

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

Francis Banville<sup>1,2,3</sup> Dominique Gravel<sup>2,3</sup> Timothée Poisot<sup>1,3</sup>

<sup>1</sup> Université de Montréal <sup>2</sup> Université de Sherbrooke <sup>3</sup> Quebec Centre for Biodiversity Science

## **Correspondance to:**

Francis Banville — francis.banville@umontreal.ca

**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 difference 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). Given the constrained nature of ecolog-  
51 ical networks, it is surprising that the principle of maximum entropy, a rigorous mathematical  
52 method designed for both the analysis and prediction of constrained systems, has been barely  
53 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  $\lambda_i$   
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). Thus, to the  
 95 best of our knowledge, MaxEnt has never been used to predict food-web structure directly, even  
 96 though food webs are among the most documented and widespread ecological networks (Ings  
 97 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 preys). 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 informa-

tion available and on our capacity to find the set of state variables that best represent natural systems and to translate them into appropriate statistical constraints. Having a validated maximum entropy model for the system at hand allows us to make least-biased predictions using a minimal amount of data, as well as identify the most important ecological processes shaping that system.

## 115 Analytical and heuristic approaches

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

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

For the second approach (heuristic), we focus on network level properties. We used a flexible and heuristic model based on simulated annealing (an optimization algorithm) to find the network configuration *close* to maximum entropy and measured its structure. We developed this heuristic model because the analytical derivation of a maximum entropy graph model of food webs is difficult, and because this model is readily applicable to other types of ecological networks and measures. Indeed, the mathematical representation of food webs (i.e. directed simple graphs

138 frequently having self-loops) makes the optimization of maximum entropy graph models more  
139 complicated than with many other types of (non-ecological) networks. In other words, deriving  
140 a probability distribution on the graphs themselves is difficult when working with food webs.  
141 We built two types of heuristic MaxEnt models depending on the constraint used. Our type I  
142 MaxEnt model uses the connectance of the network (i.e. the ratio  $L/S^2$ ) as a constraint, whereas  
143 our type II MaxEnt model uses the whole joint degree sequence as a constraint.

## 144 Data and code

145 We tested our analytical and heuristic MaxEnt models against open food-web data queried from  
146 three different sources and integrated into what we call our *complete dataset*. These sources  
147 include (1) terrestrial and aquatic food webs sampled globally and archived on the ecologi-  
148 cal interactions database Mangal; (2) freshwater stream food webs from New Zealand; and (3)  
149 aquatic food webs from Tuesday Lake (Michigan, United States). First, all food webs archived  
150 on `mangal.io` (Timothée Poisot et al. 2016; Banville, Vissault, and Poisot 2021) were directly  
151 queried from the database ( $n = 235$ ). Most ecological networks archived on Mangal are multi-  
152 layer networks, i.e. networks that describe different types of interactions. We kept all networks  
153 whose interactions were mainly of predation and herbivory types, and removed the largest net-  
154 work ( $S = 714$ ) for computational efficiency reasons. Then, to this set we added food webs  
155 from two different sources: the New-Zealand dataset ( $n = 21$ ; Pomeranz et al. 2018) and the  
156 Tuesday Lake dataset ( $n = 2$ ; Cohen, Jonsson, and Carpenter 2003). Our complete dataset thus  
157 contained a total of 257 food webs. Of the New-Zealand and Tuesday Lake datasets, 19 networks  
158 had data on species' relative abundances that were used in the neutral model (Box 2). These 19  
159 food webs constitute our *abundance dataset*, which is a subset of our complete dataset.

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

162 **Analytical maximum entropy models**

163 **Joint degree distribution**

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

170 We want to maximize Shannon's entropy

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

171 subject to the following constraints:

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

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

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

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

<sup>179</sup> The joint probability distribution of maximum entropy given these constraints is found using the  
<sup>180</sup> method of Lagrange multipliers. To do so, we seek to maximize the following expression:

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

<sup>181</sup> where  $\lambda_1$ ,  $\lambda_2$ , and  $\lambda_3$  are the Lagrange multipliers. The probability distribution that maximizes  
<sup>182</sup> entropy is obtained by finding these values. As pointed out in the introduction,  $F$  is just Shan-  
<sup>183</sup> non's entropy to which we added terms that each sums to zero (our constraints).  $F$  is maximized  
<sup>184</sup> by setting to 0 its partial derivative with respect to  $p(k_{in}, k_{out})$ . Because the derivative of a con-  
<sup>185</sup> stant is zero, this gives us:

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

<sup>186</sup> Evaluating the partial derivatives with respect to  $p(k_{in}, k_{out})$ , we obtain:

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

<sup>187</sup> Then, solving eq. 9 for  $p(k_{in}, k_{out})$ , we obtain:

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

<sup>188</sup> where  $Z = e^{1+\lambda_1}$  is called the partition function. The partition function ensures that probabilities  
<sup>189</sup> sum to 1 (our normalization constraint). It can be expressed in terms of  $\lambda_2$  and  $\lambda_3$  as follows:

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

<sup>190</sup> After substituting  $p(k_{in}, k_{out})$  in eq. 5 and eq. 6, we get a nonlinear system of two equations and  
<sup>191</sup> two unknowns:

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

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

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

197 We predicted the joint degree distribution of maximum entropy for each food web in our com-  
 198 plete dataset, i.e. using their numbers of species and numbers of interactions as state variables.  
 199 We then sampled one realization of the degree sequence for each network using the probabil-  
 200 ities given by the joint degree distribution. In fig. 1 (left panels), we show the relationship  
 201 between  $k_{out}$  and  $k_{in}$  standardized by the number of species in their networks, for empirical and  
 202 maximum entropy joint degree distributions. We see that our model predicts higher values of  
 203 generality and vulnerability compared to empirical food webs (i.e. relative values of  $k_{out}$  and  
 204  $k_{in}$  closer to 1). However, plotting the difference between predicted and empirical values for  
 205 each species gives a different perspective. The right panel of fig. 1 presents these differences  
 206 when species are ordered by their total degree in their network (i.e. by the sum of their in and  
 207 out-degrees). Indeed, our predicted joint degree sequences have the same number of species as  
 208 their empirical counterparts, but they are species agnostic; in other words, instead of predicting  
 209 a value for each species directly, we predicted the entire joint degree sequence without taking  
 210 into account species' identity. The challenge is to associate predictions with empirical data. If  
 211 we associate each node according to their rank in total degrees, we see that species predicted  
 212 to be have a higher generality (number of preys) generally have a lower vulnerability (number  
 213 of preys) than what is observed (and conversely). This is because the difference in total degree  
 214 ( $k_{out} + k_{in}$ ) is minimized when species are ordered by their total degrees in both predicted and  
 215 empirical sets (i.e. the average sum of relative  $k_{out}$  and  $k_{in}$  is close to 0 across all species). This

216 result shows that the differences between predicted and empirical degrees (in and out) are low  
217 for most species when ordered by their total degrees and that there is no apparent biases towards  
218 in or out degrees. In fig. S1, we show how these differences change when species are instead  
219 ordered by their out-degrees (left panel) and in-degrees (right panel), respectively.

220 [Figure 1 about here.]

221 We can describe the shape of the joint degree distribution by comparing its marginal distribu-  
222 tions with one another. Doing so allows us to evaluate how much the shape of the joint degree  
223 distribution of maximum entropy differs from empirical data. We plotted the Kullback–Leibler  
224 (KL) divergence between in and out-degree sequences to compare the symmetry of empirical  
225 and maximum entropy joint degree sequences fig. 2. As we expected, our model predicted more  
226 similar in-degree and out-degree distributions than empirical data (shown by a lower KL diver-  
227 gence). However, this difference decreased with connectance right panel of 2. This suggests  
228 that other ecological constraints might be needed to account for the asymmetry of the joint de-  
229 gree distribution, especially for networks with a lower connectance. This might be due to the  
230 fact that food webs with low connectance are typically harder to predict than food webs with  
231 high connectance. Indeed, in low connectance systems, what makes two species interact might  
232 be more important for predictions than in high connectance systems, in which what prevents  
233 species from interacting might be more meaningful. This implies that more ecological informa-  
234 tion might be needed in food webs with fewer numbers of interactions because more nuances  
235 determine interactions compared to non-interactions.

236 [Figure 2 about here.]

## 237 Degree distribution

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

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

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

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

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

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

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

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

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

257 In this section, we showed how important measures of food-web structure, namely the degree  
 258 distribution and the joint degree distribution, could be derived with the principle of maximum  
 259 entropy using minimal knowledge on a biological community. This type of models, although  
 260 useful to make least-biased predictions on many network properties, can be hard to apply for  
 261 other measures. Indeed, there are dozens of measures of network structure (Delmas et al. 2019)  
 262 and many are not calculated with mathematical equations, but with algorithms. Moreover, the

263 applicability of this method to empirical systems is limited by the state variables we can actu-  
264 ally measure and use. In the next section, we propose a more flexible method to predict many  
265 measures of network structure simultaneously, i.e. by finding heuristically the configuration of  
266 the network having maximum entropy given partial knowledge of its emerging structure.

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

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

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

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

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

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

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

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

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

298 [Figure 3 about here.]

## 299 Box 2 - Corresponding null and neutral models

### 300 Null models (types I and II)

301 Our heuristic MaxEnt models, predicting adjacency matrices, were compared with two topolog-  
 302 ical null models. The first is the type I null model of Fortuna and Bascompte (2006), in which  
 303 the probability that a species  $i$  predares on another species  $j$  is given by

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

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

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

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

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

### 316 Neutral model

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

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

319 where  $n_i$  and  $n_j$  are the abundances (or biomass) of both species, and  $N$  is the total abundance  
320 (or biomass) of all species in the network. We predicted neutral abundance matrices for all  
321 empirical networks in our abundance dataset ( $n = 19$ ), and converted these weighted matrices  
322 to Boolean networks using an approach analogue to the one we used for our null models.

323 **Heuristic maximum entropy models**

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

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

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

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

347 where  $s_i$  are the relative singular values of the adjacency matrix ( $s_i = \sigma_i / \sum_{i=1}^R \sigma_i$ , where  $\sigma_i$

348 are the singular values). Note that the distribution of relative singular values is analogous to  
349 a probability distribution, with  $0 < s_i < 1$  and  $\sum s_i = 1$ . Thus, this measure also satisfies  
350 all four properties of an appropriate entropy measure (see introduction), while being a proper  
351 measure of the internal complexity of food webs (Strydom, Dalla Riva, and Poisot 2021). Fol-  
352 lowing Strydom, Dalla Riva, and Poisot (2021), we standardized this measure with the rank  $R$  of  
353 the matrix (i.e.  $J / \ln(R)$ ) to account for the difference in dimensions between networks (*sensu*  
354 Pielou's evenness; Pielou 1975). We used SVD entropy to predict the network configuration  
355 of maximum entropy (i.e. of maximum complexity) heuristically given a predetermined set of  
356 constraints.

### 357 MaxEnt network models (types I and II)

358 We built two types of MaxEnt network models: one based on connectance (type I MaxEnt net-  
359 work model) and the other based on the joint degree sequence (type II MaxEnt network model).  
360 They are based on the same constraints as the types I and II null models presented above. For  
361 both models, we used a simulated annealing algorithm with 4 chains, 2000 steps and an initial  
362 temperature of 0.2. For each chain, we first generated one random Boolean matrix with the same  
363 order (number of species) as empirical webs, while maintaining the total number of interactions  
364 (type I MaxEnt network model) or rows and columns sums (type II MaxEnt network model).  
365 These are our initial configurations. Then, we swapped interactions sequentially while main-  
366 taining the original connectance or the joint degree sequence for types I and II MaxEnt network  
367 model, respectively. Configurations with a higher SVD entropy than the previous one in the  
368 chain were always accepted, whereas they were accepted with a probability conditional to a de-  
369 creasing temperature when lower. The final configuration with the highest SVD entropy among  
370 the four chains constitute our estimated MaxEnt network. Even though we decided to work with  
371 point estimates, it is possible to have a (non MaxEnt) probability distribution of networks when  
372 working with the entire chains (or part of the chains). For each network in our complete and  
373 abundance datasets, we estimated their configuration with maximum entropy using both types  
374 of MaxEnt network models.

375 **Structure of MaxEnt networks**

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

387 Overall, we found that models based on the joint degree sequence (type II null and MaxEnt  
388 network models) reproduced the structure of empirical networks much better than the ones based  
389 on connectance and the neutral model of relative abundances. On average, the type II MaxEnt  
390 network model was better at predicting nestedness ( $0.62 \pm 0.08$ ) than its corresponding null  
391 model ( $0.73 \pm 0.05$ ; empirical networks:  $0.63 \pm 0.09$ ), as well as the proportion of cannibal  
392 species. This might in part be due because nestedness was calculated using the spectral radius  
393 of the adjacency matrix, which leverages information on the network itself just like the MaxEnt  
394 network models. However, the type II null model was better at predicting network diameter and  
395 average maximum similarity between species pairs. Predictions were similar between both type  
396 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 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.  $\rho$ : nestedness measured by the spectral radius of the adjacency matrix. *maxtl*: maximum trophic level. *diam*: network diameter. *MxSim*: average maximum similarity between species pairs. *Cannib*: proportion of cannibal species (self loops). *Omniv*: proportion of omnivorous species. *entropy*: SVD entropy.

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

Table 2: Standardized mean 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.  $\rho$ : nestedness measured by the spectral radius of the adjacency matrix. *maxtl*: maximum trophic level. *diam*: network diameter. *MxSim*: average maximum similarity between species pairs. *Cannib*: proportion of cannibal species (self loops). *Omniv*: proportion of omnivorous species. *entropy*: SVD entropy.

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

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

399 be considered as simple building blocks of ecological networks (Milo et al. 2002; Stouffer et al.  
400 2007). Motifs are the backbone of complex ecological networks from which network structure  
401 is built upon and play a crucial role in community dynamics and assembly (Bastolla et al. 2009;  
402 Stouffer and Bascompte 2011). In fig. 4, we show that the motifs profile of networks generated  
403 using the type II MaxEnt network model was very close to the one of empirical data, and that  
404 they made better predictions than the type II null model. This is also shown in fig. 5, where we  
405 see that relationships between motifs pairs of empirical food webs are very similar to the ones  
406 of the type II MaxEnt networks. Overall, these results suggest that the type II MaxEnt network  
407 model can reproduce many aspects of network structure. This highlights the importance of the  
408 joint degree sequence in shaping ecological networks.

409 [Figure 4 about here.]

410 [Figure 5 about here.]

411 Moreover, we found that empirical networks are close to their maximum entropy considering a  
412 fixed joint degree sequence (fig. S3). Empirical networks had an SVD entropy of  $0.89 \pm 0.04$ ,  
413 compared to type II MaxEnt networks which had values of  $0.94 \pm 0.03$ . The relationship between  
414 the SVD entropy of empirical food webs and their maximum entropy configuration is plotted in  
415 the last panel of fig. 6. We also found no relationship between the difference in SVD entropy  
416 between empirical and type II MaxEnt networks and species richness, the number of interactions,  
417 or connectance (fig. S4). Similarly, we found no correlation between the difference in SVD  
418 entropy and the Jaccard distance of empirical and type II MaxEnt networks.

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

427 **Discussion**

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

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

453 predictions than in these properties themselves.

#### 454 Alternative MaxEnt models

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

466 Another method generating adjacency matrices are maximum entropy graph models, which pre-  
467 dict a probability distribution of networks under soft or hard constraints (e.g., Park and Newman  
468 2004; Cimini et al. 2019). Under hard constraints, every network with a non-zero probability  
469 exactly satisfies the constraints on its structure. This is in contrast with soft constraints, which  
470 require that networks satisfy them on average (i.e. many networks with a non-zero probability do  
471 not have the exact structure set by the constraints). Maximum entropy graph models are helpful  
472 because they can provide probability distributions for many network properties, by measuring  
473 the structure of all adjacency matrices with a non-zero probability. However, we consider that  
474 our approach based on simulated annealing is more flexible and more computationally efficient.  
475 Indeed, many measures of food-web structure are hard to translate into mathematical constraints.  
476 Moreover, because food webs are directed networks with self-loops, it makes the mathematical  
477 derivation of maximum entropy graph models difficult. We believe that identifying heuristically  
478 what really constrains the topology of food webs is a useful first step before attempting to derive  
479 the mathematical formulation of a maximum entropy graph model adapted to food webs.

480 **Applications**

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

492 **Conclusion**

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

500 **Acknowledgments**

501 We acknowledge that this study was conducted on land within the traditional unceded territory  
502 of the Saint Lawrence Iroquoian, Anishinabewaki, Mohawk, Huron-Wendat, and Omàmiwinini-  
503 wak nations. This work was supported by the Institute for Data Valorisation (IVADO) and the  
504 Natural Sciences and Engineering Research Council of Canada (NSERC) Collaborative Re-

505 search and Training Experience (CREATE) program, through the Computational Biodiversity  
506 Science and Services (BIOS<sup>2</sup>) program.

## 507 References

- 508 Albert, R., and A. L. Barabasi. 2002. “Statistical Mechanics of Complex Networks.” *Reviews*  
509 *of Modern Physics* 74 (1): 47–97. <https://doi.org/10.1103/RevModPhys.74.47>.
- 510 Banville, Francis, Steve Vissault, and Timothée Poisot. 2021. “Mangal.jl and EcologicalNet-  
511 works.jl: Two Complementary Packages for Analyzing Ecological Networks in Julia.” *Journal*  
512 *of Open Source Software* 6 (61): 2721. <https://doi.org/10.21105/joss.02721>.
- 513 Bascompte, J., P. Jordano, C. J. Melian, and J. M. Olesen. 2003. “The Nested Assembly of  
514 Plant-Animal Mutualistic Networks.” *Proceedings of the National Academy of Sciences*  
515 *of the United States of America* 100 (16): 9383–87. <https://doi.org/10.1073/pnas.1633576100>.
- 517 Bastolla, Ugo, Miguel A. Fortuna, Alberto Pascual-Garcia, Antonio Ferrera, Bartolo Luque, and  
518 Jordi Bascompte. 2009. “The Architecture of Mutualistic Networks Minimizes Competition  
519 and Increases Biodiversity.” *Nature* 458 (7241): 1018–U91. <https://doi.org/10.1038/nature07950>.
- 521 Beck, Christian. 2009. “Generalised Information and Entropy Measures in Physics.” *Contem-  
522 porary Physics* 50 (4): 495–510. <https://doi.org/10.1080/00107510902823517>.
- 523 Cimini, Giulio, Tiziano Squartini, Fabio Saracco, Diego Garlaschelli, Andrea Gabrielli, and  
524 Guido Caldarelli. 2019. “The Statistical Physics of Real-World Networks.” *Nature Reviews*  
525 *Physics* 1 (1): 58–71. <https://doi.org/10.1038/s42254-018-0002-6>.
- 526 Cirtwill, Alyssa R., Anna Eklof, Tomas Roslin, Kate Wootton, and Dominique Gravel. 2019.  
527 “A Quantitative Framework for Investigating the Reliability of Empirical Network Construc-  
528 tion.” *Methods in Ecology and Evolution* 10 (6): 902–11. <https://doi.org/10.1111/2041-210X.13180>.

- 530 Cohen, Joel E., Tomas Jonsson, and Stephen R. Carpenter. 2003. "Ecological Community  
531 Description Using the Food Web, Species Abundance, and Body Size." *Proceedings of  
532 the National Academy of Sciences* 100 (4): 1781–86. [https://doi.org/10.1073/pnas.  
533 232715699](https://doi.org/10.1073/pnas.232715699).
- 534 Delmas, Eva, Mathilde Besson, Marie Hélène Brice, Laura A. Burkle, Giulio V. Dalla Riva,  
535 Marie Josée Fortin, Dominique Gravel, et al. 2019. "Analysing Ecological Networks of  
536 Species Interactions." *Biological Reviews*. <https://doi.org/10.1111/brv.12433>.
- 537 Dunne, Jennifer A., Richard J. Williams, and Neo D. Martinez. 2002. "Network Structure and  
538 Biodiversity Loss in Food Webs: Robustness Increases with Connectance." *Ecology Letters*  
539 5 (4): 558–67. <https://doi.org/10.1046/j.1461-0248.2002.00354.x>.
- 540 Dunning, Iain, Joey Huchette, and Miles Lubin. 2017. "JuMP: A Modeling Language for  
541 Mathematical Optimization." *SIAM Review* 59 (2): 295–320. [https://doi.org/10.1137/  
542 15M1020575](https://doi.org/10.1137/15M1020575).
- 543 Fortuna, M. A., and J. Bascompte. 2006. "Habitat Loss and the Structure of Plant-Animal  
544 Mutualistic Networks." *Ecology Letters* 9 (3): 278–83. [https://doi.org/10.1111/j.  
545 1461-0248.2005.00868.x](https://doi.org/10.1111/j.1461-0248.2005.00868.x).
- 546 Fortuna, M. A., Daniel B. Stouffer, Jens M. Olesen, Pedro Jordano, David Mouillot, Boris R.  
547 Krasnov, Robert Poulin, and Jordi Bascompte. 2010. "Nestedness Versus Modularity in  
548 Ecological Networks: Two Sides of the Same Coin?" *Journal of Animal Ecology* 79 (4):  
549 811–17. <https://doi.org/10.1111/j.1365-2656.2010.01688.x>.
- 550 Frank, S. A., and E. Smith. 2011. "A Simple Derivation and Classification of Common Prob-  
551 ability Distributions Based on Information Symmetry and Measurement Scale." *Journal of  
552 Evolutionary Biology* 24 (3): 469–84. [https://doi.org/10.1111/j.1420-9101.2010.02204.x](https://doi.org/10.1111/j.1420-9101.2010.<br/>553 02204.x).
- 554 Gómez, José M., Francisco Perfectti, and Pedro Jordano. 2011. "The Functional Consequences  
555 of Mutualistic Network Architecture." *PLOS ONE* 6 (1): e16143. [https://doi.org/10.1371/journal.pone.0016143](https://doi.org/10.<br/>556 1371/journal.pone.0016143).

- 557 Harremoës, Peter, and Flemming Topsøe. 2001. “Maximum Entropy Fundamentals.” *Entropy*  
558 3 (3): 191–226. <https://doi.org/10.3390/e3030191>.
- 559 Harte, J., and Erica A. Newman. 2014. “Maximum Information Entropy: A Foundation for  
560 Ecological Theory.” *Trends in Ecology & Evolution* 29 (7): 384–89. <https://doi.org/10.1016/j.tree.2014.04.009>.
- 562 Harte, J., T. Zillio, E. Conlisk, and A. B. Smith. 2008. “Maximum Entropy and the State-  
563 Variable Approach to Macroecology.” *Ecology* 89 (10): 2700–2711. <https://doi.org/10.1890/07-1369.1>.
- 565 Hoorn, Pim van der, Gabor Lippner, and Dmitri Krioukov. 2018. “Sparse Maximum-Entropy  
566 Random Graphs with a Given Power-Law Degree Distribution.” *Journal of Statistical Physics*  
567 173 (3): 806–44. <https://doi.org/10.1007/s10955-017-1887-7>.
- 568 Hortal, Joaquín, Francesco de Bello, José Alexandre F. Diniz-Filho, Thomas M. Lewinsohn,  
569 Jorge M. Lobo, and Richard J. Ladle. 2015. “Seven Shortfalls That Beset Large-Scale  
570 Knowledge of Biodiversity.” *Annual Review of Ecology, Evolution, and Systematics* 46 (1):  
571 523–49. <https://doi.org/10.1146/annurev-ecolsys-112414-054400>.
- 572 Ings, Thomas C., José M. Montoya, Jordi Bascompte, Nico Blüthgen, Lee Brown, Carsten F.  
573 Dormann, François Edwards, et al. 2009. “Review: Ecological Networks Beyond Food  
574 Webs.” *Journal of Animal Ecology* 78 (1): 253–69. <https://doi.org/10.1111/j.1365-2656.2008.01460.x>.
- 576 Jaynes, E. T. 1957a. “Information Theory and Statistical Mechanics.” *Physical Review* 106 (4):  
577 620–30. <https://doi.org/10.1103/PhysRev.106.620>.
- 578 ———. 1957b. “Information Theory and Statistical Mechanics. II.” *Physical Review* 108 (2):  
579 171–90. <https://doi.org/10.1103/PhysRev.108.171>.
- 580 Jordano, Pedro. 2016. “Sampling Networks of Ecological Interactions.” *Functional Ecology* 30  
581 (12): 1883–93. <https://doi.org/10.1111/1365-2435.12763>.
- 582 Khinchin, A. Ya. 2013. *Mathematical Foundations of Information Theory*. Courier Corpora-  
583 tion.

- 584 MacDonald, Arthur Andrew Meahan, Francis Banville, and Timothée Poisot. 2020. “Revisiting  
585 the Links-Species Scaling Relationship in Food Webs.” *Patterns* 0 (0). <https://doi.org/10.1016/j.patter.2020.100079>.
- 586
- 587 Martyushev, L. M., and V. D. Seleznev. 2006. “Maximum Entropy Production Principle in  
588 Physics, Chemistry and Biology.” *Physics Reports-Review Section of Physics Letters* 426  
589 (1): 1–45. <https://doi.org/10.1016/j.physrep.2005.12.001>.
- 590 Milo, R., S. Shen-Orr, S. Itzkovitz, N. Kashtan, D. Chklovskii, and U. Alon. 2002. “Net-  
591 work Motifs: Simple Building Blocks of Complex Networks.” *Science* 298 (5594): 824–27.  
592 <https://doi.org/10.1126/science.298.5594.824>.
- 593 Park, Juyong, and M. E. J. Newman. 2004. “Statistical Mechanics of Networks.” *Physical  
594 Review E* 70 (6): 066117. <https://doi.org/10.1103/PhysRevE.70.066117>.
- 595 Pascual, Department of Ecology and Evolutionary Biology Mercedes, and Visiting Professor  
596 Jennifer A. Dunne. 2006. *Ecological Networks: Linking Structure to Dynamics in Food  
597 Webs*. Oxford University Press, USA.
- 598 Phillips, Steven J., Robert P. Anderson, and Robert E. Schapire. 2006. “Maximum Entropy  
599 Modeling of Species Geographic Distributions.” *Ecological Modelling* 190 (3): 231–59.  
600 <https://doi.org/10.1016/j.ecolmodel.2005.03.026>.
- 601 Pielou, Evelyn C. 1975. “Ecological Diversity.” In. 574.524018 P5.
- 602 Poisot, Timothee, Benjamin Baiser, Jennifer A. Dunne, Sonia Kefi, Francois Massol, Nico-  
603 las Mouquet, Tamara N. Romanuk, Daniel B. Stouffer, Spencer A. Wood, and Dominique  
604 Gravel. 2016. “Mangal - Making Ecological Network Analysis Simple.” *Ecography* 39 (4):  
605 384–90. <https://doi.org/10.1111/ecog.00976>.
- 606 Poisot, Timothée, Gabriel Bergeron, Kevin Cazelles, Tad Dallas, Dominique Gravel, Andrew  
607 MacDonald, Benjamin Mercier, Clément Violet, and Steve Vissault. 2021. “Global Knowl-  
608 edge Gaps in Species Interaction Networks Data.” *Journal of Biogeography* 48 (7): 1552–  
609 63. <https://doi.org/10.1111/jbi.14127>.
- 610 Poisot, Timothée, and Dominique Gravel. 2014. “When Is an Ecological Network Complex?  
611 Connectance Drives Degree Distribution and Emerging Network Properties.” *PeerJ* 2: e251.

- 612        <https://doi.org/10.7717/peerj.251>.
- 613    Pomeranz, Justin Page, Ross M. Thompson, Timothée Poisot, Jon S. Harding, and Justin P. F.  
614            Pomeranz. 2018. “Data from: Inferring Predator-Prey Interactions in Food Webs.” Dryad.  
615            <https://doi.org/10.5061/DRYAD.K59M37F>.
- 616    Shannon, C. E. 1948. “A Mathematical Theory of Communication.” *The Bell System Technical  
617            Journal* 27 (3): 379–423. <https://doi.org/10.1002/j.1538-7305.1948.tb01338.x>.
- 618    Staniczenko, Phillip P. A., Jason C. Kopp, and Stefano Allesina. 2013. “The Ghost of Nested-  
619            ness in Ecological Networks.” *Nature Communications* 4 (1): 1391. <https://doi.org/10.1038/ncomms2422>.
- 620    Stock, Michiel, Timothée Poisot, and Bernard De Baets. 2021. “Optimal Transportation Theory  
621            for Species Interaction Networks.” *Ecology and Evolution* 11 (9): 3841–55. <https://doi.org/10.1002/ece3.7254>.
- 622    Stouffer, Daniel B., and Jordi Bascompte. 2011. “Compartmentalization Increases Food-Web  
623            Persistence.” *Proceedings of the National Academy of Sciences* 108 (9): 3648–52. <https://doi.org/10.1073/pnas.1014353108>.
- 624    Stouffer, Daniel B., Juan Camacho, Wenxin Jiang, and Luis A. Nunes Amaral. 2007. “Evidence  
625            for the Existence of a Robust Pattern of Prey Selection in Food Webs.” *Proceedings of the  
626            Royal Society B-Biological Sciences* 274 (1621): 1931–40. <https://doi.org/10.1098/rspb.2007.0571>.
- 627    Strydom, Tanya, Michael D. Catchen, Francis Banville, Dominique Caron, Gabriel Dansereau,  
628            Philippe Desjardins-Proulx, Norma R. Forero-Muñoz, et al. 2021. “A Roadmap Towards  
629            Predicting Species Interaction Networks (across Space and Time).” *Philosophical Transactions of the Royal Society B: Biological Sciences* 376 (1837): 20210063. <https://doi.org/10.1098/rstb.2021.0063>.
- 630    Strydom, Tanya, Giulio V. Dalla Riva, and Timothee Poisot. 2021. “SVD Entropy Reveals the  
631            High Complexity of Ecological Networks.” *Frontiers in Ecology and Evolution* 9: 623141.  
632            <https://doi.org/10.3389/fevo.2021.623141>.

639 Williams, Richard J. 2011. "Biology, Methodology or Chance? The Degree Distributions of  
640 Bipartite Ecological Networks." *PLOS ONE* 6 (3): e17645. <https://doi.org/10.1371/journal.pone.0017645>.

642 Williams, Richard J., and Neo D. Martinez. 2000. "Simple Rules Yield Complex Food Webs."  
643 *Nature* 404 (6774): 180–83. <https://doi.org/10.1038/35004572>.

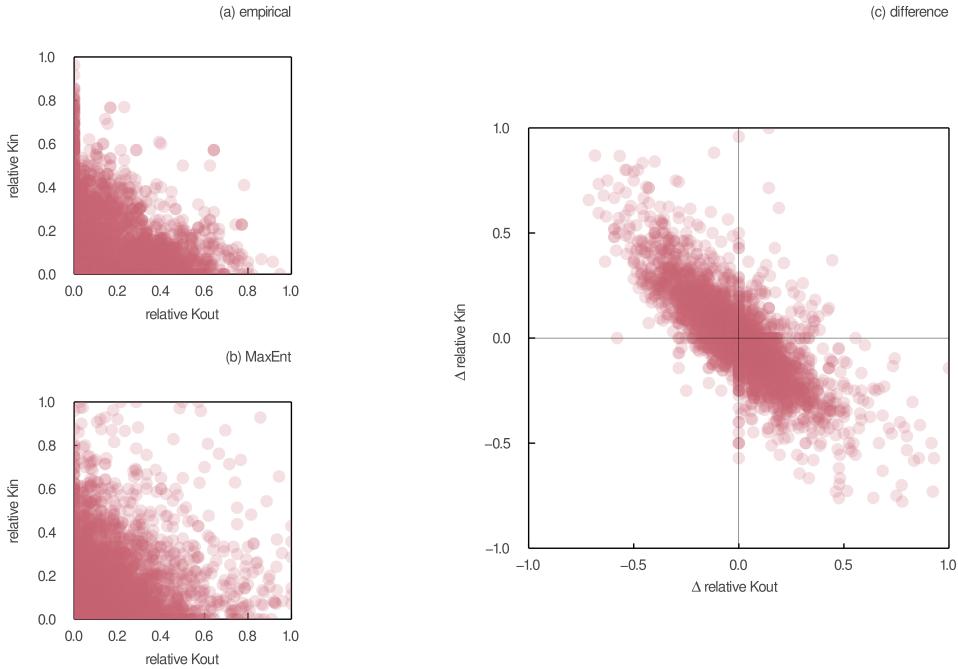


Figure 1: Relative number of predators ( $k_{in}$ ) as a function of the relative number of preys ( $k_{out}$ ) for each species in (a) empirical and (b) maximum entropy joint degree sequences. Empirical networks include all food webs archived on Mangal, as well as the New-Zealand and Tuesday Lake datasets (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.

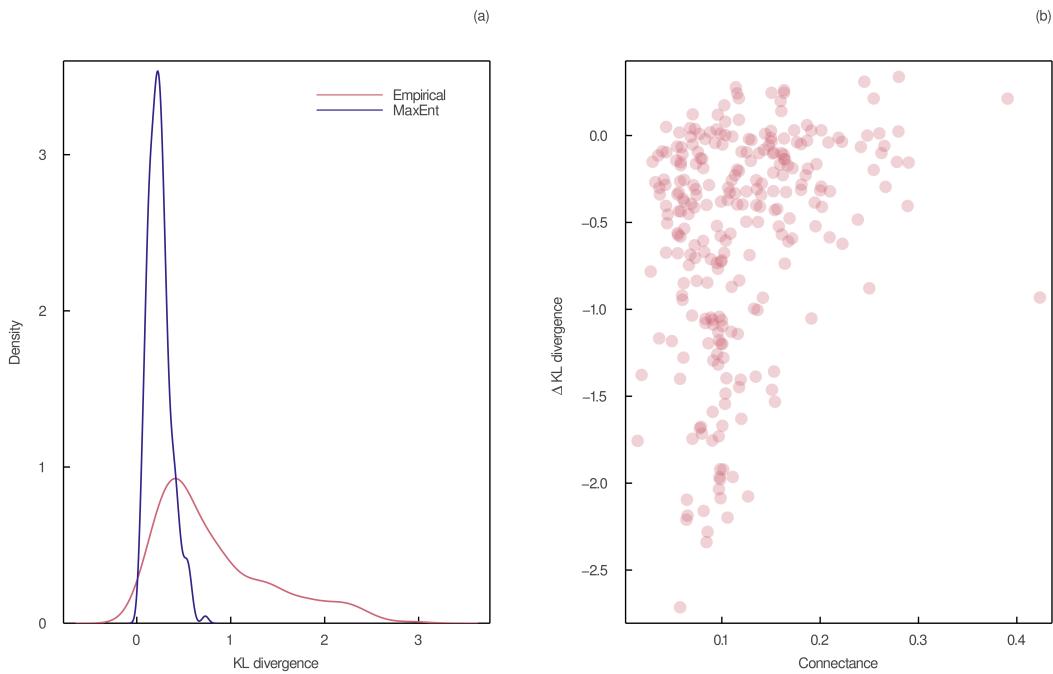


Figure 2: (a) Probability density of KL divergence between in and out-degree sequences of empirical and maximum entropy joint degree sequences. (b) Difference between the KL divergence of empirical and predicted networks as a function of connectance. In both panels, empirical networks include all food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

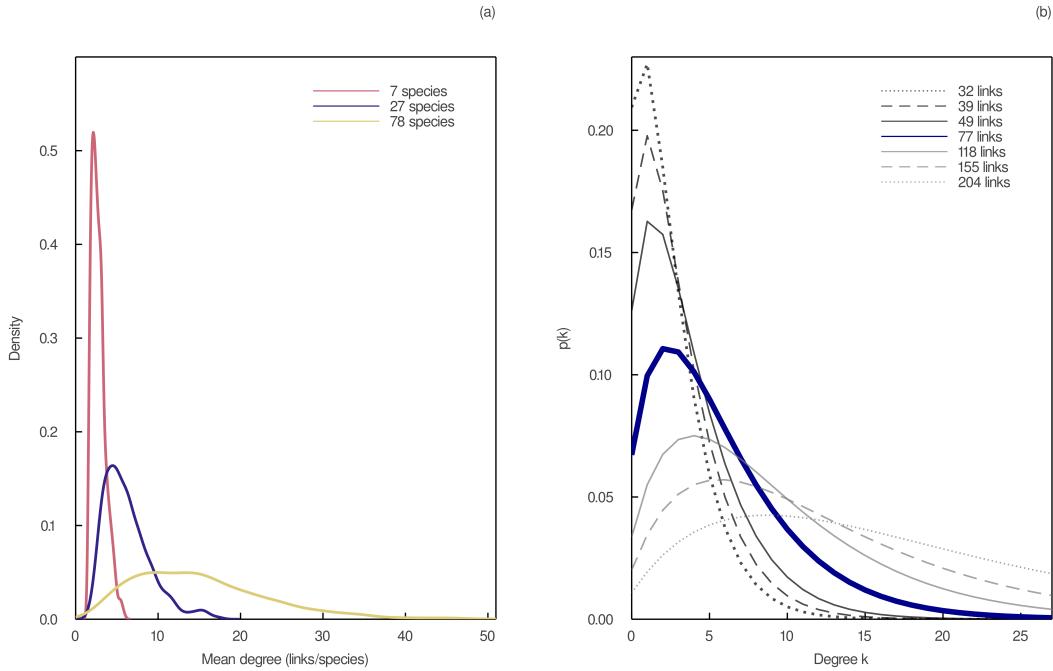


Figure 3: (a) Probability density of the predicted mean degree for different values of species richness. The number of interactions was predicted using the flexible links model fitted to all empirical networks in our complete dataset (eq. 17). (b) Degree distributions of maximum entropy for a network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

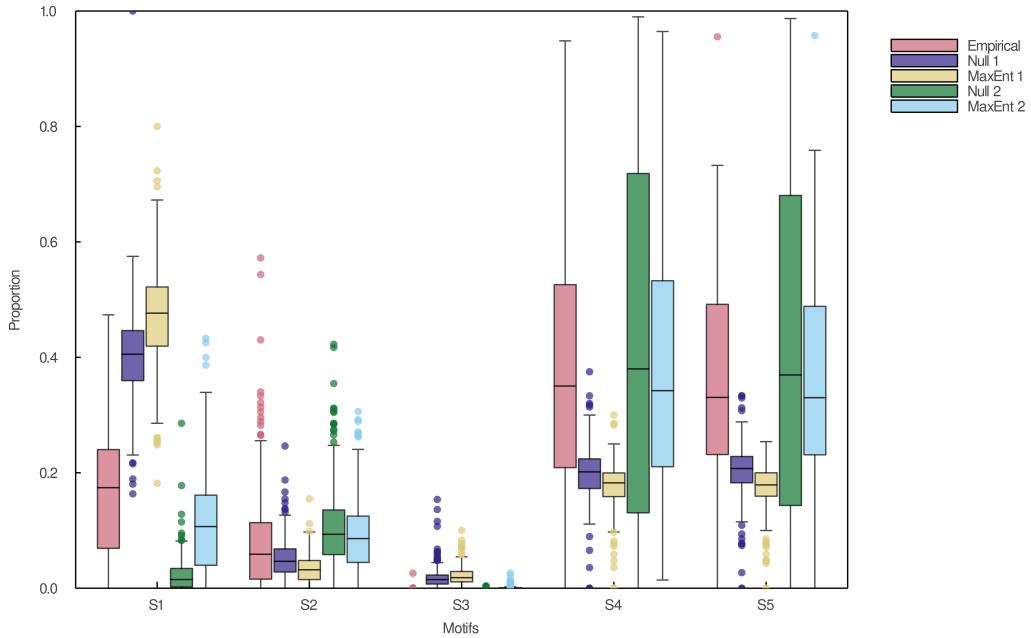


Figure 4: Motifs profile of empirical, maximum entropy, and null food webs. Empirical networks include all food webs archived on Mangal, as well as the New-Zealand and Tuesday Lake datasets (our complete dataset). Maximum entropy networks were estimated using a simulated annealing algorithm to find the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

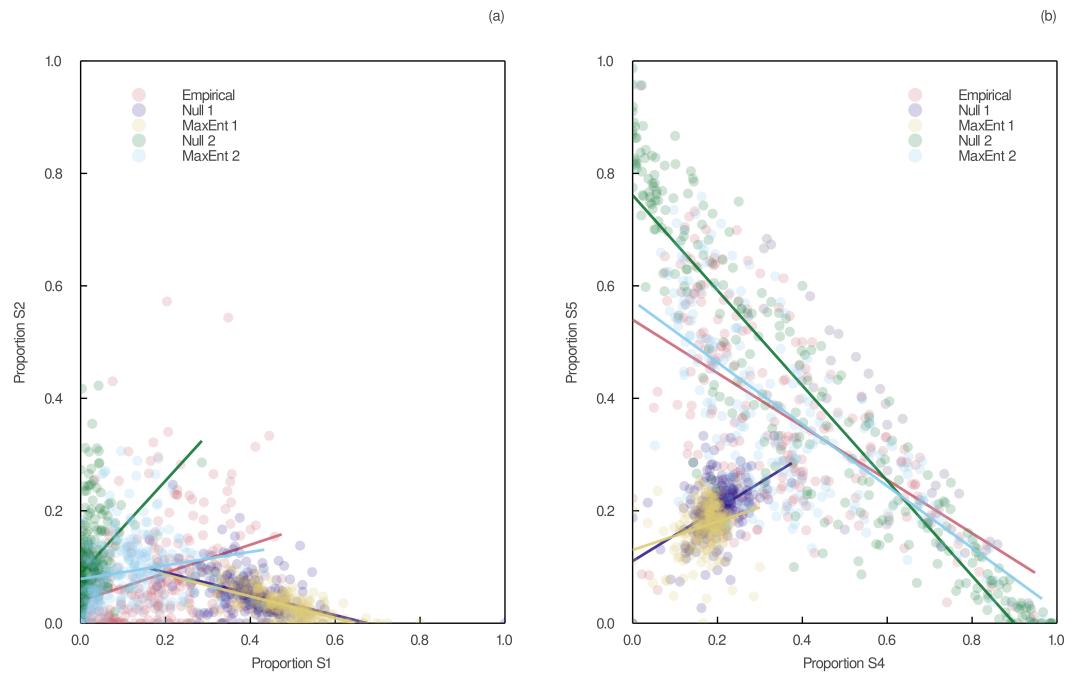


Figure 5: Relationship between motifs proportions of empirical, maximum entropy, and null food webs. Empirical networks include all food webs archived on Mangal, as well as the New-Zealand and Tuesday Lake datasets (our complete dataset). Maximum entropy networks were estimated using a simulated annealing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

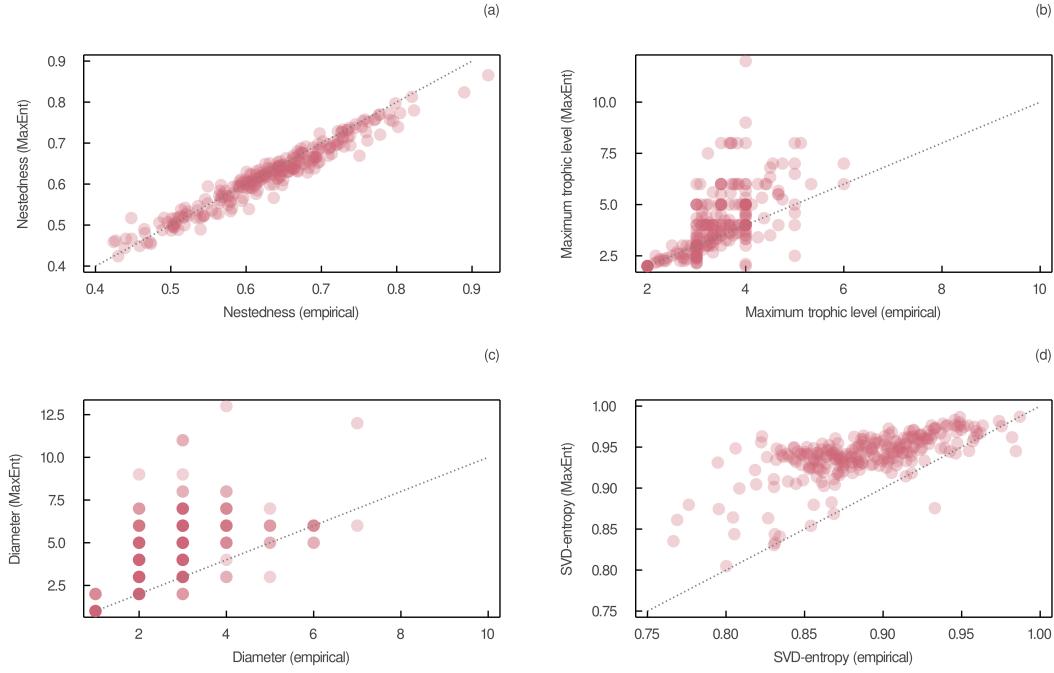


Figure 6: Relationship between the structure of empirical and maximum entropy food webs. Empirical networks include all food webs archived on Mangal, as well as the New-Zealand and Tuesday Lake datasets (our complete dataset). Maximum entropy networks were estimated using a simulated annealing algorithm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