shape and matrix size. Such a robust algorithm should identify all vertices that fulfill the criterion of nested neighborhoods (i.e. a higher degree vertex includes the neighborhood of a lower degree vertex). Therefore, we can evaluate an algorithm's robustness on such a benchmark graphs, in which all vertices belong to a single nested component. We create these graphs with the network formation process, which we already discussed in section "The Notion of Nestedness".

4.1 Calibration of NESTLON

Before we compare the values of robustness among the algorithms we need to calibrate the two exogenous parameters of the NESTLON algorithm (i.e. θ_{con} and θ_{nest}). The parameter θ_{con} is the confirmation threshold of neighborhood similarity and the parameter θ_{nest} is the threshold for counting a focal vertex to the nested component.

Calibration of NESTLON: Variation of θ_{con} and θ_{nest}

In fig. 4.1 we show the values of Nestedness for the NESTLON algorithm under variation of both parameters θ_{con} and θ_{nest}. The number of vertices the algorithm counts as nested does not differ for $\theta_{con} < 1$ but decreases for $\theta_{nest} \geq 0.5$. Because we deal with a perfectly nested graph (i.e. benchmark graph with $\alpha = 0.49$, $\rho_{rew} = 0$) both parameters shall be set so that NESTLON measures full nestedness (i.e. $\mu_{NEST} \overset{!}{=} 1$). Thus, we choose $\theta_{con} < 1$ and $\theta_{nest} < 0.5$ as reasonable for detecting nestedness.

Calibration of NESTLON: Adding Noise

In fig. 2 we show the NESTLON's ability in detecting the nested component on a benchmark graph with added noise (i.e. random rewiring of edges). In absence of rewiring (i.e. $\rho_{rew} = 0$) the algorithm includes all vertices as members of the nested component. For increasing random rewiring (i.e. $\rho_{rew} > 0$) the algorithm counts fewer vertices as part of the the nested component. This behavior is expected because the graph looses its nested structure with an increasing number of edge rewiring.

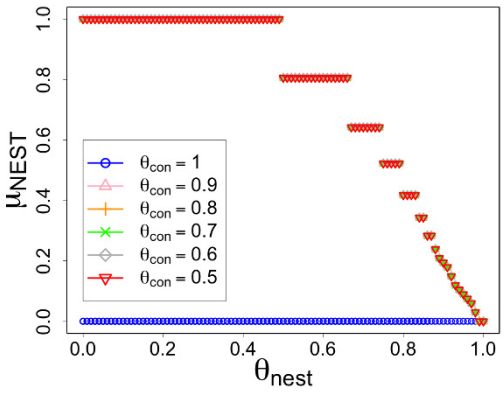

Fig. 1: Values of Nestedness for the NESTLON algorithm under variation of both exogenous parameters θ_{con} and θ_{nest}. We perform the computation on a benchmark graph of size $n = 500$ and $\alpha = 0.49$. Thus, all vertices belong to a single nested component. As we can see in the figure the thresholds are too rigid for $\theta_{con} = 1$ and $\theta_{nest} \geq 0.5$. Therefore, we choose $\theta_{con} < 1$ and $\theta_{nest} < 0.5$ as reasonable detection thresholds.

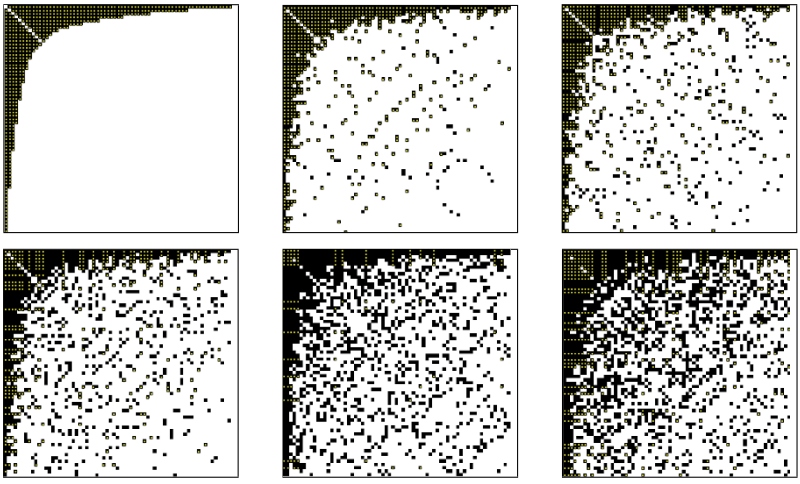

Fig. 2: Adjacency matrices of the benchmark graphs with additional noise: $\rho_{rew} = 0.0$ (top left), $\rho_{rew} = 1.0$ (top center), $\rho_{rew} = 2.0$ (top right), $\rho_{rew} = 3.0$ (bottom left), $\rho_{rew} = 5.0$ (bottom center), $\rho_{rew} = 7.0$ (bottom right). The vertices that are counted towards to the nested component by *NESTLON* are indicated by a yellow dot.

Robustness Analysis: Filling Matrix

In fig. 3 we show the values of robustness measured among the three methods BINMATNEST, NODF and NESTLON on the benchmark graphs. By increasing α the matrix filling (i.e. network density γ_d) will increase, too. The benchmark graphs are nested by definition for every value of $\alpha \in [0, 1]$.

Although every benchmark graph is perfectly nested, BINMATNEST misses to detect all vertices as belonging to the nested component beyond the phase transition (i.e. $\alpha > 1/2$). For a fully connected network its genetic algorithm can not establish a

better packing by reordering rows and columns. NODF fails in detecting nestedness for graphs with low (i.e. $\alpha < 1/2$) and high density (i.e. $\alpha > 1/2$). Because this method cancels out all rows and columns of same degree it has a strong bias towards low nestedness for both low and high density graphs. However, NESTLON indicates an entirely nested network for every graph density (i.e. $\mu_{NEST} = 1$ for every value of $\alpha \in [0,1]$).

Robustness Analysis: Adding Noise

In fig. 4 we compare the measured values of robustness among the three algorithms for increasing random rewiring ρ_{rew}. In absence of rewiring (i.e. $\rho_{rew} = 0$) the graph is still perfectly nested and, thus, we expect nestedness close to $\mu = 1$. For increasing rewiring (i.e. $\rho_{rew} > 0$) we expect that the nestedness decreases because the density of holes increases. BINMATNEST and NESTLON count all vertices to the nested component for $\rho_{rew} = 0$, whereas NODF recognizes only less than half of the vertices. By increasing noise NESTLON is significantly more parsimonious than the two other methods in judging vertices as nested. NODF has even a minimum at $\rho_{rew} \approx 4.5$. Beyond this minimum NODF detects a larger fraction of nested vertices although the graph increasingly converges to a random graph.

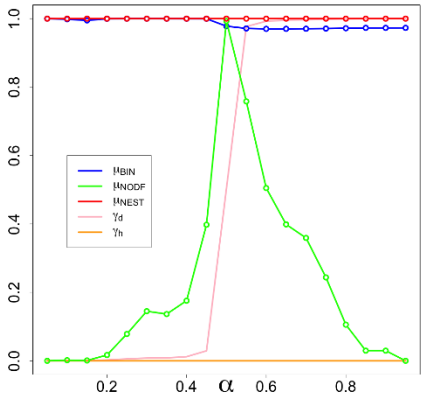

Fig. 3: Robustness in detecting the nested component among BINMATNEST, NODF and NESTLON on a benchmark graph. By definition all realizations of the benchmark graph are nested for all values of α. We perform the computation on a graph of size $n = 200$. The graph density (i.e. γ_d) increases with α, whereas the density of holes (i.e. γ_h) stays zero.

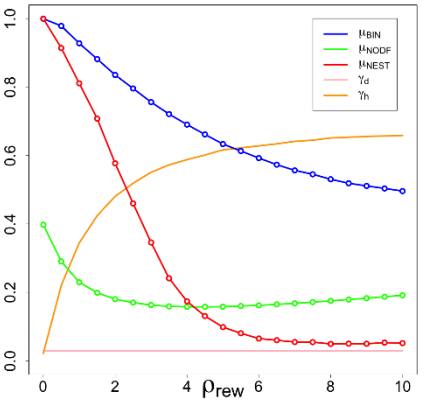

Fig. 4: Robustness in detecting the nested component among BINMATNEST, NODF and NESTLON on a benchmark graph with added noise. With increasing random rewiring ρ_{rew} the nested structure of the benchmark graph dissolves (i.e. increasing density of holes γ_h). We perform the computation on a graph of size $n = 200$ and with $\alpha = 0.45$ (i.e. $\gamma_d \approx 0.029$).

Conclusion

In this contribution we reviewed the novel method termed NESTLON for detecting a nested component in graphs. As shown, widely-used algorithms such as BINMATNEST and NODF compute unreasonable low values of nestedness on benchmark graphs with either low density (i.e. $\gamma_d < \frac{1}{2}$), NODF, or high density (i.e. $\gamma_d > \frac{1}{2}$), NODF and BINMATNEST. The method NESTLON overcomes these limitations and is applicable on both bipartite and non-bipartite graphs. The algorithm is purely based on the mathematical definition of nestedness and utilizes, thus, only local information. For the robustness analysis we created benchmark graphs with a network formation process. This network formation process allows us to tune the degree of nestedness in a controlled manner. In future work, we want to extend NESTLON to graphs with more than a single nested component.

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