

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.

1 Introduction

2 Statistical and mathematical models can help fill many gaps in our knowledge about species in-
3 teractions. Predictive and null models are two complementary types of models that have been
4 developed in network ecology for this purpose. On one hand, predictive models can partially
5 alleviate the Eltonian shortfall, which describes our current lack of knowledge on food webs
6 and other ecological networks (Hortal et al. 2015). A variety of such models have recently
7 been developed using machine learning and other statistical tools, most of which are presented
8 in Strydom et al. (2021). On the other hand, null models help us identify potential ecological
9 mechanisms that drive species interactions. They do so by comparing empirical data with an
10 unbiased distribution of measures generated using a set of rules that exclude the mechanism of
11 interest (Fortuna and Bascompte 2006; Delmas et al. 2019). Both types of models are frequently
12 topological, i.e. they often predict the adjacency matrix or specific measures of network struc-
13 ture without taking into account species' identity. According to Strydom et al. (2021), these
14 topological models could be used to make better predictions of pairwise species interactions by
15 constraining the space of feasible networks.

16 The principle of maximum entropy (MaxEnt) is a statistical and topological model that can be
17 used for both of these purposes, i.e. to make predictions of network structure and to better un-
18 derstand processes shaping ecological networks. Food-web properties that can be derived using
19 MaxEnt are varied and pertain to different elements of the network (i.e. at the species (node),
20 the interaction (edge) or the community (network) levels). Because MaxEnt is a method of find-
21 ing probability distributions that are least biased given partial knowledge about a system, these
22 properties need to be represented probabilistically. Otherwise, some data transformation might
23 be needed. For example, at the species level, MaxEnt can be used to predict the distribution
24 of trophic levels among species, as well as the distribution of species' vulnerability (number of
25 predators) and generality (number of preys). By contrast, at the interaction level, predictions
26 can be made on the distribution of interaction strengths in weighted food webs. At the commu-
27 nity level, it can give us a probability distribution of potential networks or of specific measures
28 of their emerging structure. The applicability and performance of this method depend on the
29 ecological information available and on our capacity to find the set of state variables that best

30 represent natural systems and to translate them into appropriate statistical constraints. MaxEnt
31 has been used in a wide range of disciplines, from thermodynamics to chemistry and biology
32 (Martyushev and Seleznev 2006). It has also been proven useful in ecology, e.g. in species dis-
33 tribution models (Phillips, Anderson, and Schapire 2006) and macroecological models (Harte
34 et al. 2008; Harte and Newman 2014). The probability distribution of the variable of interest
35 with the maximum entropy value is unique and least biased under the set of constraints used.
36 These constraints are built using state variables, i.e. variables that represent the macrostate of
37 the system. Having a validated maximum entropy model for the system at hand allows us to
38 make rigorous predictions using a minimal amount of data, as well as helping us describe the
39 most important factors driving that system.

40 Despite its extensive use in graph and network theories (e.g., Park and Newman 2004; van der
41 Hoorn, Lippner, and Krioukov 2018), MaxEnt has in comparison been little used in network
42 ecology. Like other real system networks, food webs and other ecological networks are repre-
43 sented mathematically as graphs. However, the very nature of food webs (directed simple graphs
44 frequently having self-loops) makes the mathematical optimization of maximum entropy graph
45 models more complicated than with many other types of (non-ecological) networks. MaxEnt has
46 nevertheless been used to predict the degree distribution of bipartite ecological networks from
47 the number of species and the number of interactions (Williams 2011) and to predict interaction
48 strengths between species pairs using their relative abundances within an optimal transportation
49 theory regularized with information entropy (Stock, Poisot, and De Baets 2021). However, to
50 the best of our knowledge, MaxEnt has never been used to predict food-web structure directly,
51 even though food webs are among the most documented and widespread ecological networks.

52 In this contribution, we used two complementary approaches to predict the structure of food
53 webs using the principle of maximum entropy. We then compared our predictions against em-
54 pirical data and null and neutral models commonly used in network ecology. The first approach
55 consists in deriving constrained probability distributions of given network properties directly.
56 We derived the joint degree distribution (the joint probability distribution that a species has a
57 given number of prey and predators in a food web) of maximum entropy using only the number
58 of species S and the number of interactions L as state variables. Then, we predicted the degree

59 distribution of maximum entropy directly from the joint degree distribution since the first is the
60 sum of the marginal distributions of the second (a species' degree is the sum of its in and out-
61 degrees). Because of the scarcity of empirical data on the number of interactions in ecological
62 networks, we present a method to predict L from S (Box 1), thus allowing the prediction of the
63 joint degree distribution from S solely. In turn, the second approach consists in finding, using
64 different constraints, the adjacency matrix of maximum entropy from which network properties
65 can be measured. To do so, we used a flexible and heuristic approach based on simulated an-
66 nealing (an optimization algorithm) to find networks *close* to maximum entropy. As discussed
67 above, our choice of algorithm stands from the very nature of food webs (i.e. simple directed
68 networks allowing self-loops) that makes the analytical derivation of a maximum entropy graph
69 model difficult. We first built our type I MaxEnt network model constrained by the connectance
70 of the network (i.e. the ratio L/S^2). A comparison of this model against empirical data indi-
71 cated that connectance alone was not sufficient to predict many aspects of network structure.
72 For this reason, we built our type II MaxEnt network model, which instead uses the whole joint
73 degree sequence as a constraint. Overall, we found that this second model was much better at
74 predicting food-web structure than the one based on connectance.

75 **The principle of maximum entropy: A primer for ecologists**

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

87 distributions found in nature.

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

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

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

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

104 where g_i is the mathematical formulation of the constraint i and c_i , its value. Note that F is just
105 Shannon's entropy to which we added terms that each sums to zero ($g_i = c_i$). F is maximized
106 by setting to 0 its partial derivative with respect to $p(n)$. In this contribution, we show how this
107 can be done by deriving the joint degree distribution analytically from the number of species
108 and the number of interactions in food webs.

109 **Data and code**

110 We tested our analytical and heuristic MaxEnt models against open food-web data queried from
111 three different sources and integrated into what we call our *complete dataset*. These sources
112 include (1) terrestrial and aquatic food webs sampled globally and archived on the ecologi-
113 cal interactions database Mangal; (2) freshwater stream food webs from New Zealand; and (3)
114 aquatic food webs from Tuesday Lake (Michigan, United States). First, all food webs archived
115 on mangal.io (Poisot et al. 2016; Banville, Vissault, and Poisot 2021) were directly queried
116 from the database ($n = 235$). Most ecological networks archived on Mangal are multilayer net-
117 works, i.e. networks that describe different types of interactions. We kept all networks whose
118 interactions were mainly of predation and herbivory types, and removed the largest network
119 ($S = 714$) for computational efficiency reasons. Then, to this set we added food webs from two
120 different sources: the New-Zealand dataset ($n = 21$; Pomeranz et al. 2018) and the Tuesday
121 lake dataset ($n = 2$; Cohen, Jonsson, and Carpenter 2003). Of these two datasets, 19 networks
122 had data on species' relative abundances that were used in the neutral model (Box 2). These 19
123 networks constitute our *abundance dataset*, which is a subset of our complete dataset.

124 All code and data to reproduce this article are available at the Open Science Framework. Data
125 cleaning, simulations and analyses were conducted in Julia v1.5.4.

126 **Analytical models: Measures of maximum entropy**

127 **Joint degree distribution**

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

134 We want to maximize Shannon's entropy

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

¹³⁵ subject to the following constraints:

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

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

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

¹³⁶ The first constraint g_1 is our normalizing constraint, whereas the other two (g_2 and g_3) fix the
¹³⁷ average of the marginal distributions of k_{in} and k_{out} to the linkage density L/S . It is important
¹³⁸ to notice that $\langle k_{in} \rangle = \langle k_{out} \rangle$ because every edge is associated to a predator and a prey. Therefore,
¹³⁹ without any further constraints, we expect the joint degree distribution of maximum entropy to
¹⁴⁰ be a symmetric probability distribution with regards to k_{in} and k_{out} . However, this does not mean
¹⁴¹ that the joint degree *sequence* will be symmetric, since the joint degree sequence is essentially
¹⁴² a random realization of its probabilistic counterpart.

¹⁴³ The joint probability distribution of maximum entropy given these constraints is found using the
¹⁴⁴ method of Lagrange multipliers. To do so, we seek to maximize the following expression:

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

¹⁴⁵ where λ_1 , λ_2 , and λ_3 are the Lagrange multipliers. The probability distribution that maximizes
¹⁴⁶ entropy is obtained by finding these values. As pointed out in the introduction, F is just Shan-
¹⁴⁷non's entropy to which we added terms that each sums to zero (our constraints). F is maximized
¹⁴⁸ by setting to 0 its partial derivative with respect to $p(k_{in}, k_{out})$. Because the derivative of a con-
¹⁴⁹stant is zero, this gives us:

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

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

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

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

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

152 where $Z = e^{1+\lambda_1}$ is called the partition function. The partition function ensures that probabilities

153 sum to 1 (our normalization constraint). It can be expressed in terms of λ_2 and λ_3 as follows:

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

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

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

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

156 We solved eq. 12 and eq. 13 numerically using the Julia library JuMP.jl v0.21.8 (Dunning,
157 Huchette, and Lubin 2017). JuMP.jl supports nonlinear optimization problems by providing
158 exact second derivatives that increase the accuracy and performance of its solvers. The estimated
159 values of λ_2 and λ_3 can be substituted in eq. 10 to have a more workable expression for the joint
160 degree distribution.

161 We predicted the joint degree distribution of maximum entropy for each food web in our com-

plete dataset, i.e. using their numbers of species and numbers of interactions as state variables.
We then sampled one realization of the degree sequence for each network using the probabilities given by the joint degree distribution. In fig. 1 (left panels), we show the relationship between k_{out} and k_{in} standardized by the number of species in their networks, for empirical and maximum entropy joint degree distributions. We see 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} closer to 1). However, plotting the difference between predicted and empirical values for each species gives a different perspective. The right panel of fig. 1 presents these differences when species are ordered by their total degree in their network (i.e. by the sum of their in and out-degrees). Indeed, our predicted joint degree sequences have the same number of species 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. When we associate predictions and empirical data according to their rank in total degrees, we see that species predicted to have a higher generality (number of preys) generally have a lower vulnerability (number of preys) than what is observed (and conversely). 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.

[Figure 1 about here.]

We plotted the Kullback–Leibler divergence between in and out-degree distributions to compare the symmetry of empirical and maximum entropy joint degree sequences fig. 2. As we expected, our model predicted more similar in-degree and out-degree distributions than empirical data. However, this difference decreased with connectance right panel of 2. Overall, this suggests that other ecological constraints might be needed to account for the asymmetry of the joint degree distribution, especially for networks with a lower connectance.

[Figure 2 about here.]

187 **Degree distribution**

188 The degree distribution $p(k)$ represents the probability that a species has k interactions in a food
189 web, with $k = k_{in} + k_{out}$. It can thus be directly obtained from the joint degree distribution:

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

190 In fig. S2, we show that the degree distribution of maximum entropy, given S and L , predicts
191 very low probabilities that a species will be isolated in its food web (i.e. having $k = 0$). As
192 MacDonald, Banville, and Poisot (2020) pointed out, the size of food webs should at least be
193 of $S - 1$ interactions, since a lower number would yield isolated species, i.e. species without
194 any predators or preys. Our results show that, under our purely information-theoretic model,
195 the probability that a species is isolated is quite high when the total number of interactions is
196 below this threshold. The expected proportion of isolated species rapidly declines by orders of
197 magnitude with increasing numbers of species and interactions.

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

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

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

201 This can be solved numerically using the constraint of the average degree $\langle k \rangle = \frac{2L}{S}$ of a species.
202 Note that the mean degree is twice the value of the linkage density, because every link must be
203 counted twice when we add in and out-degrees together.

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

204 The numerical solution is identical to the one we obtained using the joint degree distribution
205 as an intermediate. Ecologists wanting to model a system without considering isolated species
206 could simply change the lower limit of k to 1 and solve the resulting equation numerically.

207 In this section, we showed how important measures of food-web structure, namely the degree
208 distribution and the joint degree distribution, could be derived with the principle of maximum
209 entropy using minimal knowledge on a biological community. This type of models, although
210 useful to make least-biased predictions on many network properties, can be hard to apply for
211 other measures. Indeed, there are dozens of measures of network structure (Delmas et al. 2019)
212 and many are not calculated with mathematical equations, but with algorithms. Moreover, the
213 applicability of this method to empirical systems is limited by the state variables we can actu-
214 ally measure and use. In the next section, we propose a more flexible method to predict many
215 measures of network structure simultaneously, i.e. by finding heuristically the configuration of
216 the network having maximum entropy given partial knowledge of its emerging structure.

217 **Box 1 - Working with predicted numbers of interactions**

218 Our models need information on the number of species and the number of interactions. However,
219 since the later is rarely estimated empirically, ecologists might need to use predictive methods
220 to estimate the total number of interactions in a food web.

221 We used the flexible links model of MacDonald, Banville, and Poisot (2020) to predict the
222 number of interactions from the number of species. The flexible links model, in contrast to other
223 predictive models of the number of interactions, incorporates meaningful ecological constraints
224 into the prediction of L , namely the minimum $S - 1$ and maximum S^2 numbers of interactions
225 in food webs. It estimates the proportion of the $S^2 - (S - 1)$ *flexible links* that are realized.
226 More precisely, this model states that the number of *realized* flexible links (or interactions)
227 L_{FL} in a food web represents the number of realized interactions above the minimum (i.e. $L =$
228 $L_{FL} + S - 1$) and is obtained from a beta-binomial distribution with $S^2 - (S - 1)$ trials and
229 parameters $\alpha = \mu e^\phi$ and $\beta = (1 - \mu)e^\phi$:

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

230 where μ is the average probability across food webs that a flexible link is realized, and ϕ is the

231 concentration parameter around μ .

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

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

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

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

248 [Figure 3 about here.]

249 **Box 2 - Corresponding null and neutral models**

250 **Null models (types I and II)**

251 Our heuristic MaxEnt models, predicting adjacency matrices, were compared with two topolog-
252 ical null models. The first is the type I null model of Fortuna and Bascompte (2006), in which

253 the probability that a species i predares on another species j is given by

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

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

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

256 where k_{in} and k_{out} are the in and out-degrees, respectively. The type I null model is based on
257 connectance, whereas the type II null model is based on the joint degree sequence. Therefore,
258 the type I and II topological null models correspond with our type I and II MaxEnt network
259 models, respectively, since they use similar constraints.

260 We predicted both types of null networks for all empirical networks in our complete dataset
261 ($n = 257$). We converted all probabilistic networks to Boolean networks by generating 100
262 random Boolean networks for each of these probabilistic webs. Then, we counted the number
263 of times each interaction was sampled, and kept the L entries that were drawn the most amount
264 of time, with L given by the number of interactions in each food web. This ensured that the
265 resulting null networks had the same number of interactions as their empirical counterparts.

266 Neutral model

267 We also compared our MaxEnt network models with a neutral model of relative abundances, in
268 which the probabilities of interaction are given by

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

269 where n_i and n_j are the abundances (or biomass) of both species, and N is the total abundance
270 (or biomass) of all species in the network. We predicted neutral abundance matrices for all

271 empirical networks in our abundance dataset ($n = 19$), and converted these weighted matrices
272 to Boolean networks using an approach analogue to the one we used for our null models.

273 **Heuristic models: Networks of maximum entropy**

274 **From Shannon's to SVD entropy**

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

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

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

297 where s_i are the relative singular values of the adjacency matrix ($s_i = \sigma_i / \sum_{i=1}^R \sigma_i$, where σ_i
 298 are the singular values). Note that the distribution of relative singular values is analogous to
 299 a probability distribution, with $0 < s_i < 1$ and $\sum s_i = 1$. Thus, this measure also satisfies
 300 all four properties of an appropriate entropy measure (see introduction), while being a proper
 301 measure of the internal complexity of food webs (Strydom, Dalla Riva, and Poisot 2021). Fol-
 302 lowing Strydom, Dalla Riva, and Poisot (2021), we standardized this measure with the rank R of
 303 the matrix (i.e. $J / \ln(R)$) to account for the difference in dimensions between networks (*sensu*
 304 Pielou's evenness; Pielou 1975). We used SVD entropy to predict the network configuration
 305 of maximum entropy (i.e. of maximum complexity) heuristically given a predetermined set of
 306 constraints.

307 MaxEnt network models (types I and II)

308 We built two types of MaxEnt network models: one based on connectance (type I MaxEnt net-
 309 work model) and the other based on the joint degree sequence (type II MaxEnt network model).
 310 They are based on the same constraints as the types I and II null models presented above. For
 311 both models, we used a simulated annealing algorithm with 4 chains, 2000 steps and an initial
 312 temperature of 0.2. For each chain, we first generated one random Boolean matrix with the same
 313 order (number of species) as empirical webs, while maintaining the total number of interactions
 314 (type I MaxEnt network model) or rows and columns sums (type II MaxEnt network model).
 315 These are our initial configurations. Then, we swapped interactions sequentially while main-
 316 taining the original connectance or the joint degree sequence for types I and II MaxEnt network
 317 model, respectively. Configurations with a higher SVD entropy than the previous one in the
 318 chain were always accepted, whereas they were accepted with a probability conditional to a de-
 319 creasing temperature when lower. The final configuration with the highest SVD entropy among
 320 the four chains constitute our estimated MaxEnt network. Even though we decided to work with
 321 point estimates, it is possible to have a (non MaxEnt) probability distribution of networks when

322 working with the entire chains (or part of the chains). For each network in our complete and
323 abundance datasets, we estimated their configuration with maximum entropy using both types
324 of MaxEnt network models.

325 **Structure of MaxEnt networks**

326 We compared different measures of the structure of empirical food webs with the ones of null,
327 neutral, and MaxEnt networks [tbl. 1](#), and [2](#). For instance, we measured the nestedness ρ accord-
328 ing to Staniczenko, Kopp, and Allesina (2013), i.e. using the spectral radius of the adjacency
329 matrix. Nestedness indicates how much the diet of specialist species is a subset of the one of
330 generalists, and is strongly associated with network modularity (Fortuna et al. 2010). We also
331 measured the maximum trophic level *maxtl*, network diameter *diam* (i.e. the longest of the short-
332 est paths between all species pairs; Albert and Barabasi 2002), the average maximum similarity
333 between species pairs *MxSim*, the proportion of cannibal species *Cannib* (i.e. the proportion of
334 self loops), and the proportion of omnivorous species *Omniv* (i.e. species whose preys are of
335 different trophic levels). *MxSim*, *Cannib*, and *Omniv* are more deeply defined in Williams and
336 Martinez (2000).

337 Overall, we found that models based on the joint degree sequence (type II null and MaxEnt
338 network models) reproduced the structure of empirical networks much better than the ones based
339 on connectance and the neutral model of relative abundances. On average, the type II MaxEnt
340 network model was better at predicting nestedness (0.62 ± 0.08) than its corresponding null model
341 (0.73 ± 0.05 ; empirical networks: 0.63 ± 0.09), as well as the proportion of cannibal species.
342 However, the type II null model was better at predicting network diameter and average maximum
343 similarity between species pairs. Predictions were similar between both type II models for the
344 maximum trophic level and the proportion of omnivorous species.

Table 1: Standardized mean differences of predicted network measures with empirical data for all networks ($n = 257$). Positive (negative) values indicate that the measure is overestimated (underestimated) on average. Empirical networks are all food webs archived on Mangal, as well as the New Zealand and Tuesday lake food webs (our complete dataset). Null 1: Type I null model based on connectance. MaxEnt 1: Type I MaxEnt network model based on connectance. Null 2: Type II null model based on the joint degree sequence. MaxEnt 2: Type II MaxEnt network model based on the joint degree sequence. ρ : 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 differences of predicted network measures with empirical data for networks having abundance data ($n = 19$). Positive (negative) values indicate that the measure is overestimated (underestimated) on average. Empirical networks are all New Zealand and Tuesday lake food webs with abundance data (our abundance dataset). Null 1: Type I null model based on connectance. MaxEnt 1: Type I MaxEnt network model based on connectance. Null 2: Type II null model based on the joint degree sequence. MaxEnt 2: Type II MaxEnt network model based on the joint degree sequence. ρ : 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

³⁴⁵ The picture slightly changes when we consider another important property of ecological networks, i.e. their motifs profile. We measured the proportion of three-species motifs, which can

347 be considered as simple building blocks of ecological networks (Milo et al. 2002; Stouffer et al.
348 2007). Motifs are the backbone of complex ecological networks from which network structure
349 is built upon and play a crucial role in community dynamics and assembly (Bastolla et al. 2009;
350 Stouffer and Bascompte 2011). In fig. 4, we show that the motifs profile of networks generated
351 using the type II MaxEnt network model was very close to the one of empirical data, and that
352 they made better predictions than the type II null model. This is also shown in fig. 5, where we
353 see that relationships between motifs pairs of empirical food webs are very similar to the ones
354 of the type II MaxEnt networks. Overall, these results suggest that the type II MaxEnt network
355 model can reproduce many aspects of network structure. This highlights the importance of the
356 joint degree sequence in shaping ecological networks.

357 [Figure 4 about here.]

358 [Figure 5 about here.]

359 Moreover, we found that empirical networks are close to their maximum entropy considering a
360 fixed joint degree sequence (fig. S3). Empirical networks had an SVD entropy of 0.89 ± 0.04 ,
361 compared to type II MaxEnt networks which had values of 0.94 ± 0.03 . The relationship between
362 the SVD entropy of empirical food webs and their maximum entropy configuration is plotted in
363 the last panel of fig. 6. We also found no relationship between the difference in SVD entropy
364 between empirical and type II MaxEnt networks and species richness, the number of interactions,
365 or connectance (fig. S4). Similarly, we found no correlation between the difference in SVD
366 entropy and the Jaccard distance of empirical and type II MaxEnt networks.

367 Finally, in fig. 6 we also show how well empirical measures are predicted using the type II
368 MaxEnt network model. In accordance with our previous results, we found that nestedness was
369 very well predicted by our model. However, the type II MaxEnt network model overestimated
370 the maximum trophic level and network diameter, especially for networks with high empirical
371 values. In fig. S5, we show that the pairwise relationships between these four measures and
372 species richness in empirical food webs are similar (in magnitude and sign) to the ones in type
373 II MaxEnt networks.

375 **Conclusion**

376 The principle of maximum entropy is a robust mathematical method of finding least-biased
 377 probability distributions that have some desired properties given by prior knowledge on a sys-
 378 tem. We first used MaxEnt to predict the joint degree distribution and the degree distribution
 379 of maximum entropy given known numbers of species and of interactions. We found that the
 380 resulting joint degree distributions were more symmetric than the ones of empirical food webs,
 381 which suggests that other constraints might be needed to improve those predictions. We also
 382 used MaxEnt to predict networks of maximum entropy with a specified structure. These net-
 383 works are the most complex, or random, given the constraints used. Likewise, we found that
 384 knowledge of species richness and of the number of interactions were not sufficient to reproduce
 385 many aspects of network structure found in nature. However, a model based on the entire joint
 386 degree sequence, i.e. on the number of preys and predators for each species, gave more con-
 387 vincing results. Our type II MaxEnt network model yielded better or similar predictions than
 388 the type II null model, also based on the joint degree sequence, for most measures considered
 389 including the motifs profile. This suggests that the joint degree sequence drives many aspects of
 390 network structure. Indeed, considering our findings that empirical networks are close to max-
 391 imum entropy for a given joint degree sequence, our results suggest that food-web topology is
 392 configured almost entirely randomly around these marginal numbers of predators and preys.

393 **Alternative MaxEnt models**

394 There are different ways to generate food webs using MaxEnt. In this contribution, we used a
 395 method based on simulated annealing to find the network configuration with the highest SVD
 396 entropy while fixing some aspects of its structure. Another technique, also based on simulated
 397 annealing, could start by generating a food web randomly with fixed numbers of species and
 398 interactions and calculating its joint degree distribution. Pairs of interactions could be swapped
 399 sequentially until we minimize the divergence between the calculated joint degree distribution

400 and the one of maximum entropy obtained analytically. In that case, this is the entropy of the
401 joint degree distribution that would be maximized, not the one of the network's topology. To a
402 certain extent, this method would thus bridge the gap between the two approaches presented in
403 this article (i.e. analytical and heuristic MaxEnt models). More research is needed to compare
404 the quality of different methods generating adjacency matrices of food webs using MaxEnt.

405 Another method generating adjacency matrices are maximum entropy graph models, which pre-
406 dict a probability distribution of networks under soft or hard constraints (e.g., Park and Newman
407 2004; Cimini et al. 2019). Under hard constraints, every network with a non-zero probability
408 exactly satisfies the constraints on its structure. This is in contrast with soft constraints, which
409 require that networks satisfy them on average (i.e. many networks with a non-zero probability do
410 not have the exact structure set by the constraints). Maximum entropy graph models are helpful
411 because they can provide probability distributions for many network properties, by measuring
412 the structure of all adjacency matrices with a non-zero probability. However, we consider that
413 our approach based on simulated annealing is more flexible and more computationally efficient.
414 Indeed, many measures of food-web structure are hard to translate into mathematical constraints.
415 Moreover, because food webs are directed networks with self-loops, it makes the mathematical
416 derivation of maximum entropy graph models difficult. We believe that identifying heuristically
417 what really constrains the topology of food webs is a useful first step before attempting to derive
418 the mathematical formulation of a maximum entropy graph model adapted to food webs.

419 Applications

420 Our method and results could be used for different purposes. First, they could be used as first-
421 order approximations of network structure when only state variables are known. This could
422 prove useful when predicting network structure at large spatial scales, where few ecological in-
423 formation is known at that scale. Second, they could be used as informative priors in Bayesian
424 analyses of the structure of ecological networks (e.g., Cirtwill et al. 2019). Third, they could
425 be used to make better predictions of pairwise species interactions by constraining the space of
426 feasible networks, as discussed in Strydom et al. (2021). Finally, they could be used as alter-
427 native null models of ecological networks to better understand ecological mechanisms driving

428 food-web structure. In that case, our model might need to be slightly adapted to give a proba-
429 bility distribution of Boolean networks (in contrast with point estimates of maximum entropy
430 networks).

431 One of the biggest challenges in using the principle of maximum entropy is to identify the set
432 of state variables that best reproduce empirical data. We found that the numbers of preys and
433 predators for each species are important state variables for the prediction of maximum entropy
434 networks. However, our predictions overestimated some measures of network structure, espe-
435 cially the maximum trophic level and network diameter. Therefore, we should continue playing
436 the ecological detective to find these other topological constraints that would improve the pre-
437 dictions of our MaxEnt network models.

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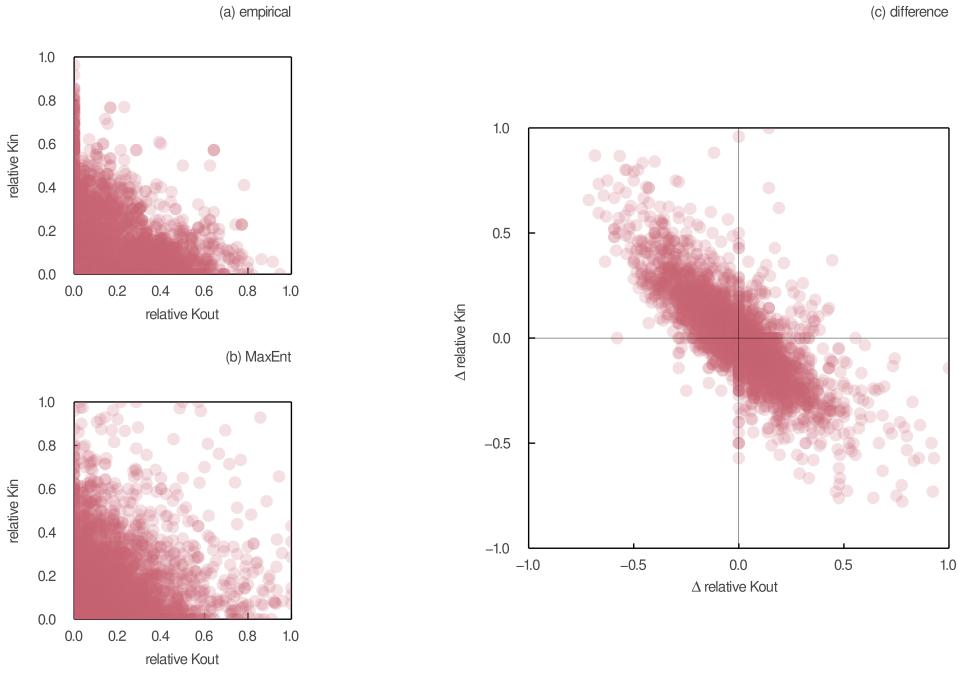


Figure 1: Relative number of predators (k_{in}) as a function of the relative number of preys (k_{out}) for each species in (a) empirical and (b) maximum entropy joint degree sequences. Empirical networks include all food webs archived on Mangal, as well as the New-Zealand and Tuesday lake datasets (our complete dataset). The predicted joint degree sequences were obtained after sampling one realization of the joint degree distribution of maximum entropy for each network. (c) Difference between predicted and empirical values when species are ordered according to their total degrees. In all panels, each dot corresponds to a single species in one of the network of our complete dataset.

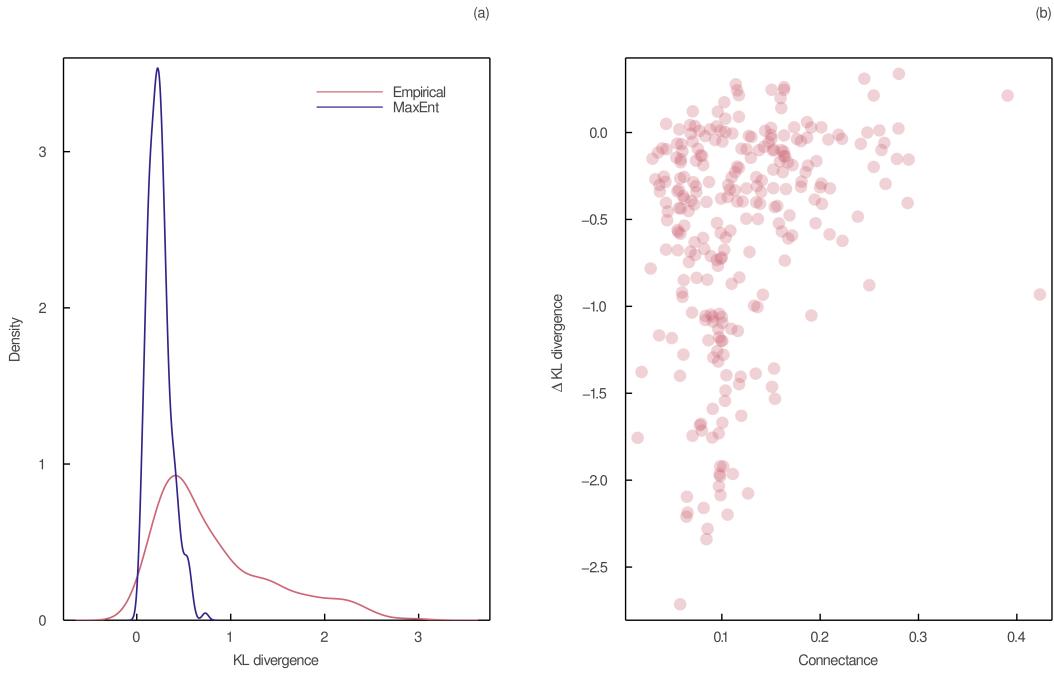


Figure 2: (a) Probability density of KL divergence between in and out-degree sequences of empirical and maximum entropy joint degree sequences. (b) Difference between the KL divergence of empirical and predicted networks as a function of connectance. In both panels, empirical networks include all food webs archived on Mangal, as well as the New-Zealand and Tuesday lake datasets (our complete dataset). The joint degree sequence of simulated networks was obtained after sampling one realization of the joint degree distribution of maximum entropy for each network.

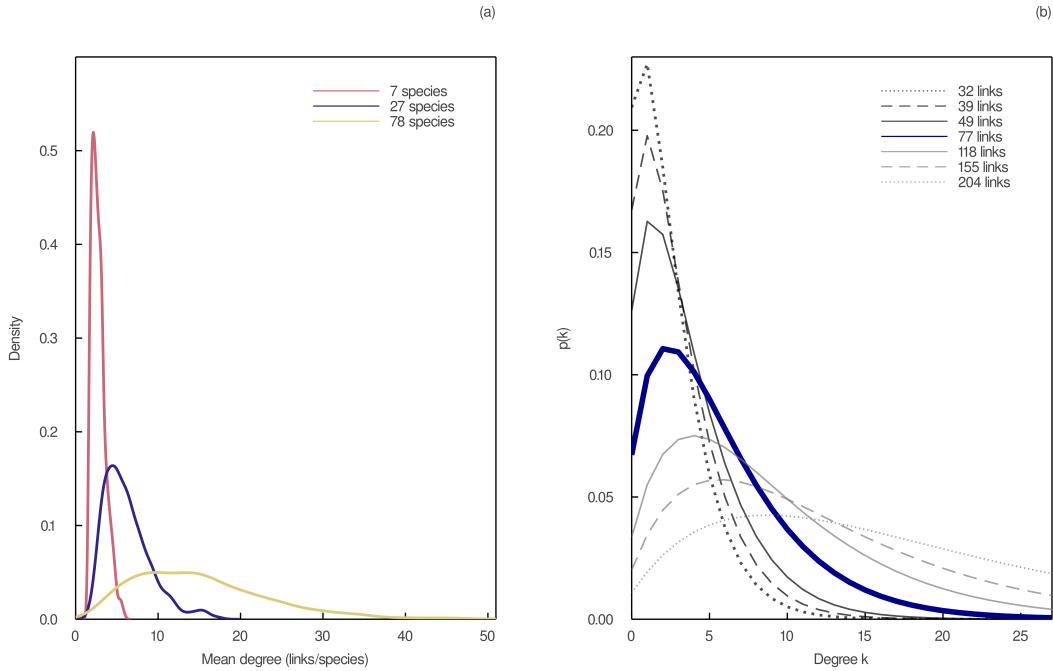


Figure 3: (a) Probability density of the predicted mean degree for different values of species richness. The number of interactions was predicted using the flexible links model fitted to all empirical networks in our complete dataset (eq. 17). (b) Degree distributions of maximum entropy for a network of $S = 27$ species and different numbers of interactions L . 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 was obtained using eq. 14 after solving numerically eq. 15 using different values for the mean degree constraint $2L/S$.

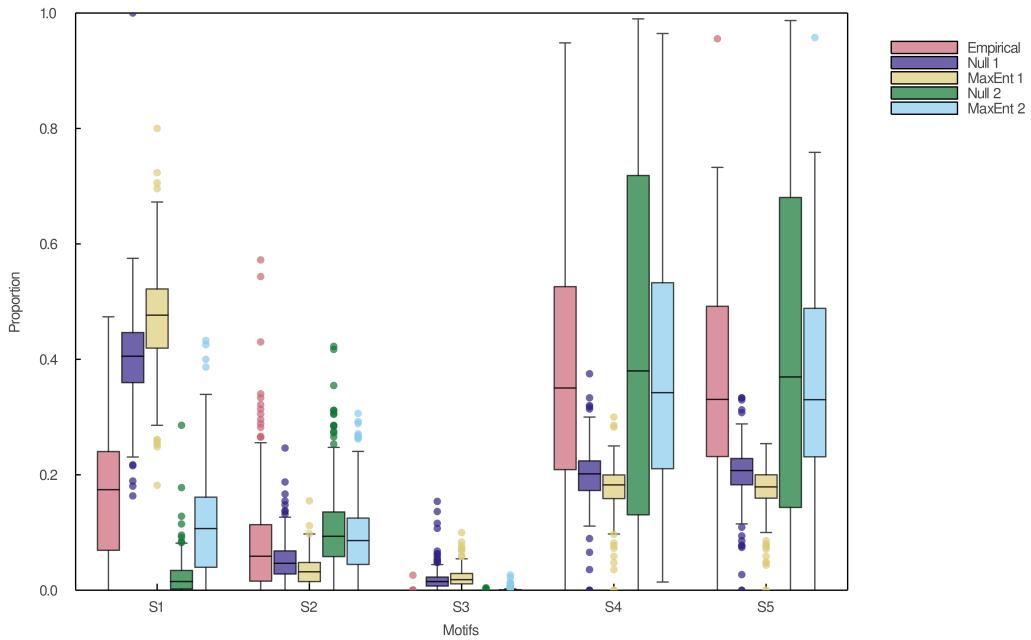


Figure 4: Motifs profile of empirical, maximum entropy, and null food webs. Empirical networks include all food webs archived on Mangal, as well as the New-Zealand and Tuesday lake datasets (our complete dataset). Maximum entropy networks were estimated using a simulated annealing algorithm to find the network of maximum SVD entropy while maintaining the connectance (type I MaxEnt network model) or the joint degree sequence (type II MaxEnt network model). The predictions of the types I and II null models are also plotted. Boxplots display the median proportions 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).

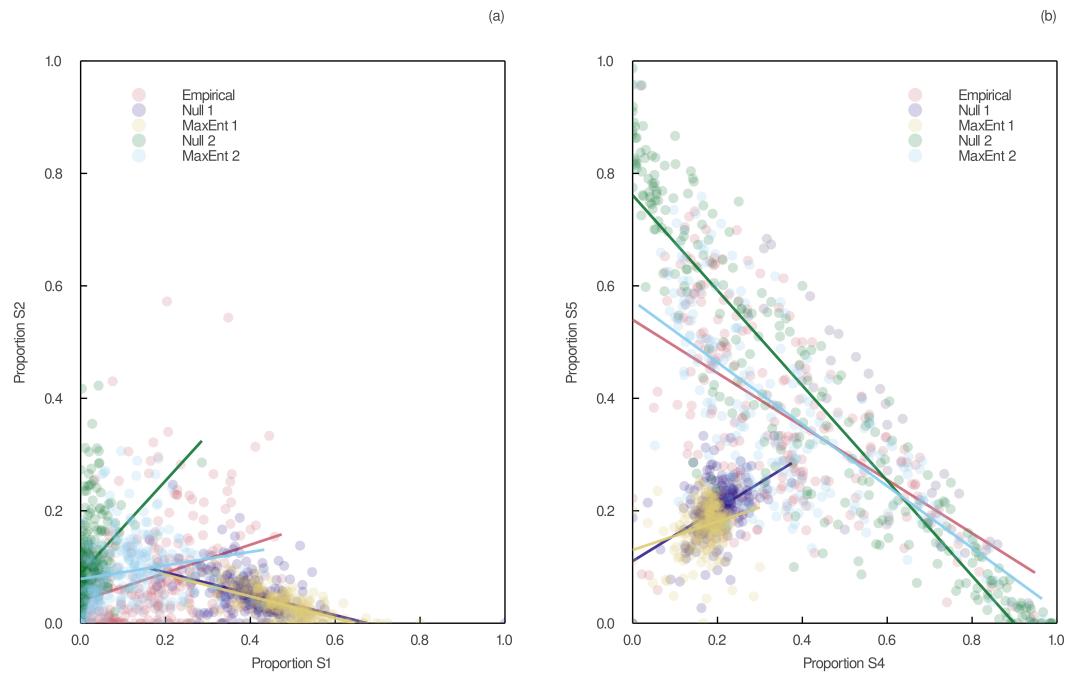


Figure 5: Relationship between motifs proportions of empirical, maximum entropy, and null food webs. Empirical networks include all food webs archived on Mangal, as well as the New-Zealand and Tuesday lake datasets (our complete dataset). Maximum entropy networks were estimated using a simulated annealing algorithm to find the network of maximum SVD entropy while maintaining the connectance (type I MaxEnt network model) or the joint degree sequence (type II MaxEnt network model). The predictions of the types I and II null models are also plotted. Regression lines are plotted in each panel. Motifs names are from Stouffer et al. (2007).

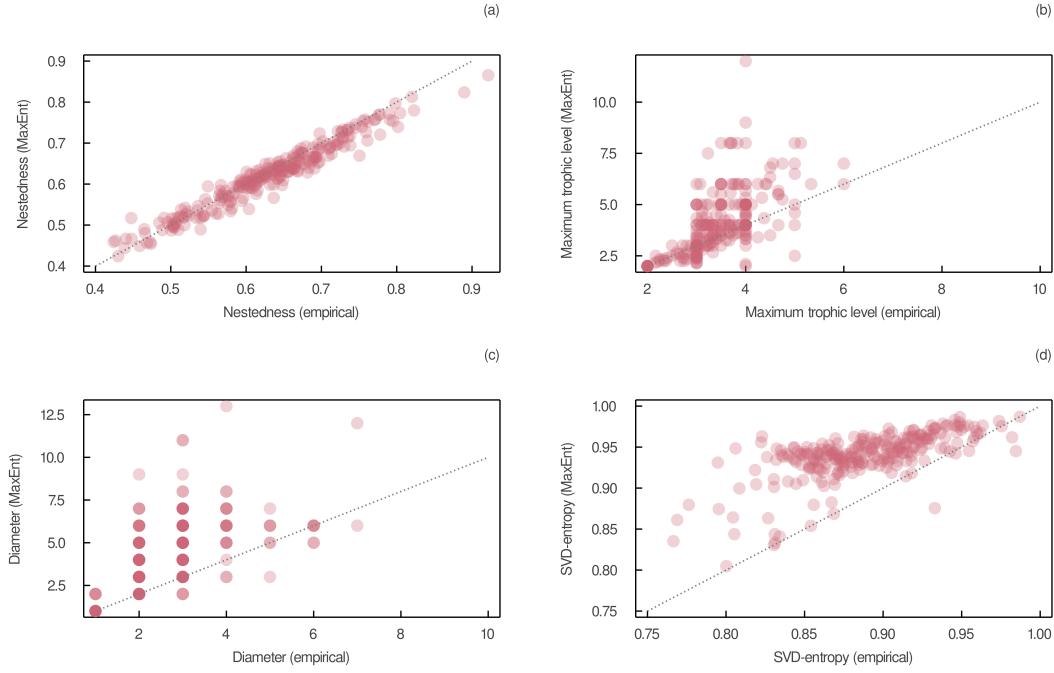


Figure 6: Relationship between the structure of empirical and maximum entropy food webs. Empirical networks include all food webs archived on Mangal, as well as the New-Zealand and Tuesday lake datasets (our complete dataset). Maximum entropy networks were estimated using a simulated annealing algorithm to find the network of maximum SVD entropy while maintaining the joint degree sequence (type II MaxEnt network model). (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.