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# **RESEARCH ARTICLE**

# An appraisal of graph embeddings for comparing trophic network architectures

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# Abstract

- 1. Comparing the architecture of interaction networks in space or time is essential for understanding the assembly, trajectory, functioning and persistence of species communities. Graph embedding methods, which position networks into a vector space where nearby networks have similar architectures, could be ideal tools for this purposes.
- 2. Here, we evaluated the ability of seven graph embedding methods to disentangle architectural similarities of interactions networks for supervised and unsupervised posterior analytic tasks. The evaluation was carried out over a large number of simulated trophic networks representing variations around six ecological properties and size.
- 3. We did not find an overall best method and instead showed that the performance of the methods depended on the targeted ecological properties and thus on the research questions. We also highlighted the importance of normalising the embedding for network sizes for meaningful posterior unsupervised analyses.
- 4. We concluded by orientating potential users to the most suited methods given the question, the targeted network ecological property, and outlined links between those ecological properties and three ecological processes: robustness to extinction, community persistence and ecosystem functioning. We hope this study will stimulate the appropriation of graph embedding methods by ecologists.

#### KEYWORDS

dimension reduction, ecological interaction networks, evaluation, food webs, graph embedding, species interactions, trophic groups, trophic networks

# **1** | INTRODUCTION

Community ecology is entering a new era, where data are becoming multi-species, multi-trophic and integrate species interactions (Pellissier et al., 2018). So far, ecologists have compared community composition data on the basis of species identity, functional traits or phylogenetic similarities (reviewed in Münkemüller et al., 2020). With the ever-increasing availability of interaction knowledge, we are now facing the opportunity to also compare communities based on their interaction network architecture, that is, the configuration of the interaction links between species of a community. This might provide crucial insights to describe biodiversity variations across environments (Pellissier et al., 2018), unveil network architecture similarities across communities composed of different species (Ohlmann et al., 2019) or understand the assembly rules behind multi-trophic assemblages (Münkemüller et al., 2020). In addition, the ecological properties that can be described from the architecture of a trophic network (e.g. degree of omnivory, generalism, compartmentalization, number of trophic levels) are important to characterise ecosystem functioning, resilience and robustness to extinctions (Monteiro & Faria, 2016; Tylianakis et al., 2010). To address these objectives, graph embedding methods that cast many networks into a common multi-dimensional vector space reflecting many aspects of architectural variations across the networks (e.g. Narayanan et al., 2017), are appealing. They allow standard multivariate analyses to be applied a posteriori to a set of networks, including descriptive analyses (e.g. dimension reduction techniques for visualization) and supervised learning (i.e. predicting an external characteristic from a network embedding coordinates based on knowledge of its values over a sample of network examples). Despite the diversity of individual network metrics or motifs studied in ecology (Lau et al., 2017), a small number of multi-dimensional graph embedding methods have been applied to trophic networks, and there has been no comparison of their abilities to capture the signatures of ecological processes on network architectures.

The ecological properties of a trophic network partially determine its dynamics, especially its persistence, its robustness to extinctions and other ecological processes. The distribution of species across trophic levels in a network especially impacts its robustness to extinctions (Pimm et al., 1991). For example, a lower proportion of basal species induces less prey per predators in higher trophic levels and thus increases the likelihood of secondary extinctions and extinction cascades. Regarding community persistence, longer trophic chains are also suggested to decrease the recovering rate of species populations after disturbance (Pimm et al., 1991), which explains shorter chains in fluctuating environments like for insect food webs. The length of trophic chains may also impact the global balance of carbon fluxes in the ecosystem through compensation of primary production and respiration as shown for lake ecosystems (Schindler et al., 1997). Compartmentalization has been theoretically shown to favour robustness to extinctions in food webs because it limits the effect of extinction cascades across modules (Thébault & Fontaine, 2010; Tylianakis et al., 2010). Compartmentalization can also impact ecosystem functioning, for instance by decreasing parasitism rate in plant-herbivore-parasite system (Montoya et al., 2003). Regarding more local ecological properties, predator generalism (number of preys), which is related to connectance, increases robustness to extinctions (Thébault & Fontaine, 2010). Moreover, theory suggests a strong link between generalism and the long-term persistence of community (Pimm et al., 1991; Thébault & Fontaine, 2010; Tylianakis et al., 2010), even though the precise mechanism behind this phenomenon still appears ambiguous. While it is often documented that generalism negatively affects community persistence (Thébault & Fontaine, 2010; Torres-Alruiz & Rodrguez, 2013), it may also provide a buffer in the response of individual predators to stochastic fluctuations of prey abundances (Tylianakis et al., 2010). This paradox is apparently resolved when high generalism is composed of many weak links which favours persistence (McCann et al., 1998). While generalism makes a species less sensitive to varying prey populations, vulnerability increases its population control. When both increase, the biomass transfer

rates are optimised at the network scale and may improve ecosystem resilience. For instance, the vulnerability of herbivores to many predators improved their population control in a collard-aphid system (Snyder et al., 2006), but excessive competition can lead to the opposite effect (Montoya et al., 2003). Omnivory is another local property known to influence parasitism rate (Montoya et al., 2003) and community persistence (Borrelli, 2015; Pimm et al., 1991). Loop patterns are suggested to destabilise trophic networks and decrease the persistence of species participating in them. Indeed, triangular motifs containing loops are less stable compared to other triangular motifs which was proposed as an explanation of their rarity in empirical food webs (Borrelli, 2015; Monteiro & Faria, 2016). As those ecological properties can be measured from network architectures and are important for many ecological processes, they provide a solid ground for comparing networks through graph embedding methods.

Among the few methods used to analyse the spatial variation of interaction networks, most quantify interaction turnover (i.e. turnover of links) between pairs of species (Ohlmann et al., 2019; Poisot et al., 2012). However, these methods do not account for the ecological properties that involve more than two species like omnivory and generalism degrees, trophic levels, loops or compartmentalization. Yet, it is crucial to compare these properties across distant ecosystems, independently of pure species and interaction turnover. Thus, measuring more complex network ecological properties requires to look at sub-structures composed of more than two species, often interlinked and very numerous. These characterizations of network architectures may be simplified by finding a suited vector space where each network will be represented as a vector, which is exactly the purpose of graph embedding methods. Some common network metrics in ecology (e.g. connectance) may be seen as components of graph embedding methods (Braga et al., 2019; Kortsch et al., 2019; Thompson & Townsend, 2005; Wood et al., 2015). Ecologists have indeed already used node level metrics (e.g. average number of links per node), node distances (e.g. diameter, mean distance) and whole networks metrics (e.g. connectance, modularity or nestedness) that measure specific properties of the network architecture. However, it is notoriously difficult to select the right metric to measure the variability of an ecological property (Braga et al., 2019) and one may also miss variations that are not explicitly dealt with the selected metrics. Counts of subgraphs with fixed number of nodes, called motifs, are also used in ecology. For instance, counts of triangular and bipartite motifs were applied to compare trophic network (Camacho et al., 2007) and plant-pollinator mutualistic network architectures (Simmons et al., 2019). However, these methods are restricted to small motif sizes due to computational complexity (i.e. up to four nodes in food webs, see Monteiro and Faria (2016), up to six nodes in bipartite mutualistic networks, see Simmons et al. (2019)).

Interestingly, a spectrum of efficient graph embedding methods has been developed in other domains to represent networks based on different types of sub-structures. Some methods may further integrate information on node labels to which we could feed information on trophic groups (Cirtwill et al., 2018), that is, sets of species sharing similar prey and predators, or any other relevant external information that classifies species into groups. Several sophisticated unsupervised machine learning algorithms (e.g. UGRAPHEMB (Bai et al., 2019), Graph2Vec (Narayanan et al., 2017)) have been proposed to produce graph embeddings. Particularly, Graph2Vec (Narayanan et al., 2017) is an interesting candidate for ecological applications. In this method, networks composed of similar node neigbourhoods are represented by embedding coordinates that are close in terms of Euclidean distance. Shortest path lengths have also been used to compare network architectures (Borgwardt & Kriegel, 2005). Comparing shortest path lengths across trophic networks is also interesting from a functional point of view. Indeed, shortest path lengths encode information related to trophic chain lengths or energy flows and are at the root of centrality measures (Costa et al., 2019). These methods might bring different and relevant perspectives to ecological network analyses, but they require a comprehensive and contextual understanding to be successfully applied.

To compare graph embedding methods for their use in ecology, we need to define their usage scenarios. They may be used for different posterior analytic tasks on networks including supervised and unsupervised learning. An unsupervised learning task would typically consist in identifying gradients or clusters of variation through visualization after reducing the embedding space dimensionality (e.g. two dimensions). In this visualization space, a set of networks that appear clustered, are thus neighbours in the embedding and share similarities in their architectures. This task requires depicting, in the embedding matrix, the main architectural variations existing across networks while reducing the effects of non-interesting sources of variability (e.g. network size). Alternatively, supervised learning aims to predict a given property of a network as a function of its embedding coordinates. For instance, one may want to predict the robustness to extinction (Dunne et al., 2002) as a function of the counts of shortest path lengths. We therefore appraise the ability of graph embedding methods to represent important architectural variations across trophic networks and for posterior supervised and unsupervised analyses. We first introduce five graph embedding methods that are relevant to trophic network analyses and based on different architectural characteristics (e.g. motifs or paths lengths). Since two of these methods can handle node labels information, we thus moreover test the use of known trophic groups as node labels. Second, we illustrate the dimension reduction step for visualization (unspervised learning) with a recent nonlinear dimension reduction technique called Uniform Manifold Approximation and Projection (UMAP; McInnes et al., 2018). Third, we detail our simulation procedure of trophic networks where we control the variation of six important categorical ecological properties (maximum trophic length, trophic group composition, compartmentalization, omnivory, generalism and intra-trophic group predation) and, independently, species richness. Fourth, we introduce several measures to evaluate the relative performances of the embedding methods for supervised and unsupervised scenarios, including robustness to species richness variability for the latter. This methodological workflow is summarised by Figure 1. We finally guide the user towards the most suited method given the general aim of the analysis and the network

ecological properties focused on, and further relate these properties to important ecological processes.

### 2 | MATERIALS AND METHODS

#### 2.1 | Embedding methods

Among the available graph embedding methods, we selected five of them that should prove useful for ecological data and are relatively easy to use (Table 1). Two of them (Graph2Vec and ShortPaths2Vec) can also use prior information on species (node labels) like the belonging to a trophic group. These methods all apply to directed unweighted graphs and thus account for the asymmetry of interactions between species' pairs. We consider by convention that interactions are directed from prey to predators.

### 2.1.1 | Groups2Vec

The underlying idea is that all species of the metanetwork (which describes potential interactions between the union of species over all networks) can be sorted by their belonging to trophic groups, meant to represent their topological role in the metanetwork (Cirtwill et al., 2018). In general, there exist many ways to define a partition of species into trophic groups. For instance, one could rely on predefined known guilds or trophic groups, build a classification from species functional traits or use a statistical approach that group species behaving in the same way in the network, like a stochastic block model (SBM, see Allesina et al., 2008; Kéfi et al., 2016) applied on the metanetwork as done by Ohlmann et al. (2019). In this study, for the sake of simplicity, we rely on the trophic groups used for the construction of the simulated networks. Thus, we do not infer those groups from the data but rather use the already known group structure. Groups2Vec simply builds its embedding matrix by computing the vector of group proportions (species richness in each group divided by total richness) for each network.

#### 2.1.2 | Metrics2Vec

Several metrics have long been used to characterise variations of trophic networks in space (see e.g. Braga et al., 2019; Kortsch et al., 2019; Thompson & Townsend, 2005; Wood et al., 2015) or in time (Albouy et al., 2014). We selected a total of 17 classical metrics (detailed in Table S1) including the average trophic level (Williams & Martinez, 2004), the average generalism, the frequency of omnivore species (defined as species that pre-date other species across more than one trophic level), proportions of top and basal species, modularity (Newman, 2006) and trophic length. Note that for our following analyses, we centred and scaled each metric (i.e. each column of the embedding matrix) so that metrics had equivalent contributions in analyses based on Euclidean distances.



**FIGURE 1** Study workflow. We used a group model to simulate 5,000 trophic networks with controlled ecological properties, cast them in a graph embedding matrix using various methods, reduced the embedding matrix dimension to generate a 2D visualization space, and compare the embedding methods qualities for supervised and unsupervised posterior analysis tasks

# 2.1.3 | Motifs2Vec

This embedding method gathers the frequencies of the 13 directed connected triangular motifs (see Figure S3), without self-loop (i.e. their count divided by the number of possible species triplets which is n(n - 1)(n - 2)/6 for a network of size *n*). These small motifs have been regularly used to characterise local architectures in trophic networks (Camacho et al., 2007). This normalization allows to correct for the effect of network size on motifs counts when comparing different networks. Larger motifs would give more precise representation of the whole network structure, but the computational complexity of motifs count,  $O(n^k)$  for *k*-nodes motifs, is prohibitive (Shervashidze et al., 2009).

# 2.1.4 | Graph2Vec

Graph2Vec (Narayanan et al., 2017) is an approach based on the description of the local neighbourhood of each node. Practically, the algorithm decomposes each network into trees rooted at each of its nodes. It takes as input a maximal depth, which corresponds to the distance up to which the neighbours of each node will be explored. Then, the description of the local neighbourhood of each node is used to generate an embedding matrix, whose dimensionality is chosen a priori by the user and where networks with similar node neighbourhoods tend to be close (more details in Section A.3 of Supporting Information). Graph2Vec has the possibility to account (or not) for prior information on node labels. In the case of no prior information, TABLE 1 Graph embedding methods tested in this study

Acronym	Principle	Reference
Groups2Vec	Trophic group proportions	This study
Metrics2Vec	Seventeen classic food web metrics	Thompson and Townsend (2005)
Motifs2Vec	Directed triangular motif proportions	Camacho et al. (2007)
Graph2Vec	Decomposition into local neighbourhoods	Narayanan et al. (2017)
Graph2Vec_lab	Graph2Vec + trophic groups as node labels	Narayanan et al. (2017)
ShortPaths2Vec	Shortest path lengths distribution	This study
ShortPaths2Vec_lab	ShortPaths2Vec + trophic groups as node labels	This study

TABLE 2The six ecological propertiescontrolled in our networks simulation andtheir categories

Property acronym	Effect	Possible values (categories)
nModules	Number of modules (compartments)	{1, 2}
trophLens	Trophic length in each module	see Section B from Supporting Information
maxTrophLen	Maximal trophic length across modules	{2, 3, 4, 5}
omni	Activates interactions between non- successive trophic levels in a module	{TRUE, FALSE}
generalism	Favours interactions between successive trophic levels in a module	{TRUE, FALSE}
loop	Allows intra-group interactions and thus favours loops	{TRUE, FALSE}

it takes the node degree as a label. In this study, we compared the embedding method (hereafter called Graph2Vec) with no prior information on node labels, with Graph2Vec\_lab that directly uses the species trophic group as node label (the same than in Groups2Vec). Since Graph2Vec was originally designed for undirected graphs, we forced the method to take into account edges direction when building a node neighbourhood. By default, it explores the network from prey to predators. We also tested to concatenate this default embedding matrix with the one derived from the network transposed adjacency matrix (exploration from predators to prey) to better represent the directed architecture of the trophic network. We compared the concatenated version to the default embedding matrix and also the effect of the maximal depth choice (Section A.4 from of Supporting Information). In the following application, we used the concatenated version of Graph2Vec (with an embedding matrix dimension of 30 for both the default and transposed version) with a maximal depth of 2.

# 2.1.5 | ShortPaths2Vec

This embedding method gathers the frequencies of the directed shortest path lengths. For a network, we first computed the length of the shortest path between all pairs of nodes, following edges direction. When there is no path between two nodes, it is counted as an infinite length. Then, the frequency vector of this set of lengths is constructed (for each length, its occurrence count is divided by n(n - 1), the total number of ordered pairs of distinct nodes for a size-n graph). When considering several networks, the columns of this embedding matrix correspond to the set of all lengths observed across the different networks. This embedding method gathers information related to the notion of trophic length, sometimes computed as the length of the longest directed shortest path. The ratio of shortest paths with infinite length may also encode information on compartmentalization in the network. As for Graph2Vec, our proposed ShortPaths2Vec approach is generalised to account for prior information on node label in a second version called ShortPaths2Vec\_lab. In ShortPaths2Vec\_lab, the counts of shortest paths of any given length is decomposed per combination of source and target node labels. In other words, any column of the embedding matrix corresponds to the count of shortest paths of a given length k starting from a node with a given label l and going to a node with a given label l' divided by n(n - 1), as for ShortPaths2Vec. We again use trophic groups as node labels (the same than in Groups2Vec).

# 2.2 | From embedding space to visualization space using UMAP dimension reduction

Once an embedding matrix is obtained from a set of networks, dimension reduction techniques can be used to visualise the networks in a lower dimensional vector space (here two dimensions) called the visualization space. Indeed, our embedding matrices have dimensionality ranging from 13 (Motifs2vec) to 60 (Graph2Vec in both directions) and above (dimension of ShortPaths2Vec/ ShortPaths2Vec\_lab depends on the networks shortest paths). We thus used a nonlinear dimension reduction technique called UMAP(McInnes et al., 2018) that was recently popularised for the analysis of biological data (Becht et al., 2019). UMAP relies on a user-defined distance metric (e.g. here the Euclidean distance) computed between all pairs of networks using their embedding coordinates. For any embedded network, UMAP considers its closest neighbours (we selected 150 neighbours here), and aims to find a projection into the visualization space such that, in this new space, these neighbouring networks are also close to the targeted one. This property has to be satisfied for every embedded network, and a mathematical criterion is numerically optimised to achieve this goal.

#### 2.3 | Simulation experiment

To compare these seven embedding methods, we carried out a simulation study to generate 5,000 trophic interaction networks (i.e. food webs). Each network was drawn from a parametric random network model (a SBM, see Allesina et al., 2008), hereafter called a group model, where species are divided into trophic groups and where the probabilities of interaction between species depend on their belonging to trophic groups. A group model is defined by its trophic groups (here, between 2 and 10 groups), the interaction probabilities between groups and the distribution of nodes (species) in groups. For each simulated network, we first randomly draw the network size and six parameters, hereafter called ecological properties (Table 2), determining the group model structure. As illustrated in Figure 2, our group model splits species in trophic groups which organise the network vertically in trophic levels and horizontally in one or two modules, in which case there are less interactions between modules than inside modules. As ecological properties varied across the networks, our procedure allowed generating networks with contrasted ecological characteristics. More details on the construction of the group models are provided in Section B from Supporting Information. We defined the number of species (network size) in {60, 120} and independently of the other properties. We affected one species per group (to avoid emptiness) and then randomly distributed the remaining species among the groups. Lastly, we randomly drew the presence of a directed interaction between each ordered pair of species through the probability of interaction of their groups as defined by the group model. Figure 2 illustrates the variety of our simulated networks and the effects of the variations in ecological properties through some examples.

We then applied the seven embedding methods to the 5,000 simulated networks. Practically, the 10 trophic groups resulting from the largest possible group model (see details in Section B from Supporting Information) were used as the groups for Groups2Vec and also as the node labels in Graph2Vec\_lab and ShortPaths2Vec\_lab.

#### 2.4 | Quality assessment of the embedding methods

We evaluated the ability of the seven embedding methods to disentangle the network ecological properties (maxTrophLen, trophlens, nModules, generalism, omni and loop) of the simulated networks for posterior supervised and unsupervised analysis tasks with several criteria (detailed in Section D from Supporting Information). In all that follows, we call categories the possible values taken by an ecological property as shown in the right column of Table 2, for example, 1 and 2 are the categories of the property **nModules**. For posterior supervised learning tasks, we used the predictive accuracy as a measure of quality to evaluate how well each property is predicted from network embedding coordinates. For a given property, we used the classification accuracy of a Random Forest (Breiman, 2001) trained to predict the category of a network from its coordinates in the embedding (e.g. predict the category of nModules using the 13 motifs proportions provided by Motifs2Vec). For unsupervised analyses, we aimed at evaluating how well the segregation between categories can be detected by human eyes in the visualization space. We assumed that if each category forms a cluster of networks well separated from other categories in the embedding space, the user has more chances to detect a structure with a clustering method or visually on the visualization space. For that purpose, three criteria were used. First, we measured how well networks of the same category aggregate into clusters, that is, how well distinct categories were segregated, in (a) the embedding space using a metric called R2-ebd and (b) in the 2D visualization space obtained from dimension reduction of the embedding matrix using UMAP using a metric called R2-umap (see Sections D.2 and D.3 from Supporting Information). The third criterion evaluated how the segregation of categories (in the embedding space and in the visualization space respectively) is blurred due to variation in network sizes (see Section D.4 from Supporting Information for the definitions of the two metrics R2-loss-ebd and R2-loss-umap). Note that, given the simulation design, Groups2Vec, Graph2Vec\_lab and ShortPaths2Vec\_lab were unfairly favoured for all criteria on properties maxTrophLen, trophlens and nModules compared to other embedding methods because they directly encoded trophic group composition that generated the network. Groups2Vec was also disfavoured compared to other methods for the omni, generalism and loop properties because, by our simulation design the trophic group proportions were not affected by changes in these three properties.

#### 3 | RESULTS

# 3.1 | Evaluation for supervised learning task: Predictive accuracy

The relative ability of the different embedding methods to predict the categories varied across ecological properties (Table 3). Among the different methods, Metrics2Vec had the highest predictive accuracy for maxTrophLen, trophlens and nModules





nModules=2; loop=FALSE trophLens=2,3; omni=FALSE; generalism=FALSE



nModules=1; loop=TRUE trophLens=3; omni=FALSE; generalism=FALSE



nModules=2; loop=TRUE trophLens=4,4; omni=TRUE; generalism=TRUE



FIGURE 2 Examples of simulated trophic networks of size 60 and their group model parameters (ecological properties). These networks span the four possible combinations of values for **nModules** (compartmentalization) and **loop** (intra-group predation). Nodes are coloured according to their trophic group

(excluding methods that integrate a priori information on trophic groups), closely followed by ShortPaths2Vec. For **omni**, the methods with the highest predictive accuracy were Graph2Vec\_ lab, ShortPaths2Vec\_lab and Motifs2Vec. Metrics2Vec and ShortPaths2Vec had the best predictive accuracy for **generalism**, and the latter was even more efficient when using trophic groups as node labels (ShortPaths2Vec\_lab, Table 3). **loop** was almost perfectly predicted by all embedding methods. Unlike its extension with node labels, we found that Graph2Vec had a relatively weak predictive accuracy for all properties except **loop** (Table 3, also visible on Figure 3d). This relatively low predictive accuracy persisted when applying the algorithm with more iterations FIGURE 3 UMAP 2D plans, Part 1. Each plane, that is, visualization space, is output by UMAP applied to an embedding of the simulated networks. Axes UMAP1 and UMAP2 may be read as the principal axes in multivariate linear analyses, without notion of importance ranking. Each point represents a network and the color (resp. shape) indicates the category of the ecological property at stake (resp. species richness  $n \in \{60, 120\}$ ). For visualization clarity, we randomly subsampled 600 points out of 5,000

TABLE 3 Predictive accuracy percentage for each ecological property and embedding method. This is the Out-Of-Bag classification accuracy of a Random Forest trained to predict the category of the ecological property from the coordinates of the network in the embedding. Some coefficients are shaded because their comparison with other embedding methods would be unfair, see our methodology. Bold values correspond to the best performance for each property (per column)

Method	maxTrophLen	trophlens	nModules	omni	generalism	loop
Groups2Vec	100	100	100	52	50	49
Metrics2Vec	93	71	99	89	95	100
Motifs2Vec	85	64	98	90	93	100
Graph2Vec	67	49	89	83	75	100
Graph2Vec_lab	100	99	100	92	88	100
ShortPaths2Vec	93	69	99	82	94	100
ShortPaths2Vec_lab	100	99	100	91	96	100

(higher order neighbourhood exploration, see Section A.4 from Supporting Information).

# 3.2 | Evaluation for unsupervised learning task: Segregation of categories

Motifs2Vec had the best segregation of categories in the embedding space (highest R2-ebd) for maxTrophLen, trophlens and nModules (Table 4). However, this relative performance was not consistently preserved in the UMAP plane. Indeed, its R2-umap was significantly inferior to the one of Metrics2Vec for nModules (Table 4, and see Figure 3b/f). Even though the categories of maxTrophLen and nModules were well separated in the UMAP plans of Metrics2Vec, ShortPaths2Vec and Motifs2Vec, this separation was always nonlinear and would not allow us to distinguish visually the categories without knowing them a priori (see Figures 3b/f and 4d as examples, or more comprehensively Figures S7 and S8). Specifically, Motifs2Vec had a higher R2-ebd than Metrics2Vec (Table 4) whereas it had a lower predictive accuracy for the same three properties (Table 3). These apparent conflicting results showed that the most suited approach clearly depends on the research questions and the task scenario (unsupervised vs. supervised analysis). Surprisingly, categories of maxTrophLen seemed much less segregated in the embedding space than in the visualization space for ShortPaths2Vec (R2-ebd < R2-umap, Table 4). This shows that even though a small portion of this embedding matrix variability was related to max-TrophLen, it was well retained after UMAP compression (see Figure 3d). Properties omni and generalism had an overall much weaker effect on the embedding matrix structures than nModules, loop and n (R2-ebd and R2-umap close to 0, see Table 4), even if they had the same number of categories. Here, the heterogeneity of results between methods was not meaningful enough to recommend

one method over another. This result might arise from our simulation model and might not be generalised to other datasets. For **loop**, the segregation of categories was heterogeneous across methods both in the embedding spaces and visualization spaces. ShortPaths2Vec showed the highest performance in the embedding space (R2-ebd, Table 4), but not in the visualization space where Graph2Vec and Graph2Vec\_lab had the highest R2-umap. Visually, all embeddings except ShortPaths2Vec\_lab exhibited a clean segregation of categories for **loop** in their visualization space, as shown in Figures 3d/e and 4b/c. Note, however, that it is certain that ShortPaths2Vec\_lab separates linearly **loop** in its embedding space (non-infinite shortest path lengths exist between species of a same trophic group when **loop** is activated), but its R2-ebd does not reflect it and remains relatively small probably because this embedding space contains mostly dimensions unrelated to **loop**.

#### 3.3 | Robustness to size variability

Groups2Vec and Motif2Vec were almost insensitive to network sizes variability and were thus the most robust methods both in the embedding and visualization spaces (R2-loss-ebd and R2-lossumap almost null in Tables S3 and S4) for all ecological properties, revealing the efficiency of their normalization for size. For other methods, network size variability decreased more or less the segregation of categories in their embedding and visualization spaces for all properties (R2-loss-ebd > 0 and R2-loss-umap > 0). Indeed, for Metrics2Vec, ShortPaths2Vec and ShortPaths2Vec\_lab, the segregation of categories decreased by around 10% in the embedding space and visualization space (i.e. R2-loss-ebd and R2-loss-umap are around 10 in Tables S3 and S4) when networks of size 60 and 120 were all considered together compared to the average segregation of categories when considering only one size at a time. This shows



TABLE 4 Segregation of categories for each ecological property (column) in each embedding space and 2D visualization space (measured
through R2-ebd and R2-umap). This measure reflects the level of clustering of networks of a same category compared to the average
distance. Shaded values should not be compared with other embeddings (in the same column) as it would be unfair, see Section 2.4. Bold
values correspond to the best performance for each property (per column)

	maxTro	phLen	trophle	ens	nModu	ıles	omni		genera	lism	loop	
Method	ebd	umap	ebd	umap	ebd	umap	ebd	umap	ebd	umap	ebd	umap
Groups2Vec	0.42	0.60	0.90	0.99	0.38	0.30	0.00	0.00	0.00	0.00	0.00	0.00
Metrics2Vec	0.19	0.10	0.32	0.20	0.20	0.14	0.02	0.00	0.02	0.00	0.30	0.48
Motifs2Vec	0.39	0.19	0.62	0.25	0.32	0.05	0.01	0.00	0.07	0.01	0.09	0.25
Graph2Vec	0.06	0.08	0.12	0.13	0.07	0.08	0.00	0.00	0.01	0.01	0.09	0.61
Graph2Vec_lab	0.10	0.09	0.30	0.13	0.09	0.07	0.04	0.00	0.00	0.00	0.08	0.61
ShortPaths2Vec	0.03	0.21	0.15	0.24	0.13	0.04	0.01	0.01	0.01	0.00	0.61	0.48
ShortPaths2Vec_lab	0.35	0.04	0.64	0.35	0.22	0.22	0.01	0.01	0.00	0.00	0.10	0.15

that ShortPaths2Vec normalization for size is not fully working. Finally, Graph2Vec and Graph2Vec\_lab appeared as the least robust methods as they showed the highest R2-loss-ebd and R2-loss-umap for all properties (resp. Tables S3 and S4). For instance, networks with the same size tended to be clustered in the UMAP plane of Graph2Vec (see Figure 3d). This strongly suggested that Graph2Vec and Graph2Vec\_lab are not suitable to compare networks with different sizes (when the effect of size was not a feature of interest) in posterior unsupervised analysis tasks. On the other hand, one can observe how the positions of networks of different size were mixed on the visualization planes of Groups2Vec and Motif2Vec (e.g. Figure S6 for Groups2Ved and Figure 3a for Motifs2Vec).

# 4 | DISCUSSION

This study proposed a critical evaluation of the ability of different graph embedding methods to detect ecological property variations between simulated trophic networks. We introduced two methods that have never been used to analyse ecological networks (Graph2Vec and ShortPaths2Vec) and proposed to use trophic groups as node labels to enrich the description of network architecture for these two methods. We evaluated seven embedding methods for posterior use in supervised and unsupervised analysis tasks focusing on six important network ecological properties, and testing their robustness to network sizes variability for the unsupervised setting.

Depending on the type of task, supervised or not, and the ecological property targeted, the relative performances of the embedding methods differed. Overall, Motifs2Vec and ShortPaths2Vec, which have a relatively small dimensionality (here 13 and 15), interpretable dimensions, and are relatively robust to network sizes variability, often proved to be more suitable for unsupervised analysis. Other embedding methods either poorly captured the properties of interest (e.g. Graph2Vec), or captured them in a nonlinear way which reduces their potential interpretability in visualization steps of unsupervised task (e.g. ShortPaths2Vec\_lab in Figure 3f). Metrics2Vec, ShortPaths2Vec\_lab and Graph2Vec\_lab, revealed their potential for posterior supervised learning tasks (Table 3). Moreover, predictive accuracy increased when architecturally relevant information (here trophic groups) was integrated as node labels in the embedding methods (ShortPaths2Vec\_lab and Graph2Vec\_lab, Table 3). In the following paragraphs, we suggest the most appropriate approach for a given targeted ecological property, and further motivate the study of a given property in the light of the ecological processes of interest (Table 5).

Motifs2Vec and Metrics2Vec proved to be the most suitable, respectively for unsupervised and supervised tasks, for maximum trophic length, trophic group composition and compartmentalization. As relationships between compartmentalization and robustness to extinction are mainly theoretical (Dunne et al., 2002; Thébault & Fontaine, 2010), supervised methods could be applied to predict the robustness to extinctions from an embedding coordinates that contains compartmentalization descriptors (e.g. modularity, clustering coefficient and nestedness). As noted earlier, trophic levels were suggested to impact resilience to perturbations and carbon flux balance (Pimm et al., 1991; Schindler et al., 1997). To test hypotheses on the effect of these environmental factors, we could apply ShortPaths2Vec combined with dimension reduction to a large set of trophic networks spatially distributed in various conditions of perturbation frequency and primary productivity in order to visualise potential patterns of association with trophic chain lengths.

Concerning generalism, ShortPaths2Vec\_lab and Metrics2Vec were the most suitable methods for supervised analysis while there was no efficient approach for unsupervised analyses (but Motifs2Vec performed best in R2-ebd, Table 4). This suggests that the effect of generalism appeared as a minor driver of the embedding matrices and one might probably specify another embedding method describing the joint distribution of in/out degrees across species to better capture variations of generalism. It might enable to better understand the still ambiguous relationship between generalism, vulnerability and robustness to extinctions (Dunne et al., 2002; Thébault & Fontaine, 2010). For instance, we hypothesise that a stronger negative relationship



Property	Supervised	Unsupervised	Ecological processes
maxTrophLen	Metrics2Vec	Motifs2Vec	CP, CFB
TrophLens	Metrics2Vec	Motifs2Vec	RE, CP, CFB
nModules	Metrics2Vec	Motifs2Vec	RE, PC
omni	Graph2Vec_lab/ ShortPaths2Vec_ lab/ Motifs2Vec		CP, PC
generalism	ShortPaths2Vec(_lab)		RE, CP, PC
loop		ShortPaths2Vec/ Metrics2Vec	

TABLE 5 Guide table summarising which embedding method to use according to the network ecological property that is targeted, the supervised or unsupervised nature of the analysis. Ecological processes demonstrably linked to each property are listed in the last column. We used the following acronyms, CFB, carbon flux balance; CP, community persistence; PC: population control; RE, robustness to extinctions

between species generalism and vulnerability within a network, for a fixed connectance, makes it more robust to extinctions. Furthermore, the change of these relationships in trophic networks along long time-scales have the potential to reveal signatures of community level selection related to mass extinction events (Roopnarine et al., 2007). For omnivory, Graph2Vec lab appears as the most adapted method for supervised learning, while no approach yielded significant performances for posterior unsupervised analyses. We might improve unsupervised analysis applications by combining some triangular motifs proportions related to omnivory and some dedicated metrics (e.g. omnivore proportion, average degree of omnivory) in order to unveil contrasts in omnivory patterns across networks that are known to influence parasitism rate (Montoya et al., 2003) and community persistence (Pimm et al., 1991). Finally, the predictive accuracy for the loop property was almost perfect for all methods, so that we cannot discriminate between them for a supervised learning application. For the unsupervised case, ShortPaths2Vec turned out to be the most suitable. Lastly, it might be important to note that the tested food web Metrics and Graph2Vec require less computational effort than the shortest paths embeddings. Indeed, the complexity of the former is linear with the number of nodes, while it is cubic for the latter using the Floyd-Warshall algorithm (Floyd, 1962).

Most graph embedding developments concerned supervised learning problems and especially graph classification (Li et al., 2017; Xu et al., 2018). Even the unsupervised graph embedding methods (Ivanov & Burnaev, 2018; Verma & Zhang, 2017) have been mostly evaluated on supervised learning tasks. Furthermore, the evaluation is most often done on multiple benchmark datasets coming from different research domains (e.g. bioinformatics or social networks) and weakly related to research questions of these domains, thus questioning the relevance of the evaluation for the end-users of these methods. Here, we took a different perspective since our comparative analysis and evaluation focused on the usefulness of graph embedding methods to address explicit research questions based on trophic network analyses, especially in the unsupervised context which is probably the most common case in ecology. This perspective comes at the price of some questions regarding the generality of our evaluation methodology and the potential limits of our simulation experiments. Regarding network simulation, omnivory and generalism were especially difficult to segregate for all embedding methods suggesting that our simulation model did not make their variations salient. Besides, two species belonging to the same trophic group in our simulation model tend to interact with the same other groups and with an equal proportion of species in each of these groups. This is a way to model trophic Eltonian niches (O'Connor et al., 2020), but it induces very similar positions of species belonging to a given group in the network. Regarding the evaluation methodology, the UMAP dimension reduction step has sometimes drastically reduced the segregation of categories of some property in the visualization space compared to the embedding space, while preserving it for others (e.g. nModules with Motifs2Vec, see Table 4). This behaviour might have been different using another dimension reduction technique.

Some lessons have been learnt and some questions have been raised on different embedding methods during this study. First, Groups2Vec did not allow us to segregate omnivory, generalism and loop because these properties were considered independently to generate the simulated trophic groups in our design. However, real studies demonstrated that some trophic groups can highlight differences in omnivory, the presence of loops or generalism. For example, Kéfi et al. (2016) fitted a SBM on a large interaction network including trophic interactions and showed that some identified groups included more omnivore species than others. Then, networks having higher species richness for these groups would have a higher degree of omnivory. We therefore point out that the relevance of Groups2Vec entirely depends on the ecological properties captured by the trophic groups so that results for this approach are very context dependent. We also showed that Graph2Vec was strongly affected by network size and thus not suitable for unsupervised analyses. Indeed, the distribution of the local neighbourhoods that are present in a network is affected by network size. For instance, deeper node neighbourhoods are more likely in larger networks. However, to our knowledge, no suitable size normalization procedure is available for this embedding method and its use in unsupervised analyses should thus be restricted to the comparison of networks with similar size. Even though ShortPaths2Vec was

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more robust to size variability, finding the right normalisation for this embedding method is not simple either. The normalisation we used revealed to not be fully efficient. This is probably because the frequencies of shortest path lengths are affected by network size, and not only their average count. Another important lesson regarding Graph2Vec concerns its parameterization. It is crucial to adapt the number of iterations (depth) to the average size of networks because the diversity of subtrees increases exponentially with the number of iterations. Then, applying a large depth to small graphs will tend to increase similarities between networks and thus induce approximately equally spaced points in the embedding space. In our experiment, we standardised each column of the Metrics2Vec embedding matrix so that they have equal contribution to the Euclidean distance computed in the embedding space. This impacts the arrangement of networks in the UMAP plane and the measure of segregation of categories. Without standardization, we would have favoured properties discriminated by the columns with highest variance. Interestingly, we can use standardization to control the relative importance of the metrics by multiplying each column by a specific coefficient depending on the targeted network ecological contrasts that we want to distinguish in the visualization space. Recently, graph neural networks (GNNs, see e.g. Gilmer et al., 2017; Kipf & Welling, 2016) have been proposed to produce more expressive and flexible graph embedding methods. Most GNNs are designed for supervised learning tasks, such as graphs classification, rather than unsupervised graph embedding methods (but see e.g. Bandyopadhyay et al., 2020). Supervised graph embedding with GNNs may be a way forward to find more general representations of interaction networks, as a GNN embedding may be trained, for instance, to predict several network ecological features such as dynamical behaviours or robustness to extinctions.

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#### AUTHORS' CONTRIBUTIONS

Everyone conceived the ideas and designed methodology. C.B., V.M., C.M. and S.D. carried out the formal analyses. Everyone carried the investigation. C.B. developed the software, produced visualizations and wrote the original draft. Everyone validated and reviewed. V.M., C.M., W.T. and S.D. supervised.

#### DATA AVAILABILITY STATEMENT

All the R and Python code necessary to reproduce our results is accessible from Zenodo (Botella, 2021) and Github https://github.com/ ChrisBotella/TrophicNetEncoder. The graph embedding methods except Graph2Vec are available as part of the R package econetwork available at CRAN, the Comprehensive R Archive Network (https:// cran.r-project.org/web/packages/econetwork/).

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