Nested mess: thermodynamics disentangles conflicting notions of nestedness in ecological networks

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Many real networks feature the property of nestedness, i.e. the neighbours of nodes with a few connections are hierarchically nested within the neighbours of nodes with more connections. Despite the abstract simplicity of this notion, different mathematical definitions of nestedness have been proposed, sometimes giving contrasting results. Moreover, there is an ongoing debate on the statistical significance of nestedness, since even random networks where the number of connections (degree) of each node is fixed to its empirical value are typically as nested as real-world ones. Here we propose a clarification that exploits the recent finding that random networks where the degrees are enforced as hard constraints (microcanonical ensembles) are thermodynamically different from random networks where the degrees are enforced as soft constraints (canonical ensembles). We show that if the real network is perfectly nested, then the two ensembles are trivially equivalent and the observed nestedness, independently of its definition, is indeed an unavoidable consequence of the empirical degrees. On the other hand, if the real network is not perfectly nested, then the two ensembles are not equivalent and alternative definitions of nestedness can be even positively correlated in the canonical ensemble and negatively correlated in the microcanonical one. This result disentangles distinct notions of nestedness captured by different metrics and highlights the importance of making a principled choice between hard and soft constraints in null models of ecological networks.

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I. INTRODUCTION

Network theory provides a simplified representation of a variety of complex systems, i.e. systems composed by many elements whose mutual interactions create new and emergent behaviours. The network description, despite its simplification, allows to detect and measure collective patterns, independently of the nature of the underlying interactions [1–3].

Amongst the quantities analysed in network theory, nestedness [4] is one of the most elusive. It was originally observed in biogeography [5–7] where less frequently observed species are assumed to occupy a niche of the habitats occupied by more ubiquitous species. In terms of the resulting ecological network, nestedness is loosely defined as the observation that the neighbours of nodes with a few connections (lower degree) are typically a subset of the neighbours of nodes with more connections (higher degree). Generalized as such, nestedness has been detected in other networks as well, e.g. in trade networks [8–10], interbank networks [9, 11], social-media information networks [12], and mutualistic ecological networks [4, 13]. In Bascompte et al. [13], nestedness has been found to be highly correlated with the stability of the ecosystem under different types of disturbances and perturbations. The ubiquity and structural importance of nestedness naturally raises some fundamental questions regarding the possible mechanism generating nested patterns in real networks. Actually, while the intuitive notion of nestedness is straightforward, its mathematical definition is not trivial and different metrics, focusing on different aspects, have been proposed. One of the most popular metrics is NODF (Nestedness measure based on Overlap and Decreasing Fill, [14]), which considers the (normalised) overlap between pairs of nodes in the same layer of a bipartite network. Such a definition was later adjusted in order to increase its robustness [4, 15]. An alternative definition has been proposed by looking at certain spectral properties of the adjacency matrix of a bipartite network. Since it can be shown that, when the degree sequence is constrained on one of the two layers of the network, the spectral radius is maximum for the perfectly nested network [16], in [17] the spectral radius itself was proposed as a measure of nestedness (in the following SNES, i.e. Spectral NEStedness).

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Other researchers looked even closer at the effect of the degree sequence. Ref. [18] compared the metric introduced in Ref. [15] with a null model preserving the degree sequence (and valid only in the sparse regime) and found that in most of the cases the degree sequence is responsible for the the high value of the nestedness. The recent contribution of Ref. [19] came to similar conclusions, using an improved null model still preserving the degree sequence, but valid for any level of density of the network.

In the present paper, we shed more light on the intimate meaning of the various nestedness measures and on the role of the degree sequence. In order to tackle the problem, we use two different network null models, both enforcing the degree sequence. On the one hand, we define an ensemble of graphs in which all elements have exactly the same degree sequence [20], following a prescription similar to the microcanonical ensemble in statistical mechanics. On the other hand, continuing with the analogy, we follow a canonical approach, in which we define an ensemble of graphs in which all elements have fixed degree sequence on average over the ensemble [3, 21]. First, we observe that for both null models, a perfectly nested network (PNN) is singular, i.e. both the microcanonical and the canonical ensembles include just a single network with the given degree sequence, i.e. the PNN itself. Thus, the realized nestedness is an unavoidable consequence of the degree sequence itself and it is impossible to draw conclusions about the statistical significance of the nested pattern. Next, we examine the statistical significance of the different nestedness definition as measured on a set of mutualistic biological bipartite networks, according to the various null-models. Indeed, we observe substantial discrepancies in the two cases, essentially due to the presence of non-zero variances in the canonical approach: such contributions introduce an overestimation on all superlinear quantities that appear in the NODF and SNES definitions. Furthermore, focusing on the canonical approach, one may conclude that NODF and SNES correlate, but a different picture appears once we focus on the results obtained via the comparison with the microcanonical approach.

In this latter case, we observe that actually the SNES and the NODF are anticorrelated, an effect that is screened by the fluctuations of the degree sequence in the canonical ensemble. More in details, the SNES tends to prefer assortative networks, i.e. those in which highly connected nodes are connected with highly connected ones; on the other hand, the NODF rewards nodes in which poorly connected nodes are connected with highly connected ones. Finally, we can safely state, by looking at the table in Fig. 3 that in most of the cases, even in the microcanonical approach, beside the chosen measure, the degree sequence is mostly responsible of the nestedness of the system. Indeed, 12 on 40 real ecological mutualistic networks, the NODF is statistically significant ($z \geq 2$), while for the SNES this ratio reduces to $4 \over 40$. Actually, the SNES seems to be more tied with the degree sequence.

Given these results, we cannot state which measure should be used, since it depends on the features that could be relevant for the description of the system. Nevertheless, the degree sequence should be analysed carefully in order to understand if it is nested per se, thus being responsible of the nested nature of the system. Moreover, the choice of the proper null-model is not trivial too: in the case in which the data are completely safe, i.e. there are not any possible issue about the reliability of the data, the microcanonical approach should be considered. Instead, if the data are likely to include some uncontrolled noise, a canonical approach has to be preferred, even if it may introduce a bias in the analyses.

II. METHODS

A bipartite network is a graph where the set of vertices can be divided in two parts, so that all the edge connect one element of the first subset with one element of the second subset. In practice a bipartite network is defined by two sets of nodes $L$ (of size $N_L$) and $\Gamma$ (of size $N_\Gamma$) called layers and by the prescription that connections are allowed only between the layers and not inside them. Thus, a bipartite network can be univocally described by its biadjacency matrix $M$, i.e. an $(N_L \times N_\Gamma)$-matrix, whose entries $m_{i\alpha} = 1$ if a link exists between $i \in N_L$ and $\alpha \in \Gamma$ and $m_{i\alpha} = 0$ otherwise. In the following we shall use the previous definitions for generic biadjacency matrices and related quantities, but we shall add an asterisk $\ast$ whenever considering quantities measured on real networks.

A. Nestedness measures

1. NODF

One of the most popular measure of nestedness, namely the Nestedness as a measure of Overlap and Decreasing Fill (NODF) was introduced in 2008 by Almeida-Neto et al. [14]. Such measure is based on the overlap between the neighborhoods of nodes with different degrees. Given a generic bipartite graph
with given $n$ nodes and $L$ links is a perfectly nested network [22];

- Among all bipartite networks with a given degree sequence on one of the two layers, the one that maximises the spectral radius is the perfectly nested one [16].

4. Normalised spectral nestedness

The spectral radius, though, has a strong dependence on the size of the network and on its density. It is well known that the maximum eigenvalue of a bipartite network with $L$ links is bounded from above by $\sqrt{L}$ and that the only network for which $\lambda(M) = \sqrt{L(M)}$ (if it exists) is a complete bipartite network [16, 22].

For this reason we decide to introduce $nSNES$ where we normalize the measure with the square root of the number of edges and we have

$$nSNES(M) = \frac{SNES(M)}{\sqrt{L(M)}} = \frac{\lambda(M)}{\sqrt{L(M)}}.$$  \hspace{1cm} (3)

Although the $nSNES$ ranges from 0 to 1, the drawback of this normalization is that a perfectly nested matrix that is not full will not have a perfect score of 1.

B. Null-models

In the present paper, we aim at understanding the role of the degree sequence in the formation of bipartite nested structures. In order to measure the amount of nestedness which is not due to the node degrees, we would need a sort of network benchmark with the same degree sequence, but otherwise maximally random. This approach has strong similarities with Statistical Mechanics: actually, the recipe is to build an ensemble and fix the node degrees on it. As in the standard Statistical Mechanics, those constraints can be imposed on average, as in the canonical construction [3, 21, 23–25], or considering stricter constraints, as in the microcanonical formulation [20, 26]. The two approaches are known to be non equivalent [27–33] and indeed such non equivalence is going to be crucial in the following.

1. The canonical approach: the Bipartite Configuration Model

The Bipartite Configuration Model (BtCM, [34]) is the bipartite extension of the entropy based null-model [3, 21, 23–25]. The strategy is inspired by work by Jaynes [35], which derived the canonical ensemble of Statistical Mechanics from Information
Theory principles. The recipe is pretty simple: first, define an ensemble of all possible physical configurations, and then maximise its Shannon entropy constraining the relevant information about the system (in this case, the energy): the result is exactly the canonical ensemble. The maximisation of the Shannon entropy represents the crucial step: it can be interpreted as assuming maximal ignorance about the the non constrained degrees of freedom of the system.

Following the same strategy, starting from a real network, we can define $\mathcal{M}$ the ensemble of all possible biadjacency matrices with the same number of nodes (nodes represent the volume in Statistical Mechanics). The Shannon entropy associated to the ensemble is

$$S = -\sum_{\mathcal{M} \in \mathcal{M}} P(\mathcal{M}) \ln P(\mathcal{M})$$

and maximise it, constraining the degree sequence $\{k_i\}$.

The entropy maximisation leads to an exponential likelihood-maximisation equations:

The numerical value is determined by solving the constraint degree sequence $\{k_i\}$.

Their numerical value is determined by solving the Lagrange multipliers $\{\lambda_i\}$ associated Lagrangian multipliers $\{\lambda_i\}$.

Interestingly enough, constraints linear in the adjacency matrix (as the degree sequence) allow us to factorize the probability $P(\mathcal{M})$ as the product of probability per possible link:

$$P(\mathcal{M}) = \prod_{i,\alpha} p_{i\alpha}^{m_{i\alpha}} (1 - p_{i\alpha})^{1 - m_{i\alpha}},$$

where $p_{i\alpha}$ is the probability of existence of the link connecting nodes $i$ and $\alpha$.

In the case of the BiCM, $p_{i\alpha}$ is a function of $x_i$ and $y_\alpha$, which are simple reparametrisations of the Lagrange multipliers associated to the observed degrees ($k_i$ and $h_\alpha$ respectively):

$$p_{i\alpha} = \frac{x_i y_\alpha}{1 + x_i y_\alpha},$$

Their numerical value is determined by solving the likelihood-maximisation equations:

$$\begin{align*}
\langle k_i \rangle &= \sum_\alpha p_{i\alpha} = k_i^*, \quad i = 1 \ldots N_L, \\
\langle h_\alpha \rangle &= \sum_i p_{i\alpha} = h_\alpha^*, \quad \alpha = 1 \ldots N_\Gamma,
\end{align*}$$

$k_i$ and $h_\alpha$ being the degree of the node $i$ and $\alpha$ respectively.

2. The microcanonical approach: the Curveball algorithm

The microcanonical approach, differently from the BiCM, keeps the degrees of all nodes in the system constant. In a sense, it has a stricter ensemble (just all configurations with the given degree sequence are allowed) and all allowed configurations have the same probability. Such approach is computationally costly since the probabilities of links in the system are not pairwise independent and the fastest way of spanning the ensemble of networks with a given degree sequence relies on swapping endpoints of links iteratively. In the present manuscript, the ensemble was sampled using the strategy of [20]; the algorithm works as follows:

1. Select at random a couple of nodes on the same layer (for making the example clearer let us consider, in full generality, $i, j \in N_L$);

2. Check that the neighborhoods of the nodes are not perfectly overlapping: if so, start again.

3. Take the set of uncommon neighbors $U(i, j) = \{\alpha \in N_\Gamma | (m_{i\alpha} = 0 \& \& k_\alpha = 1) \| (m_{i\alpha} = 1 \& \& m_{j\alpha} = 0)\}$ and remove them from the neighborhood of both;

4. Assign $k_i - \sum_\alpha m_{i\alpha} m_{j\alpha}$ new neighbors to node $i$, chosen at random from $U(i, j)$ and the rest of the nodes in $U(i, j)$ to node $j$.

We will refer to these model and algorithm as Curveball, as in the original paper [20]; in [26] it was shown that such approach is ergodic.

III. RESULTS

In this section we are going to present the results of our analyses on artificial and real networks. To test the measures and models, we analyze a set of 40 pollination networks taken from the Web of Life database [42]. They represent ecological mutualistic networks of plant-pollinators. In the following, we compare the various measures and state their significance respect to the various null-models.

A. Measure differences

First, in order to study the behaviours of the previous measures, we compare them on the above-mentioned dataset. The Fig. 1 shows that indeed the normalised SNES is highly correlated with NODF.
FIG. 1: NODF vs SNES (top) and vs nSNES (bottom) for the 40 networks of the Bascompte dataset. Spearman correlation coefficients are, respectively, -0.23 and 0.96.

(actually, it is not true for the non normalised version of the spectral nestedness, due to its dependence on the total number of link). In a sense we may think that indeed, while they differ in the philosophy, the two measures are capturing the same structure. After a detailed comparison with the appropriate null-models, we will see that it is not the case.

B. Degree sequence vs. nestedness

The degree sequence of the network carries some information about the nestedness of the system, the extreme case being the Perfectly Nested Network (PNN in the following) one. Actually, in this case, the degree sequence identifies completely the network and both the micro- and the canonical ensembles are composed by a single network, i.e. the PNN one. Let us show the PNN issue in more details.

Let us start from the microcanonical ensemble. First, consider the case in which $k_i = k_j$: due to PNN nature, $U(i,j) = \emptyset$ and the algorithm stops at the step 2. Then, consider the case $k_i > k_j$: $U(i,j)$ contains only the connections that $i$ has and $j$ has not (due to the perfect nestedness of the network, all connections of $j$ are connections of $i$ too). Then, at step 4, the number of new neighbours of $j$ is $k_j - \sum_m m_i \alpha m_j \alpha = 0$, while the same quantity is exactly $|U(i,j)|$ for $i$, thus the algorithm is stuck in the present configuration.

In the canonical ensemble the situation is a little more involved. Let us consider, as an example, the biadjacency matrix in Fig. 2 representing a PNN; the presented arguments can be generalised to any PNN. Due to the ordering we imposed on the biadjacency, if rows and columns represent respectively the $L$ and the $\Gamma$ layers, we have:

$$\langle k_1 \rangle = \sum_{\alpha} p_{1\alpha} = k_1^* = N_\Gamma;$$

$$\langle h_1 \rangle = \sum_{i} p_i 1 = h_1^* = N_L,$$

which can be satisfied if and only if $p_{1\alpha} = 1$, $\forall \alpha \in \Gamma$ and $p_{i1} = 1$, $\forall i \in L$. Thus all entries involving the fully connected nodes are deterministic. Such a conclusion has implications, on the opposite side of the biadjacency matrix:

$$\langle k_{N_L} \rangle = \sum_{\alpha>1} p_{N_L\alpha} + 1 = k_{N_L}^* = N_\Gamma - 1;$$

$$\langle h_{N_L} \rangle = \sum_{i>1} p_{iN_L} + 1 = h_{N_L}^* = N_L,$$

which, in turns, implies $p_{N_L\alpha} = 0$, $\forall \alpha > 1 \in \Gamma$ and $p_{iN_L} = 0$, $\forall i > 1 \in L$, i.e. the entries of nodes with only a single connection are deterministic too. Then let us pass to consider again the first nodes:

$$\langle k_2 \rangle = 1 + \sum_{\alpha>1} p_{2\alpha} + 0 = k_2^* = N_\Gamma - 1;$$

$$\langle h_2 \rangle = \langle h_3 \rangle = 1 + \sum_{i>1} p_{i2} + 0$$

$$= 1 + \sum_{i>1} p_{i3} + 0$$

$$= h_2^* = h_3^* = N_L - 1.$$
FIG. 2: An example of a perfectly nested network with its probabilities per link from the BiCM: at the first step, the first row and column are full, and the degree is respectively 12 and 8. So the link probabilities must be exactly one, for preserving the row sum and the column sum. At the second step, since the last row and column have degree 1, the remaining entries must sum to 0, yielding all zeros. At the end of this process, the link probabilities are all set to 0 or 1, so the corresponding canonical ensemble contains only one matrix.

(in the second line we use the fact that columns 2 and 3 have the same degree, thus their Lagrangian multipliers are equal and so $p_{2i} = p_{3i}, \forall i \in L$). Let us first focus on equation (9): we have $N_{\Gamma} - 2$ unknown probabilities, summing to $N_{\Gamma} - 2$. Thus $p_{2\alpha} = 1$ for $1 < \alpha < N_{\Gamma}$. Analogous considerations are valid for all $p_{2\alpha}$ and $p_{3\alpha}$ and thus these entries are again deterministic. Iteratively discounting the information obtained at the previous steps, it is possible to show that the canonical ensemble of a PNN is composed by a single graph, or, more correctly, the probability for every representative in the ensemble is 0 but for the PNN itself (which, instead has $P(PNN) = 1$).

Thus, for both the micro- and the canonical ensembles, the degree sequence of a PNN defines a singular ensemble and thus the degree sequence captures the level of nestedness of the whole system. Actually, even when the network is close to a perfectly nested one, its configuration model ensembles contain all networks that are highly nested. Thus, a real network may show a high value of the nestedness measure (whatever it is), which is, nevertheless, statistically non significant respect to a null-model discounting the degree sequence: actually in such a case the high value of the nestedness is already captured by the degree sequence. We will examine in more details the role of the null-model in the following sections.

C. Measure and models differences

1. Null-model differences: micro- vs. canonical ensemble

In Fig. 3 we compare the z-scores relative to the different measures and null-models introduced in the Sec. II.

The averages of the measures are systematically different when using a microcanonical model or a canonical one, since, in the latter case, the variance in the degrees of the nodes generates a bias in all quantities that scales superlinearly (or sublinearly) in the number of links. Such behaviour can be explained following Jensen’s inequality [36, 37]. Let $L = \sum_{\alpha} m_{\alpha}$ be the total number of links in a bipartite network: for any convex function $\phi$ we have

$$\langle \phi(L) \rangle \geq \phi(\langle L \rangle),$$

with the strict inequality holding if the function is
FIG. 3: Measures and z-scores of each of the networks in the Web of Life pollination dataset. The microcanonical z-scores of the nSNES are omitted because they are identical to the SNES ones. The color scales have been normalized linearly in the respective measures' domains for the measures, while for the z-scores there is a unique color scale, blue for the negative and red for the positive scores. The SNES measure does not have a color scale since they are not comparable given the different sizes.

strictly convex, while if the function is concave (in the case of sublinear dependence) the opposite inequality holds. So we have:

\[ \langle L^x \rangle > \langle L \rangle^x \text{ if } x > 1 \lor x < 0, \]  
\[ \langle L^x \rangle < \langle L \rangle^x \text{ if } 0 < x < 1. \]  

Actually the situation is a little subtler for \( x < 0 \), since in the canonical ensemble even the configuration with \( L = 0 \) has a non zero probability, thus \( \langle L^x \rangle = \infty \). We will take care of possible issues related to negative exponents in the following.
FIG. 4: Micro- vs canonical measures for all 40 Web of Life pollination datasets: the error bars represent the standard deviations of the respective ensemble.

a. NODF vs. null-models The displacement of the NODF measures between the two ensembles can be explained by the overestimation of the total number of V-motifs by the BiCM. As mentioned in the previous section, both ensembles contain only one configuration in the case of a perfectly nested degree sequence and their measures are trivially exactly the same. When the two ensembles separate for a non-perfectly nested matrix, the canonical ensemble produces some variance in the degrees of the nodes, which generates the effect of (12). This effect is not present in the microcanonical ensemble, where the degrees of all nodes are fixed deterministically. The average number of V-motifs \[ N^*_V \] scales quadratically in \[ L \] and is therefore actually overestimated in the canonical ensemble. Indeed, the number of observed V-motifs is

\[
N^*_V = \frac{1}{2} \sum_{\alpha} \left( h^*_\alpha - h^*_\alpha \right) = \frac{1}{2} \sum_{\alpha} \left( h^*_\alpha - h^*_\alpha \right)^2 (14)
\]

and thus we have

\[
\langle N_V \rangle - N^*_V = \sum_{\alpha} \left( \langle h^2_\alpha \rangle - \langle h^*_\alpha \rangle \right) - \left( \langle h^*_\alpha \rangle^2 - \langle h^*_\alpha \rangle \right) \\
= \sum_{\alpha} \left( \langle h^2_\alpha \rangle - \langle h^*_\alpha \rangle^2 \right) \\
= \sum_{\alpha} \frac{\sigma^2_\alpha}{2} = \frac{\sigma^2}{2} \geq 0, (15)
\]

and the average total number of V-motifs is systematically overestimated in the canonical ensemble. Such an effect has an impact on the NODF: while in the formula the total number of V-motifs does not appear explicitly, it contributes nevertheless. Moreover, the extra factor at the denominator of each contribution, i.e. the minimum degree of two nodes, is underestimated by the canonical model, since

\[
\langle \min\{k_i, k_j\} \rangle \leq \min\{k^*_i, k^*_j\}, (16)
\]

(where we use that in the BiCM \( \langle k_i \rangle = k^*_i \)) and thus it contributes to the overestimation of the NODF.

In a sense, calculating the average NODF of the ensemble simply replacing the quantities in (1) with their averages introduces a bias in the calculation and takes to incorrect conclusions. On the other hand, there is not a closed form for the expected NODF in the microcanonical approach either: indeed, while the denominator does not represent an issue (since it is fixed), the numerator is. Actually the probability of observing the V-motif \( V_{ij}^\alpha \) cannot be replaced by the probabilities of observing both links forming the motif, since in this model the probabilities of the two links composing the motif are not independent.
b. SNES vs. null-models We observe that the spectral radius is slightly overestimated in the canonical model. Some first evidences say that on average, out of two matrices with the same number of links, the one with the smallest number of nodes has the largest radius, so when a sample of the canonical model has an empty row or column it has, on average, a higher radius. Still, we are not able to evaluate such discrepancy. Regarding the normalized SNES, instead, the quantity is depending sublinearly on \( L \), due to the normalization by \( \sqrt{L} \). For the Jensen’s inequality in (12), the measures on the canonical sample are all overestimated, causing this upper shift. As mentioned above, in principle \( \langle L^{−\frac{1}{2}} \rangle = \infty \), since \( P(L = 0) > 0 \), but since the numerator is exactly equal to zero when \( L = 0 \), there is no singularity for an empty graph.

c. The significance of the nestedness measures with respect to the different statistical ensembles Bearing in mind all of the considerations of the previous paragraphs, we can interpret the z-scores of the table in Fig. 3. The two NODF columns of the table refer to the z-score of the two variants of NODF with respect to the canonical ensemble; they contain all negative high z-scores, because of the overestimation of the two measures in the ensemble. There are, though, important differences between the NODF and sNODF measures in some cases. This is mainly due to the presence of many nodes with the same degree, and with degree 1, in particular. For instance, dataset 21 has 500 columns of degree 1 out of 677 total columns and thus the two measures are very distant on the real network (its NODF score is 0.07, while the sNODF is 0.12), but the averages over the ensemble are closer (0.08 vs. 0.11). Such feature is common to many networks, given their power law distribution of the degrees. Then we have the columns of SNES: even in this case, the canonical null-model has all negative z-scores, due to the slight overestimation of the SNES. The normalized SNES column also contains all negative z-scores due to its sublinear dependence on \( L \), as discussed before. The second-last column contains the microcanonical SNES z-scores.

As it can be observed from the matrix, there is no agreement between the column of the SNES [43] and the sNODF columns in the microcanonical ensemble. A hint is given by the assortativity z-scores, whose Pearson correlation coefficient with the SNES scores is 0.84, while SNES and NODF anti-correlate with a score of -0.88.

In order to investigate this difference, we generate a scatter plot of the realizations of the different ensembles (Fig. 5), plotting the NODF against the SNES of the sampled networks. The results are striking: the two measures are highly anti-correlated on the microcanonical ensemble, while this effect is hindered by the overestimates in the canonical ensemble.

Using the other proposed measures, the results are always similar when comparing a NODF measure and a spectral nestedness measure. NODF and SNES are actually capturing different ways of be-
order to discount the information carried by the degree sequence only. Therefore, we can define null models that maximise NODF and SNES are made (Fig. 6).

Actually the NODF-maximising matrix has one of the smallest value of assortativity, while the one that maximises the SNES presents a big hub of the highest degree nodes and two smaller disconnected subgraphs, see Fig. 6. Roughly speaking, on the one hand, the SNES prefers networks in which highly connected nodes link to highly connected nodes, since they are sort of carrying the “mass” of the adjacency matrix (which is what the spectral radius is measuring). On the other hand the NODF, due to the denominator of its contributions, prefers to link poorly connected nodes with highly connected ones, thus focusing on disassortative configurations. Regarding the anti-correlation between the NODF (or similar definition) and the assortativity, other studies got similar conclusions [18, 39]: as far as we know, there were no evidences regarding the opposite behaviour of the SNES.

IV. DISCUSSION

While the abstract idea of nestedness in networks is quite straightforward, its mathematical definition is less trivial. As a consequence, while nested structures are ubiquitously observed across several networks, measuring the actual level of nestedness along with its statistical significance remains a challenging task.

In the present manuscript we have investigated in details different metrics of nestedness in both real-world and synthetic networks. In particular, we mainly focused on two measures, NODF [14] and SNES [17], and some of their modifications [4]. When applied to real networks, these metrics go in the same direction, as they give positively correlated results.

We then moved to discount the contribution of the degree sequence to the different nestedness measures. Literally, according to the case of study and to the available information on our system we can create suitably chosen series of randomized copies of our graph (ensembles). This procedure allows us to use the machinery of Statistical Physics to assess the significance of our measurements.

Thus, for our aim, we can define null models preserving the degrees of nodes either as hard (microcanonical ensembles [20]) or as soft (canonical ensembles [3, 21]) constraints. Otherwise stated, we are using the extensions of the microcanonical and canonical ensembles to complex networks in order to discount the information carried by the node degree: the degree sequence is known to have an effect they have on the nestedness [18, 19], thus we want to focus on the information carried by the different metrics that cannot be explained by the degree sequence only.

First, we concentrated our attention on Perfectly Nested Networks (PNN). A PNN has a degree sequence that admits only a single network, i.e. the PNN itself, irrespective of whether the degrees are treated as hard or soft constraints: both the microcanonical and canonical ensembles of a PNN are composed by the PNN network only. Otherwise stated, there exist perfectly nested degree sequences and each of them defines univocally a single network, i.e. the PNN one. In the case of PNNs, thus, the value of the nestedness is completely due to the degree sequence only. But what happens when the network is not perfectly nested?

We compared the value of NODF and SNES measured on real networks with the expectations of, respectively, the microcanonical and canonical ensembles. As theoretically predicted in other studies [27–33], the two ensembles are not equivalent, thus they should be characterized by different macroscopic properties. Literally, we found that the two families of definitions (NODF and SNES') are negatively correlated when the microcanonical ensemble is used, while they are positively correlated in the canonical ensemble. Actually, the fluctuations of the canonical ensemble cover the real behaviours of the NODF and SNES. Instead, once the degree sequence is fixed as a hard constraint, the level of nestedness is influenced by higher-order correlations between the degrees themselves, and in particular the assortativity of the network. In fact, the two classes of measures of nestedness give different results in the microcanonical ensemble, when considering networks with different assortativity: NODF tends to give larger values of nestedness when the network is disassortative, while SNES tends to give larger values of nestedness when the network is assortative.

These results illustrate that statistical ensembles disentangle certain conflicting notions of nestedness. An important implication is that one should make a principled choice of the ensemble used as a null model in the analysis [32, 33]. The microcanonical ensemble, which treats degrees as hard constraints, should be preferred if one is sure that the observed degrees are error-free, i.e. if they are the actual values of the property to be kept fixed in the null hypothesis. If one suspects that the observed degrees are instead subject to some sort of error (e.g. measurement errors, incomplete data collection, poor sampling, etc.), then the microcanonical
ensemble should be avoided, as it would give zero probability to the true (undistorted) configuration and to any configuration with the same degree sequence as the true configuration. Therefore, if the observed degrees are possibly ‘noisy’, one should prefer the canonical ensemble, which treats degrees as soft constraints and can access the true configuration with nonzero probability (as desirable, this probability is higher for lower levels of ‘noise’, i.e. for a lower distortion in the values of the degrees).

Beside the choice of the null-model, there are still two main problems. The first one is natural, at the end of the this manuscript: which measure captures at best our idea of nestedness? As we saw, NODF rewards more low degree nodes connecting with high degree ones, the SNES favors the links among high degree nodes and both ideas are compatible with our basic intuition. Thus, the choice of the metric should be done in light of the phenomenon that one wants to capture.

The second issue is subtler, and probably more crucial: we saw that perfectly nested networks have a peculiar degree sequence, but how can we relate the degree sequence with the nestedness? In the present manuscript we saw that, given a non perfect nested degree sequence, the NODF and SNES preferred different regions of the phase space (and this allowed to distinguish the behaviour of each measure), but we were not able to univocally measure the amount of nestedness already contained in the degree sequence. Due to the evidences shown, it is a crucial issue in addressing the problem of measuring the nestedness of a system and it is going to be the subject for future work.

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[41] Note that while in the Jaynes derivation of the Statistical Mechanics, the constraints, i.e. the energy, was a global one, the degree sequence represent a local one. Actually, the local constraint is responsible for the nonequivalence of the microcanonical and canonical ensembles.
[42] www.web-of-life.es
For the microcanonical null-model, the z-scores of the nSNES were not reported since they correspond to the one of the SNES (the normalising factor can-