

# What constrains food webs? A maximum entropy framework for predicting their structure with minimal biases

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**Abstract:** Food webs are complex ecological networks whose structure is both ecologically and statistically constrained, with many network properties being correlated with each other. Despite the recognition of these invariable relationships in food webs, the use of the principle of maximum entropy (MaxEnt) in network ecology is still rare. This is surprising considering that MaxEnt is a renowned and rigorous statistical tool precisely designed for understanding and predicting many different types of constrained systems. Precisely, this principle asserts that the least-biased probability distribution of a system's property, constrained by prior knowledge about that system, is the one with maximum information entropy. MaxEnt has been proven useful in many ecological modelling problems, but its application in food webs and other ecological networks is limited. Here we show how MaxEnt can be used to derive many food-web properties both analytically and heuristically. First, we show how the joint degree distribution (the joint probability distribution of the numbers of prey and predators for each species in the network) can be derived analytically using the number of species and the number of interactions in food webs. Second, we present a heuristic and flexible approach of finding a network's adjacency matrix (the network's representation in matrix format) based on simulated annealing and SVD entropy. We built two heuristic models using the connectance and the joint degree sequence as statistical constraints, respectively. We compared both models' predictions against corresponding null and neutral models commonly used in network ecology using open access data of terrestrial and aquatic food webs sampled globally ( $N = 257$ ). We found that the heuristic model constrained by the joint degree sequence was a good predictor of many measures of food-web structure, especially the nestedness and motifs distribution. Specifically, our results suggest that the structure of terrestrial and aquatic food webs is mainly driven by their joint degree distribution.

**Keywords:**  
ecological modelling  
ecological networks  
food webs  
maximum entropy  
null models

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## Introduction

**1.1. The constrained structure of ecological networks** A variety of measures of the structure of ecological networks have been used to describe the organization of species interac-

tions in a biological community (Delmas et al. 2019). These measures provide valuable information on the functioning of ecosystems and their responses to environmental change (e.g., Pascual and Dunne 2006; Gómez, Perfectti, and Jordano 2011). For instance, Bascompte et al. (2003) suggest that plant–pollinator and seed-disperser networks have a highly nested structure that can promote species persistence. Another example, in food webs, shows that a high connectance can promote the robustness of the system to species lost (Dunne, Williams, and Martinez 2002). However, despite the growing literature on the ecological implications of network structure, the association between many of these measures impedes our ability to fully understand what drives the structure and behavior of ecological networks. In particular, nestedness and modularity are strongly associated in ecological networks (Fortuna et al. 2010), and network connectance has been shown to be an important driver of many other emerging network properties (Poisot and Gravel 2014). In light of these observations, it is difficult to assess whether attributed effects of given properties are the artifacts of other, perhaps simpler, measures.

One way to tackle this issue is first to recognize that food webs and other ecological networks are constrained systems. In other words, the space of possible network configurations shrinks as we know more about a network structure. For example, there is a finite number of networks with specified numbers of nodes and edges. Indeed, the structure of ecological networks is first and above all constrained by the number of species, or nodes, present. Food webs with high species richness typically have a lower connectance (MacDonald, Banville, and Poisot 2020) than smaller networks. This is because the number of realized interactions in empirical food webs scales slower than the number of possible species pairs (MacDonald, Banville, and Poisot 2020). As shown by Poisot and Gravel (2014), connectance itself can constrain different aspects of network structure such as the degree distribution (i.e. the probability distribution of the number of interspecific interactions realized by a species). Other measures, such as the maximum trophic level, can also constrain the space of feasible networks.

Prior knowledge on the structure of ecological networks is thus especially useful in the current context of data scarcity about species interactions (Jordano 2016). Indeed, this Eltonian shortfall (Hortal et al. 2015) can be partially alleviated using known information about an ecological network. As suggested by Strydom et al. (2021), network structure can be used to improve the prediction of pairwise species interactions when data is lacking by constraining the space of feasible networks. Similarly, partial knowledge on the structure of an ecological network can also be used to predict others of its properties by constraining their range of possible values. This is important given that many aspects of network structure cannot be measured empirically without data on pairwise species interactions, a prevailing situation worldwide (Poisot et al. 2021).

Understanding the ecological constraints that shape species interactions networks and predicting their emerging structure are thus two complementary aims of network ecology. This distinction between understanding and predicting is essential when using statistical and mathematical models in network ecology and interpreting them. On one hand, null models help us identify potential ecological mechanisms that drive species interactions and constrain ecological networks. Null models generate a distribution for a target measure using a set of rules that exclude the mechanism of interest (Fortuna and Bascompte 2006; Delmas et al. 2019). The deviation between the model and empirical data helps us evaluate the effect of this ecological process in nature. On the other hand, predictive models can help fill many gaps on species interactions data. A variety of such models have recently been developed using machine learning and other statistical tools, most of which are presented in Strydom et al. (2021). However, given the constrained nature of ecological networks, it is surprising that the principle of maximum entropy, a rigorous mathematical method designed for both the analysis and prediction of constrained systems, has been barely used in network ecology.

**1.2. The principle of maximum entropy: A primer for ecologists** The principle of maximum entropy (MaxEnt) is a mathematical method of finding probability distributions, strongly rooted in statistical mechanics and information theory (Jaynes 1957a, 1957b; Harremoës and Topsøe 2001). Starting from a set of constraints given by prior knowledge of a system (i.e. what we call state variables), this method helps us find least-biased probability distributions subject to the constraints. These probability distributions are guaranteed to be unique given our prior knowledge and represent the most we can say about a system without making more assumptions. For example, if the only thing we know about a biological community is its average number of individuals per species, the least-biased inference we could make on its species abundance distribution is the exponential distribution (Frank and Smith 2011; Harte and Newman 2014). However, this does not imply that this distribution will be the best fit to empirical data. The challenge is to find the right set of constraints that would best reproduce distributions found in nature.

MaxEnt states that the least-biased probability distribution given the constraints used is the one with the highest entropy among all probability distributions that satisfy these constraints. Entropy is a measure of the average amount of information given by the outcome of a random variable. Many measures of entropy have been developed in physics (Beck 2009), but only a fraction of them could be used as an optimization measure with the principle of maximum entropy. According to Beck (2009) and Khinchin (2013), a measure of entropy  $H$  should satisfy four properties in the discrete case: (1) it should be a function of a probability distribution  $p(n)$  only; (2) it should be maximized when  $p(n)$  is uniform; (3) it should not be influenced by outcomes with a null probability; and (4) it should be independent of the order of information acquisition. The Shannon's entropy (Shannon 1948)

$$H = - \sum_n p(n) \log p(n) \quad (1)$$

satisfies all of these properties. Finding the probability distribution  $p(n)$  that maximizes  $H$  under a set of  $m$  constraints  $g$  can be done using the method of Lagrange multipliers. These constraints could include one or many properties of the probability distribution (e.g., its mean, variance, and range). However, the normalization constraint always need to be included in  $g$  in order to make sure that  $p(n)$  sums to 1. The objective is then to find the values of the Lagrange multipliers  $\lambda_i$  that optimize a function  $F$ :

$$F = H - \sum_{i=1}^m \lambda_i (g_i - c_i), \quad (2)$$

where  $g_i$  is the mathematical formulation of the constraint  $i$  and  $c_i$ , its value. Note that  $F$  is just Shannon's entropy to which we added terms that each sums to zero ( $g_i = c_i$ ).  $F$  is maximized by setting to 0 its partial derivative with respect to  $p(n)$ .

The principle of maximum entropy has been used in a wide range of disciplines, from thermodynamics, chemistry and biology (Martyushev and Seleznev 2006) to graph and network theory (e.g., Park and Newman 2004; van der Hoorn, Lippner, and Krioukov 2018). It has also been proven useful in ecology, e.g. in species distribution models (Phillips, Anderson, and Schapire 2006) and macroecological models (Harte et al. 2008; Harte and Newman 2014). In network ecology, MaxEnt has been used to predict the degree distribution of bipartite networks from the number of species and the number of interactions (Williams 2011) and to predict interaction strengths between species pairs using their relative abundances within an optimal transportation theory regularized with information entropy (Stock, Poisot, and De Baets 2021). However, to the best of our knowledge, MaxEnt has never been used to predict food-web structure directly, even though food webs are among the most documented and widespread ecological networks (Ings et al. 2009).

Food-web properties that can be derived using MaxEnt are varied and pertain to different elements of the network (i.e. at the species (node), the interaction (edge) or the community (network) levels). Because MaxEnt is a method of finding least-biased probability distributions given partial knowledge about a system, these properties need to be represented probabilistically. For example, at the species level, MaxEnt can be used to predict the distribution of trophic levels among species, as well as the distribution of species' vulnerability (number of predators) and generality (number of prey). By contrast, at the interaction level, predictions can be made on the distribution of interaction strengths in weighted food webs. At the community level, it can generate probability distributions of many measures of their emerging structure and of networks themselves (i.e. a probability distribution that specific network configurations are realized given the model and constraints). Overall, the potential of this method in the study of food webs is broad. The applicability and performance of MaxEnt mostly depend on the ecological information available and on our capacity to find the right set of state variables that best represent natural systems and to translate them into appropriate statistical constraints. Having a validated maximum entropy model for the system at hand allows us to make least-biased predictions using a minimal amount of data, as well as identify the most important ecological processes shaping that system. In other words, MaxEnt is a valuable and underexploited tool in network ecology that allows us to better understand and predict the structure of ecological networks.

**1.3. Analytical and heuristic approaches** In this contribution, we used two complementary approaches to predict the structure of food webs using the principle of maximum entropy. The first approach consists in deriving constrained probability distributions of given network properties analytically, whereas the second approach consists in finding the adjacency matrix of maximum entropy heuristically, from which network properties can be measured. We compared our predictions against empirical data and null and neutral models commonly used in network ecology. We focus on deterministic and unweighted (Boolean) food webs in both approaches for data availability reasons. However, our framework can be applied to all types of ecological networks and a wide variety of measures.

For the first approach (analytic), we focus on species level properties. Specifically, we derived the joint degree distribution (i.e. the joint probability distribution that a species has a given number of prey and predators in its network) of maximum entropy using only the number of species  $S$  and the number of interactions  $L$  as state variables. Then, we predicted the degree distribution of maximum entropy directly from the joint degree distribution since the first is the sum of the marginal distributions of the second. Because of the scarcity of empirical data on the number of interactions in food webs, we present a method to predict  $L$  from  $S$  (Box 1), thus allowing the prediction of the joint degree distribution from  $S$  solely.

For the second approach (heuristic), we focus on network level properties. We used a flexible and heuristic model based on simulated annealing (an optimization algorithm) to find the network configuration *close* to maximum entropy and measured its structure. We developed this heuristic model because the analytical derivation of a maximum entropy graph model of food webs is difficult, and because this model is readily applicable to other types of ecological networks and measures. Indeed, the mathematical representation of food webs (i.e. directed simple graphs frequently having self-loops) makes the optimization of maximum entropy graph models more complicated than with many other types of (non-ecological) networks. In other words, deriving a probability distribution on the graphs themselves is difficult when working with food webs. We built two types of heuristic MaxEnt models depending on the constraint used. Our type I MaxEnt model uses the connectance of the network (i.e. the ratio  $L/S^2$ ) as a constraint, whereas our type II MaxEnt model uses the whole joint degree sequence as a constraint.

## Analytical maximum entropy models

Our analytical approach is the most common way to use and develop maximum entropy models. As shown above, starting from a defined set of constraints, a mathematical expression for the target distribution is derived using the method of Lagrange multipliers. The derived distribution of maximum entropy is unique and least biased given the constraints used. Although we refer to this approach as analytic, finding the values of the Lagrange multipliers usually requires the use of numerical methods. Here we use MaxEnt to derive two species level properties in food webs: the joint degree distribution and the degree distribution. The degree distribution has driven the attention of ecologists because of its role in determining the assembly of ecological networks (Vázquez 2005), shaping their emerging structure (Fortuna et al. 2010), and understanding interaction mechanisms (Williams 2011). As noted above, although the degree distribution of maximum entropy has already been derived in bipartite networks (Williams 2011), we show in much greater details its mathematical derivation in food webs. But first, we derive the joint degree distribution, a related property that holds significantly more ecological information than the degree distribution.

We tested our analytical MaxEnt model against open food-web data queried from three different sources and integrated into what we call our *complete dataset*. These sources include (1) terrestrial and aquatic food webs sampled globally and archived on the ecological interactions database Mangal; (2) freshwater stream food webs from New Zealand; and (3) aquatic food webs from Tuesday Lake (Michigan, United States). First, all food webs archived on mangal.io (Poisot et al. 2016; Banville, Vissault, and Poisot 2021) were directly queried from the database ( $N = 235$ ). Most ecological networks archived on Mangal are multilayer networks, i.e. networks that describe different types of interactions. We kept all networks whose interactions were mainly of predation and herbivory types, and removed the largest network ( $S = 714$ ) for computational efficiency reasons. Then, to this set we added food webs from two different sources: the New Zealand dataset ( $N = 21$ ; J. P. Pomeranz et al. 2018) and the Tuesday Lake dataset ( $N = 2$ ; Cohen, Jonsson, and Carpenter 2003). Our complete dataset thus contained a total of 257 food webs. All code and data to reproduce this article are available at the Open Science Framework (OSF.IO/KT4GS). Data cleaning, simulations and analyses were conducted in Julia v1.8.0.

**2.1. Joint degree distribution** The joint degree distribution  $p(k_{in}, k_{out})$  of a food web with  $S$  species is a joint discrete probability distribution describing the probability that a species has  $k_{in}$  predators and  $k_{out}$  prey, with  $k_{in}$  and  $k_{out} \in [0, S]$ . Basal species (e.g., plants) have a  $k_{out}$  of 0, whereas top predators have a  $k_{in}$  of 0. In contrast, the maximum number of prey and predators a species can have is set by the number of species in the food web. Here we show how the joint degree distribution of maximum entropy can be obtained given knowledge of the number of species  $S$  and the number of interactions  $L$ .

We want to maximize Shannon's entropy

$$H = - \sum_{k_{in}=0}^S \sum_{k_{out}=0}^S p(k_{in}, k_{out}) \log p(k_{in}, k_{out}) \quad (3)$$

subject to the following constraints:

$$g_1 = \sum_{k_{in}=0}^S \sum_{k_{out}=0}^S p(k_{in}, k_{out}) = 1; \quad (4)$$

$$g_2 = \sum_{k_{in}=0}^S \sum_{k_{out}=0}^S k_{in} p(k_{in}, k_{out}) = \langle k_{in} \rangle = \frac{L}{S}; \quad (5)$$

$$g_3 = \sum_{k_{in}=0}^S \sum_{k_{out}=0}^S k_{out} p(k_{in}, k_{out}) = \langle k_{out} \rangle = \frac{L}{S}. \quad (6)$$

The first constraint  $g_1$  is our normalizing constraint, whereas the other two ( $g_2$  and  $g_3$ ) fix the average of the marginal distributions of  $k_{in}$  and  $k_{out}$  to the linkage density  $L/S$ . It is important to notice that  $\langle k_{in} \rangle = \langle k_{out} \rangle$  because every edge is associated to a predator and a prey. Therefore, without using any further constraints, we would expect the joint degree distribution of maximum entropy to be a symmetric probability distribution with regards to  $k_{in}$  and  $k_{out}$ . However, this does not mean that the joint degree *sequence* will be symmetric, since the joint degree sequence is essentially a random realization of its probabilistic counterpart.

The joint probability distribution of maximum entropy given these constraints is found using the method of Lagrange multipliers. To do so, we seek to maximize the following expression:

$$F = H - \lambda_1(g_1 - 1) - \lambda_2 \left( g_2 - \frac{L}{S} \right) - \lambda_3 \left( g_3 - \frac{L}{S} \right), \quad (7)$$

where  $\lambda_1$ ,  $\lambda_2$ , and  $\lambda_3$  are the Lagrange multipliers. The probability distribution that maximizes entropy is obtained by finding these values. As pointed out above,  $F$  is just Shannon's entropy to which we added terms that each sums to zero (our constraints).  $F$  is maximized by setting to 0 its partial derivative with respect to  $p(k_{in}, k_{out})$ . Because the derivative of a constant is zero, this gives us:

$$\frac{\partial H}{\partial p(k_{in}, k_{out})} = \lambda_1 \frac{\partial g_1}{\partial p(k_{in}, k_{out})} + \lambda_2 \frac{\partial g_2}{\partial p(k_{in}, k_{out})} + \lambda_3 \frac{\partial g_3}{\partial p(k_{in}, k_{out})}. \quad (8)$$

Evaluating the partial derivatives with respect to  $p(k_{in}, k_{out})$ , we obtain:

$$-\log p(k_{in}, k_{out}) - 1 = \lambda_1 + \lambda_2 k_{in} + \lambda_3 k_{out}. \quad (9)$$

Then, solving eq. 9 for  $p(k_{in}, k_{out})$ , we obtain:

$$p(k_{in}, k_{out}) = \frac{e^{-\lambda_2 k_{in} - \lambda_3 k_{out}}}{Z}, \quad (10)$$

where  $Z = e^{1+\lambda_1}$  is called the partition function. The partition function ensures that probabilities sum to 1 (our normalization constraint). It can be expressed in terms of  $\lambda_2$  and  $\lambda_3$  as follows:

$$Z = \sum_{k_{in}=0}^S \sum_{k_{out}=0}^S e^{-\lambda_2 k_{in} - \lambda_3 k_{out}}. \quad (11)$$

After substituting  $p(k_{in}, k_{out})$  in eq. 5 and eq. 6, we get a nonlinear system of two equations and two unknowns:

$$\frac{1}{Z} \sum_{k_{in}=0}^S \sum_{k_{out}=0}^S k_{in} e^{-\lambda_2 k_{in} - \lambda_3 k_{out}} = \frac{L}{S}; \quad (12)$$

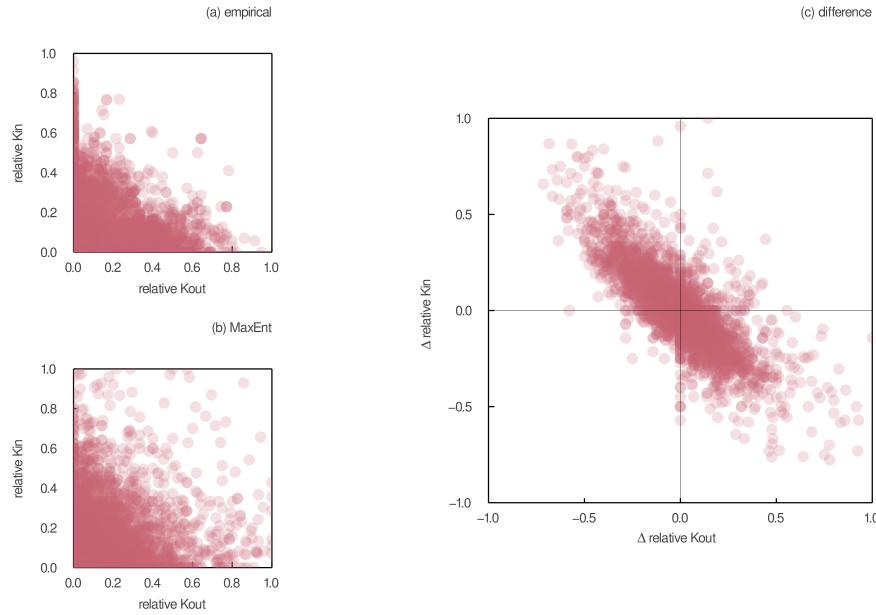
$$\frac{1}{Z} \sum_{k_{in}=0}^S \sum_{k_{out}=0}^S k_{out} e^{-\lambda_2 k_{in} - \lambda_3 k_{out}} = \frac{L}{S}. \quad (13)$$

We solved eq. 12 and eq. 13 numerically using the Julia library JuMP.jl v0.21.8 (Dunning, Huchette, and Lubin 2017). JuMP.jl supports nonlinear optimization problems by providing exact second derivatives that increase the accuracy and performance of its solvers. The estimated values of  $\lambda_2$  and  $\lambda_3$  can be substituted in eq. 10 to have a more workable expression for the joint degree distribution.

We assessed the empirical support of this expression using all food webs in our complete dataset. First, we predicted the joint degree distribution of maximum entropy for each of these food webs, i.e. using their number of species and number of interactions as state variables. Then, we sampled one realization of the joint degree sequence for each network using the probabilities given by the joint degree distribution of maximum entropy, while fixing the total number of interactions. This gave us a random realization of the number of prey and predators for each species in each network. We standardized the predicted  $k_{out}$  and  $k_{in}$  of each species by the total number of species in their network to generate relative values, which can be compared across networks. In fig. 1 (left panels), we show the relationship between these relative  $k_{out}$  and  $k_{in}$  obtained from the joint degree distributions of maximum entropy (bottom panel) and this relationship using empirical values (top panel). We observe that our model predicts higher values of generality and vulnerability compared to empirical food webs (i.e. relative values of  $k_{out}$  and  $k_{in}$  both closer to 1) for many species. In other words, our model predicts that species that have many predators also have more prey than what is observed empirically (and conversely). This is not surprising, given that our model did not include biological factors preventing generalist predators from having many prey. Nevertheless, with the exception of these generalist species, MaxEnt adequately predicts that most species have low generality and vulnerability values.

Examining the difference between predicted and empirical values for each species gives a slightly different perspective (right panel of fig. 1). To do so, we must first associate each of our predictions to a specific species in a network in order to make that comparison. Indeed, our predicted joint degree sequences have the same number of species (elements) as their empirical counterparts, but they are species agnostic. In other words, instead of predicting a value for each species directly, we predicted the entire joint degree sequence without taking into account species' identity. The challenge is thus to adequately associate predictions with empirical data. In fig. 1, we present these differences when species are ordered by their total degree in their respective networks (i.e. by the sum of their in and out-degrees). This means that the species with the highest total degree in its network will be associated with the highest prediction, and so forth. Doing so, we see that species predicted to have a higher number of predators than what is observed generally have a lower number of prey than what is observed (and conversely). This is because the difference in total degree ( $k_{out} + k_{in}$ ) between predictions and empirical data is minimized when species are ranked by their total degree (i.e. the average deviation of the sum of relative  $k_{out}$  and  $k_{in}$  is close to 0 across all species). This result thus shows that the difference between predicted and empirical total degrees is low for most species when ordered by their total degrees. There are no apparent biases towards in or out degrees. In fig. S1, we show how these differences change when species are instead ordered by their out-degrees (left panel) and in-degrees (right panel), respectively.

Another way to evaluate the empirical support of the predicted joint degree sequences is to compare their shape with the ones of empirical food webs. We can describe the shape of a joint degree sequence by comparing its marginal distributions with one another. To do so, we calculated the Kullback–Leibler (KL) divergence between the in and out-degree sequences sampled from the joint degree distribution of maximum entropy. Similarly, we calculated the divergence between the in and out-degree sequences obtained empirically. This allows us to compare the symmetry



**Figure 1** Relative number of predators ( $k_{in}$ ) as a function of their relative number of prey ( $k_{out}$ ) for each species in (a) empirical and (b) joint degree sequences obtained from the analytical MaxEnt model. Empirical networks include most food webs archived on Mangal, as well as the New Zealand and Tuesday Lake datasets (our complete dataset). The predicted joint degree sequences were obtained after sampling one realization of the joint degree distribution of maximum entropy for each network, while keeping the total number of interactions constant. (c) Difference between predicted and empirical values when species are ordered according to their total degrees. In each panel, each dot corresponds to a single species in one of the networks.

of empirical and predicted joint degree sequences (left panel of fig. 2). As we expected, our model predicts more similar in-degree and out-degree sequences than empirical data (shown by lower KL divergence values). However, this difference decreases with connectance (right panel of fig. 2). This might be due to the fact that food webs with a low connectance are harder to predict than food webs with a high connectance. Indeed, in low connectance systems, what makes two species interact might be more important for prediction than in high connectance systems, in which what prevents species from interacting might be more meaningful. This implies that more ecological information might be needed in food webs with a low connectance because more ecological processes determine interactions compared to non-interactions. Therefore, other ecological constraints might be needed to account for the asymmetry of the joint degree distribution, especially for networks with a lower connectance. However, our MaxEnt model was able to capture quite well the shape of the joint degree sequence for networks having a high connectance.

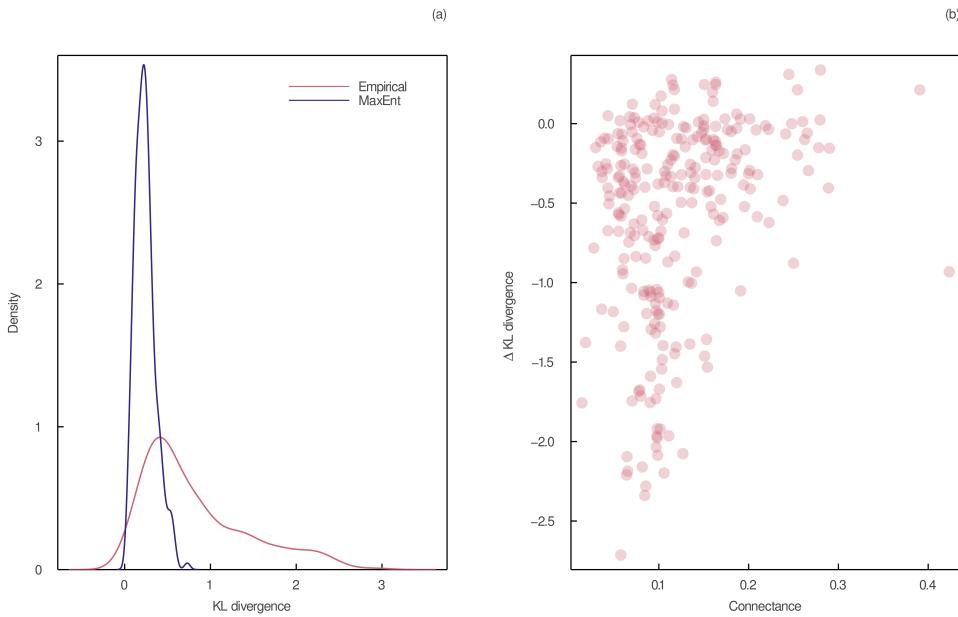
**2.2. Degree distribution** The joint degree distribution derived using MaxEnt (eq. 10) can be used to obtain the degree distribution of maximum entropy. Indeed, the degree distribution  $p(k)$  represents the probability that a species has  $k$  interactions in its food web, with  $k = k_{in} + k_{out}$ . It can thus be obtained from the joint degree distribution as follows:

$$p(k) = \sum_{i=0}^k p(k_{in} = k - i, k_{out} = i).$$

The degree distribution could have also been obtained directly using the principle of maximum entropy, as discussed in Williams (2011). This gives the following distribution:

$$p(k) = \frac{e^{-\lambda_2 k}}{Z}, \quad (14)$$

with  $Z = \sum_{k=0}^S e^{-\lambda_2 k}$ .



**Figure 2** (a) Probability density of KL divergence between in and out-degree sequences of empirical and predicted joint degree sequences. (b) Difference between the KL divergence of empirical and predicted joint degree sequences as a function of connectance. In both panels, empirical networks include most food webs archived on Mangan, as well as the New Zealand and Tuesday Lake datasets (our complete dataset). The predicted joint degree sequences were obtained after sampling one realization of the joint degree distribution of maximum entropy for each network, while keeping the total number of interactions constant.

This can be solved numerically using the constraint of the average degree  $\langle k \rangle = \frac{2L}{S}$  of a species, yielding an identical solution to the one obtained using the joint degree distribution as an intermediate. Note that the mean degree is twice the value of the linkage density, because every link must be counted twice when we add in and out-degrees together.

$$\frac{1}{Z} \sum_{k=0}^S k e^{-\lambda_2 k} = \frac{2L}{S} \quad (15)$$

One aspect of the degree distribution that informs us of its ecological realism is the number of isolated species it predicts. As MacDonald, Banville, and Poisot (2020) pointed out, the size of food webs should at least be of  $S - 1$  interactions, since a lower number would yield isolated species, i.e. species without any predators or prey. Because non-basal species must eat to survive, isolated species could indicate that other species are missing or they could simply be removed from the food web. In fig. S2, we show that the degree distribution of maximum entropy, given  $S$  and  $L$ , gives very low probabilities that a species will be isolated in its food web (i.e. having  $k = 0$ ) above the  $S - 1$  threshold. However, under our purely information-theoretic model, the probability that a species is isolated is quite high when the total number of interactions is below  $S - 1$ . Moreover, the expected proportion of isolated species rapidly declines by orders of magnitude with increasing numbers of species and interactions. This supports the ecological realism of the degree distribution of maximum entropy derived above. Nevertheless, ecologists wanting to model a system without allowing isolated species could simply change the lower limit of  $k$  to 1 in eq. 15 and solve the resulting equation numerically.

### 3

#### Box 1 - Working with predicted numbers of interactions

Our analytical MaxEnt models require information on the number of species and the number of interactions. However, since the later is rarely measured empirically, ecologists might need to

use predictive models to estimate the total number of interactions in a food web before using MaxEnt. Here we illustrate how this can be done by combining both models sequentially.

We used the flexible links model of MacDonald, Banville, and Poisot (2020) to predict the number of interactions from the number of species. The flexible links model, in contrast to other predictive models of the number of interactions, incorporates meaningful ecological constraints into the prediction of  $L$ , namely the minimum  $S - 1$  and maximum  $S^2$  numbers of interactions in food webs. It estimates the proportion of the  $S^2 - (S - 1)$  *flexible links* that are realized. More precisely, this model states that the number of *realized* flexible links (or interactions)  $L_{FL}$  in a food web represents the number of realized interactions above the minimum (i.e.  $L = L_{FL} + S - 1$ ) and is obtained from a beta-binomial distribution with  $S^2 - (S - 1)$  trials and parameters  $\alpha = \mu e^\phi$  and  $\beta = (1 - \mu)e^\phi$ :

$$L_{FL} \sim \text{BB}(S^2 - (S - 1), \mu e^\phi, (1 - \mu)e^\phi), \quad (16)$$

where  $\mu$  is the average probability across food webs that a flexible link is realized, and  $\phi$  is the concentration parameter around  $\mu$ .

We fitted the flexible links model on all food webs in our complete dataset, and estimated the parameters of eq. 16 using a Hamiltonian Monte Carlo sampler with static trajectory (1 chain and 3000 iterations):

$$[\mu, \phi | \mathbf{L}, \mathbf{S}] \propto \prod_{i=1}^m \text{BB}(L_i - (S_i - 1) | S_i^2 - (S_i - 1)), \mu e^\phi, (1 - \mu)e^\phi \times \text{B}(\mu | 3, 7) \times \mathcal{N}(\phi | 3, 0.5), \quad (17)$$

where  $m$  is the number of food webs ( $m = 257$ ) and  $\mathbf{L}$  and  $\mathbf{S}$  are respectively the vectors of their numbers of interactions and numbers of species. Our weakly-informative prior distributions were chosen following MacDonald, Banville, and Poisot (2020), i.e. a beta distribution for  $\mu$  and a normal distribution for  $\phi$ . The Monte Carlo sampling of the posterior distribution was conducted using the Julia library Turing v0.15.12.

The flexible links model is a generative model, i.e. it can generate plausible values of the predicted variable. We thus simulated 1000 values of  $L$  for different values of  $S$  using the joint posterior distribution of our model parameters (eq. 17), and calculated the mean degree for each simulated value. The resulting distributions are shown in the left panel of fig. 3 for three different values of species richness. In the right panel of fig. 3, we show how the probability distribution for the mean degree constraints can be used to generate a distribution of maximum entropy degree distributions, since each simulated value of mean degree generates a different maximum entropy degree distribution (eq. 14 and eq. 15).

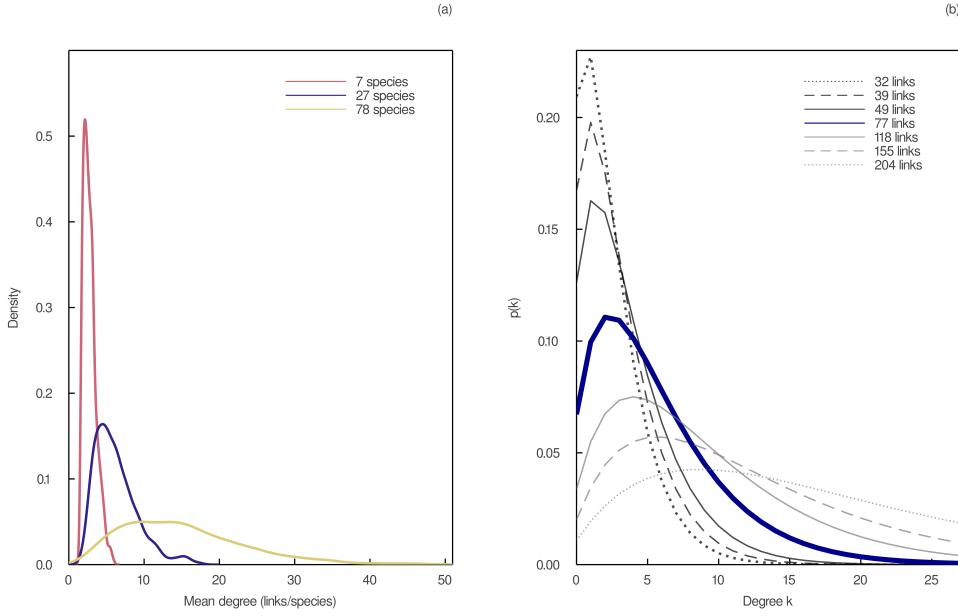
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### Box 2 - Corresponding null and neutral models

**4.1. Null models (types I and II)** The predictions of our heuristic maximum entropy models were compared against two topological null models. These null models use the same ecological information as our heuristic models and thus constitute an adequate baseline for comparison. The first is the type I null model of Fortuna and Bascompte (2006), in which the probability that a species  $i$  predares on another species  $j$  is given by

$$p(i \rightarrow j) = \frac{L}{S^2}. \quad (18)$$



**Figure 3** (a) Probability density of the mean degree of a food web obtained using different values of species richness  $S$ . The number of interactions  $L$  was simulated 1000 times using the flexible links model fitted to all empirical networks in our complete dataset (eq. 17). The mean degrees  $2L/S$  were then obtained from these simulated values. (b) Degree distributions of maximum entropy for a network of  $S = 27$  species and different numbers of interactions. The numbers of interactions correspond to the lower and upper bounds of the 67, 89, and 97 percentile intervals (PI), as well as the median (in blue), of the counterfactuals of the flexible links model. Each degree distribution of maximum entropy was obtained using eq. 14 after solving numerically eq. 15 using different values of the mean degree constraint.

The second is the type II null model of Bascompte et al. (2003), in which the probability of interaction is instead given by

$$p(i \rightarrow j) = \frac{1}{2} \left( \frac{k_{in}(j)}{S} + \frac{k_{out}(i)}{S} \right), \quad (19)$$

where  $k_{in}(j)$  and  $k_{out}(i)$  are the in and out-degrees of species  $j$  and  $i$ , respectively. The type I null model is based on connectance, whereas the type II null model is based on the joint degree sequence. Therefore, the type I and II topological null models correspond to our type I and II heuristic MaxEnt models, respectively, since they use similar constraints.

We generated probabilistic networks using both types of null models for all empirical food webs in our complete dataset. Then, we converted these networks to adjacency matrices of Boolean values by generating 100 random networks for each of these probabilistic webs, and kept the  $L$  entries that were sampled the most amount of times, with  $L$  given by the number of interactions in each food web. This ensured that the resulting null networks had the same number of interactions as their empirical counterparts. Thus, for each null model, we ended up with one null adjacency matrix for each empirical network.

**4.2. Neutral model** We also compared our heuristic MaxEnt models with a neutral model of relative abundances, in which the probabilities of interaction are given by

$$p(i \rightarrow j) \propto \frac{n_i}{N} \times \frac{n_j}{N}, \quad (20)$$

where  $n_i$  and  $n_j$  are the abundances (or biomass) of both species, and  $N$  is the total abundance (or biomass) of all species in the network. We generated neutral abundance matrices for all empirical food webs in our abundance dataset, and converted these weighted networks to adjacency matrices of Boolean values using the same method as the one we used for our null models.

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## Heuristic maximum entropy models

With the analytical approach, we showed how important measures of food-web structure (e.g., the degree distribution and the joint degree distribution) can be derived with the principle of maximum entropy using minimal knowledge about a biological community. This type of models, although useful to make least-biased predictions of many network properties, can be hard to apply for other measures. Indeed, there are dozens of measures of network structure (Delmas et al. 2019) and many are not directly calculated with mathematical equations, but are instead estimated algorithmically. Moreover, the applicability of this method to empirical systems is limited by the state variables we can actually measure and use. Here, we propose a more flexible method to predict many measures of network structure simultaneously, i.e. by finding heuristically the network configuration having maximum entropy given partial knowledge of its emerging structure.

**5.1. From Shannon's to SVD entropy** The principle of maximum entropy can be applied on the network itself if we decompose its adjacency matrix into a non-zero vector of relative values. This is a necessary step when working with food webs, which are frequently expressed as a matrix  $A = [a_{ij}]$  of Boolean values representing the presence ( $a_{ij} = 1$ ) or absence ( $a_{ij} = 0$ ) of an interaction between two species  $i$  and  $j$ . Knowing one or many properties of a food web of interest (e.g., its number of species and number of interactions), we can simulate its adjacency matrix randomly by using these known ecological information to constrain the space of potential networks. The entropy of this hypothetical matrix can then be measured after decomposing it into appropriate values. Simulating a series of networks until we find the one having the highest entropy allows us to search for the most complex food-web configuration given the ecological constraints used. This configuration is the least biased one considering the information available. In other words, the most we can say about a network's adjacency matrix, without making more assumptions than the ones given by our incomplete knowledge of its structure, is the one of maximum entropy. Generating the most complex network that corresponds to this structure allows us to explore more easily other properties of food webs under MaxEnt.

Shannon's entropy can only be calculated on conventional probability distributions such as the joint degree distribution. This is an issue when working with the adjacency matrix of ecological networks. For this reason, we need to use another measure of entropy if we want to predict a network's configuration directly using MaxEnt. We used the SVD entropy as our measure of entropy, which is an application of Shannon's entropy to the relative non-zero singular values of a truncated singular value decomposition (t-SVD; Strydom, Dalla Riva, and Poisot 2021) of a food web's Boolean adjacency matrix. We measured SVD entropy as follows:

$$J = - \sum_{i=1}^R s_i \log s_i, \quad (21)$$

where  $s_i$  are the relative singular values of the adjacency matrix ( $s_i = \sigma_i / \sum_{i=1}^R \sigma_i$ , where  $\sigma_i$  are the singular values). Note that the distribution of relative singular values is analogous to a probability distribution, with  $0 < s_i < 1$  and  $\sum s_i = 1$ . This measure also satisfies all four properties of an appropriate entropy measure above-mentioned, while being a proper measure of the internal complexity of food webs (Strydom, Dalla Riva, and Poisot 2021). Following Strydom, Dalla Riva, and Poisot (2021), we standardized this measure with the rank  $R$  of the matrix (i.e.  $J / \ln(R)$ ) to account for the difference in dimensions between networks (*sensu* Pielou's evenness; Pielou 1975).

**5.2. Types I and II heuristic MaxEnt models** We used SVD entropy to predict the network configuration of maximum entropy (i.e. of maximum complexity) heuristically given different constraints for all food webs in our complete dataset. We built two types of heuristic MaxEnt models that differ on the constraint used. The type I heuristic MaxEnt model is based on connectance, whereas the type II heuristic MaxEnt model is based on the joint degree sequence. These models are thus based on the same constraints as the types I (Fortuna and Bascompte 2006) and II (Bascompte et al. 2003) null models (Box 2) frequently used to generate random networks topologically. This allows direct comparison of the performance of null and heuristic MaxEnt models in reproducing the emerging structure of empirical food webs.

For each network in our complete dataset, we estimated their configuration of maximum entropy given each of these constraints. For both types of heuristic MaxEnt models, we used a simulated annealing algorithm with 4 chains, 2000 steps and an initial temperature of 0.2. For each food web, we first generated one random Boolean matrix per chain while fixing the number of species. We also maintained the total number of interactions (i.e. the sum of all elements in the matrix) in the type I MaxEnt model and the joint degree sequence (i.e. the rows and columns sums) in the type II MaxEnt model. These were our initial configurations. Then, we swapped interactions sequentially while maintaining the original connectance or joint degree sequence. Configurations with a higher SVD entropy than the previous one in the chain were always accepted, whereas they were accepted with a probability conditional to a decreasing temperature when lower. The final configuration with the highest SVD entropy among the four chains constitute the estimated maximum entropy configuration of a food web given the constraint used.

**5.3. Structure of MaxEnt food webs** We measured various properties of these configurations of maximum entropy to evaluate how well they reproduce the structure of sampled food webs. Specifically, we evaluated their nestedness  $\rho$ , their maximum trophic level  $maxtl$ , their network diameter  $diam$ , their average maximum similarity between species pairs  $MxSim$  (Williams and Martinez 2000), their proportion of cannibal species  $Cannib$ , their proportion of omnivorous species  $Omniv$ , their SVD entropy, and their motifs profile. Nestedness indicates how much the diet of specialist species is a subset of the one of generalists (Delmas et al. 2019) and was measured using the spectral radius of the adjacency matrix (Staniczenko, Kopp, and Allesina 2013). In turn, the network diameter represents the longest of the shortest paths between all species pair (Albert and Barabasi 2002). Further, cannibal species are species that can eat individuals of their own species (i.e. species having self loops), whereas omnivorous species can prey on different trophic levels (Williams and Martinez 2000). Finally, a motifs profile represents the proportion of three-species motifs (subnetworks), which can be considered as simple building blocks of ecological networks (Milo et al. 2002; Stouffer et al. 2007). All of these properties are relatively easy to measure and were chosen based on their ecological importance and prevalent use in network ecology (McCann 2011; Delmas et al. 2019).

We compared the performance of both heuristic MaxEnt models in predicting these measures to the one of the null and neutral models (Box 2). We conducted these comparisons using two different datasets: (1) our complete dataset including most food webs archived on Mangal, as well as all food webs in the New Zealand and Tuesday Lake datasets, and (2) our *abundance dataset*, a subset of the complete dataset comprising all food webs having data on their species' relative abundances ( $N = 19$ ). Indeed, of the New Zealand and Tuesday Lake datasets, 19 networks had data on species' relative abundances that were used in the neutral model to better assess the performance of our heuristic models. We compared our models' predictions using these two datasets separately to minimize biases and to better represent food webs with abundance data (tbl. 1 and tbl. 2).

Overall, we found that the models based on the joint degree sequence (i.e. the type II null and heuristic MaxEnt models) reproduced the structure of empirical food webs much better than the ones based on connectance (i.e. the type I null and heuristic MaxEnt models). This suggests that

the predictive power of connectance might be more limited than what was previously suggested (Poisot and Gravel 2014). On the other hand, the neutral model of relative abundances was surprisingly good at predicting the maximum trophic level and the network diameter. However, with the exception of the network diameter, the type II heuristic MaxEnt model was better at predicting network structure than the neutral model for most measures considered. This might be because, although neutral processes are important, they act in concert with niche processes in determining species interactions Canard et al. (2014). The joint degree sequence encodes information on both neutral and niche processes because the number of prey and predators a species has is determined by its relative abundance and biological traits. These results thus show that having information on the number of prey and predators for each species substantially improves the prediction of food-web structure, both compared to models solely based on connectance and to the ones solely based on species relative abundances.

Next, the predictions of the type II heuristic MaxEnt model can be compared to its null model counterpart. On average, the type II heuristic MaxEnt model was better at predicting nestedness ( $0.62 \pm 0.08$ ) than its corresponding null model ( $0.73 \pm 0.05$ ; empirical networks:  $0.63 \pm 0.09$ ) for networks in our complete dataset (tbl. 1). This might in part be due to the fact that nestedness was calculated using the spectral radius of the adjacency matrix, which directly leverages information on the network itself just like the heuristic MaxEnt model. The proportion of self-loops (cannibal species) was also better predicted by the type II heuristic MaxEnt model in comparison to the type II null model. However, the type II null model was better at predicting network diameter and average maximum similarity between species pairs, and predictions of the maximum trophic level and the proportion of omnivorous species were similar between both types of models. We believe that this is because increasing the complexity of a food web might increase its average and maximum food-chain lengths. In comparison, the null model was more stochastic and does not necessarily produce more complex food webs with longer food-chain lengths.

**Table 1** Standardized mean difference between predicted network measures and empirical data for all food webs in our complete dataset ( $N = 257$ ). Positive (negative) values indicate that the measure is overestimated (underestimated) on average. Empirical networks include most food webs archived on Mangal, as well as the New Zealand and Tuesday Lake food webs. Null 1: Type I null model based on connectance. MaxEnt 1: Type I heuristic MaxEnt model based on connectance. Null 2: Type II null model based on the joint degree sequence. MaxEnt 2: Type II heuristic MaxEnt model based on the joint degree sequence.  $\rho$ : nestedness measured by the spectral radius of the adjacency matrix. *maxtl*: maximum trophic level. *diam*: network diameter. *MxSim*: average maximum similarity between species pairs. *Cannib*: proportion of cannibal species (self loops). *Omniv*: proportion of omnivorous species. *entropy*: SVD entropy.

model	rho	maxtl	diam	MxSim	Cannib	Omniv	entropy
null 1	-0.167	0.980	1.428	-0.502	2.007	1.493	0.056
MaxEnt 1	-0.226	0.831	1.274	-0.524	1.982	1.863	0.106
null 2	0.160	-0.125	0.016	0.007	1.078	0.559	-0.023
MaxEnt 2	-0.015	0.178	0.565	-0.282	0.698	0.589	0.058

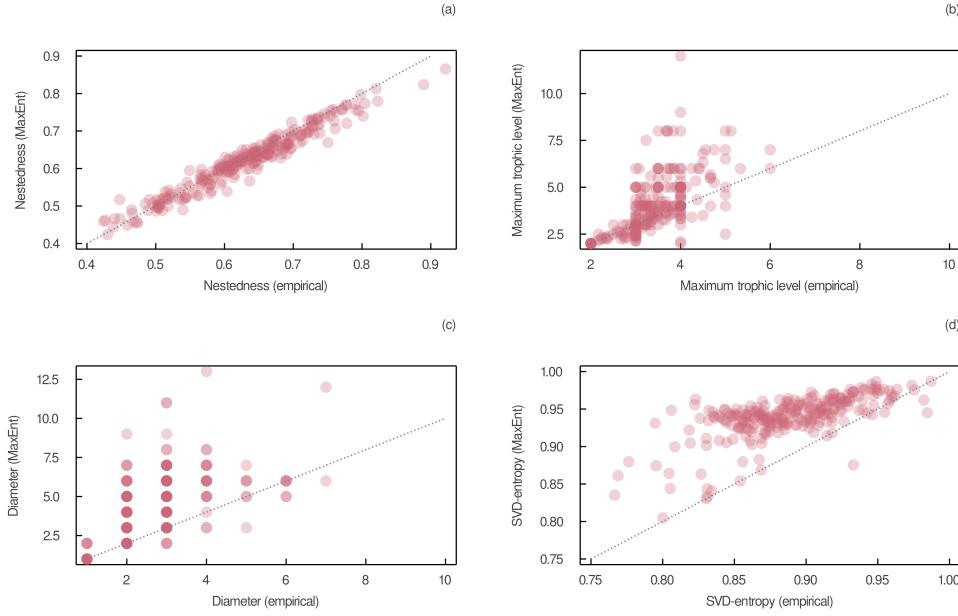
**Table 2** Standardized mean difference between predicted network measures and empirical data for all food webs in our abundance dataset ( $N = 19$ ). Positive (negative) values indicate that the measure is overestimated (underestimated) on average. Empirical networks include the New Zealand and Tuesday Lake food webs having abundance data. Neutral: Neutral model of relative abundances. Null 1: Type I null model based on connectance. MaxEnt 1: Type I heuristic MaxEnt model based on connectance. Null 2: Type II null model based on the joint degree sequence. MaxEnt 2: Type II heuristic MaxEnt model based on the joint degree sequence.  $\rho$ : nestedness measured by the spectral radius of the adjacency matrix. *maxtl*: maximum trophic level. *diam*: network diameter. *MxSim*: average maximum similarity between species pairs. *Cannib*: proportion of cannibal species (self loops). *Omniv*: proportion of omnivorous species. *entropy*: SVD entropy.

model	rho	maxtl	diam	MxSim	Cannib	Omniv	entropy
neutral	0.367	-0.090	0.027	0.266	6.870	0.576	-0.083
null 1	-0.134	0.950	1.919	-0.369	2.077	0.614	0.068
MaxEnt 1	-0.229	1.020	1.946	-0.355	2.215	0.801	0.121
null 2	0.128	-0.115	-0.135	0.157	1.444	0.029	-0.021
MaxEnt 2	-0.010	0.054	0.243	-0.062	-0.038	0.083	0.038

Despite this increase in maximum trophic level and network diameter in MaxEnt food webs, we found that empirical food webs are close to their maximum entropy given a fixed joint degree sequence (fig. S3). Empirical food webs in the complete dataset had an SVD entropy of  $0.89 \pm 0.04$ , compared to an SVD entropy of  $0.94 \pm 0.03$  for networks generated using the type II heuristic MaxEnt model. The relationship between the SVD entropy of empirical food webs and their maximum entropy is plotted in the last panel of fig. 4. As expected, the SVD entropy of maximum entropy food webs was higher than that of empirical food webs for almost all networks, confirming that our method indeed generated more complex networks. Moreover, we found no to a weak relationship between the increase in SVD entropy and the number of species, the number of interactions, and connectance (fig. S4). This suggests that the slight increase in entropy between empirical food webs and their maximum entropy configuration was sufficient to modify some of their properties, regardless of their number of species and their number of interactions.

A direct comparison of the structure of maximum entropy food webs, constrained by the joint degree sequence, with empirical data also supports the results depicted in fig. 1. Indeed, in fig. 4 we show how well empirical measures are predicted by the type II heuristic MaxEnt model. In accordance with our previous results, we found that nestedness was very well predicted by our model. However, the model overestimated the maximum trophic level and network diameter, especially when the sampled food web had intermediate values of these measures. In fig. S5, we show that the pairwise relationships between the four measures in fig. 4 and species richness in empirical food webs are similar (in magnitude and sign) to the ones found in food webs generated using the type II heuristic MaxEnt model. This indicates that the number of species in the network does not seem to impact the ability of the model to reproduce food-web structure.

Notwithstanding its difficulties in reproducing adequate measures of food-chain lengths, the type II heuristic MaxEnt model can predict surprisingly well the motifs profile. Motifs are the backbone of complex ecological networks from which network structure is built upon and play a crucial role in community dynamics and assembly (Stouffer and Bascompte 2011). For this reason, the motifs profile can act as an effective ecological constraint shaping species interactions networks, and thus constitute a substantial source of ecological information. In fig. 5, we show that the motifs profile of networks generated using the type II heuristic MaxEnt model accurately reproduced the one of empirical data. This model made significantly better predictions than the ones based on connectance and the type II null model based on the joint degree sequence. This is also shown in fig. 6, where we see that the relationships between motifs proportions in empirical food webs are very similar to the ones in networks generated using the type II heuristic



**Figure 4** Relationship between the structure of empirical and maximum entropy food webs. Empirical networks include most food webs archived on Mangal, as well as the New Zealand and Tuesday Lake food webs (our complete dataset). Maximum entropy networks were obtained using the type II heuristic MaxEnt model based on the joint degree sequence. (a) Nestedness (estimated using the spectral radius of the adjacency matrix), (b) the maximum trophic level, (c) the network diameter, and (d) the SVD entropy were measured on these empirical and maximum entropy food webs. The identity line is plotted in each panel.

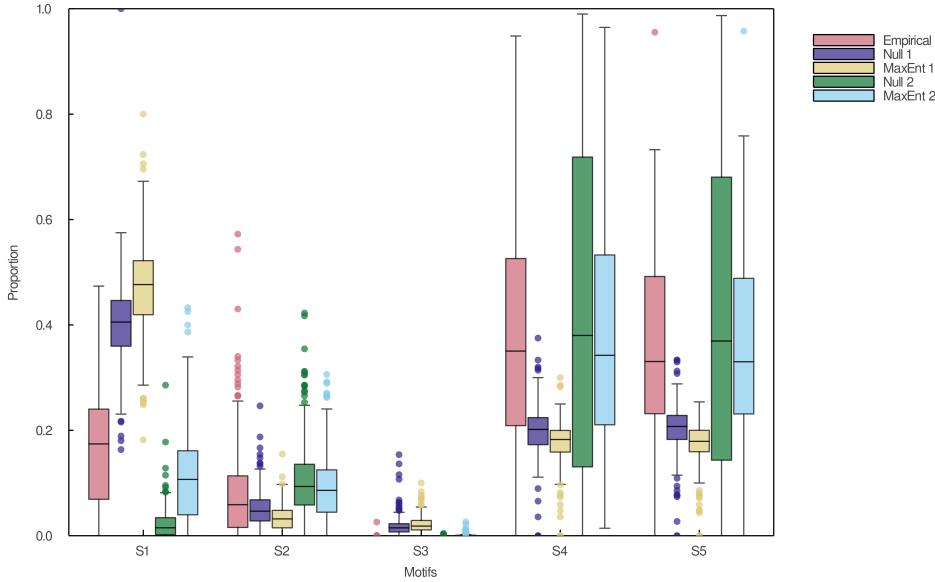
MaxEnt model. This is in contrast with the type I null and MaxEnt models based on connectance, which produced opposite relationships than what was observed empirically. Our findings thus suggest that increasing food-web complexity within a maximum entropy framework based on the joint degree sequence does not alter the proportion of three-species motifs, but might alter their position relative to one another.

One of the challenges in implementing and validating a maximum entropy model is to discover where its predictions break down. The results depicted in [tbl. 1](#) and [fig. 4](#) show that our type II heuristic MaxEnt model can capture many high-level properties of food webs, but does a poor job of capturing others. This suggests that, although the joint degree sequence is an important driver of food-web structure, other ecological constraints might be needed to account for some emerging food-web properties, especially the ones regarding food-chain lengths. Nevertheless, [fig. 5](#) and [fig. 6](#) show that the model can reproduce surprisingly well the motifs profile, one of the most ecologically informative properties of food webs. This suggests that the emerging structure of food webs is mainly driven by their joint degree sequence, although higher-level properties might be needed to ensure that food-chain lengths fall within realistic values.

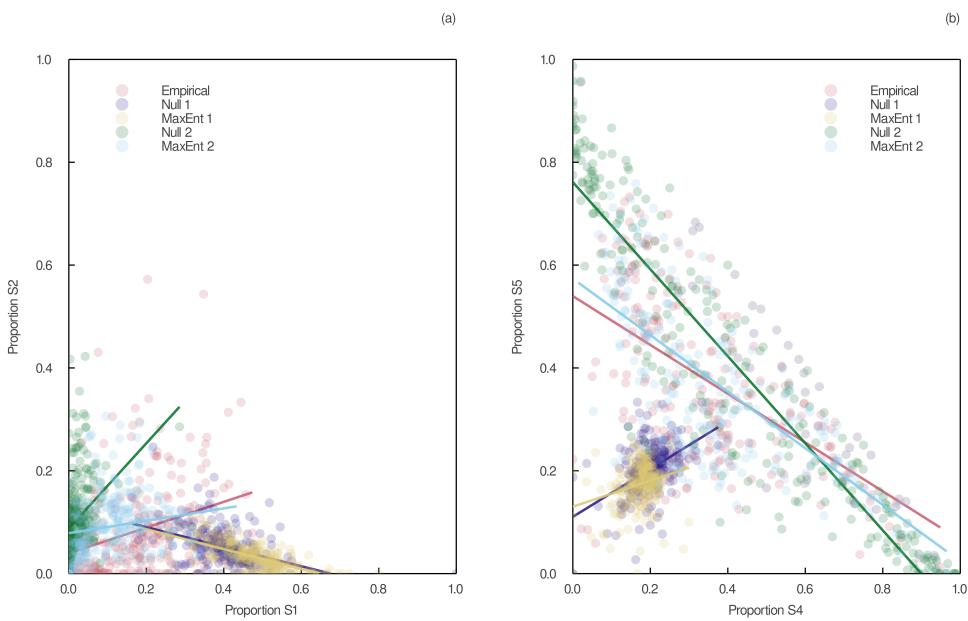
## 6

## Conclusion

The principle of maximum entropy is a robust mathematical method of finding least-biased probability distributions that have some specified properties given by prior knowledge about a system. We first applied this conventional MaxEnt approach on food webs to predict species level properties, namely the joint degree distribution and the degree distribution of maximum entropy given known numbers of species and interactions. We found that the joint degree distributions of maximum entropy had a similar shape to the ones of empirical food webs in high-connectance systems. However, these MaxEnt distributions were more symmetric than the ones of empirical food webs when connectance was low, which suggests that other constraints might be needed to improve these predictions in low-connectance systems. Then, we used a slightly different approach that aimed at finding heuristically the network configuration with the highest SVD



**Figure 5** Motifs profile of empirical and predicted food webs. Empirical networks include most food webs archived on Mangal, as well as the New Zealand and Tuesday Lake datasets (our complete dataset). Null 1: Type I null model based on connectance. MaxEnt 1: Type I heuristic MaxEnt model based on connectance. Null 2: Type II null model based on the joint degree sequence. MaxEnt 2: Type II heuristic MaxEnt model based on the joint degree sequence. Boxplots display the median proportion of each motif (middle horizontal lines), as well as the first (bottom horizontal lines) and third (top horizontal lines) quartiles. Vertical lines encompass all data points that fall within 1.5 times the interquartile range from both quartiles, and dots are data points that fall outside this range. Motifs names are from Stouffer et al. (2007).



**Figure 6** Pairwise relationships between motifs proportions of empirical and predicted food webs. Empirical networks include most food webs archived on Mangal, as well as the New Zealand and Tuesday Lake datasets (our complete dataset). Null 1: Type I null model based on connectance. MaxEnt 1: Type I heuristic MaxEnt model based on connectance. Null 2: Type II null model based on the joint degree sequence. MaxEnt 2: Type II heuristic MaxEnt model based on the joint degree sequence. Regression lines are plotted in each panel. Motifs names are from Stouffer et al. (2007).

entropy, i.e. whose vector of relative singular values has maximum entropy. This network of maximum entropy is the most complex, or random, given the specified structure. We found that the heuristic maximum entropy model based on connectance did not predict the structure of sampled food webs very well. However, the heuristic maximum entropy model based on the entire joint degree sequence, i.e. on the number of prey and predators for each species, gave more convincing results. Indeed, this model reproduced food-web structure surprisingly well, including the highly informative motifs profile. Nevertheless, it was not able to predict realistic food-chain lengths.

Our results bring to the forefront the role of the joint degree distribution in shaping food-web structure. This echoes the work of Fortuna et al. (2010), who found that the degree distribution of ecological networks drive their emerging structure such as their nestedness and modularity. Network ecologists tend to focus on several measures of food webs when studying the ecological consequences of their structure (McCann 2011; Delmas et al. 2019). In fact, following Williams (2011), we believe there is a lot more ecological information in the deviation between these properties in empirical systems and in their maximum entropy configuration given a fixed joint degree sequence.

**6.1. Alternative MaxEnt models** In this contribution, we used a method based on simulated annealing to find the network configuration with the highest SVD entropy while fixing some aspects of its structure. However, there are different ways to generate adjacency matrices using MaxEnt. Another technique, also based on simulated annealing, could begin by generating a food web randomly with fixed numbers of species and interactions and calculating its joint degree distribution. Pairs of interactions could then be swapped sequentially until we minimize the divergence between the calculated joint degree distribution and the one of maximum entropy obtained analytically. In that case, this is the entropy of the joint degree distribution that would be maximized, not the one of the network's topology. To a certain extent, this method would thus bridge the gap between the analytical and heuristic approaches presented in this article. More research is needed to compare the quality of different methods generating adjacency matrices of food webs using MaxEnt.

Maximum entropy graph models are another type of methods that predict a distribution of adjacency matrices under soft or hard constraints (e.g., Park and Newman 2004; Cimini et al. 2019). Under hard constraints, every network with a non-zero probability exactly satisfies the constraints on its structure. This is in contrast with soft constraints, which require that networks satisfy them on average (i.e. many networks with a non-zero probability do not have the exact structure set by the constraints). Maximum entropy graph models are helpful because they can provide probability distributions for many network properties by measuring the structure of all adjacency matrices with a non-zero probability. However, we consider that our approach based on simulated annealing is more flexible and more computationally efficient. Indeed, many measures of food-web structure are hard to translate into mathematical constraints. Moreover, because food webs are directed networks that can have self-loops, it makes the mathematical derivation of maximum entropy graph models difficult. We believe that identifying heuristically what really constrains the topology of food webs is a useful first step before attempting to derive the mathematical formulation of a maximum entropy graph model for food webs.

**6.2. Applications** Our analytical and heuristic models can be applied for different purposes. First, they could be used to generate first-order approximations of a network's properties when state variables are known empirically. For example, knowing the number of species in an ecological community, we can predict its number of interactions using the flexible links model and then predict its joint degree distribution with minimal biases using the principle of maximum entropy. This could prove particularly useful when predicting network structure at large spatial scales, subdividing the study area into smaller communities (e.g., grid cells). Indeed, because

species richness and other ecological data are increasingly abundant (e.g., Dickinson, Zuckerberg, and Bonter 2010), validated MaxEnt models can be used to respond to a wider range of macroecological questions regarding food webs.

Second, our analytical model can be used to generate informative priors in Bayesian analyses of the structure of ecological networks (e.g., Cirtwill et al. 2019). Indeed, the probability distribution of maximum entropy derived using MaxEnt can be used as a prior that can be constantly updated with novel data. For instance, if we know the number of species and the number of interactions, we can get the degree distribution of maximum entropy, as shown in this contribution. The degree distribution represents the probability that a species can interact (as a predator or a prey) with a number of other species. Data on species interactions can be used to update the prior degree distribution to generate a more accurate posterior distribution, thus improving our description and understanding of the system.

Third, our analytical and heuristic models can be used to make better predictions of pairwise species interactions by constraining the space of feasible networks, as discussed in Strydom et al. (2021). In other words, we can use the network configuration and/or specific measures of food-web structure derived using MaxEnt to ensure that our predictions of interspecific interactions form feasible networks. This means that the probability that two species interact can be conditional on the network structure and on the probability of interactions of all other species pairs. For that purpose, MaxEnt can be used to predict network structure when other data is lacking.

Finally, our analytical and heuristic models can be used as alternative null models of ecological networks to better understand and identify the ecological processes driving food-web structure. Indeed, these mechanisms can be better described when analyzing the deviation of empirical data from MaxEnt predictions. A strong deviation would indicate that ecological mechanisms not encoded in the statistical constraints is at play for the system at hand. If deviations are systematic, the maximum entropy model might need to be revised to include appropriate ecological constraints. This revision process helps us reflect on and identify what really constrains food-web structure.

The principle of maximum entropy can thus be applied for both the prediction and understanding of natural systems. Therefore, the model interpretation depends on how we use it. It can be used as a baseline distribution to identify the ecological constraints organizing natural systems. It can also be used as predictions of ecological systems. This distinction between understanding and predicting is essential when using and interpreting MaxEnt models.

**6.3. Final remarks** One of the biggest challenges in using the principle of maximum entropy is to identify the set of state variables that best reproduce empirical data. We found that the number of species and the number of interactions are important state variables for the prediction of the joint degree distribution. Similarly, we found that the numbers of prey and predators for each species in a food web are important state variables for the prediction of the network configuration. However, our predictions overestimated the symmetry of the joint degree distribution for our analytical model and the maximum trophic level and network diameter for our heuristic model. We should thus continue to play the ecological detective to find these other topological constraints that would improve the predictions of MaxEnt models and help us understand better what really drives food-web structure.

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