

# Predicting metawebs: graph embeddings can help alleviate spatial data deficiencies

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1. Metawebs, i.e. networks of potential interactions within a species pool, are a powerful abstraction to understand how large-scales species interaction networks are structured.
2. Because metawebs are typically expressed at large spatial and taxonomic scales, assembling them is a tedious and costly process; predictive methods can help circumvent the limitations in data deficiencies, by providing 'draft' metawebs.
3. One way to improve the predictive ability is to maximize the information used for prediction, by using graph embeddings rather than the list of species interactions. Graph embedding is an emerging field in machine learning that holds great potential for ecological problems.
4. In this perspective, we outline how the challenges associated with inferring metawebs line-up with the advantages of graph embeddings; furthermore, because metawebs are inherently spatial objects, we discuss how the choice of the species pool has consequences on the reconstructed network, but also embeds hypotheses about which human-made boundaries are ecologically meaningful.

1 Having a general solution for inferring *potential* interactions (despite the unavailability of interaction data)  
2 could be the catalyst for significant breakthroughs in our ability to start thinking about species interaction  
3 networks over large spatial scales. In a recent overview of the field of ecological network prediction,  
4 Strydom et al. (2021) identified two challenges of interest to the prediction of interactions at large scales.  
5 First, there is a relative scarcity of relevant data in most places globally – paradoxically, this restricts our  
6 ability to infer interactions to locations where inference is perhaps the least required; second, accurate  
7 predictions often demand accurate predictors, and the lack of methods that can leverage small amount of  
8 data is a serious impediment to our predictive ability globally.

9 Following the definition of Dunne (2006), a metaweb is a network analogue to the regional species pool;  
10 specifically, it is an inventory of all *potential* interactions between species from a spatially delimited area  
11 (and so captures the  $\gamma$  diversity of interactions). The metaweb is, therefore, *not* a prediction of the food  
12 web at a specific locale within the spatial area it covers, and will have a different structure (notably by  
13 having a larger connectance; see e.g. Wood et al., 2015). These local food webs (which captures the  $\alpha$   
14 diversity of interactions) are a subset of the metaweb’s species and interactions, and have been called  
15 “metaweb realizations” (Poisot et al., 2015). Differences between local food web and their metaweb are  
16 due to chance, species abundance and co-occurrence, local environmental conditions, and local  
17 distribution of functional traits, among others.

18 Because the metaweb represents the joint effect of functional, phylogenetic, and macroecological  
19 processes (Morales-Castilla et al., 2015), it holds valuable ecological information. Specifically, it is the  
20 “upper bounds” on what the composition of the local networks can be (see e.g. McLeod et al., 2021). These  
21 local networks, in turn, can be reconstructed given appropriate knowledge of local species composition,  
22 providing information on structure of food webs at finer spatial scales. This has been done for example for  
23 tree-galler-parasitoid systems (Gravel et al., 2018), fish trophic interactions (Albouy et al., 2019), tetrapod  
24 trophic interactions (O’Connor et al., 2020), and crop-pest networks (Grünig et al., 2020). Whereas the  
25 original metaweb definition, and indeed most past uses of metawebs, was based on the presence/absence  
26 of interactions, we focus on *probabilistic* metawebs where interactions are represented as the chance of  
27 success of a Bernoulli trial (see e.g. Poisot et al., 2016); therefore, not only does our method recommend  
28 interactions that may exist, it gives each interaction a score, allowing us to properly weigh them.

## **The metaweb is an inherently probabilistic object**

Yet, owing to the inherent plasticity of interactions, there have been documented instances of food webs undergoing rapid collapse/recovery cycles over short periods of time (Pedersen et al., 2017). The embedding of a network, in a sense, embeds its macro-evolutionary history, especially as RDPG captures ecological signal (Dalla Riva & Stouffer, 2016); at this point, it is important to recall that a metaweb is intended as a catalogue of all potential interactions, which should then be filtered (Morales-Castilla et al., 2015). In practice (and in this instance) the reconstructed metaweb will predict interactions that are plausible based on the species' evolutionary history, however some interactions would/would not be realized due to human impact.

Dallas et al. (2017) suggested that most links in ecological networks may be cryptic, *i.e.* uncommon or otherwise hard to observe. This argument essentially echoes Jordano (2016): the sampling of ecological interactions is difficult because it requires first the joint observation of two species, and then the observation of their interaction. In addition, it is generally expected that weak or rare links would be more common in networks (Csermely, 2004), compared to strong, persistent links; this is notably the case in food chains, wherein many weaker links are key to the stability of a system (Neutel et al., 2002). In the light of these observations, the results in fig. ?? are not particularly surprising: we expect to see a surge in these low-probability interactions under a model that has a good predictive accuracy. Because the predictions we generate are by design probabilistic, then one can weigh these rare links appropriately. In a sense, that most ecological interactions are elusive can call for a slightly different approach to sampling: once the common interactions are documented, the effort required in documenting each rare interaction may increase exponentially. Recent proposals suggest that machine learning algorithms, in these situations, can act as data generators (Hoffmann et al., 2019): in this perspective, high quality observational data can be supplemented with synthetic data coming from predictive models, which increases the volume of information available for inference. Indeed, Strydom et al. (2021) suggested that knowing the metaweb may render the prediction of local networks easier, because it fixes an “upper bound” on which interactions can exist; indeed, with a probabilistic metaweb, we can consider that the metaweb represents an aggregation of informative priors on the interactions.

## 56 Graph embedding offers promises for the inference of potential 57 interactions

58 Graph embedding is a varied family of machine learning techniques aiming to transform nodes and edges  
59 into a vector space, usually of a lower dimension, whilst maximally retaining key properties of the graph  
60 (Yan et al., 2005). Ecological networks are an interesting candidate for the widespread application of  
61 embeddings, as they tend to possess a shared structural backbone (Mora et al., 2018), which hints at  
62 structural invariants that can be revealed at lower dimensions. Indeed, previous work by Eklöf et al. (2013)  
63 suggests that food webs are inherently low-dimensional objects, and can be adequately represented with  
64 less than ten dimensions. Simulation results by Botella et al. (2022) suggest that there is no best method to  
65 identify architectural similarities between networks, and that multiple approaches need to be tested and  
66 compared to the network descriptor of interest.

67 But the popularity of graph embedding techniques in machine learning is rather more intuitive than the  
68 search for structural invariants: while graphs are discrete objects, machine learning techniques tend to  
69 handle continuous data better. Therefore, bringing a discrete graph into a continuous vector space opens  
70 up a broader variety of predictive algorithms.

Table 1: Overview of some common graph embedding approaches, by time of publication, alongside examples of their use in the prediction of species interactions. Surprisingly, these methods have not yet been used routinely to predict species interactions; most of the examples we identified were either statistical associations, or analogues to joint species distribution models. <sup>a</sup>: statistical interactions; <sup>b</sup>: joint-SDM-like approach.

Method	Embedding approach	Reference	Species interactions
			application
RDPG	graphs through SVD	Young & Scheinerman (2007)	Poisot et al. (2021)
tSNE	nodes through statistical divergence	Hinton & Roweis (2002)	Cieslak et al. (2020) <sup>a</sup>
DeepWalk	graph walk	Perozzi et al. (2014)	Wardeh et al. (2021)

Method	Embedding approach	Reference	Species interactions application
FastEmbed	graph through PCA/SVD analogue	Ramasamy & Madhow (2015)	
LINE	nodes through statistical divergence	Tang et al. (2015)	
SDNE	nodes through auto-encoding	D. Wang et al. (2016)	
node2vec	node embedding	Grover & Leskovec (2016)	
graph2vec	sub-graph embedding	Narayanan et al. (2017)	
DMSE	joint node embedding	D. Chen et al. (2017)	D. Chen et al. (2017) <sup>b</sup>
HARP	nodes through a meta-strategy	H. Chen et al. (2017)	
GraphKKE	graph embedding	Melnyk et al. (2020)	Melnyk et al. (2020) <sup>a</sup>
Joint methods	multiple graphs	S. Wang et al. (2021)	

71 **The metaweb embeds hypotheses about which spatial boundaries are**  
72 **meaningful**

73 As Herbert (1965) rightfully pointed out, “[y]ou can’t draw neat lines around planet-wide problems”; in  
74 this regard, our approach (and indeed, any inference of a metaweb at large scales) must contend with  
75 several interesting and interwoven families of problems. The first is the limit of the metaweb to embed  
76 and transfer. If the initial metaweb is too narrow in scope, notably from a taxonomic point of view, the  
77 chances of finding another area with enough related species to make a reliable inference decreases; this

would likely be indicated by large confidence intervals during ancestral character estimation, but the lack of well documented metawebs is currently preventing the development of more concrete guidelines. The question of phylogenetic relatedness and dispersal is notably true if the metaweb is assembled in an area with mostly endemic species, and as with every predictive algorithm, there is room for the application of our best ecological judgement. Conversely, the metaweb should be reliably filled, which assumes that the  $S^2$  interactions in a pool of  $S$  species have been examined, either through literature surveys or expert elicitation. Supp. Mat. 1 provides some guidance as to the type of sampling effort that should be prioritized. While RDPG was able to maintain very high predictive power when interactions were missing, the addition of false positive interactions was immediately detected; this suggests that it may be appropriate to err on the side of “too many” interactions when constructing the initial metaweb to be transferred. The second series of problems are related to determining which area should be used to infer the new metaweb in, as this determines the species pool that must be used.

In our application, we focused on the mammals of Canada. The upside of this approach is that information at the country level is likely to be required by policy makers and stakeholders for their biodiversity assessment, as each country tends to set goals at the national level (Buxton et al., 2021) for which quantitative instruments are designed (Turak et al., 2017), with specific strategies often enacted at smaller scales (Ray et al., 2021). And yet, we do not really have a satisfying answer to the question of “where does a food web stop?”; the current most satisfying solutions involve examining the spatial consistency of network area relationships (see e.g. Galiana et al., 2018, 2019, 2021; **Fortin2021NetEco?**), which is of course impossible in the absence of enough information about the network itself. This suggests that an *a posteriori* refinement of the results may be required, based on a downscaling of the metaweb. The final family of problems relates less to the availability of data or quantitative tools, and more to the praxis of spatial ecology. Operating under the context of national divisions, in large parts of the world, reflects nothing more than the legacy of settler colonialism. Indeed, the use of ecological data is not an apolitical act (Nost & Goldstein, 2021), as data infrastructures tend to be designed to answer questions within national boundaries, and their use both draws upon and reinforces territorial statecraft; as per Machen & Nost (2021), this is particularly true when the output of “algorithmic thinking” (e.g. relying on machine learning to generate knowledge) can be re-used for governance (e.g. enacting conservation decisions at the national scale). We therefore recognize that methods such as we propose operate under the framework that contributed to the ongoing biodiversity crisis (Adam, 2014), reinforced

108 environmental injustice (Choudry, 2013; Domínguez & Luoma, 2020), and on Turtle Island especially,  
109 should be replaced by Indigenous principles of land management (Eichhorn et al., 2019; No'kmaq et al.,  
110 2021). As we see AI/ML being increasingly mobilized to generate knowledge that is lacking for  
111 conservation decisions (e.g. Lamba et al., 2019; Mosebo Fernandes et al., 2020), our discussion of these  
112 tools need to go beyond the technical, and into the governance consequences they can have.

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