

REVIEW

Fluctuating ecological networks: A synthesis of maximum-entropy approaches for pattern detection and process inference

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Abstract

1. Ecological networks such as plant–pollinator systems and food webs vary in space and time. This variability includes fluctuations in global properties such as the total number and intensity of interactions in the network but also in the number and intensity of local (i.e. node level) species interactions.
2. Fluctuations of species' properties can significantly affect higher-order network features, for example, robustness and nestedness, and should therefore be taken into account in null models for pattern detection and hypothesis testing.
3. In ecological research, classical null models treat node-level properties as 'hard' constraints that cannot fluctuate. Here, we review and synthesize a set of maximum-entropy methods that allow for fluctuating ('soft') constraints, offering a new addition to the classical toolkit of the ecologist. We illustrate the methods with some practical examples, pointing to currently available open-source computer codes. We clarify how this approach can be used by experimental ecologists to detect non-random patterns with null models that not only rewire, but also redistribute interaction strengths by allowing fluctuations in the enforced constraints.
4. Explicit modelling of interspecific heterogeneity through local (i.e. species level) fluctuations of topological and quantitative constraints offers a statistically robust and expanded (e.g. including weighted links) set of tools to understand the assembly and resilience of ecological networks.

KEYWORDS

ecological networks, maximum entropy, network fluctuations, network pattern detection, network reconstruction, null models, soft constraints

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1 | INTRODUCTION

In recent years, there has been increasing recognition of the spatial and temporal variability of ecological networks, for example in terms of network rewiring (i.e. changes in who is connected to whom) caused by seasonality and perturbations (CaraDonna et al., 2017; Evans et al., 2013). At the same time, there are some network features that remain rather stable. For example, plant-animal mutualistic networks can be highly variable in terms of which species is connected to which other species (i.e. their topology) and yet maintain a clear core-periphery structure where a small number of generalist species (i.e. the core) interact with a large number of specialized species (i.e. the periphery; Miele et al., 2020).

The question of how ecological networks assemble and what controls their stability has been intensely investigated (Aizen et al., 2016; Allesina & Pascual, 2008; Evans et al., 2013; Fortuna et al., 2010; James et al., 2012; Säterberg et al., 2013; Valdovinos, 2019; Valverde et al., 2020), typically by comparing network models to observed networks. Network models are generally constructed from data that describe who is interacting with whom (adjacency matrix) and possibly the intensity of interactions, that is, link weights (interaction or weight matrix). The modelling usually starts from the observed interaction matrix and aims to synthetically summarize general, structural patterns such as nestedness or the abundance of specific subgraphs/motifs. Also, models are often used to simulate general structural changes such as those due to species extinctions. In all these cases, changes in network structure are very often assessed with null models (Evans et al., 2013; Pascual & Dunne, 2006; Valdovinos, 2019).

Tailored null models based on constrained permutations of the values observed in the data matrix have become central to hypothesis testing and pattern detection in ecological networks. One central goal is testing whether basic properties measurable at the node level (see Glossary) can explain higher-order properties such as nestedness (Bruno et al., 2020; Dormann et al., 2009; Dormann & Strauss, 2014; Payrató-Borrás et al., 2019; Strona et al., 2014). Ecological null models generally permute, randomize or sample the entries of network matrices by keeping the values of certain quantities, also known as *constraints*, fixed. Constraints can, for instance, be total sums over the entire matrix (e.g. total interaction strengths, or total number of links), or local sums along each row and/or column (e.g. the number of links of each node, known as the *degree*). The constraints can be measured on the empirical matrix and are generally enforced strictly, that is, treated as 'hard' constraints, in the construction of the null model. Hard constraints are appropriate if the properties they embody are expected not to fluctuate (or have negligibly small fluctuations). In addition, the randomization algorithms used to construct null models with hard constraints should not bias the estimate of the statistics used to describe the structure of the network (Bruno et al., 2020; Dormann et al., 2009; Dormann & Strauss, 2014; Payrató-Borrás et al., 2019; Strona et al., 2014).

Here, however, we illustrate a different approach that suits the much less explored and yet arguably very frequent case of

fluctuating constraints, that is the case when the constraints have values that vary around the measured ones. If constraints fluctuate, for example due to spatial and temporal variance in species ecology, the measured values used in the null models should be interpreted as a 'characteristic' but definitely not unique value for each node (species) in the network. Indeed, in many systems, the intrinsic variability of species-level activity, diet or behaviour implies that observed links are a particular snapshot of a larger set of possible realizations, which is very evident in time series of the same system (e.g. Miele et al., 2020). For example, two species can be linked in one snapshot of the network and not linked in another. Or, a species might have a certain number of connections in one snapshot and a different number in another snapshot. Also, experimental observations are necessarily collected with some measurement errors such as spurious associations and missing data. In all these cases, it is reasonable to assume that the constraints themselves fluctuate around a characteristic value. The models we propose allow implementing that assumption. This perspective, while poorly explored in ecology (but see references we review in the next sections), is actually well established in statistical mechanics and its applications to network modelling (Squartini & Garlaschelli, 2017). Indeed, over the last two decades, the so-called maximum-entropy ensembles of networks with fluctuating constraints have been developed theoretically in the general context of the statistical physics of complex networks (Cimini et al., 2019; Newman, 2018; Park & Newman, 2004), with applications mainly to large social, economic and financial networks. Some seminal applications to ecological networks have been recently proposed in the specific context of the property of nestedness (Bruno et al., 2020; Payrató-Borrás et al., 2019; Payrató-Borrás et al., 2020).

Here, we review and illustrate the existing theory to propose applications of the available models to ecological datasets for which the assumption of fluctuations in node-level properties is appropriate. We emphasize that the approach we review here has important practical consequences for empirical analyses. This review specifically focuses on the assumptions of the classical approach as well as of the approach we present here, for the benefit of the practicing ecologists. We make the point that models with different assumptions may produce very different results. The importance of the assumptions we discuss here for null models (specifically 'hard' vs. 'soft' constraints; see glossary) is generically analogous to the difference that exists between assuming uncorrelated errors and homogeneity of variance in standard linear models or, rather, explicitly model error correlation and heterogeneity of variance in mixed effect linear models (Zuur et al., 2009). For certain systems, treating null constraints as fixed ('hard') or fluctuating ('soft') makes little difference when constraints represent *global* quantities (e.g. total number of links) and the matrix is very large. This property is known as *ensemble equivalence* (Touchette, 2015). A number of recent works have, however, shown that ensemble equivalence does not hold when constraints are *local* (i.e. node specific or species specific), which is often the case of interest in modern applications dealing with networks with high levels of heterogeneity in local

properties (Garlaschelli et al., 2016; Squartini et al., 2015; Zhang & Garlaschelli, 2020). This heterogeneity typically coexists with, and is often responsible for, other forms of hierarchy and structure such as core–periphery structure, the presence of network communities or other types of modular organization. Why is network heterogeneity and the violation of *ensemble equivalence* important to the experimentalist? Recent analyses have shown that, when networks are heterogeneous, statistical analyses based on models with hard local constraints (e.g. row and/or column sums that are kept exactly fixed) produce results that can be even opposite to those obtained from models based on fluctuating constraints (Bruno et al., 2020). We stress that the fact that null models based on hard and soft constraints may lead to very different results does not mean that soft constraints are ‘correct’ and hard constraints are ‘wrong’. The difference in results simply reflects different assumptions. Therefore, the data analyst must make a principled choice on the nature of the constraints, taking into consideration the tested ecological hypotheses. In this review, we illustrate the relatively less known framework based on soft constraints and discuss how it can be applied and further expanded to offer additional tools that become necessary whenever the constraints are expected to fluctuate. The approach suits virtually all types of ecological datasets, from binary bipartite networks to weighted soil food webs. Moreover, it is also computationally efficient, a feature that is becoming increasingly important for molecular datasets such as those linking plants to their symbiont microbes. Also, the approach we propose can be fully applied not only to presence/absence network data, but also to networks with weighted links, which is a very important generalization filling a major gap in the current ecologist's toolkit. The possibility of generating null models for networks with weighted links is of major significance to systems such as food webs, where links typically have (very) heterogeneous intensities. Finally, we also propose various future research lines that we argue will help ecologists shed light on the processes that structure ecological networks with high variability over space and time.

2 | ENSEMBLES OF NETWORKS

2.1 | Formulation of null models

The approach we illustrate here interprets the observed network matrix as a typical, but not unique, state of the system, which is assumed to be intrinsically fluctuating. Accordingly, the network is best described by a large ensemble of possible states ‘fluctuating around’ the observed typical state (Figure 1). Each state is a particular matrix realization and is assigned a probability of occurrence. How to derive this probability? The first step is the choice of the constraints (Figure 1), which are structural network properties that are expected to be robust across possible alternative realizations of the state of the system. The constraints we consider here apply to local properties of nodes (e.g. number of links of each node) and not just to global network-wide properties (e.g. total number of links

in the network). Locality of constraints is vital because real-world networks are neither homogeneous (Caldarelli, 2007) nor symmetric upon arbitrary permutations of species (Miele et al., 2020). Some of the empirical signatures of heterogeneity include the intrinsically hierarchical structure of ecological networks, for example, the trophic hierarchy and allometric scaling of food webs (Garlaschelli et al., 2003), and the fact that most networks have broad distributions of the number of links per node (Bascompte, 2010).

In ecological null models, the most typical constraint is the number of neighbours (degree) of a species, to be enforced for each species separately. The resulting vector of the degrees of all species is also known as *degree sequence*. In the most popular implementation of this null model, the randomized matrices respect the degree sequence constraint exactly: if a species has, say, 10 partners in the observed matrix, it will retain exactly 10 partners in all randomized matrices. These constraints are therefore ‘hard’. After defining the hard constraints, traditional ecological null models generate an arbitrarily large set of random matrices computationally through a permutation rule or randomization algorithm (Camacho et al., 2007; Dormann et al., 2009; Gotelli, 2000). These techniques are also qualified as ‘rewiring algorithms’ as they are fundamentally based on repositioning quantities within the original matrix so that links and/or their weights are effectively rewired. Besides the fact that the randomization procedure must ensure that locally exact constraints (e.g. numbers of pollinator species associated with each plant species) are preserved in the randomly rewired matrices, there is another important criterion that the null model should respect: the generated set of random matrices must be an unbiased sample from the probability distribution implied by the model, which typically has a non-closed form. ‘Unbiased sample’ means that the sample should purely reflect the model hypotheses so that no other hidden or unjustified assumption is (either explicitly or implicitly) made in the generation of the sample, given the data. For instance, if the null hypothesis does not discriminate between two network realizations having different topology but the same values of the constraints (i.e. having the same sufficient statistics), then the two realizations are naturally assigned the same probability by the null model, and the algorithm implementing the model should rigorously ensure this equiprobability. Under hard local constraints, requiring an unbiased sampling of the set of matrices while ensuring computational efficiency becomes a challenging algorithmic and combinatorics problem for increasingly large networks (Squartini et al., 2015). Basically, one has to check whether the algorithms sample the ensemble in an unbiased way. Rewiring algorithms have in the past been used to generate such ensembles computationally, with applications that include analyses of food webs (Camacho et al., 2007; Stouffer et al., 2007). Approaches allowing for the randomization of other types of binary matrices (e.g. co-occurrence matrices) relevant to ecology have also been developed (Carstens, 2015; Strona et al., 2014, 2018; Ulrich & Gotelli, 2012). In relative terms, computational efficiency is ultimately not a major issue for many ecological networks, especially if binary, because networks encountered in ecology are typically much smaller in size with respect to other (e.g. social or financial)

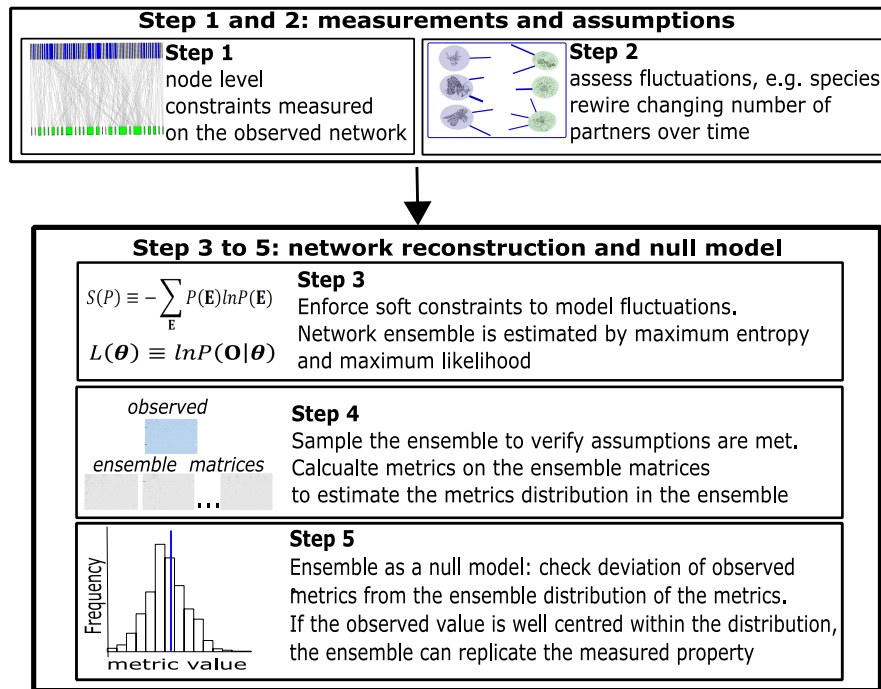


FIGURE 1 Overview of the construction of a statistical mechanics ensemble of a network, from the observed network (step 1) to the final ensemble (step 4) and null model analysis (step 5). Starting from the observed network, node-level properties such as the node degree (number of connections to the node) are enforced to construct the ensemble. The illustration is based on animal pollinators (light blue) and their plants (light green). The constraint is used to find the probability distribution $P(E)$ that maximizes the entropy S as per step 3. See also Table 1 for a summary of currently available models (and their acronym) that can be fit to ecological datasets, including weighted bipartite network and food webs. In the canonical ensemble, the constraint is 'soft' (step 2 and 3), meaning it is enforced only on average. In this case, the maximization of the log-likelihood function defined through $P(E)$ is used to find the $P(E)$ parameterization that also maximizes entropy given the constraint (step 3). In step 4, many matrices can be sampled from the ensemble to create a null distribution (step 5) for any network property. For example, metrics such as NODF (a measure of nestedness) can be computed for each of the n matrices sampled from the ensemble as well as for the single matrix of the observed network (blue vertical line). A z-score can then be calculated to quantify how metrics measured on the observed matrix deviates from the central tendency of the null distribution of that metrics.

networks for which algorithms have been developed. Issues related to biased estimates of statistics sampled from randomly rewired matrices may, nevertheless, arise for large and highly heterogeneous networks (Artzy-Randrup & Stone, 2005; Roberts & Coolen, 2012), with the exception of particular types of data structures and randomization algorithms (Carstens, 2015; Strona et al., 2014, 2018; Ulrich & Gotelli, 2012). In general, if untested for unbiasedness, local randomization algorithms carry a risk of not sampling the ensemble uniformly—the bias becoming unavoidable if the values of the local constraints are too heterogeneously distributed across the network (Roberts & Coolen, 2012). Solutions that correct the bias of local rewiring algorithms are computationally intensive and apply only to specific conditions (Roberts & Coolen, 2012). Moreover, the randomization models typically available to the ecologist apply only to network topology (binary data) and the underlying heuristics cannot be easily generalized to networks with weighted links or with a combination of purely topological and weighted constraints (Squartini & Garlaschelli, 2017).

On the other hand, as we discuss below and in the Supporting Information, soft constraints are mathematically and computationally easier to work with, and the corresponding ensembles can be constructed in a rigorously unbiased fashion. Before we enter these

details, the main point we address here is that a 'hard constraints' approach is appropriate as long as it is reasonable to assume that the constraints themselves do not fluctuate, or that their fluctuations are so small that they can be ignored. When this is not the case, ensembles with soft constraints have to be used. This distinction has major implications because soft and hard constraints are guaranteed to asymptotically (i.e. in the limit of a large number of nodes) return the same results only when the chosen constraints are global (e.g. the total number of links). For local constraints, such as the degree sequence (see Glossary), ensembles with soft constraints are not equivalent to ensembles with hard constraints (Squartini et al., 2015; Zhang & Garlaschelli, 2020): null model outcomes will be different because the model assumptions are different. This means that there are certain structural properties that display necessarily different expected values in the two types of ensembles (Touchette, 2015), a difference that may even lead to opposite statistical conclusions—as recently shown explicitly for the nestedness of plant–pollinator networks (Bruno et al., 2020). Choosing between soft and hard constraints is a fundamental modelling decision that will affect the final results of the analysis (Squartini & Garlaschelli, 2017). We thus emphasize that the most important question is not which constraints are 'computationally easier' or 'more mathematically appealing' but,

rather, what constraints should be used given the system and hypotheses under investigation.

2.2 | The statistical mechanics formulation of null models

The approach to the construction of the network null models we review here is based on statistical mechanics, which offers a general and unified treatment of ensembles built from both hard and soft constraints (Cimini et al., 2019; Park & Newman, 2004; Squartini & Garlaschelli, 2017). The basic quantity to construct a statistical mechanics ensemble is entropy, and the key procedure is entropy maximization. Entropy quantifies the uncertainty encoded in a probability distribution (see Glossary). The best known expressions of entropy are Shannon entropy and Renyi's generalization through the so-called Hill numbers. In ecology, these expressions have been applied to various statistical distributions, for example to measure community diversity in terms of the balance between species richness and evenness (Hill, 1973; Magurran, 2013). Relatedly, the maximum-entropy theory of ecology has been introduced to parsimoniously synthesize patterns such as relative species' abundances in ecological communities (Harte, 2011; Harte & Newman, 2014). In the context of networks and statistical mechanics, Shannon (or equivalently Gibbs) entropy is applied to the probability of observing a particular graph in an ensemble of possible ones. The graph probability distribution that maximizes the entropy under certain constraints reflects maximal ignorance of all network properties, except for those used to set the constraints themselves. In other words, the maximization of entropy corresponds to the construction of networks that are maximally random, apart from the imposed constraints.

In line with our discussion above, there are two fundamentally different ways in which constraints can be applied to derive a statistical mechanics ensemble. One way is the so-called *microcanonical ensemble* (see Glossary), which enforces the constraint exactly on

each randomly generated matrix. The microcanonical ensemble corresponds to the enforcement of hard constraints as used in classical ecological null models. For hard constraints, the maximum-entropy probability is uniform over the compatible configurations and the maximized entropy reduces to Boltzmann's definition of entropy, that is, it equals the logarithm of the number of allowed configurations. For example, if the constraint is the degree sequence as observed in a real-world network, then all the networks in the ensemble will have exactly the same degree sequence as the observed one. For binary networks, this model is known as the *microcanonical* (or 'hard') *configuration model*, and its entropy is the logarithm of the number of graphs with that particular degree sequence. Calculating this number remains a challenging combinatorial enumeration problem, not solved in closed form yet. The alternative way of enforcing the constraints in statistical physics is in the 'soft' way (Squartini & Garlaschelli, 2017), which leads to the so-called *canonical ensemble* (see Glossary). In the canonical ensemble, the constraint is respected by the ensemble only on average and the investigator is looking at a system that fluctuates around a set of 'typical' configurations, which are collectively the most likely. Again, when the constraint is the degree sequence, the corresponding model is known as the *canonical* (or 'soft') *configuration model*. Its entropy can be interpreted as the logarithm of the *effective* number of typical configurations. When ensemble equivalence does not hold, this entropy is significantly different from the entropy of the corresponding microcanonical ensemble (Squartini et al., 2015). For example, in the real network, plant A might have five known pollinators, that is, a degree equal to 5. Across the individual networks generated in the corresponding canonical ensemble, the same species A will have a fluctuating number of pollinators, for example, sometimes 3, sometimes 6 or any other integer number; however, the ensemble average of the degree of species A will be exactly 5. This will hold simultaneously for all nodes in the network so that the degree of each node will be on average exactly equal to the empirical degree for the same node. Unlike its corresponding microcanonical ensemble, this canonical ensemble can be exactly characterized mathematically, but

Network type	Soft constraints: Canonical ensemble	Hard constraints: Rewiring algorithms in ecological null models
Undirected		
Binary	UBCM [1]	e.g.: swap sequential algorithms, fixed margins
Weighted	UWCM, CReM [1] [2]	e.g.: swap sequential algorithms, fixed
Binary + weighted	UECM, CReM [1] [2]	only partially developed (e.g. swap and shuffle algorithms)
Directed		
Binary	DBCM, BiCM [1] [2] [3]	Implicit within algorithms for undirected matrices
Weighted	DWCM, CReM [1] [2]	Implicit within algorithms for undirected matrices
Binary + Weighted	DECM, CReM [1] [2]	Not developed

Note: [1] Squartini et al. (2015); [2] Parisi et al. (2020). [3] Saracco et al. (2015).

TABLE 1 Summary of existing canonical models that can be fitted to an ecological network matrix, using just the degree sequence (binary), the strength sequence (weighted) or both sequences as 'soft' constraints. The models are compared to counterparts with 'hard' constraints, in particular some illustrative (but not exhaustive) examples of the most popular rewiring algorithms used by ecologists

also easily sampled in an unbiased way (Squartini et al., 2015). In our example above, if the ensemble is sampled numerically and the expected degree of plant A is estimated as an arithmetic average over independently sampled matrices (i.e. using the realized frequencies), then that sample average will converge to 5 as the number of sampled matrices increases.

The most used constraints in the ecological literature, being local in nature, have been found to break the asymptotic ensemble equivalence (Squartini et al., 2015; Squartini & Garlaschelli, 2017). Specifically for plant–pollinator networks, this breakdown has been shown to imply opposite conclusions on the statistical significance of nestedness (Bruno et al., 2020). As we anticipated, this situation calls for a principled choice of the ensemble to be used in practical applications. In what follows, we will therefore offer an extended illustration of canonical ensembles as constructed in statistical physics from soft local constraints, thereby complementing the more established discussion of models with hard constraints that have become popular in ecology. Armed with this addition, the ecologist will be able to opt for the most appropriate (either hard or soft) set of models to use in statistical analyses, depending on the data and question at hand.

3 | CANONICAL ENSEMBLES FROM SOFT CONSTRAINTS TO MODEL ECOLOGICAL NETWORKS

3.1 | Matrix formalization

Let us call \mathbf{O} ('observed') the matrix that describes the observed network with S species or nodes. The ensemble we are looking for consists of a large number of matrices, each of them denoted by \mathbf{E}_m ('ensemble' matrices) and labelled by an integer number m . Each \mathbf{E}_m has the same size, that is, the same number S of nodes, as \mathbf{O} . Moreover, across the entire ensemble, we preserve the identity of all nodes by attaching a unique label i to each of them, that is, the corresponding networks or matrices are *labelled*. In general, the difference between each \mathbf{E}_m and \mathbf{O} is in terms of who is connected to whom and/or the strength of these connections. The set of all ensemble matrices contains all the possible states of the network. Among them, only one is exactly \mathbf{O} . What characterizes the ensemble is the probability $P(\mathbf{E})$ over the entire set of matrices, and we want this probability to depend on some set of structural properties of \mathbf{O} . In particular, we choose a set of constraining properties and enforce their values as empirically observed in \mathbf{O} . As we want each constraining property to apply locally to each species, our constraint has the form of a vector, that is, a vector having at least as many elements as the number of species in \mathbf{O} . We say 'at least' because we may want to have multiple constraints for each species, for example, the number of incoming links (in-degree) and separately the number of outgoing links (out-degree) for each node in a directed network such as a food web. We denote the vector of constraints by \mathbf{C} . We denote the value of property \mathbf{C} attained on a generic network \mathbf{E}_m

as $\mathbf{C}(\mathbf{E}_m)$, and so the empirical value of the constraint is denoted as $\mathbf{C}^* = \mathbf{C}(\mathbf{O})$, where the star means the special value of the constraining property as measured in the observed network \mathbf{O} . For example, if \mathbf{O} represents an undirected network and \mathbf{C} is the degree sequence, then \mathbf{C}^* will be the degree sequence of matrix \mathbf{O} , that is, the list of empirical degrees of all species, which would look something like $\mathbf{C}^* = [k_1, k_2, \dots, k_S]$, where k_i is the degree (number of interacting species) of each species i (for all $i = 1, S$).

3.2 | Entropy maximization

The main objective of statistical mechanics is finding the probability distribution $P(\mathbf{E})$ that fulfils the constraint by guarantying maximum randomness of all other properties. With this probability distribution, we can formulate a statistical expectation of all observable quantities. Mathematically, finding the distribution $P(\mathbf{E})$ that maximizes the randomness, given the constraints \mathbf{C}^* plus the unavoidable additional constraint that $P(\mathbf{E})$ has to be normalized, requires a quantitative definition of the randomness (i.e. uncertainty) encoded in $P(\mathbf{E})$ in the first place. The statistical mechanics definition is Shannon (or Gibbs) entropy, defined as

$$S(P) \equiv - \sum_{\mathbf{E}} P(\mathbf{E}) \ln P(\mathbf{E}),$$

which is familiar to ecologists as a diversity index. It is obvious from this equation that entropy would just count the number of allowed states if $P(\mathbf{E})$ were uniform. Maximizing $S(P)$ given the constraints conceptually corresponds to the requirement of unbiasedness: given the measured constraint, the ensemble must be maximally random. Technically, this maximization requires a choice on how specifically the matrices \mathbf{E}_m 'realize' the constraint \mathbf{C}^* measured on the observed matrix \mathbf{O} . The two main options are the aforementioned microcanonical (hard constraints) and canonical (soft constraints) ensembles. In the Supporting Information, we provide the analytical details of how to formalize and derive the microcanonical and canonical probabilities (part A) and how to estimate the model parameters (part B). More information can be found in the original references (Cimini et al., 2019; Park & Newman, 2004; Squartini & Garlaschelli, 2017).

Here, we want to highlight that under soft constraints the probability distribution that maximizes the entropy can be derived analytically and the corresponding parameters can be estimated from the dataset using the maximum likelihood approach. To visualize the difference between the 'soft constraints' approach and most existing rewiring methods, one could imagine the case in which a small tolerance (say, delta) is introduced around the hard constraints, that is, the hard constraints are preliminary perturbed by (at most) an amount delta, and for each such perturbation a microcanonical ensemble is generated. That approach would not be equivalent to the soft constraint approach of the canonical ensemble, for at least three reasons. First, the choice of any delta would be arbitrary. Second, the resulting perturbed constraints

will need to be realizable in some graphs, for example, they will have to respect the conditions set by the Erdős–Gallai theorem (Bollobás, 1998) for a sequence of natural numbers to be the degree sequence of a graph. Meeting these conditions is a non-trivial combinatorics problem (and, in our example, incompatible with an arbitrarily small, hence necessarily non-integer delta). And third (and most importantly), even if one could meet the Erdős–Gallai conditions, one should also specify the probability with which each perturbed constraint is selected within the delta interval, thus introducing another level of arbitrariness. By contrast, the canonical ensemble automatically specifies, without any arbitrary assumption, the appropriate probability of any configuration, for each amount of departure of the constraints from the corresponding observed value.

4 | EXPANDING THE ECOLOGIST'S TOOLKIT

4.1 | Applications

The form of the equations formalizing the construction of a canonical ensemble (Supporting Information A) is very general. For applications, specific forms of the equations must enforce the desired constraints. Those equations (Supporting Information) clarify that the randomized matrices of the ensemble will have to respect the constraints only on average ('soft'). Two specific examples of a model derivation are given in the Supporting Information (parts C and D), but there are many 'off the shelf' models that ecologists can already fit to their data. The currently developed models are based on the so-called exponential family of random graphs. This important family of graphs has been used to derive not only the ensemble corresponding to the usual constraints currently implemented by ecological null models, but also many others (Table 1). A novel point is that the available models apply not only to binary matrices (representing the mere topology of the network), but also to weighted matrices (which include information about link intensities). In weighted networks, each node is characterized not only by its degree, but also by its strength (total weight of all links attached to that node, see Glossary). Canonical models can thus be fit by imposing constraints on the degree sequence, the strength sequence, and also combined degree and strength sequences (Squartini et al., 2015; Squartini & Garlaschelli, 2017), thereby filling a major gap in the current ecologist's toolkit, which is mostly based on binary models or on debated quantitative models. Canonical models can be fit by maximum likelihood using either the entire observed matrix or just partial information available on the constraints (e.g. just the degree and/or strength sequence) as input. The existing models can easily be fit using publicly available and computationally efficient routines written in Python, MatLab and C (see <https://meh.imtlucca.it/> and the Python codes we made available at <https://doi.org/10.6084/m9.figshare.20531655.v1>, which were used to generate the network ensembles of Figures 2–4).

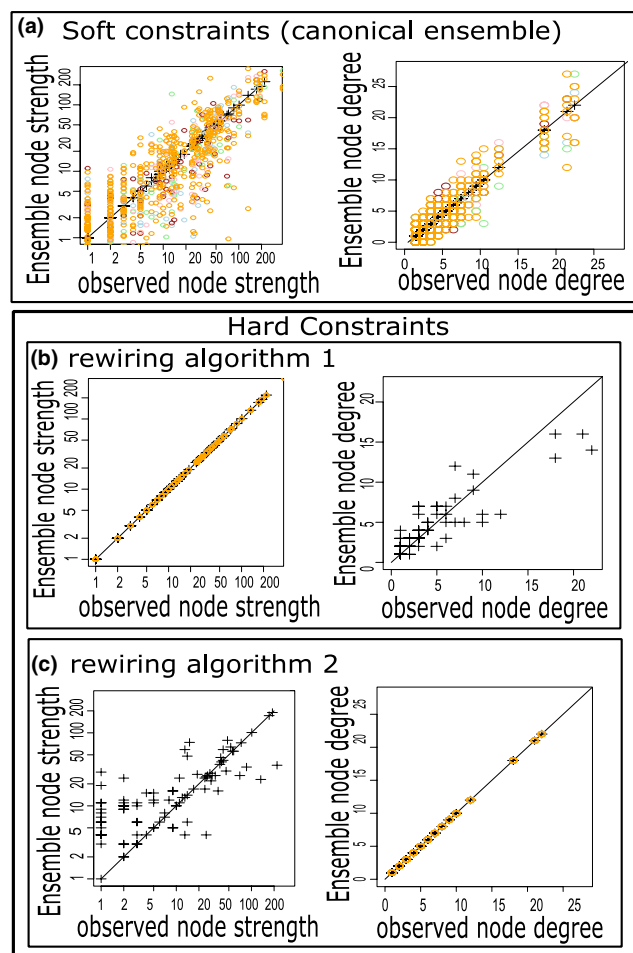
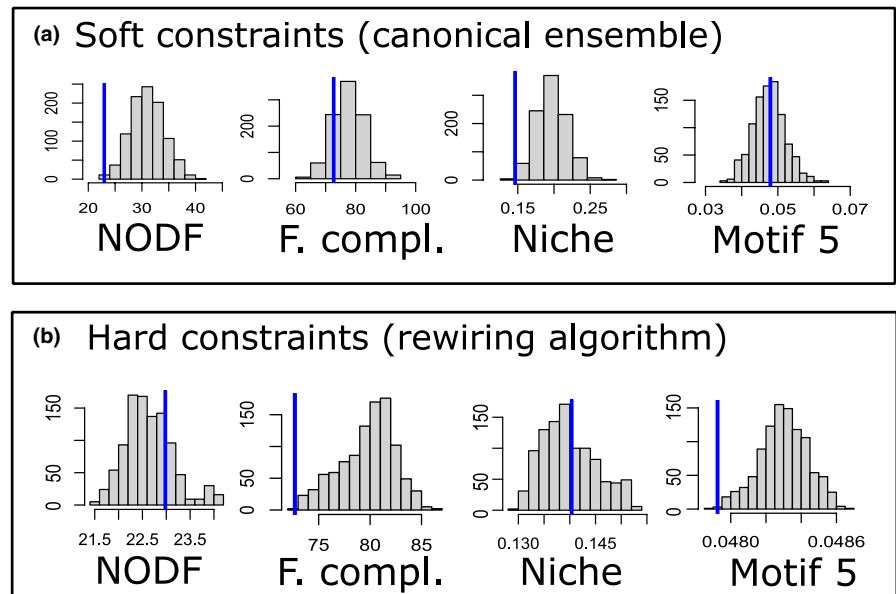


FIGURE 2 Node degrees and node strengths of the observed network are jointly used as constraints to derive the canonical ensemble of the network (panel a). If the ensemble is estimated correctly, by construction the theoretical expected value of both degree and strength sequences should be exactly equal to the observed value (computationally, this should happen for an average over a large number of sampled matrices). Here, the cross symbols correspond to an average over 999 matrices from the canonical ensemble of the 8th matrix of the general plant–pollinator dataset of (Miele et al., 2020), used here as an example. Those averages fall on the identity line, confirming that the ensemble respects the key assumptions. The coloured dots correspond to various randomly chosen sampled matrices, showing that the ensemble built from soft constraint is a set of networks whose properties (coloured dots) fluctuate around a mean, 'equilibrium' state (cross symbols) which inherits the observed node level-properties. In (b, c), the same representation of a) but, respectively, for an ensemble obtained either with the 'swap_count' algorithm (1) or with the 'abuswap_' algorithm (2) available in the nullmodel function of 'vegan' in R. These quantitative swap algorithms preserve either the strength or the degree sequence exactly but not both strength and degree sequence at the same time.

4.2 | Types of existing canonical or 'soft' models

The most important types of models of interest to ecologists can be categorized in directed and undirect binary models (degree sequence as constraint, other topological properties are randomized), directed

FIGURE 3 Four binary network metrics calculated for the (a) canonical ensemble of the binary version of the network of Figure 2, from Miele et al. (2020) and (b) the classical null model ensemble obtained with the 'swap algorithm' of 'nullmodel' in vegan, which preserves row and column margins and is traditionally considered a robust model to test for the pure effect of species composition. The most evident result is that the two ensembles return opposite output and we advocate for soft constraints if there is uncertainty on the experimental measurement of the constraints and/or if the constraint is known to fluctuate.



and undirected weighted models (strength sequence as constraint, other weighted and structural properties, including the degree sequence, are free to vary), and directed or undirected models where both degree sequence(s) and strength sequence(s) are constrained. Finally, the bipartite version of all these models, important for mutualist and host–parasite networks, can also be implemented by simple reparameterizations of the monopartite models. The possibility of implementing weighted null models is particularly important for weighted mutualistic network and food webs, where there typically is information on link weights. Also, the theory is flexible and general enough to generate new models and so test more specific ecological hypotheses.

5 | EXAMPLES

As an example, we applied bipartite models to a publicly available database of a plant–pollinator network (<https://orcid.org/0000-0002-3449-5748>), which has been recently proposed and analysed in the context of core–periphery models (Miele et al., 2020). This dataset consists of 6 years of data with three sampling time points each year, and the network links are weighted. This is useful to illustrate how both binary and weighted models can be fit. We provide the following application files at <https://doi.org/10.6084/m9.figshare.20531655.v1> (Caruso et al., 2022): two Python codes to fit a binary configuration model to a bipartite network and a weighted, bipartite configuration model to a quantitative bipartite network; two R codes used for downstream analysis. These codes, if applied to the data also provided in the repository, can altogether fully reproduce the results we present here from Figures 2–4. In the repository, we also provide guidelines documents that explain all the key steps of the Python codes. The guidelines also offer references for installing dependencies and testing them, which are also available at <https://pypi.org/project/bicm/> and <https://pypi.org/project/NEMtropy/>. Finally, in the repository, alongside the analysed data matrices, which are given in a format that can easily be imported in Python and R, we also provide the matrices

sampled from the ensemble models that we have used here to generate the examples of Figures 2–4. The user will just need to apply the R scripts provided at <https://doi.org/10.6084/m9.figshare.20531655.v1> to the data also provided there to generate Figures 2–4 of this article. See supporting information C and D for theoretical and analytical details on the binary and weighted bipartite models used in the examples here and underlying the codes available at <https://doi.org/10.6084/m9.figshare.20531655.v1>.

For the binary case, we used well-known R routines and packages to also compute a classic null model based on hard constraints using a very well-known swap algorithm, which keeps the row and column margins fixed and randomizes the matrix otherwise (Gotelli, 2000). This comparison allows us to look for possible differences in the statistical output of models with hard and soft constraints.

We also computed two null models using two swap algorithms for weighted matrices. These algorithms can be implemented with the well-known R function 'nullmodel' in the package VEGAN. Specifically, through 'commsim', we used the method 'swap_count', which can preserve node strength sequence but not degree sequence, and the method 'abuswap_r', which preserves the node degree sequence but not the strength sequence. See implementation of these functions in the R codes accessible at <https://doi.org/10.6084/m9.figshare.20531655.v1>.

Both for the canonical ensemble and the classic null models, we sampled 999 matrices, checked that the main assumptions on the constraints were fully met by the ensembles and calculated some network metrics to compare the values measured on the observed matrix with the corresponding distributions produced by the ensemble (Supporting information E). In the case of the canonical ensemble, as the constraint is soft, the ensemble respects the constraint only on average. Instead, the ensemble created with the swap algorithm consists of matrices that all respect the imposed constraint exactly. This confirms that in both hard and soft constraint cases, the model output is respecting the assumptions perfectly. What assumption is most correct for the data at hand is

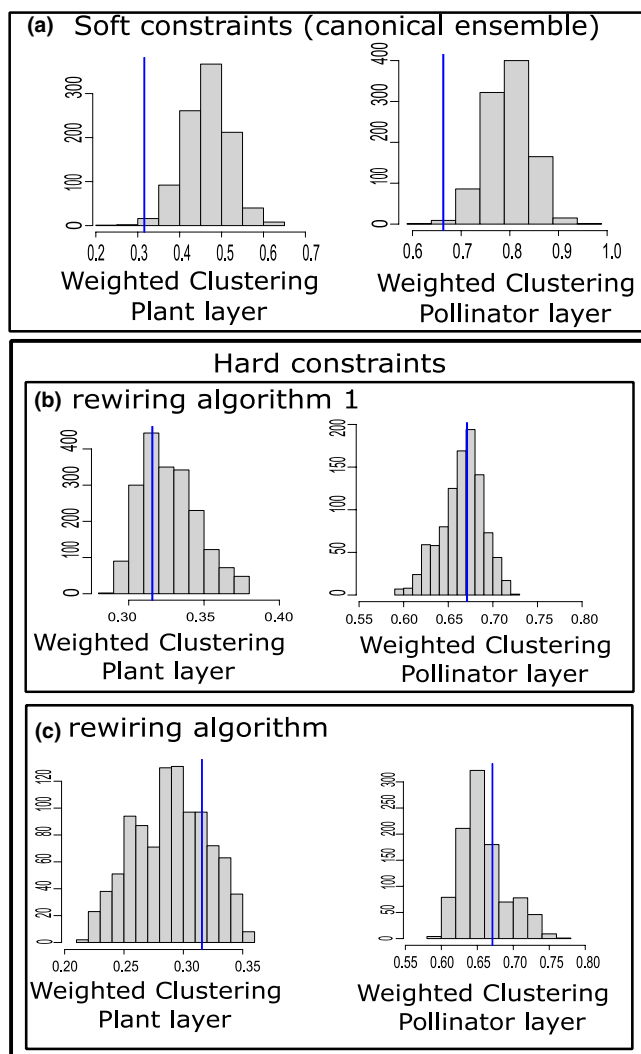


FIGURE 4 As [Figure 3](#), for the same network but with weighted links. In this case, we calculated the weighted version of the clustering coefficient for the two network layers (plants and pollinators). With soft constraints (canonical ensemble, panel a), the null model is rejected, meaning that combined strength and degree sequence alone cannot replicate the weighted clustering coefficient. The two tested quantitative swap algorithms are the same as in [Figure 2](#) and would lead to the opposite conclusion (null model retained), but we also know from [Figure 2](#) that these two ensembles are not reconstructing either the degree or weight sequence, which could bias the reconstruction of the clustering coefficient.

a very important but different question, which we discuss at the end of the paper.

For the weighted case, while the canonical ensemble can be chosen to preserve both the degree and strength sequences (soft constraints met on average, see data points labelled with cross in [Figure 2a](#)), the ensemble created with the swap algorithm can preserve either only the strength or only the degree sequence as hard constraints; see [Figure 2b,c](#). We are not aware of rewiring algorithms that are computationally efficient and that can, at the same time, preserve both degree and strength sequences while also been proved not to be biased when attempting a uniform sampling of the ensemble.

Once the ensembles are constructed, the ecologist can estimate metrics on the observed and randomized ensemble matrices, and then compare the observed metrics to the distribution of the randomized ones. Just as an example, for the binary model we chose NODF (a metric of nestedness), functional complementary, niche overlap and the so-called motif 5 as defined in Dormann and Strauss (2014) and Simmons et al. (2019), but we could have chosen many other properties. The choice of the metrics to analyse depends on the research question, and is therefore context specific. For our four metrics, we observed that the canonical ensemble provided an excellent estimate of functional complementary and the so-called motif 5 ([Figure 3a](#)). Instead niche overlap and NODF (a metric of nestedness) deviated significantly from the ensemble average. What is really important, however, is that opposite results were observed for the classic null model based on the swap algorithm ([Figure 3b](#)), which had functional complementary and motif-5 deviating from the null model to a very large extent, while NODF and niche overlap well replicated by the central tendency of the randomized matrices.

For the weighted case, we calculated the weighted version of the clustering coefficient ([Figure 4](#)). Again, we observed opposite results for the canonical ensemble ([Figure 4a](#)) and the two swap algorithms we implemented ([Figure 4b,c](#)): the observed clustering coefficients greatly diverged from the central tendency of the canonical ensemble distribution, which was not observed with both rewiring algorithms. Note that in this case there is an important additional difference between soft and hard constraint models. In the soft case, the model can respect both constraints (strengths and degrees) at the same time. Instead, at least for the algorithms we used here, the hard approach can satisfy only one of the two constraints at a time. This means that the two classes of models (soft and hard) are even less comparable than in the binary-only case.

6 | MODEL CHOICES, ECOLOGICAL IMPLICATIONS AND FUTURE DEVELOPMENTS

6.1 | Model assumptions

What model is to be chosen then? In fact, the actual question is what model assumptions to choose. Uncertainty in the measurement of node-level properties, which can be due to a combination of measurement error and natural spatial and temporal fluctuations, is a typical feature of ecological data. The soft constraint approach suits this uncertainty very well: the graph probabilities in the canonical ensemble are necessarily constructed from the 'noisy' observed values of the constraints, and maximal for the set of configurations displaying such values. But the configurations displaying the 'true' (unobserved) values of the constraints will also be assigned a comparably large probability. By contrast, in the microcanonical ensemble even a minimal error on the values of the constraints will bias the sampling enormously, and propagate the initial measurement error to the entire inference procedure. Moreover, even when constraints

are known to be error-free, an unbiased sampling of microcanonical ensembles via rewiring algorithms is achievable only after complex corrections, which are needed for heterogeneous networks (Artzy-Randrup & Stone, 2005; Roberts & Coolen, 2012).

6.2 | Going beyond the search for 'statistical significance'

The assumptions behind the choice of hard or soft constraints are crucial to hypothesis testing and connect to the concept of 'network reconstruction' from partial information. This concept moves the formulation of null models beyond the typical quest for the 'statistical significance' of a structural pattern (e.g. 'the observed network is significantly more or less nested than the set of random networks built under the constraints of some of the properties observed on the actual network'). When observed properties (e.g. metrics of nestedness) fully fall within the distribution expected under the null model ensemble, then the null model can replicate higher-order properties of the observed network (e.g. clustering coefficient, nestedness) just from the lower-level properties (e.g. degree sequence) used as constraints. In other words, the constraints used to build the null model are sufficient to reconstruct some high-level properties of the network (e.g. nestedness, clustering). There is thus a link between null-model formulation and network reconstruction, which primarily aims at reconstructing unobserved or even unobservable network properties using some of its observable features. As shown by our examples and by other examples in ecology (Bruno et al., 2020; Payrató-Borràs et al., 2019; Payrató-Borràs et al., 2020) and other disciplines (Cimini et al., 2019; Squartini & Garlaschelli, 2017), careful choices of the constraints can lead to canonical ensembles replicating many other network properties. If we interpret the canonical ensemble as a possible reconstruction of the network, the processes that control the shape of the constraints could also control the probability distribution of the network configuration. When that is the case, there are major implications for applications. For example, a perturbation affecting how the network is structured may eventually push the network away from the typical configuration observed before the perturbation. That type of structural shift can be detected with tailored null models and even used as an early-warning signal of disruption (Squartini et al., 2013). How? if the reconstruction is initially successful at predicting non-constrained properties and it then becomes unsuccessful from a certain point in time onwards, the comparison between the empirical, evolving network and the canonical null model can reveal and quantify the magnitude of the ongoing departure of the system from its typical state. This has been shown empirically on datasets that described the global financial crises of 2008 (Squartini et al., 2013). But how good should a reconstruction be for this type of applications? We note that the properties chosen as constraints can be enforced one at a time or all at the same time, making the ensemble more or less tightly dependent on the original network. The more meaningful constraints are added, the more the ensemble should be able to replicate higher-level properties. Meaningful constraints are those chosen among the general structural properties that

are directly controlled by the assembly processes that structure the network. What these properties and processes are in practice will depend on the network under investigation and will often be a matter of experimental research. We, nevertheless, expect that the general approach provided here will help ecologists formulate and enforce new sets of constraints based on hypotheses on the processes that structure ecological systems (e.g. phylogenetic correlation between nodes caused by co-evolution). The properties will be enforced as constraints one at a time or at the same time in different combinations, which will help ecologists reveal the relative roles of the factors that contribute to the formation, fluctuations and maintenance of networks in nature.

Glossary

Entropy: a fundamental concept in thermodynamics, probability theory, statistical physics and information theory, for which many definitions exist. In statistical physics, the definition of entropy quantifies the amount of uncertainty encoded in a probability distribution representing the possible microscopic states of the system. Looking for the probability distribution that maximizes the entropy, subject to certain constraints (see definition in this Glossary), is a key step in the formulation of null models of networks that are maximally random, apart from a set of properties that are enforced (i.e. the constraints).

Canonical network ensemble: a maximum-entropy ensemble in which the constraints (see definition in this Glossary) are respected only as average values. Such constraints are called 'soft'. This means that individual realizations of the system (e.g. network matrices) sampled from the ensemble will in general not meet the constraints exactly. However, as a result of entropy maximization under the enforced constraints, some configurations are much more probable than others and the probability distribution is centred around the 'typical' ensemble configurations that do meet the constraints. The ensemble average of the constraints exactly equals the enforced values. The resulting (maximized) entropy equals Gibbs's, or equivalently Shannon's, definition and can be interpreted as the logarithm of the effective number of typical configurations. The ensemble can be conceptualized as a set of networks 'fluctuating around' the typical configurations formalized through the constraints, that is, around the microcanonical configurations (*cf* microcanonical ensemble definition in this Glossary).

Constraints: a set of properties that a (null) model must obey. In the context of entropy maximization, the constraints are used to find the maximally random probability distribution while keeping certain properties fixed. The first and unavoidable constraint is the normalization condition guaranteeing that the result of the maximization is indeed a probability distribution. The additional constraints represent properties that one wants to enforce, for example, structural network features that one would like to be identical to those empirically observed in a real network, while leaving maximum randomness in all the other properties of the network. This is the basis for separating random and non-random patterns in network structure. Global constraints are network-wide properties, such as the total number of links in the matrix. Local constraints, instead, are defined

at the node level, such as the number of links to a specific node or the entire degree sequence (see definition in this Glossary).

Degree and degree sequence: in a network, the degree of a node is the number of links reaching that node. The degree sequence is a vector that, node by node, lists the degrees of all nodes, where the position in the list corresponds to the label of the node. As an example, the degree sequence {1,10,7,...} (of length S) indicates that nodes 1, 2 and 3 (out of the S nodes in the network) have degree 1, 10 and 7, respectively. If the network is directed, two distinct ('out-' and 'in-') degrees per node can be defined, as the number of outgoing and incoming links, respectively. Correspondingly, the out-degree sequence and the in-degree sequence can be defined as two separate vectors.

Microcanonical network ensemble: a maximum-entropy ensemble in which the constraints are respected exactly by each individual realization of the system (e.g. by each allowed state of the network). As a result, the constraints are called 'hard'. The maximum-entropy probability distribution of the microcanonical ensemble is uniform over all configurations that realize the hard constraints. The resulting (maximized) entropy coincides with the classic definition by Boltzmann: it equals the logarithm of the number of allowed configurations. It is generally very hard to calculate this number. For example, if the constraint is the degree sequence (see definition in this Glossary) and if the value of such constraint is set equal to the value of the degree sequence observed in a real food web, then each of the networks sampled from the microcanonical ensemble will have exactly the same degree sequence of the observed one. As a comparison, the randomization schemes usually implemented by ecologists also use 'hard' constraints, in the sense that the randomized matrices respect these constraints exactly. However, not all algorithms with hard constraints (especially in the case of weighted and/or local constraints) are guaranteed to actually sample the correct maximum-entropy (uniform) distribution, and one should be aware of the risk of bias.

Strength and strength sequence: in a network with weighted links, such as a food web where the links can be expressed in units of energy or C fluxes, the strength of a node is the sum of all the weights of the links connected to that node. If the network is directed, two separate ('out-' and 'in-') node strengths can be defined for each node. Similar to the degree sequence (see definition in this Glossary), the strength sequence is a vector that lists, node by node, the strength of that node. For directed weighted networks, the out-strength sequence and the in-strength sequence can be defined as two separate vectors.

AUTHOR CONTRIBUTIONS

Tancredi Caruso and Diego Garlaschelli developed the concept of the paper, analysed the data and equally contributed to writing. Giulio Virginio Clemente developed the Python scripts and contributed significantly to network analysis. Matthias C. Rillig critically reviewed the concepts and results of the work, and substantially contributed to writing.

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CONFLICT OF INTEREST

The authors declare no conflict of interest.

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DATA AVAILABILITY STATEMENT

Computer Codes, Application guidelines and data available at <https://doi.org/10.6084/m9.figshare.20531655.v1>.

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SUPPORTING INFORMATION

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