

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 The constrained structure of ecological networks

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

18 One way to tackle this issue is first to recognize that food webs and other ecological networks
19 are constrained systems. In other words, the space of possible network configurations shrinks
20 as we know more about a network structure. For example, there is a finite number of networks
21 with specified numbers of nodes and edges. Indeed, the structure of ecological networks is first
22 and above all constrained by the number of species, or nodes, present. Food webs with high
23 species richness typically have a lower connectance (MacDonald, Banville, and Poisot 2020)
24 than smaller networks. This is because the number of realized interactions in empirical food
25 webs scales slower than the number of possible species pairs (MacDonald, Banville, and Poisot
26 2020). As shown by Timothée Poisot and Gravel (2014), connectance itself can constrain differ-
27 ent aspects of network structure such as the degree distribution (i.e. the probability distribution
28 of the number of interspecific interactions realized by a species). Other measures, such as the

29 maximum trophic level, can also constrain the space of feasible networks.

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

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

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

55 The principle of maximum entropy (MaxEnt) is a mathematical method of finding probabil-
56 ity distributions, strongly rooted in statistical mechanics and information theory (Jaynes 1957a,

57 1957b; Harremoës and Topsøe 2001). Starting from a set of constraints given by prior knowl-
58 edge of a system (i.e. what we call state variables), this method helps us find least-biased prob-
59 ability distributions subject to the constraints. These probability distributions are guaranteed to
60 be unique given our prior knowledge and represent the most we can say about a system without
61 making more assumptions. For example, if the only thing we know about a biological commu-
62 nity is its average number of individuals per species, the least-biased inference we could make on
63 its species abundance distribution is the exponential distribution (Frank and Smith 2011; Harte
64 and Newman 2014). However, this does not imply that this distribution will be the best fit to
65 empirical data. The challenge is to find the right set of constraints that would best reproduce
66 distributions found in nature.

67 MaxEnt states that the least-biased probability distribution given the constraints used is the one
68 with the highest entropy among all probability distributions that satisfy these constraints. En-
69 tropy is a measure of the average amount of information given by the outcome of a random
70 variable. Many measures of entropy have been developed in physics (Beck 2009), but only
71 a fraction of them could be used as an optimization measure with the principle of maximum
72 entropy. According to Beck (2009) and Khinchin (2013), a measure of entropy H should sat-
73 isfy four properties in the discrete case: (1) it should be a function of a probability distribution
74 $p(n)$ only; (2) it should be maximized when $p(n)$ is uniform; (3) it should not be influenced by
75 outcomes with a null probability; and (4) it should be independent of the order of information
76 acquisition. The Shannon's entropy (Shannon 1948)

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

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

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

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

86 The principle of maximum entropy has been used in a wide range of disciplines, from thermo-
 87 dynamics, chemistry and biology (Martyushev and Seleznev 2006) to graph and network theory
 88 (e.g., Park and Newman 2004; van der Hoorn, Lippner, and Krioukov 2018). It has also been
 89 proven useful in ecology, e.g. in species distribution models (Phillips, Anderson, and Schapire
 90 2006) and macroecological models (Harte et al. 2008; Harte and Newman 2014). In network
 91 ecology, MaxEnt has been used to predict the degree distribution of bipartite networks from the
 92 number of species and the number of interactions (Williams 2011) and to predict interaction
 93 strengths between species pairs using their relative abundances within an optimal transportation
 94 theory regularized with information entropy (Stock, Poisot, and De Baets 2021). However, to
 95 the best of our knowledge, MaxEnt has never been used to predict food-web structure directly,
 96 even though food webs are among the most documented and widespread ecological networks
 97 (Ings et al. 2009).

98 Food-web properties that can be derived using MaxEnt are varied and pertain to different ele-
 99 ments of the network (i.e. at the species (node), the interaction (edge) or the community (net-
 100 work) levels). Because MaxEnt is a method of finding least-biased probability distributions
 101 given partial knowledge about a system, these properties need to be represented probabilistically.
 102 For example, at the species level, MaxEnt can be used to predict the distribution of trophic levels
 103 among species, as well as the distribution of species' vulnerability (number of predators) and
 104 generality (number of prey). By contrast, at the interaction level, predictions can be made on
 105 the distribution of interaction strengths in weighted food webs. At the community level, it can
 106 generate probability distributions of many measures of their emerging structure and of networks
 107 themselves (i.e. a probability distribution that specific network configurations are realized given
 108 the model and constraints). Overall, the potential of this method in the study of food webs is
 109 broad. The applicability and performance of MaxEnt mostly depend on the ecological infor-

110 mation available and on our capacity to find the right set of state variables that best represent
111 natural systems and to translate them into appropriate statistical constraints. Having a validated
112 maximum entropy model for the system at hand allows us to make least-biased predictions using
113 a minimal amount of data, as well as identify the most important ecological processes shaping
114 that system. In other words, MaxEnt is a valuable and underexploited tool in network ecology
115 that allows us to better understand and predict the structure of ecological networks.

116 Analytical and heuristic approaches

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

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

133 For the second approach (heuristic), we focus on network level properties. We used a flexible and
134 heuristic model based on simulated annealing (an optimization algorithm) to find the network
135 configuration *close* to maximum entropy and measured its structure. We developed this heuristic
136 model because the analytical derivation of a maximum entropy graph model of food webs is
137 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.

145 Data and code

We tested our analytical and heuristic MaxEnt models 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` (Timothée Poisot et al. 2016; Banville, Vissault, and Poisot 2021) were directly queried from the database ($N = 235$). Most ecological networks archived on Mangal are multi-layer 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 ($N = 21$; 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. Of the New Zealand and Tuesday Lake datasets, 19 networks had data on species' relative abundances that were used in the neutral model (Box 2). These 19 food webs constitute our *abundance dataset*, which is a subset of our complete dataset.

All code and data to reproduce this article are available at the Open Science Framework. Data cleaning, simulations and analyses were conducted in Julia v1.6.1.

163 **Analytical maximum entropy models**

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

178 **Joint degree distribution**

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

186 We want to maximize Shannon's entropy

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

¹⁸⁷ subject to the following constraints:

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

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

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

¹⁸⁸ The first constraint g_1 is our normalizing constraint, whereas the other two (g_2 and g_3) fix the
¹⁸⁹ average of the marginal distributions of k_{in} and k_{out} to the linkage density L/S . It is important
¹⁹⁰ to notice that $\langle k_{in} \rangle = \langle k_{out} \rangle$ because every edge is associated to a predator and a prey. Therefore,
¹⁹¹ without using any further constraints, we would expect the joint degree distribution of maximum
¹⁹² entropy to be a symmetric probability distribution with regards to k_{in} and k_{out} . However, this
¹⁹³ does not mean that the joint degree *sequence* will be symmetric, since the joint degree sequence
¹⁹⁴ is essentially a random realization of its probabilistic counterpart.

¹⁹⁵ The joint probability distribution of maximum entropy given these constraints is found using the
¹⁹⁶ method of Lagrange multipliers. To do so, we seek to maximize the following expression:

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

¹⁹⁷ where λ_1 , λ_2 , and λ_3 are the Lagrange multipliers. The probability distribution that maximizes
¹⁹⁸ entropy is obtained by finding these values. As pointed out above, F is just Shannon's entropy
¹⁹⁹ to which we added terms that each sums to zero (our constraints). F is maximized by setting to
²⁰⁰ 0 its partial derivative with respect to $p(k_{in}, k_{out})$. Because the derivative of a constant is zero,
²⁰¹ this gives us:

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

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

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

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

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

204 where $Z = e^{1+\lambda_1}$ is called the partition function. The partition function ensures that probabilities
205 sum to 1 (our normalization constraint). It can be expressed in terms of λ_2 and λ_3 as follows:

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

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

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

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

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

213 We assessed the empirical support of this expression using all food webs in our complete dataset.
214 First, we predicted the joint degree distribution of maximum entropy for each of these food webs,
215 i.e. using their number of species and number of interactions as state variables. Then, we sam-
216 pled one realization of the joint degree sequence for each network using the probabilities given

217 by the joint degree distribution of maximum entropy, while fixing the total number of interac-
218 tions. This gave us a random realization of the number of prey and predators for each species in
219 each network. We standardized the predicted k_{out} and k_{in} of each species by the total number of
220 species in their network to generate relative values, which can be compared across networks. In
221 fig. 1 (left panels), we show the relationship between these relative k_{out} and k_{in} obtained from the
222 joint degree distributions of maximum entropy (bottom panel) and this relationship using em-
223 pirical values (top panel). We observe that our model predicts higher values of generality and
224 vulnerability compared to empirical food webs (i.e. relative values of k_{out} and k_{in} both closer to
225 1) for many species. In other words, our model predicts that species that have many predators
226 also have more prey than what is observed empirically (and conversely). This is not surprising,
227 given that our model did not include biological factors preventing generalist predators from hav-
228 ing many prey. Nevertheless, with the exception of these generalist species, MaxEnt adequately
229 predicts that most species have low generality and vulnerability values.

230 Examining the difference between predicted and empirical values for each species gives a slightly
231 different perspective (right panel of fig. 1). To do so, we must first associate each of our predic-
232 tions to a specific species in a network in order to make that comparison. Indeed, our predicted
233 joint degree sequences have the same number of species (elements) as their empirical counter-
234 parts, but they are species agnostic. In other words, instead of predicting a value for each species
235 directly, we predicted the entire joint degree sequence without taking into account species' iden-
236 tity. The challenge is thus to adequately associate predictions with empirical data. In fig. 1, we
237 present these differences when species are ordered by their total degree in their respective net-
238 works (i.e. by the sum of their in and out-degrees). This means that the species with the highest
239 total degree in its network will be associated with the highest prediction, and so forth. Doing so,
240 we see that species predicted to have a higher number of predators than what is observed gen-
241 erally have a lower number of prey than what is observed (and conversely). This is because the
242 difference in total degree ($k_{out} + k_{in}$) between predictions and empirical data is minimized when
243 species are ranked by their total degree (i.e. the average deviation of the sum of relative k_{out} and
244 k_{in} is close to 0 across all species). This result thus shows that the difference between predicted
245 and empirical total degrees is low for most species when ordered by their total degrees. There

246 are no apparent biases towards in or out degrees. In fig. S1, we show how these differences
247 change when species are instead ordered by their out-degrees (left panel) and in-degrees (right
248 panel), respectively.

249 [Figure 1 about here.]

250 Another way to evaluate the empirical support of the predicted joint degree sequences is to com-
251 pare their shape with the ones of empirical food webs. We can describe the shape of a joint degree
252 sequence by comparing its marginal distributions with one another. To do so, we calculated the
253 Kullback–Leibler (KL) divergence between the in and out-degree sequences sampled from the
254 joint degree distribution of maximum entropy. Similarly, we calculated the divergence between
255 the in and out-degree sequences obtained empirically. This allows us to compare the symmetry
256 of empirical and predicted joint degree sequences (left panel of fig. 2). As we expected, our
257 model predicts more similar in-degree and out-degree sequences than empirical data (shown
258 by lower KL divergence values). However, this difference decreases with connectance (right
259 panel of fig. 2). This might be due to the fact that food webs with a low connectance are harder
260 to predict than food webs with a high connectance. Indeed, in low connectance systems, what
261 makes two species interact might be more important for prediction than in high connectance
262 systems, in which what prevents species from interacting might be more meaningful. This im-
263 plies that more ecological information might be needed in food webs with a low connectance
264 because more ecological processes determine interactions compared to non-interactions. There-
265 fore, other ecological constraints might be needed to account for the asymmetry of the joint
266 degree distribution, especially for networks with a lower connectance. However, our MaxEnt
267 model was able to capture quite well the shape of the joint degree sequence for networks having
268 a high connectance.

269 [Figure 2 about here.]

270 **Degree distribution**

271 The joint degree distribution derived using MaxEnt (eq. 10) can be used to obtain the degree
272 distribution of maximum entropy. Indeed, the degree distribution $p(k)$ represents the probability

273 that a species has k interactions in its food web, with $k = k_{in} + k_{out}$. It can thus be obtained
 274 from the joint degree distribution as follows:

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

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

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

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

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

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

282 One aspect of the degree distribution that informs us of its ecological realism is the number of
 283 isolated species it predicts. As MacDonald, Banville, and Poisot (2020) pointed out, the size of
 284 food webs should at least be of $S - 1$ interactions, since a lower number would yield isolated
 285 species, i.e. species without any predators or prey. Because non-basal species must eat to survive,
 286 isolated species could indicate that other species are missing or they could simply be removed
 287 from the food web. In fig. S2, we show that the degree distribution of maximum entropy, given
 288 S and L , gives very low probabilities that a species will be isolated in its food web (i.e. having
 289 $k = 0$) above the $S - 1$ threshold. However, under our purely information-theoretic model,
 290 the probability that a species is isolated is quite high when the total number of interactions is
 291 below $S - 1$. Moreover, the expected proportion of isolated species rapidly declines by orders
 292 of magnitude with increasing numbers of species and interactions. This supports the ecological
 293 realism of the degree distribution of maximum entropy derived above. Nevertheless, ecologists

294 wanting to model a system without allowing isolated species could simply change the lower limit
295 of k to 1 in eq. 15 and solve the resulting equation numerically.

296 Box 1 - Working with predicted numbers of interactions

297 Our analytical MaxEnt models require information on the number of species and the number of
298 interactions. However, since the later is rarely measured empirically, ecologists might need to
299 use predictive models to estimate the total number of interactions in a food web before using
300 MaxEnt. Here we illustrate how this can be done by combining both models sequentially.

301 We used the flexible links model of MacDonald, Banville, and Poisot (2020) to predict the
302 number of interactions from the number of species. The flexible links model, in contrast to other
303 predictive models of the number of interactions, incorporates meaningful ecological constraints
304 into the prediction of L , namely the minimum $S - 1$ and maximum S^2 numbers of interactions
305 in food webs. It estimates the proportion of the $S^2 - (S - 1)$ *flexible links* that are realized.
306 More precisely, this model states that the number of *realized* flexible links (or interactions)
307 L_{FL} in a food web represents the number of realized interactions above the minimum (i.e. $L =$
308 $L_{FL} + S - 1$) and is obtained from a beta-binomial distribution with $S^2 - (S - 1)$ trials and
309 parameters $\alpha = \mu e^\phi$ and $\beta = (1 - \mu) e^\phi$:

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

310 where μ is the average probability across food webs that a flexible link is realized, and ϕ is the
311 concentration parameter around μ .

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

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

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

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

328 [Figure 3 about here.]

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

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

331 The predictions of our heuristic maximum entropy models were compared against two topologi-
 332 cal null models. These null models use the same ecological information as our heuristic models
 333 and thus constitute an adequate baseline for comparison. The first is the type I null model of
 334 Fortuna and Bascompte (2006), in which the probability that a species i predares on another
 335 species j is given by

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

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

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

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

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

349 Neutral model

350 We also compared our heuristic MaxEnt models with a neutral model of relative abundances, in
 351 which the probabilities of interaction are given by

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

352 where n_i and n_j are the abundances (or biomass) of both species, and N is the total abundance
 353 (or biomass) of all species in the network. We generated neutral abundance matrices for all em-
 354 pirical food webs in our abundance dataset, and converted these weighted networks to adjacency

355 matrices of Boolean values using the same method as the one we used for our null models.

356 **Heuristic maximum entropy models**

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

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

369 The principle of maximum entropy can be applied on the network itself if we decompose its
370 adjacency matrix into a non-zero vector of relative values. This is a necessary step when work-
371 ing with food webs, which are frequently expressed as a matrix $A = [a_{ij}]$ of Boolean values
372 representing the presence ($a_{ij} = 1$) or absence ($a_{ij} = 0$) of an interaction between two species i
373 and j . Knowing one or many properties of a food web of interest (e.g., its number of species and
374 number of interactions), we can simulate its adjacency matrix randomly by using these known
375 ecological information to constrain the space of potential networks. The entropy of this hypo-
376 thetical matrix can then be measured after decomposing it into appropriate values. Simulating
377 a series of networks until we find the one having the highest entropy allows us to search for the
378 most complex food-web configuration given the ecological constraints used. This configuration
379 is the least biased one considering the information available. In other words, the most we can
380 say about a network's adjacency matrix, without making more assumptions than the ones given

381 by our incomplete knowledge of its structure, is the one of maximum entropy. Generating the
382 most complex network that corresponds to this structure allows us to explore more easily other
383 properties of food webs under MaxEnt.

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

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

391 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
392 are the singular values). Note that the distribution of relative singular values is analogous to
393 a probability distribution, with $0 < s_i < 1$ and $\sum s_i = 1$. This measure also satisfies all four
394 properties of an appropriate entropy measure above-mentioned, while being a proper measure of
395 the internal complexity of food webs (Strydom, Dalla Riva, and Poisot 2021). Following Stry-
396 dom, Dalla Riva, and Poisot (2021), we standardized this measure with the rank R of the matrix
397 (i.e. $J / \ln(R)$) to account for the difference in dimensions between networks (*sensu* Pielou's
398 evenness; Pielou 1975).

399 **Types I and II heuristic MaxEnt models**

400 We used SVD entropy to predict the network configuration of maximum entropy (i.e. of max-
401 imum complexity) heuristically given different constraints for all food webs in our complete
402 dataset. We built two types of heuristic MaxEnt models that differ on the constraint used. The
403 type I heuristic MaxEnt model is based on connectance, whereas the type II heuristic MaxEnt
404 model is based on the joint degree sequence. These models are thus based on the same con-
405 straints as the types I (Fortuna and Bascompte 2006) and II (Bascompte et al. 2003) null models

406 (Box 2) frequently used to generate random networks topologically. This allows direct com-
407 parison of the performance of null and heuristic MaxEnt models in reproducing the emerging
408 structure of empirical food webs.

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

421 **Structure of MaxEnt networks**

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

433 Overall, we found that models based on the joint degree sequence (type II null and MaxEnt

434 network models) reproduced the structure of empirical networks much better than the ones based
 435 on connectance and the neutral model of relative abundances. On average, the type II MaxEnt
 436 network model was better at predicting nestedness (0.62 ± 0.08) than its corresponding null
 437 model (0.73 ± 0.05 ; empirical networks: 0.63 ± 0.09), as well as the proportion of cannibal
 438 species. This might in part be due because nestedness was calculated using the spectral radius
 439 of the adjacency matrix, which leverages information on the network itself just like the MaxEnt
 440 network models. However, the type II null model was better at predicting network diameter and
 441 average maximum similarity between species pairs. Predictions were similar between both type
 442 II models for the 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 most 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

443 The picture slightly changes when we consider another important property of ecological net-
 444 works, i.e. their motifs profile. We measured the proportion of three-species motifs, which can
 445 be considered as simple building blocks of ecological networks (Milo et al. 2002; Stouffer et al.
 446 2007). Motifs are the backbone of complex ecological networks from which network structure
 447 is built upon and play a crucial role in community dynamics and assembly (Bastolla et al. 2009;
 448 Stouffer and Bascompte 2011). In fig. 4, we show that the motifs profile of networks generated
 449 using the type II MaxEnt network model was very close to the one of empirical data, and that
 450 they made better predictions than the type II null model. This is also shown in fig. 5, where we
 451 see that relationships between motifs pairs of empirical food webs are very similar to the ones
 452 of the type II MaxEnt networks. Overall, these results suggest that the type II MaxEnt network
 453 model can reproduce many aspects of network structure. This highlights the importance of the
 454 joint degree sequence in shaping ecological networks.

455 [Figure 4 about here.]

456 [Figure 5 about here.]

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

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

472 [Figure 6 about here.]

473 Discussion

474 The principle of maximum entropy is a robust mathematical method of finding least-biased
475 probability distributions that have some desired properties given by prior knowledge on a sys-
476 tem. We first used MaxEnt to predict the joint degree distribution and the degree distribution
477 of maximum entropy given known numbers of species and of interactions. We found that the
478 resulting joint degree distributions were more symmetric than the ones of empirical food webs,
479 which suggests that other constraints might be needed to improve those predictions. We also
480 used MaxEnt to predict networks of maximum entropy with a specified structure. These net-
481 works are the most complex, or random, given the constraints used. Likewise, we found that
482 knowledge of species richness and of the number of interactions were not sufficient to reproduce
483 many aspects of network structure found in nature. However, a model based on the entire joint

484 degree sequence, i.e. on the number of prey and predators for each species, gave more convinc-
485 ing results. Our type II MaxEnt network model yielded better or similar predictions than the
486 type II null model, also based on the joint degree sequence, for most measures considered in-
487 cluding the motifs profile. This suggests that the joint degree sequence drives many aspects of
488 network structure. Indeed, considering our findings that empirical networks are close to max-
489 imum entropy for a given joint degree sequence, our results suggest that food-web topology is
490 configured almost entirely randomly around these marginal numbers of predators and prey.

491 Our results bring to the forefront the role of the joint degree distribution in shaping food-web
492 structure. This echoes the work of Williams (2011), which shows using MaxEnt how the degree
493 distribution can drive the structure of bipartite networks. Fortuna et al. (2010) also found that
494 the degree distribution of ecological networks is associated with some of their emerging prop-
495 erties such as nestedness and modularity. Network ecologists tend to focus on several emerging
496 properties of food webs (Delmas et al. 2019), although we show that food-web structure is very
497 well predicted by the joint degree distribution. In the light of our results, there is a lot more
498 ecological information in the difference between properties of empirical networks and MaxEnt
499 predictions than in these properties themselves.

500 Alternative MaxEnt models

501 There are different ways to generate food webs using MaxEnt. In this contribution, we used a
502 method based on simulated annealing to find the network configuration with the highest SVD
503 entropy while fixing some aspects of its structure. Another technique, also based on simulated
504 annealing, could start by generating a food web randomly with fixed numbers of species and
505 interactions and calculating its joint degree distribution. Pairs of interactions could be swapped
506 sequentially until we minimize the divergence between the calculated joint degree distribution
507 and the one of maximum entropy obtained analytically. In that case, this is the entropy of the
508 joint degree distribution that would be maximized, not the one of the network's topology. To a
509 certain extent, this method would thus bridge the gap between the two approaches presented in
510 this article (i.e. analytical and heuristic MaxEnt models). More research is needed to compare
511 the quality of different methods generating adjacency matrices of food webs using MaxEnt.

512 Another method generating adjacency matrices are maximum entropy graph models, which pre-
513 dict a probability distribution of networks under soft or hard constraints (e.g., Park and Newman
514 2004; Cimini et al. 2019). Under hard constraints, every network with a non-zero probability
515 exactly satisfies the constraints on its structure. This is in contrast with soft constraints, which
516 require that networks satisfy them on average (i.e. many networks with a non-zero probability do
517 not have the exact structure set by the constraints). Maximum entropy graph models are helpful
518 because they can provide probability distributions for many network properties, by measuring
519 the structure of all adjacency matrices with a non-zero probability. However, we consider that
520 our approach based on simulated annealing is more flexible and more computationally efficient.
521 Indeed, many measures of food-web structure are hard to translate into mathematical constraints.
522 Moreover, because food webs are directed networks with self-loops, it makes the mathematical
523 derivation of maximum entropy graph models difficult. We believe that identifying heuristically
524 what really constrains the topology of food webs is a useful first step before attempting to derive
525 the mathematical formulation of a maximum entropy graph model adapted to food webs.

526 Even though we decided to work with point estimates, it is possible to have a (non MaxEnt)
527 probability distribution of networks when working with the entire chains (or part of the chains).

528 Applications

529 Our method and results could be used for different purposes. First, they could be used as first-
530 order approximations of network structure when only state variables are known. This could
531 prove useful when predicting network structure at large spatial scales, where few ecological in-
532 formation is known at that scale. Second, they could be used as informative priors in Bayesian
533 analyses of the structure of ecological networks (e.g., Cirtwill et al. 2019). Third, they could
534 be used to make better predictions of pairwise species interactions by constraining the space of
535 feasible networks, as discussed in Strydom et al. (2021). Finally, they could be used as alter-
536 native null models of ecological networks to better understand ecological mechanisms driving
537 food-web structure. In that case, our model might need to be slightly adapted to give a proba-
538 bility distribution of Boolean networks (in contrast with point estimates of maximum entropy
539 networks).

540 **Conclusion**

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

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555 **References**

- 556 Albert, R., and A. L. Barabasi. 2002. “Statistical Mechanics of Complex Networks.” *Reviews*
557 *of Modern Physics* 74 (1): 47–97. <https://doi.org/10.1103/RevModPhys.74.47>.
- 558 Banville, Francis, Steve Vissault, and Timothée Poisot. 2021. “Mangal.jl and EcologicalNet-
559 works.jl: Two Complementary Packages for Analyzing Ecological Networks in Julia.” *Jour-*
560 *nal of Open Source Software* 6 (61): 2721. <https://doi.org/10.21105/joss.02721>.
- 561 Bascompte, J., P. Jordano, C. J. Melian, and J. M. Olesen. 2003. “The Nested Assembly of
562 Plant-Animal Mutualistic Networks.” *Proceedings of the National Academy of Sciences*
563 *of the United States of America* 100 (16): 9383–87. <https://doi.org/10.1073/pnas.1633576100>.

- 565 Bastolla, Ugo, Miguel A. Fortuna, Alberto Pascual-Garcia, Antonio Ferrera, Bartolo Luque, and
566 Jordi Bascompte. 2009. “The Architecture of Mutualistic Networks Minimizes Competition
567 and Increases Biodiversity.” *Nature* 458 (7241): 1018–U91. <https://doi.org/10.1038/nature07950>.
- 569 Beck, Christian. 2009. “Generalised Information and Entropy Measures in Physics.” *Contemporary Physics* 50 (4): 495–510. <https://doi.org/10.1080/00107510902823517>.
- 571 Cimini, Giulio, Tiziano Squartini, Fabio Saracco, Diego Garlaschelli, Andrea Gabrielli, and
572 Guido Caldarelli. 2019. “The Statistical Physics of Real-World Networks.” *Nature Reviews Physics* 1 (1): 58–71. <https://doi.org/10.1038/s42254-018-0002-6>.
- 574 Cirtwill, Alyssa R., Anna Eklof, Tomas Roslin, Kate Wootton, and Dominique Gravel. 2019.
575 “A Quantitative Framework for Investigating the Reliability of Empirical Network Construc-
576 tion.” *Methods in Ecology and Evolution* 10 (6): 902–11. <https://doi.org/10.1111/2041-210X.13180>.
- 578 Cohen, Joel E., Tomas Jonsson, and Stephen R. Carpenter. 2003. “Ecological Community
579 Description Using the Food Web, Species Abundance, and Body Size.” *Proceedings of
580 the National Academy of Sciences* 100 (4): 1781–86. <https://doi.org/10.1073/pnas.232715699>.
- 582 Delmas, Eva, Mathilde Besson, Marie Hélène Brice, Laura A. Burkle, Giulio V. Dalla Riva,
583 Marie Josée Fortin, Dominique Gravel, et al. 2019. “Analysing Ecological Networks of
584 Species Interactions.” *Biological Reviews*. <https://doi.org/10.1111/brv.12433>.
- 585 Dunne, Jennifer A., Richard J. Williams, and Neo D. Martinez. 2002. “Network Structure and
586 Biodiversity Loss in Food Webs: Robustness Increases with Connectance.” *Ecology Letters*
587 5 (4): 558–67. <https://doi.org/10.1046/j.1461-0248.2002.00354.x>.
- 588 Dunning, Iain, Joey Huchette, and Miles Lubin. 2017. “JuMP: A Modeling Language for
589 Mathematical Optimization.” *SIAM Review* 59 (2): 295–320. <https://doi.org/10.1137/15M1020575>.
- 591 Fortuna, M. A., and J. Bascompte. 2006. “Habitat Loss and the Structure of Plant-Animal
592 Mutualistic Networks.” *Ecology Letters* 9 (3): 278–83. <https://doi.org/10.1111/j.1462-2920.2006.00891.x>.

- 593 1461-0248.2005.00868.x.
- 594 Fortuna, M. A., Daniel B. Stouffer, Jens M. Olesen, Pedro Jordano, David Mouillot, Boris R.
595 Krasnov, Robert Poulin, and Jordi Bascompte. 2010. “Nestedness Versus Modularity in
596 Ecological Networks: Two Sides of the Same Coin?” *Journal of Animal Ecology* 79 (4):
597 811–17. <https://doi.org/10.1111/j.1365-2656.2010.01688.x>.
- 598 Frank, S. A., and E. Smith. 2011. “A Simple Derivation and Classification of Common Prob-
599 ability Distributions Based on Information Symmetry and Measurement Scale.” *Journal of*
600 *Evolutionary Biology* 24 (3): 469–84. <https://doi.org/10.1111/j.1420-9101.2010.02204.x>.
- 601
- 602 Gómez, José M., Francisco Perfectti, and Pedro Jordano. 2011. “The Functional Consequences
603 of Mutualistic Network Architecture.” *PLOS ONE* 6 (1): e16143. <https://doi.org/10.1371/journal.pone.0016143>.
- 604
- 605 Harremoës, Peter, and Flemming Topsøe. 2001. “Maximum Entropy Fundamentals.” *Entropy*
606 3 (3): 191–226. <https://doi.org/10.3390/e3030191>.
- 607 Harte, J., and Erica A. Newman. 2014. “Maximum Information Entropy: A Foundation for
608 Ecological Theory.” *Trends in Ecology & Evolution* 29 (7): 384–89. <https://doi.org/10.1016/j.tree.2014.04.009>.
- 609
- 610 Harte, J., T. Zillio, E. Conlisk, and A. B. Smith. 2008. “Maximum Entropy and the State-
611 Variable Approach to Macroecology.” *Ecology* 89 (10): 2700–2711. <https://doi.org/10.1890/07-1369.1>.
- 612
- 613 Hoorn, Pim van der, Gabor Lippner, and Dmitri Krioukov. 2018. “Sparse Maximum-Entropy
614 Random Graphs with a Given Power-Law Degree Distribution.” *Journal of Statistical Physics*
615 173 (3): 806–44. <https://doi.org/10.1007/s10955-017-1887-7>.
- 616
- 617 Hortal, Joaquín, Francesco de Bello, José Alexandre F. Diniz-Filho, Thomas M. Lewinsohn,
618 Jorge M. Lobo, and Richard J. Ladle. 2015. “Seven Shortfalls That Beset Large-Scale
619 Knowledge of Biodiversity.” *Annual Review of Ecology, Evolution, and Systematics* 46 (1):
523–49. <https://doi.org/10.1146/annurev-ecolsys-112414-054400>.

- 620 Ings, Thomas C., José M. Montoya, Jordi Bascompte, Nico Blüthgen, Lee Brown, Carsten F.
621 Dormann, François Edwards, et al. 2009. “Review: Ecological Networks Beyond Food
622 Webs.” *Journal of Animal Ecology* 78 (1): 253–69. <https://doi.org/10.1111/j.1365-2656.2008.01460.x>.
- 624 Jaynes, E. T. 1957a. “Information Theory and Statistical Mechanics.” *Physical Review* 106 (4):
625 620–30. <https://doi.org/10.1103/PhysRev.106.620>.
- 626 ———. 1957b. “Information Theory and Statistical Mechanics. II.” *Physical Review* 108 (2):
627 171–90. <https://doi.org/10.1103/PhysRev.108.171>.
- 628 Jordano, Pedro. 2016. “Sampling Networks of Ecological Interactions.” *Functional Ecology* 30
629 (12): 1883–93. <https://doi.org/10.1111/1365-2435.12763>.
- 630 Khinchin, A. Ya. 2013. *Mathematical Foundations of Information Theory*. Courier Corpora-
631 tion.
- 632 MacDonald, Arthur Andrew Meahan, Francis Banville, and Timothée Poisot. 2020. “Revisiting
633 the Links-Species Scaling Relationship in Food Webs.” *Patterns* 0 (0). <https://doi.org/10.1016/j.patter.2020.100079>.
- 635 Martyushev, L. M., and V. D. Seleznev. 2006. “Maximum Entropy Production Principle in
636 Physics, Chemistry and Biology.” *Physics Reports-Review Section of Physics Letters* 426
637 (1): 1–45. <https://doi.org/10.1016/j.physrep.2005.12.001>.
- 638 Milo, R., S. Shen-Orr, S. Itzkovitz, N. Kashtan, D. Chklovskii, and U. Alon. 2002. “Net-
639 work Motifs: Simple Building Blocks of Complex Networks.” *Science* 298 (5594): 824–27.
640 <https://doi.org/10.1126/science.298.5594.824>.
- 641 Park, Juyong, and M. E. J. Newman. 2004. “Statistical Mechanics of Networks.” *Physical
642 Review E* 70 (6): 066117. <https://doi.org/10.1103/PhysRevE.70.066117>.
- 643 Pascual, Department of Ecology and Evolutionary Biology Mercedes, and Visiting Professor
644 Jennifer A. Dunne. 2006. *Ecological Networks: Linking Structure to Dynamics in Food
645 Webs*. Oxford University Press, USA.

- 646 Phillips, Steven J., Robert P. Anderson, and Robert E. Schapire. 2006. "Maximum Entropy
647 Modeling of Species Geographic Distributions." *Ecological Modelling* 190 (3): 231–59.
648 <https://doi.org/10.1016/j.ecolmodel.2005.03.026>.
- 649 Pielou, Evelyn C. 1975. "Ecological Diversity." In. 574.524018 P5.
- 650 Poisot, Timothee, Benjamin Baiser, Jennifer A. Dunne, Sonia Kefi, Francois Massol, Nico-
651 las Mouquet, Tamara N. Romanuk, Daniel B. Stouffer, Spencer A. Wood, and Dominique
652 Gravel. 2016. "Mangal - Making Ecological Network Analysis Simple." *Ecography* 39 (4):
653 384–90. <https://doi.org/10.1111/ecog.00976>.
- 654 Poisot, Timothée, Gabriel Bergeron, Kevin Cazelles, Tad Dallas, Dominique Gravel, Andrew
655 MacDonald, Benjamin Mercier, Clément Violet, and Steve Vissault. 2021. "Global Knowl-
656 edge Gaps in Species Interaction Networks Data." *Journal of Biogeography* 48 (7): 1552–
657 63. <https://doi.org/10.1111/jbi.14127>.
- 658 Poisot, Timothée, and Dominique Gravel. 2014. "When Is an Ecological Network Complex?
659 Connectance Drives Degree Distribution and Emerging Network Properties." *PeerJ* 2: e251.
660 <https://doi.org/10.7717/peerj.251>.
- 661 Pomeranz, Justin Page, Ross M. Thompson, Timothée Poisot, Jon S. Harding, and Justin P. F.
662 Pomeranz. 2018. "Data from: Inferring Predator-Prey Interactions in Food Webs." Dryad.
663 <https://doi.org/10.5061/DRYAD.K59M37F>.
- 664 Shannon, C. E. 1948. "A Mathematical Theory of Communication." *The Bell System Technical
665 Journal* 27 (3): 379–423. <https://doi.org/10.1002/j.1538-7305.1948.tb01338.x>.
- 666 Staniczenko, Phillip P. A., Jason C. Kopp, and Stefano Allesina. 2013. "The Ghost of Nested-
667 ness in Ecological Networks." *Nature Communications* 4 (1): 1391. <https://doi.org/10.1038/ncomms2422>.
- 669 Stock, Michiel, Timothée Poisot, and Bernard De Baets. 2021. "Optimal Transportation Theory
670 for Species Interaction Networks." *Ecology and Evolution* 11 (9): 3841–55. <https://doi.org/10.1002/ece3.7254>.
- 672 Stouffer, Daniel B., and Jordi Bascompte. 2011. "Compartmentalization Increases Food-Web
673 Persistence." *Proceedings of the National Academy of Sciences* 108 (9): 3648–52. [https://doi.org/10.1073/pnas.101811108](https://doi.org/10.1073/pnas.1018111108).

- 674 [//doi.org/10.1073/pnas.1014353108](https://doi.org/10.1073/pnas.1014353108).
- 675 Stouffer, Daniel B., Juan Camacho, Wenxin Jiang, and Luis A. Nunes Amaral. 2007. "Evidence
676 for the Existence of a Robust Pattern of Prey Selection in Food Webs." *Proceedings of the*
677 *Royal Society B-Biological Sciences* 274 (1621): 1931–40. <https://doi.org/10.1098/rspb.2007.0571>.
- 679 Strydom, Tanya, Michael D. Catchen, Francis Banville, Dominique Caron, Gabriel Dansereau,
680 Philippe Desjardins-Proulx, Norma R. Forero-Muñoz, et al. 2021. "A Roadmap Towards
681 Predicting Species Interaction Networks (across Space and Time)." *Philosophical Trans-*
682 *actions of the Royal Society B: Biological Sciences* 376 (1837): 20210063. <https://doi.org/10.1098/rstb.2021.0063>.
- 684 Strydom, Tanya, Giulio V. Dalla Riva, and Timothee Poisot. 2021. "SVD Entropy Reveals the
685 High Complexity of Ecological Networks." *Frontiers in Ecology and Evolution* 9: 623141.
686 <https://doi.org/10.3389/fevo.2021.623141>.
- 687 Vázquez, Diego P. 2005. "Degree Distribution in Plantanimal Mutualistic Networks: Forbidden
688 Links or Random Interactions?" *Oikos* 108 (2): 421–26. <https://doi.org/10.1111/j.0030-1299.2005.13619.x>.
- 690 Williams, Richard J. 2011. "Biology, Methodology or Chance? The Degree Distributions of
691 Bipartite Ecological Networks." *PLOS ONE* 6 (3): e17645. <https://doi.org/10.1371/journal.pone.0017645>.
- 693 Williams, Richard J., and Neo D. Martinez. 2000. "Simple Rules Yield Complex Food Webs."
694 *Nature* 404 (6774): 180–83. <https://doi.org/10.1038/35004572>.

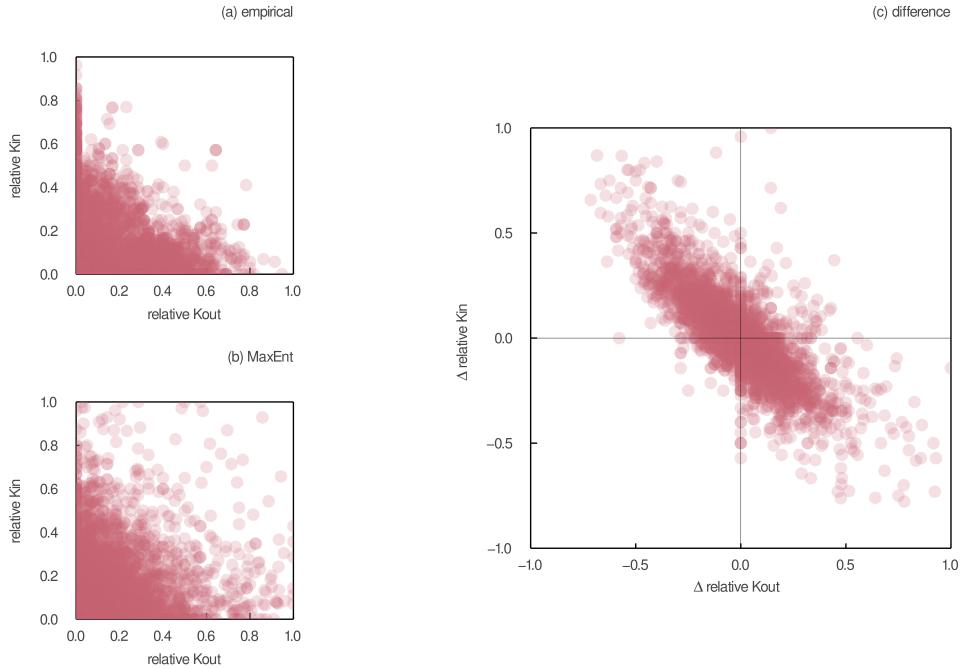


Figure 1: Relative number of predators (k_{in}) as a function of their relative number of prey (k_{out}) for each species in (a) empirical and (b) joint degree sequences obtained from the analytical MaxEnt model. Empirical networks include most food webs archived on Mangal, as well as the New Zealand 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.

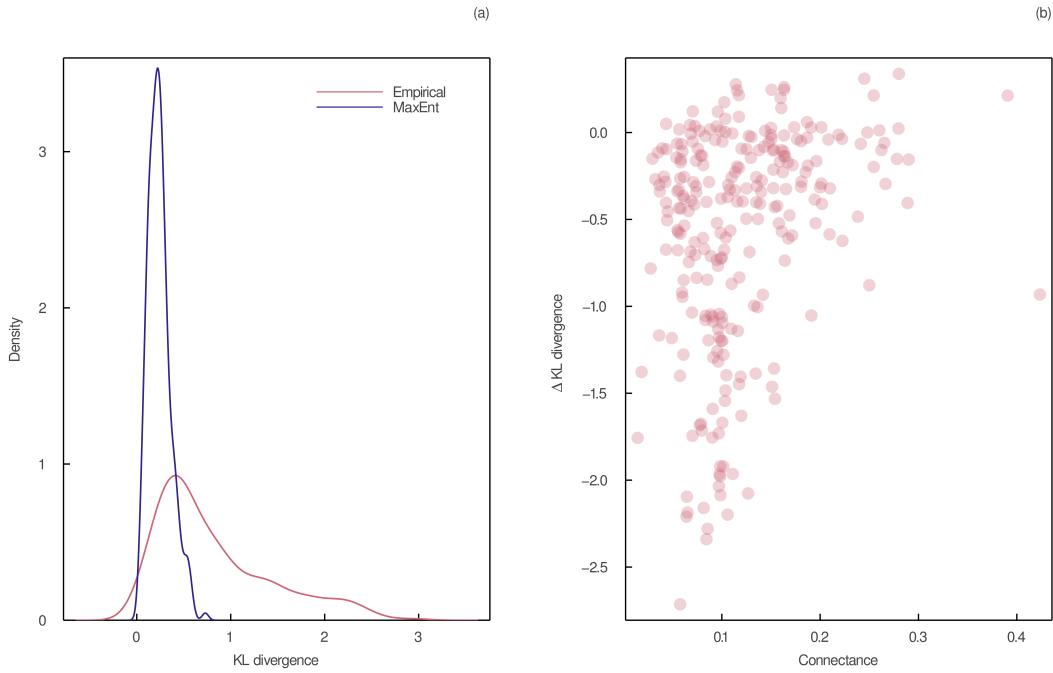


Figure 2: (a) Probability density of KL divergence between in and out-degree sequences of empirical and predicted joint degree sequences. (b) Difference between the KL divergence of empirical and predicted joint degree sequences as a function of connectance. In both panels, empirical networks include most food webs archived on 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.

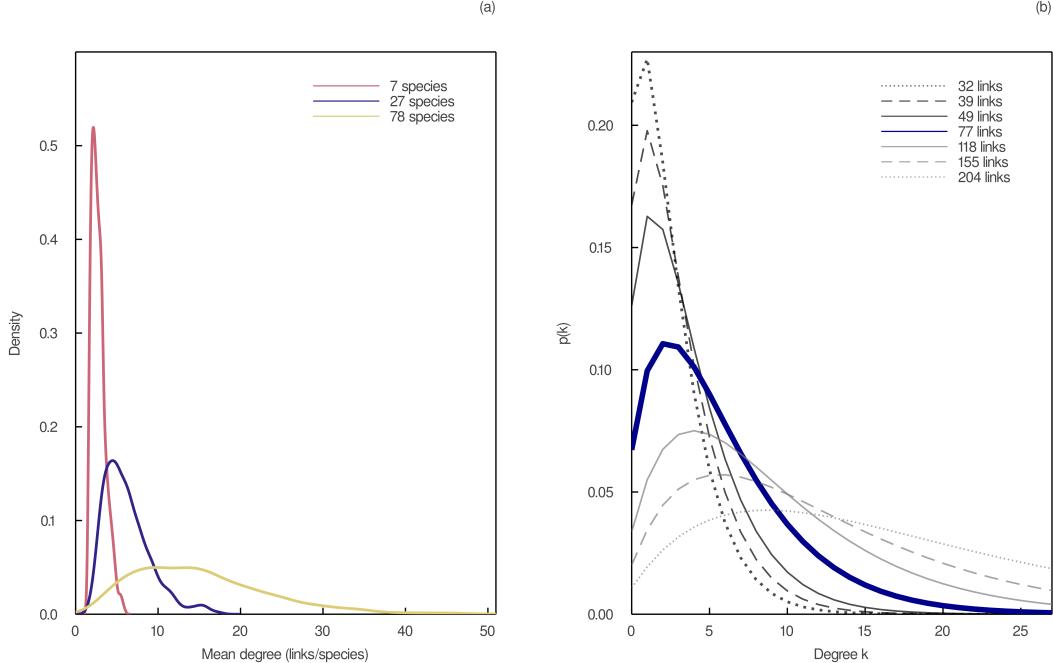


Figure 3: (a) Probability density of the mean degree of a food web obtained using different values of species richness S . The number of interactions L was simulated 1000 times using the flexible links model fitted to all empirical networks in our complete dataset (eq. 17). The mean degrees $2L/S$ were 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.

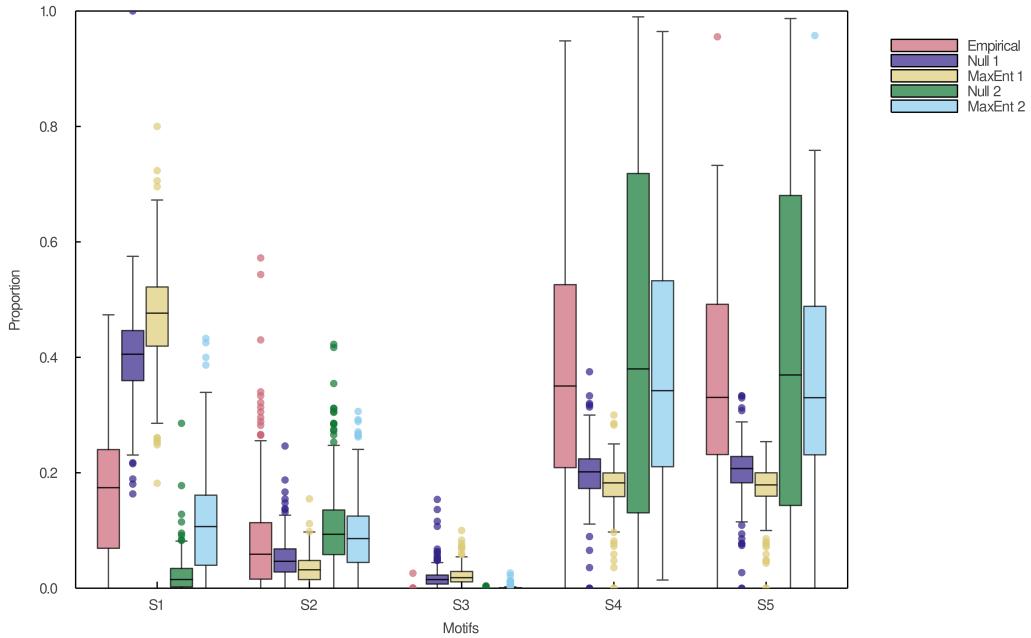


Figure 4: Motifs profile of empirical, maximum entropy, and null food webs. Empirical networks include most food webs archived on Mangal, as well as the New Zealand and Tuesday Lake datasets (our complete dataset). Maximum entropy networks were estimated using a simulated annealing algorithm to find 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).

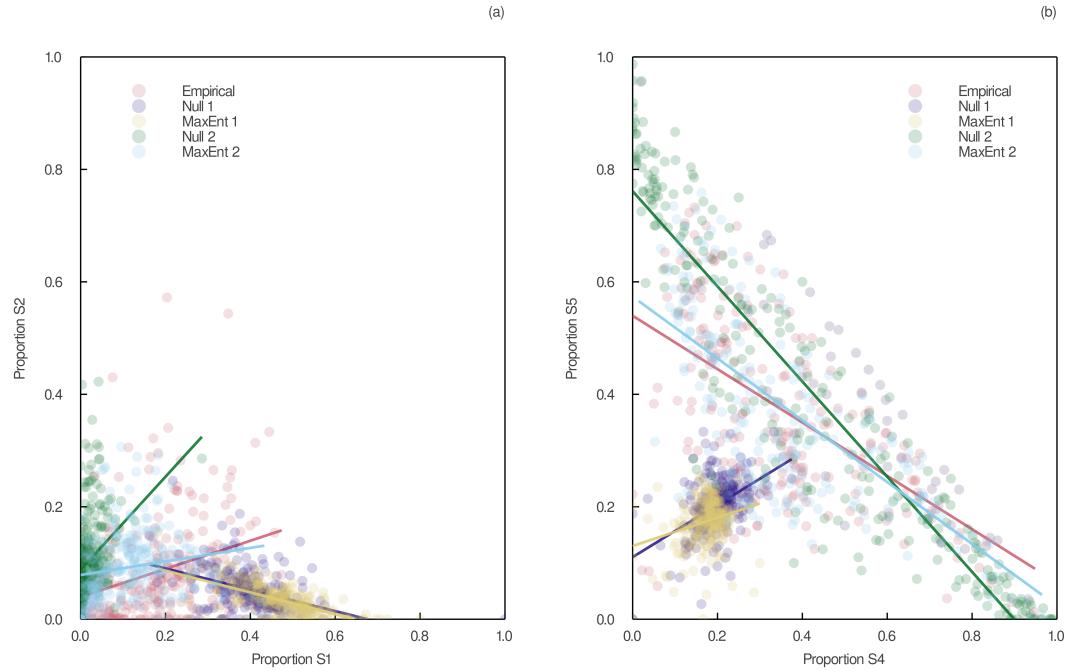


Figure 5: Relationship between motifs proportions of empirical, maximum entropy, and null food webs. Empirical networks include most food webs archived on Mangal, as well as the New Zealand and Tuesday Lake datasets (our complete dataset). Maximum entropy networks were estimated using a simulated annealing 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).

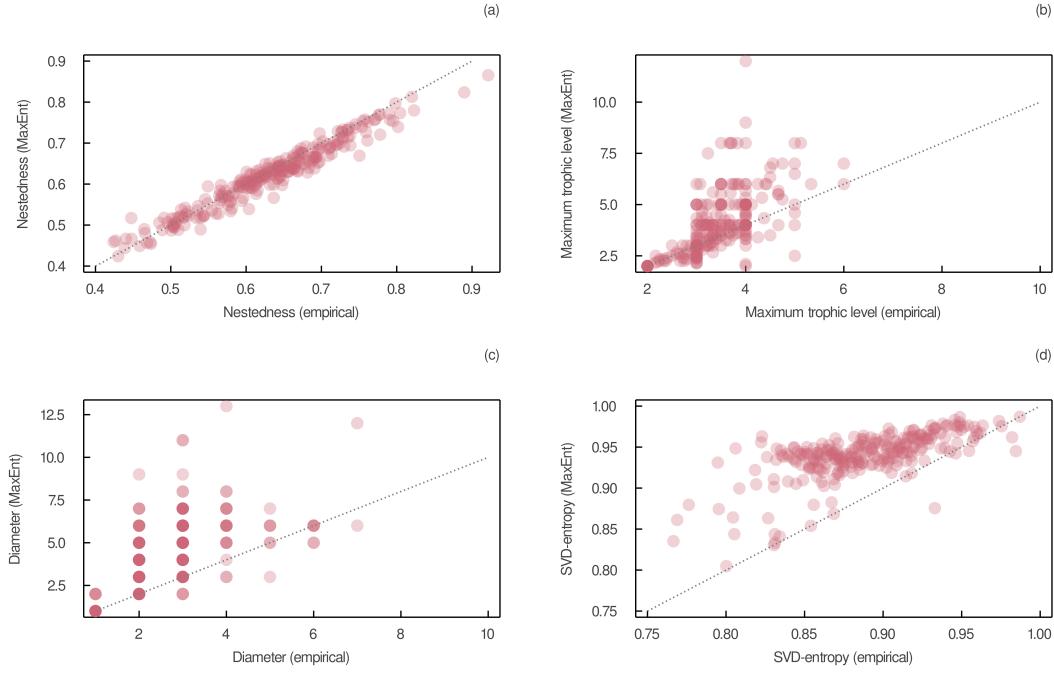


Figure 6: Relationship between the structure of empirical and maximum entropy food webs. Empirical networks include most food webs archived on Mangal, as well as the New Zealand and Tuesday Lake datasets (our complete dataset). Maximum entropy networks were estimated using a simulated annealing algorithm 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.