# Telling ecological networks apart by their structure: a computational challenge
# SUPPLEMENTARY INFORMATION

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## Contents

# S1 Network Data

In this section, we briefly describe how the ecological and non-ecological networks were collected. All the networks have been stored in a Git repository (`http://git.io/f4y4o`), with each file reporting the details on how the network was collected, as well as the reference to where it was published (if relevant).

## S1.1 Crime networks

The networks represent daily crime occurrence by neighborhood. Nodes stand for either a crime or a city neighborhood, and edges indicate which crimes took place in which neighborhood on a given day of the year. We compiled a network for each day of 2016 and for several cities: Chicago, Denver, Minneapolis, San Francisco, and Washington DC. For each network, we took the largest connected component (in case of disconnected networks).

## S1.2 Legislature networks

Annual networks of legislature voting rolls. Nodes indicate either a legislator or a bill and links indicate positive votes of a given legislator for a given bill. Data was collated for the United States (House and Senate), the United Nations General Assembly, and the European Parliament. For each network originally containing all bills voted on in a given year and all legislators who voted on at least one of those bills, the largest connected component (in case of disconnected networks) was extracted.

## S1.3 Microbiome networks

In our individual microbiome networks, nodes are either location on the body of an individual or operational taxonomic units (OTUs) of bacteria found at the body location. Edges mark the presence of a given OTU at a particular bodily site. We used OTUs based on the 16S rRNA variable region 3-5 (V35), which was analyzed for all the samples (about 5000) by the NIH Human Microbiome Project. For each of the subjects, samples were collected for 15–18 body sites. We built a network for each individual associated with more than 10 samples. In case of multiple visits by the same subject, the same body sites could have been sampled more than once, in which case we kept the samples as distinct nodes. As such, the number of nodes representing sites can be larger than 18. To build the networks, we downloaded the data on the samples and connected it with the corresponding OTU table.

## S1.4 Authorship networks

These networks connect authors to journals where they have published across their career. For example, the network ”American Naturalist 2016” takes all the authors who have published in The American Naturalist in 2016, and connects them with the journals where they have published throughout their career.

We downloaded from Scopus all the abstracts published in 10 ecological journals (*The American Naturalist*, *Ecography*, *Ecological Applications*, *Ecological Monographs*, *Ecology*, *Ecology Letters*, *Journal of Animal Ecology*, *Journal of Applied Ecology*, *Journal of Ecology*, and *Oikos*) for the years 2006 to 2016. We then extracted all authors ID found in the metatadata associated with each abstract ($31,308$ unique authors were represented). For each author, we collected from Scopus the names of the journals in which they had published their research. We retained all journals in which at least 100 of the authors had published (687 journals). Finally, we constructed the network connecting authors to journals and took the giant component, comprising $20,087$ authors and 687 journals. Each of the networks analyzed in this work is obtained subsetting this giant component, by selecting only the authors who have published in a given journal/year combination (*e.g.*, *The American Naturalist*, 2016).

## S1.5 Movie-Actor networks

These networks connect actors with the movies in which they acted. For each of the $201,346$ movies listed in the Movie Data base, we have downloaded the list of actors in the credits, as well as the production year and the genre(s) (up to four genres were recorded). We then built a network for each genre and period (spanning a few years, for example ”Action 1996-2000” or ”Crime 1900-1950”; the different periods were chosen to avoid networks that were to small or too large). For each network, we retained only the giant component.

## S1.6 Ecological interaction networks

These networks detail species interactions among two sets of species. They can be further subdivided into separate sub-types, reported below. In all cases, both classes of nodes represent species (or other taxonomic units, especially in the case of bacteria and viruses), and edges connecting the nodes stand for species' interactions (*e.g.*, pollination, parasitism). Because these networks have been taken from the ecological literature, we simply report the references to the original studies, containing a detailed description of how the data were collected.

### S1.6.1 Antagonism

- Host-Parasite (109) [Hadfield et al., 2013, Arai and Mudry, 1983, Arthur et al., 1976, Bangham, 1955, Bellay et al., 2013, Dechtiar, 1972, Krasnov et al., 2012, Leong and Holmest, 1981, Pilosof et al., 2013]
- Plant-Herbivore (41) [Basset et al., 1996, Blüthgen et al., 2006, Bodner, 2009, Coley et al., 2006, Ibanez et al., 2013, Janzen et al., 1980, 2003, Joern, 1979, Leather, 1991, Lewis et al., 2002, Loye and Zuk, 1992, Macfadyen et al., 2009, Nakagawa et al., 2015, Novotny et al., 2005, 2012, Prado and Lewinsohn, 2004, Starỳ et al., 2008, Tavakilian et al., 1997, Ueckert et al., 1976]
- Bacteria-Phage (27) [Barrangou et al., 2002, Capparelli et al., 2010, Comeau et al., 2005, 2006, Doi et al., 2003, Flores et al., 2011, Hansen et al., 2007, Holmfeldt et al., 2007, Kankila and Lindström, 1994, Krylov et al., 2006, Langley et al., 2003, Middelboe et al., 2009, Miklič and Rogelj, 2003, Poullain et al., 2008, Quiberoni et al., 2003, Rybniker et al., 2006, Seed and Dennis, 2005, Stenholm et al., 2008, Sullivan et al., 2003, Synnott et al., 2009, Wichels et al., 1998, Zinno et al., 2010]
- Host-Parasitoid (23) [Barbosa et al., 2003, Carvalheiro et al., 2008, Le Corff et al., 2000, Macfadyen et al., 2009, Stireman and Singer, 2003, Sugiura, 2007]

### S1.6.2 Mutualism

- Plant-Pollinator (217) [Brosi et al., 2017a,b, Carstensen et al., 2018, 2017, Kaiser-Bunbury et al., 2010, 2014, Magrach et al., 2018, 2017, Arroyo et al., 1982, Barrett and Helenurm, 1987, Bartomeus et al., 2008, Bezerra et al., 2009, Bundgaard, 2003, Burkle et al., 2013, Clements and Long, 1923, Dicks et al., 2002, Dupont et al., 2003, Dupont and Olesen, 2009, Elberling and Olesen, 1999, Herrera, 1988, Hocking, 1968, Inoue, 1990, Inouye and Pyke, 1988, Kaiser-Bunbury et al., 2014, Kakutani et al., 1990, Kato et al., 1990, 1993, Kato, 1996, 2000, Kevan, 1970, Lundgren and Olesen, 2005, McMullen, 1993, Medan et al., 2002, Memmott, 1999, Montero, 2005, Mosquin and Martin, 1967, Motten, 1982, Olesen et al., 2002, Ollerton et al., 2003, Percival, 1974, Petanidou, 1991, Primack, 1983, Ramirez, 1989, Ramirez and Brito, 1992, Robertson, 1929, de Mendonça Santos et al., 2010, Schemske et al., 1978, Small, 1976, Smith-Ramírez et al., 2005, Stald, 2003, Tur et al., 2013, Vázquez, 2002, Weiner et al., 2011, Yamazaki and Kato, 2003, Gilarranz et al., 2015, 2014, Orford et al., 2016b,a, Lara-Romero et al., 2016b,a, Trøjelsgaard et al., 2015, Trøjelsgaard et al., 2015]
- Plant-Seed disperser (41) [Baird, 1980, Beehler, 1983, Carlo et al., 2003, Crome, 1975, Frost, 1980, Galletti and Pizo, 1996, Guitian Rivera and Callejo Rey, 1983, Hamann and Curio, 1999, Jordano, 1985, Lambert, 1989, Mack and Wright, 1996, NOMA, 1997, Poulin et al., 1999, Schleuning et al.,

2011, Silva, 2002, Snow and Snow, 1971, 1988, Sorensen, 1981, Tutin et al., 1997, Wheelwright et al., 1984]

- Ant-Plant (11) [Blüthgen et al., 2004, Davidson et al., 1989, Fonseca and Ganade, 1996, Passmore et al., 2012]
- Anemone-Fish (1) [Ollerton et al., 2007]

### S1.7 Censoring networks

For all figures in the main text and in this supplement, any networks collected which had fewer than five nodes in either category (*e.g.*, plants or pollinators, crimes or neighborhoods) were excluded from further analysis and summary tables. In general, we believe that the type of analysis described in this work is only feasible for networks that a) are sufficiently large (because fluctuations in network metrics are going to overwhelm the "signal" in small networks); and b) sufficiently connected (if a network is close to a tree, or another barely connected graph, there is no structure to investigate; the same holds for networks where almost all edges are realized).

## S2 Randomizations

For each network we collected, we created two randomized versions. The first randomization produces a network containing exactly the same number of nodes and links, but having the links rearranged such that any two nodes have the same probability of being connected. This randomization yields an Erdős-Rényi random bipartite graph with the same size and fill as the original. Because the original networks are surely connected (for each network, we only kept the giant connected component), we repeatedly randomized each network until we obtained a connected graph. For sufficiently high connectance, the probability of obtaining a connected graph is close to one, and as such the computation is quick. For sufficiently low connectance, however, the probability of obtaining a connected graph rapidly approaches zero [Staniczenko et al., 2013], such that this naive method for randomizing the network would require an unreasonably long time. In these cases, we modified the randomization scheme by first drawing a random spanning tree through the nodes, and then randomly assigning the remaining links (to bring the total number up to that of the original network) as described above. This should not bias our randomizations, as a spanning tree is a necessary backbone of any connected network.

The second randomization produces a random bipartite graph with the same degree sequence as the original (*i.e.*, each **node** maintains the same number of connections as it had in the original network). This is known as a "configuration model". For this randomization, we utilized a fast, unbiased routine called the "curveball algoritm" [Strona et al., 2014]. In this case, it is more compuationally taxing to ensure connectedness of the randomized network, and therefore we discarded disconnected graphs and re-randomized from the original network again until a connected graph was identified. For several networks (especially the actor-movie set), despite more than 1000 attempts, we were still unable to find a connected network. This is often due to very low connectance, which reduces the number of possible connected networks with the desired degree distribution. For these cases, we omitted those networks from configuration model panels in the relevant figures. Due to the unbiased nature of the curveball algorithm, this process of discarding and re-randomizing is not expected to influence our analysis. Importantly, the curveball algorithm only produces simple graphs (*i.e.*graphs with neither links connecting a node to itself (self-links) nor multiple links connecting the same pair of nodes (hyperedges)). Since all of our empirical networks are simple graphs, this constraint increases the relevance of the network-structure-space we are sampling for comparison.

## S3 Matrix representation of bipartite networks and their spectra

Any bipartite network can be represented as a $n \times m$ incidence matrix $\mathbf{B}$, where $n$ is the number of rows (nodes of the first class), and $m$ the number of columns (nodes of the second class), and $B_{ij} = 1$ if node $i$

and $j$ are connected, and 0 otherwise. Without loss of generality, we assume $n \geq m$ in what follows. The graph can be also represented as a symmetric adjacency matrix:

$$\mathbf{A} = \begin{pmatrix} \mathbf{0} & \mathbf{B} \\ \mathbf{B}^T & \mathbf{0} \end{pmatrix} .$$

Where a superscript $T$ signifies the transpose of the associated matrix. The spectrum (*i.e.*, the set of eigenvalues) of the adjacency matrix of a bipartite network is composed of real eigenvalues and symmetric about 0: if $\lambda$ is an eigenvalue of $\mathbf{A}$, then $-\lambda$ is also an eigenvalue. Up to $2m$ eigenvalues can be different from zero, while the remaining eigenvalues are all 0. This means that in general the adjacency matrix will be rank-deficient whenever $n \neq m$. The singular values of the bipartite network, $\sigma_1, \sigma_2, \ldots \sigma_m$ are the eigenvalues of $\mathbf{B}^T\mathbf{B}$. The eigenvalues of $\mathbf{B}\mathbf{B}^T$ are the same of those of $\mathbf{B}^T\mathbf{B}$, with the addition of $n-m$ zero eigenvalues. The eigenvalues of $\mathbf{A}$ are the square roots of the singular values.

# S4 Metrics Collected

For each network, including the two randomized versions of each empirical network, we measured a number of structural properties. These included network size (number of rows and columns in the matrix representation of the bipartite network) and fill (absolute number of links as well as the ratio of the number of links to the number of possible links, termed "connectance"), and a number of other properties.

In this section, we list the metrics we collected, along with a brief explanation or references to the literature. We describe in detail how the metrics used in the main text for our example were obtained.

## S4.1 Spectral properties

For each network, we recorded the three "rightmost" (largest positive) eigenvalues of the adjacency matrix, $\lambda_1$, $\lambda_2$ and $\lambda_3$ as well as the three largest eigenvalues of the Laplacian matrix $\mathbf{L} = \mathbf{D} - \mathbf{A}$, where $\mathbf{D}$ is a diagonal matrix whose coefficients report the degrees of each node. We also measured the inverse participation ratio for the three leading eigenvectors of the adjacency matrix, quantifying localization [Pastor-Satorras and Castellano, 2016]: if $w$ is a unitary eigenvector of $\mathbf{A}$, $IPR = \sum_i w_i^4$. Finally, we measured the algebraic connectivity of the network, taken as the second smallest eigenvalue of the Laplacian matrix [Fiedler, 1973].

## S4.2 Expectation for the largest eigenvalues of the randomized networks

For each network, we want to also record the expected values of $\lambda_1$ and $\lambda_2$, which we will then use to remove the dependency on size and fill. These approximations are based on the assumption that we are estimating the eigenvalues of a random graph, either with a specified degree sequence (configuration model; only the spectral abscissa ($\lambda_1$)), or with a given size and fill (Erdős-Rényi for the spectral abscissa and Marchenko-Pastur for the second largest eigenvalue). We omit the calculations here for the expected value of the second largest eigenvalue of a configuration model random graph, as we found that, while such as estimation is accurate asymptotically, it performs quite poorly for our real-world networks.

To approximate $\lambda_1$, we use the formula provided by Chung et al. [2003] for the case of unipartite graphs with a specified degree sequence: $\lambda_1 \approx \mathbb{E}[d_i^2]/\mathbb{E}[d_i]$ where $\mathbb{E}$ is the expectation, and $d_i$ is the degree of node $i$. When working with bipartite networks, we need to account for the degrees of the nodes in the two classes. We use $r_i$ for the degree of the nodes in the first class, and $c_j$ for those in the second. By the same argument of Chung et al. [2003], the approximation for the first eigenvalue of the bipartite graph becomes:

$$\lambda_1 \approx \sqrt{\frac{\mathbb{E}[r_i^2]}{\mathbb{E}[r_i]} \frac{\mathbb{E}[c_j^2]}{\mathbb{E}[c_j]}} ,$$

which already provides an estimate for the configuration model ($\lambda_1^{cm}$), given that the statistics on the degrees are immediate to compute. We want to compute a similar approximation for the Erdős-Rényi case. One could simply assume that both $r_i$ and $c_i$ are binomially distributed, with parameters $m$ and $p = L/(nm)$ for the case of $r_i$ and $n$ and $p$ for the case of $c_i$. This would yield:

$$\lambda_1 \approx \sqrt{\frac{m^2p^2 + mp(1-p)}{mp}\frac{n^2p^2 + np(1-p)}{np}} = \sqrt{(mp + (1-p))(np + (1-p))} \; .$$

While this approximation works well for sufficiently high connectances $p$, it becomes inaccurate when the network has few connections. Because we are only considering connected networks, each row (column) must contain at least one connection (*i.e.*, $r_i \geq 1$, $c_j \geq 1$ for all $i$ and $j$. To improve the approximation, we account for this fact directly. In particular, the degree of each row follows the random variable $1 + x_r$ where $x_r$ is binomially distributed with parameters $m - 1$ and $\tilde{p}_r$, where the "excess connectance" $\tilde{p}_r = (L - n)/(n - m)$. We therefore obtain $\mathbb{E}[r_i] = 1 + \mathbb{E}[x_r] = 1 + (m-1)\tilde{p}_r$ and $\mathbb{E}[r_i^2] = \mathbb{E}[(1 + x_r)^2] = 1 + 2\mathbb{E}[x_r] + \mathbb{E}[x_r^2]$. Substituting, we get $\mathbb{E}[r_i^2] = 1 + 2(m-1)\tilde{p}_r + (m-1)^2\tilde{p}_r^2 + (m-1)\tilde{p}_r(1 - \tilde{p}_r)$. Performing the same calculation with the columns, we finally obtain:

$$\lambda_1^{er} \approx \sqrt{\frac{1 + (m-1)\tilde{p}_r(3 - \tilde{p}_r + (m-1)\tilde{p}_r)}{1 + (m-1)\tilde{p}_r} \times \frac{1 + (n-1)\tilde{p}_c(3 - \tilde{p}_c + (n-1)\tilde{p}_c)}{1 + (n-1)\tilde{p}_c}} \; ,$$

which performs better when connections are few, and converges to the previous estimate when $p$ is sufficiently large.

For completeness, we also compute the approximation for the case of a random semi-regular bipartite graph, in which all nodes in the same class have the same, average degree, and therefore $\mathbb{E}[r_i^2] = \mathbb{E}[r_i]^2$:

$$\lambda_1^{reg} \approx \sqrt{mpnp} = p\sqrt{nm} \; .$$

Having established the approximations for $\lambda_1$, we turn to $\lambda_2$.

The distribution of the singular values of an Erdős-Rényi random bipartite graph are expected to be formed by a bulk of singular values, following the Marchenko-Pastur distribution [Marchenko and Pastur, 1967], and a single outlier, accounting for the fact that the coefficients of matrix $\mathbf{B}$ have nonzero mean.

If $\mathbf{X}$ is an $n \times m$ matrix whose coefficients are i.i.d. random variables with mean zero and variance $s^2/n$, the largest singular value of $\mathbf{X}$ is approximately $\sigma_1 \approx s^2(1 + \sqrt{m/n})^2$. In our case, we want to compute the variance $s^2$ once we removed the mean ($p$). The second singular value of $\mathbf{B}$ should therefore be $\sigma_2 \approx np(1-p)(1 + \sqrt{m/n})^2$. We therefore obtain the estimate:

$$\lambda_2^{mp} \approx \left(1 + \sqrt{\frac{m}{n}}\right)\sqrt{np(1-p)}$$

## S4.3 Other network properties

We have also recorded a number of popular networks metrics, that can be used to explore the data set. Notice however that for many of these metrics, the correlation with size and fill of the matrix is unkown.

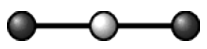
### S4.3.1 Large scale properties

- modularity[Newman, 2006] of the network (where computationally feasible)
- nestedness of the network (where computationally feasible), as measured by:
    - nestedness temperature [Atmar and Patterson, 1993]
    - NODF [Almeida-Neto et al., 2008]
    - the overlap measure of nestedness [Strona and Veech, 2015]
    - The spectral radius [Staniczenko et al., 2013]

### S4.3.2 Motif-related properies

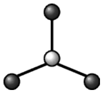
The counts of some small subgraphs present in the network can be computed directly from degree sequence:

- H2: $\sum_i \binom{d_i}{2}$

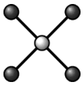


- H3: $(\boldsymbol{d}_{row} - 1) \times \mathbf{B} \times (\boldsymbol{d}_{col} - 1)$

- H4: $\sum_i \binom{d_i}{3}$



- H17: $\sum_i \binom{d_i}{4}$



### S4.3.3 Measures of centrality

We collected several measures of network centralization based on the following centrality measures:

- betweenness centrality
- closeness centrality
- eigenvector centrality

These were calculated using the ‘igraph‘ package [Csardi and Nepusz, 2006] in ‘R‘ [R Core Team, 2018]. Centralization is defined to be the sum of the normalized centrality scores of each node in the network. More precisely, the centralization $C$ of graph $G$ is

$$C(G) = \sum_v \left( \max_w (c(w)) - c(v) \right),$$

where $c(v)$ is the centrality of node $v$.

### S4.3.4 Clustering coefficient

Clustering in bipartite networks has traditionally been approached in one of two ways. First, one can use traditional measures of clustering (the proportion of completed triangles, or the proportion of a node’s connections that are also connected to one another) on one of the two unipartite projections of the bipartite network [Zhang et al., 2008, Opsahl, 2013]. Second, one can extend the foundational logic of clustering to look at paths of length four, rather than the original length three [Lind et al., 2005, Zhang et al., 2008, Opsahl, 2013].

Opsahl [2013] provides the most defensible interpretation of clustering for bipartite graphs, and details the expected value under Erdős-Rényi randomization, which we utilize in our analysis. Importantly, however, there are still significant limitations in this approach. First, this formulation depends on the orientation of the incidence matrix (*i.e.* which node class are rows and which are columns), identifying node classes as either primary or secondary, which is a subjective decision for many of the datasets being analyzed here. Second, as this technique involves counting (or at least sampling) chains of length four, it rapidly becomes computationally infeasible for moderately-sized networks. And third, the normalization proposed by Opsahl [2013] does not completely remove the relationship between size and fill for our data.

#### S4.3.5 Other properties

- network diameter (maximum distance between two nodes)
- average path length between nodes of the network
- degree heterogeneity in each of the row/column nodes (the mean degree squared divided by the mean of the squared degrees)
- degree assortativity (the correlation of degre between connected nodes)

## S5 A Note on Methodology

For the main text, we restricted our analysis in several ways. Some of these choices were dictated by clarity of presentation, while others were more principled. For instance, in the main-text figures, we used a subset of the collected metrics for clarity of presentation. Though we believe a simple solution (*i.e.*, one that utilizes relatively few measures of network structure) would be a more aesthetic solution, this is not a necessary property of a method that can classify ecological interaction networks. On the other hand, our choice to fit the PCA to the non-ecological data stemmed from more principled concerns.

First, not fitting the ecological data directly reduces the risk of overfitting our model to the particular ecological data being used.

Second, by utilizing a wide range of network types, we are able to create a more complete map of the possible space of bipartite network structures. Thus, when the bipartite networks are overlaid onto this space, we have a clearer idea of the general structure of this class as a whole. In every case we considered, the ecological networks most closely aligned with crime networks, suggesting some similarities in structure that might be worth further investigation.

Finally, a more logistical concern stemmed from the quality of currently available ecological data. Due in part to the difficulty of collecting ecological data, and in part to the fact that there are few cases of a single scientist publishing multiple networks, we are faced with a greater amount of noise in the ecological networks, compared with the other data sets. This noise can come from the study system itself (even collecting small ecological network data can be laborious), but also from more systemic sources. For instance, different networks depicting the same type of interaction will nevertheless have different sampling methodologies and span a large geographic and temporal range. Thus, utilizing the more highly and consistently replicated non-ecological data seemed to be a way of avoiding this variation/noise from disrupting the broader approach. In a later section of this supplement, we perform a PCA restricted to these data for comparison.

Each biplot throughout this text was constructed in a similar way: first the data were divided into a training set of 100 (or the size of the smallest network class (whichever was larger) networks from each class, and a testing/fitting set consisting of the remaining networks in teh dataset. A principal component (PC) space was constructed using the training set (fig. A, left panel) and this space was kept constant for each remaining figure, including the right panel of fig. A where the testing data for the PC space used in the main text are plotted. In later sections, we demonstrate alternative PC spaces stemming from including different/additional metrics and/or data.

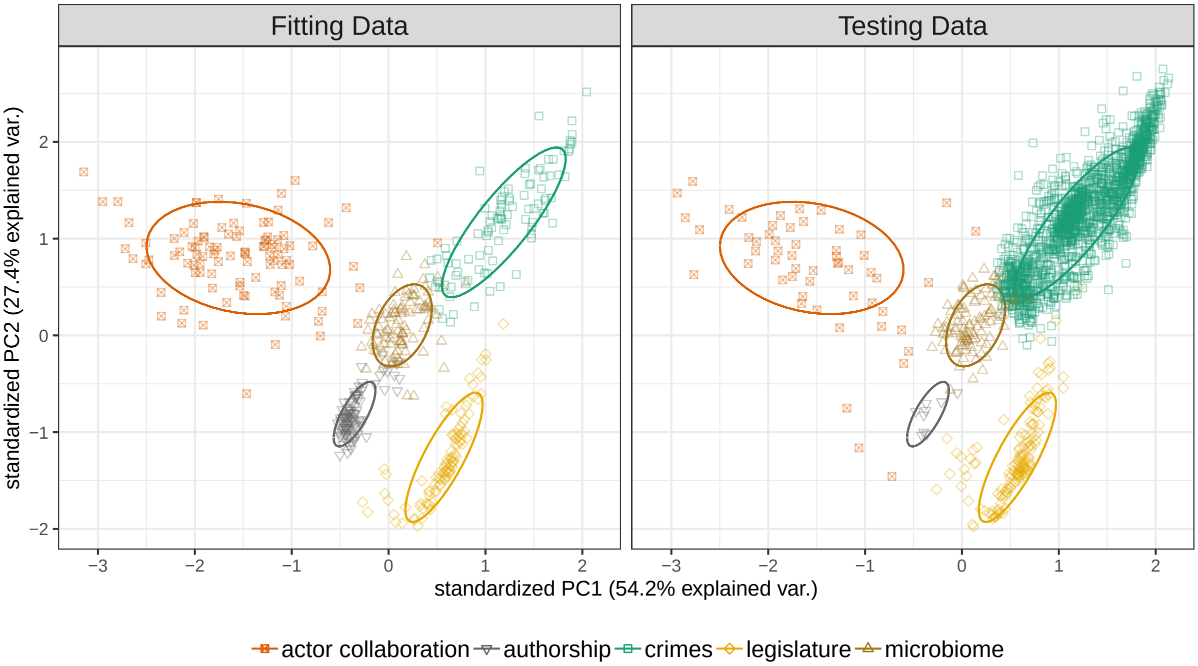


Figure A: A Principal Component Analysis (PCA) biplot of the first two principal components. Left: each point indicates a single network and the ellipses are drawn to contain ≈ 68% of the points in each network type, *i.e.*, one standard deviation if the points were to follow a bivariate normal distribution. Right: all remaining webs in each category projected onto the principal component space defined by the left pane. The fact that the remaining points generally fall within the same region as those used to fit the model is an indication that the model is sufficiently general.

## S6 Uninformative Variation

As argued in the main text, there exists some variation between different networks that is, in general, uninformative with regards to distinguishing between network types. This is because such properties are highly correlated with independent factors such as sampling effort or methodology. In the figures in the main text, we chose metrics in an effort to minimize the influence of these aspects of network structure. In fig. B we provide a visual indication of our degree of success in reducing these effects.

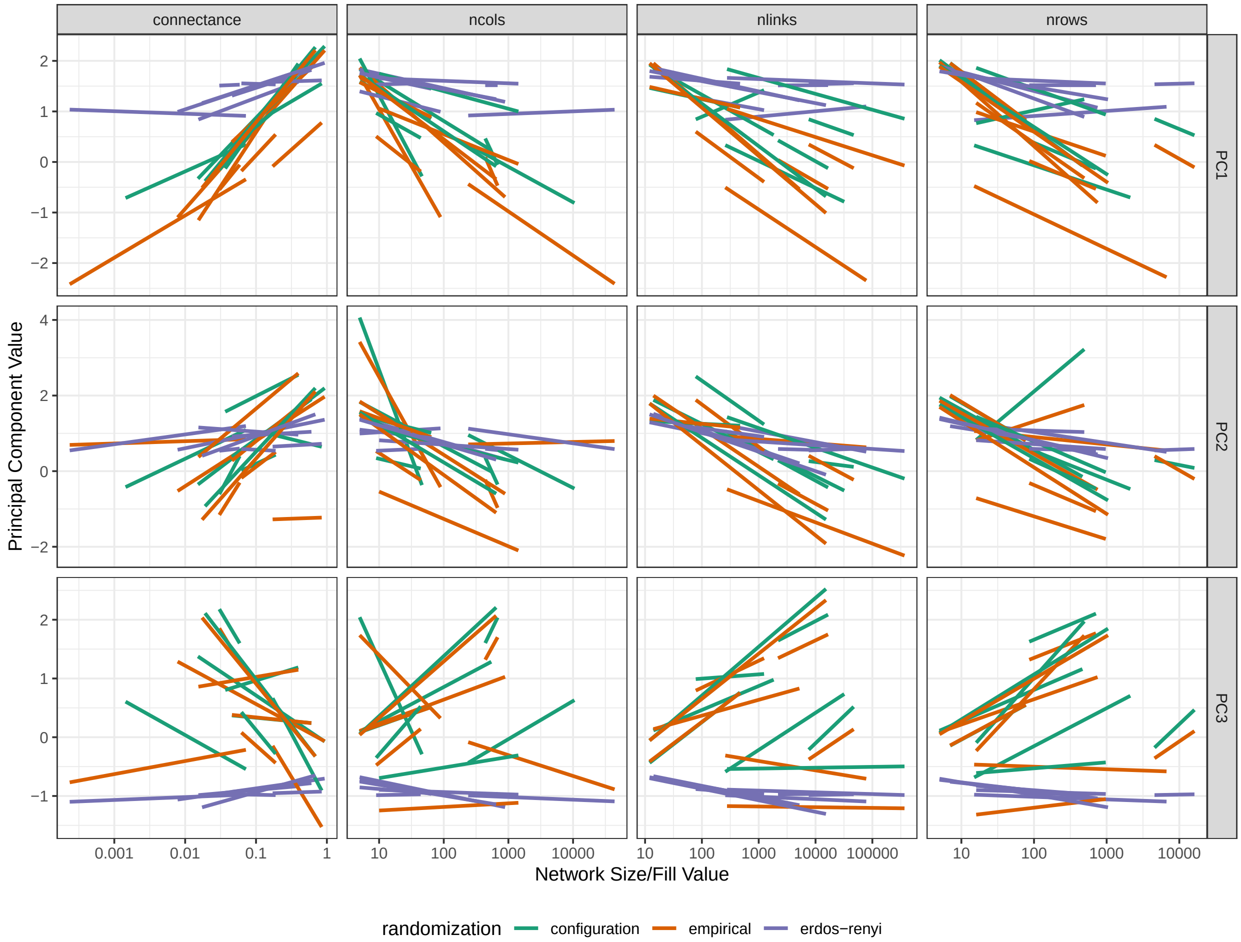


Figure B: Best fitting linear models for each network type, grouped according to randomization. In each plot, the lines indicate the best fitting linear model of the form *PC metric*, where the particular principal component (PC) is indicated by the horizontal facetting and the network metric is indicated by the vertical facetting. In each panel, each network type is represented by three lines, corresponding to the empirical networks (orange) and the sets of Erdős-Rényi and configuration model randomizations (purple and green, respectively). The reduced slopes for the Erdős-Rényi regressions indicate greater success at reducing the effect of size and fill on our map of network types.

# S7 Alternative Metrics

In this section, we provide analogous figures to those in the main text which include all colleced metrics for comparison. Note that, because several of these metrics have strong correlations with size and fill, we do not see the desired collapsing behavior in the randomized networks (figs. C to F).

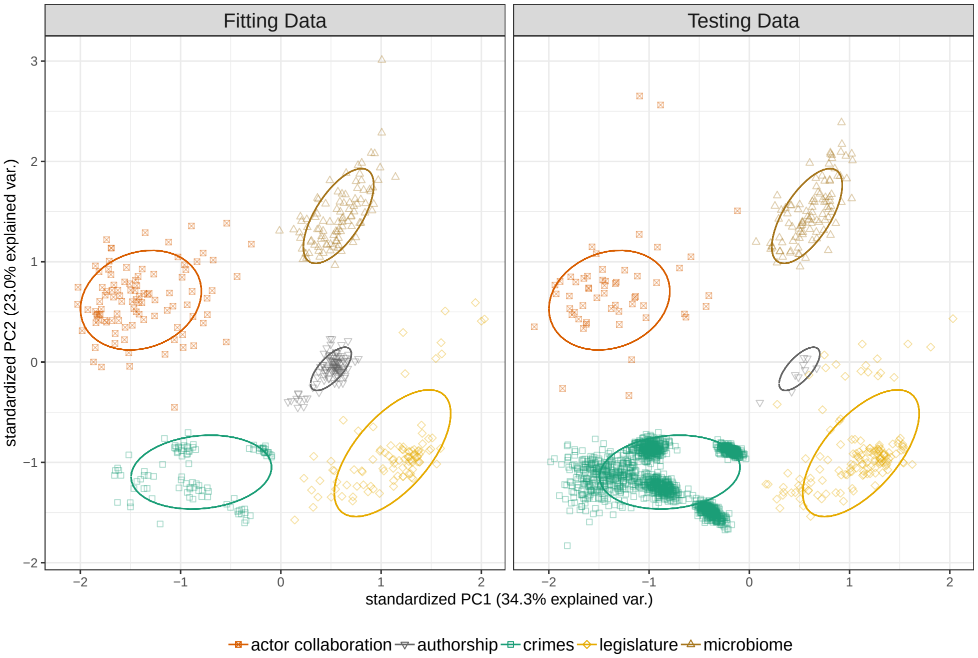


Figure C: As fig. A, but using all metrics.

Note that, while we obtain even better separation for the non-ecological networks, the mutualistic and antagonistic networks still fall nearly on top of one another. These figures also reveal a clear tradeoff between specificity and generality: this better separation for non-ecological data comes at the cost of being able to tell randomized networks apart, meaning that at least some of our ability to distinguish network types is an artifact of the different sizes and connectances of the different classes. To avoid this, one option would be to create empirical z-scores for each of the metrics employed, by taking several randomizations and computing mean and variances. The downside of this approach is that randomizing the large networks is computationally very challenging.

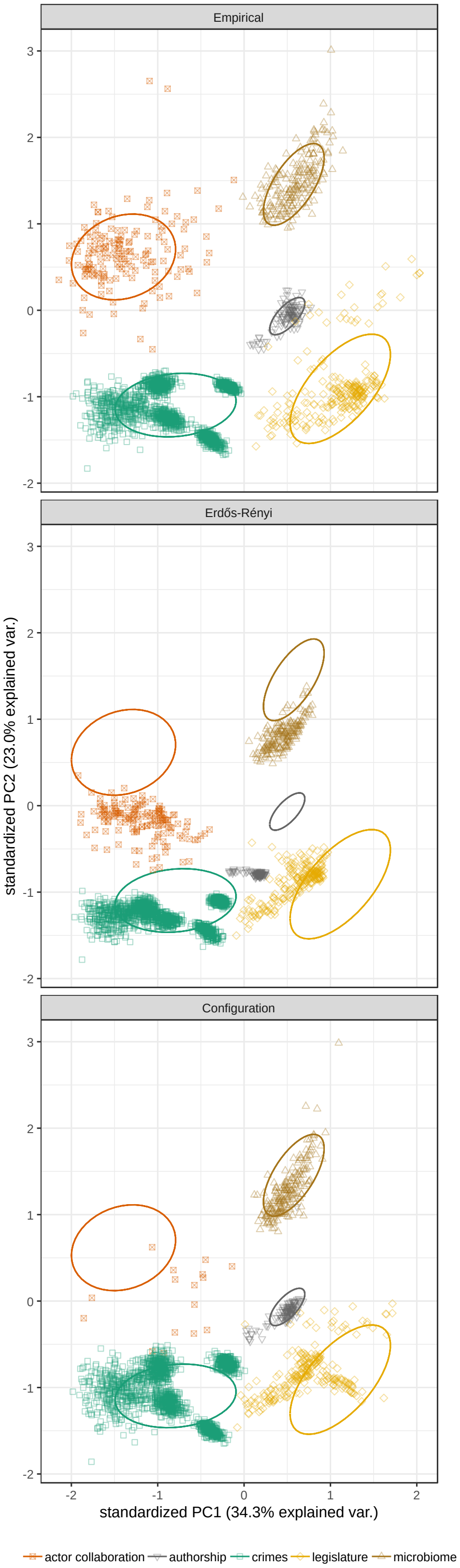


Figure D: As Figure 1 of the main text, but using all metrics.

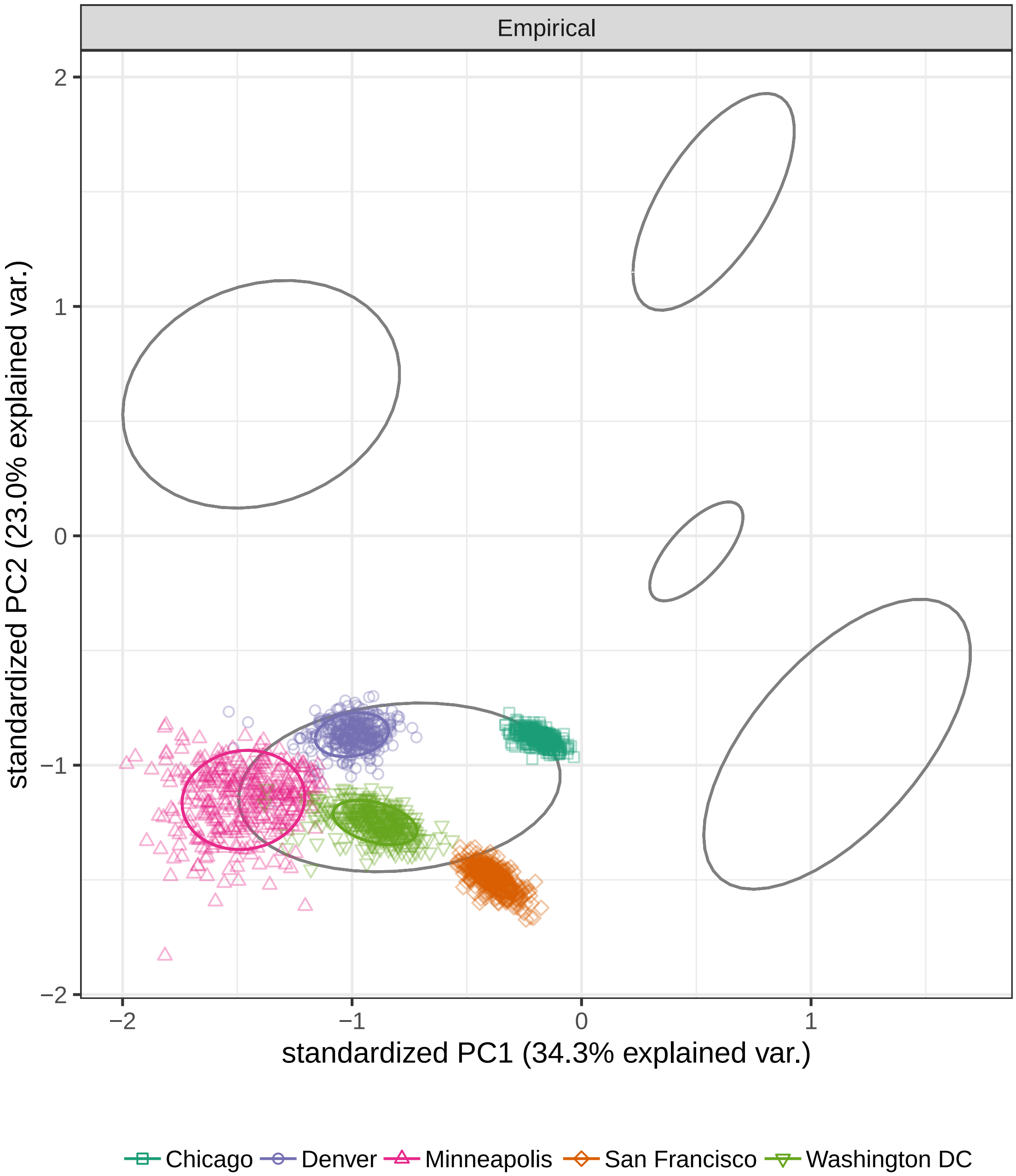


Figure E: As Figure 2 of the main text, but using all metrics.

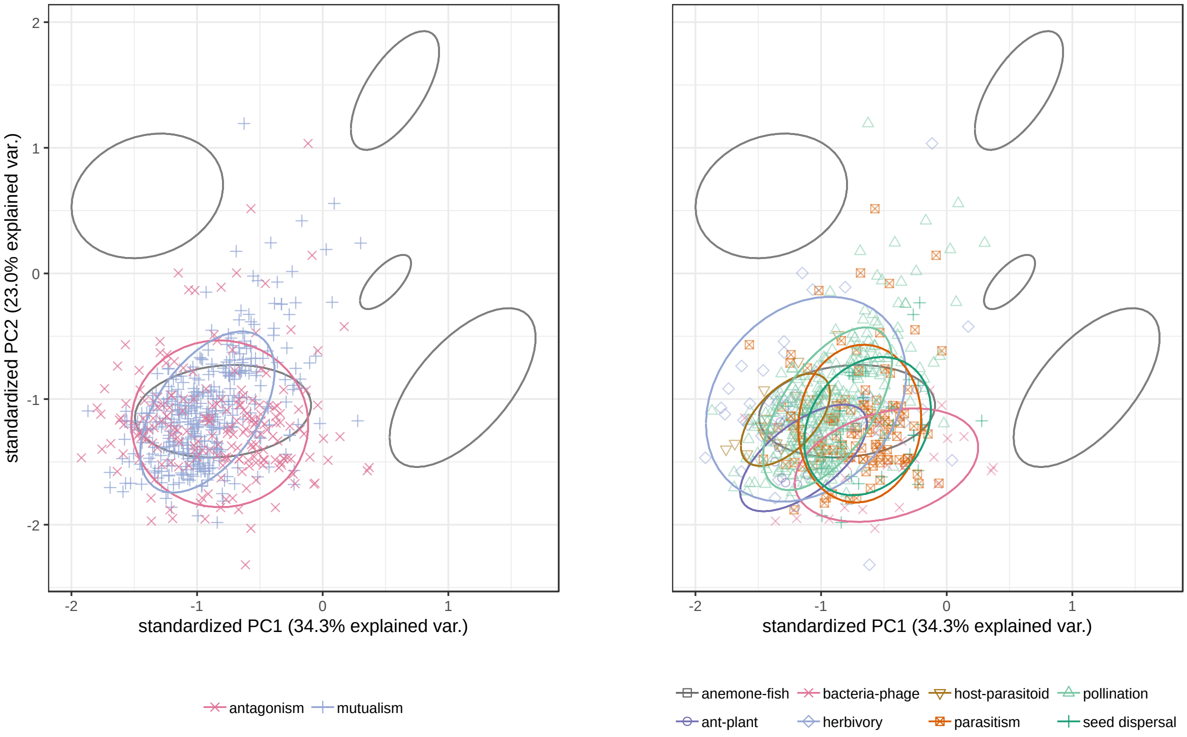


Figure F: As Figure 3 of the main text, but using all metrics.

# S8 Focusing on Nestedness and Modularity

In table A, we report the statistics run on the results presented in Figure 5 of the main text. To compare the distributions, we followed [Thébault and Fontaine, 2010] in using Welch's t-test (which accounts for different sample sizes and variances; [Welch, 1947]).

As an alternative to Figure 5 in the main text, we could investigate the role of Nestedness and Modularity in distinguishing ecological networks using PCA (fig. G). Here, we ran a PCA just on the ecological data using just measures of nestedness and modularity as input values. As before, there is no separation between interaction type.

Table A: Nestedness and modularity statistical comparison

| Null Model | Metric | mean (size) antagonism | mean (size) mutualism | degrees of freedom | P-Value |
|---|---|---|---|---|---|
| Configuration Model | NODF[1] | 0.0978(173) | 0.0839(245) | 403.0649 | 0.370 |
| | Overlap[2] | −0.2188(173) | −0.2536(245) | 214.4697 | 0.010 |
| | $\rho$[3] | −0.0178(173) | 0.0135(245) | 414.6372 | 0.827 |
| | Temperature[4] | 0.012(173) | 0.0618(245) | 271.7934 | 0.789 |
| | Modularity[5] | 0.1814(173) | 0.1949(245) | 402.6117 | 0.093 |
| Erdős-Rényi | NODF[1] | −0.2391(188) | 0.6974(248) | 433.7538 | $< 0.001$ |
| | Overlap[2] | 39.4128(188) | −1.4504(248) | 192.7469 | 0.377 |
| | $\rho$[3] | −0.0623(188) | 0.6483(248) | 423.9124 | 0.152 |
| | Temperature[4] | 0.0248(188) | −0.5723(248) | 371.7239 | 0.176 |
| | Modularity[5] | 0.0158(188) | −0.0498(248) | 282.2995 | 0.101 |

[1] Almeida-Neto et al. [2008], [2] Strona and Veech [2015], [3] Staniczenko et al. [2013], [4] Atmar and Patterson [1993], [5] Newman [2006]

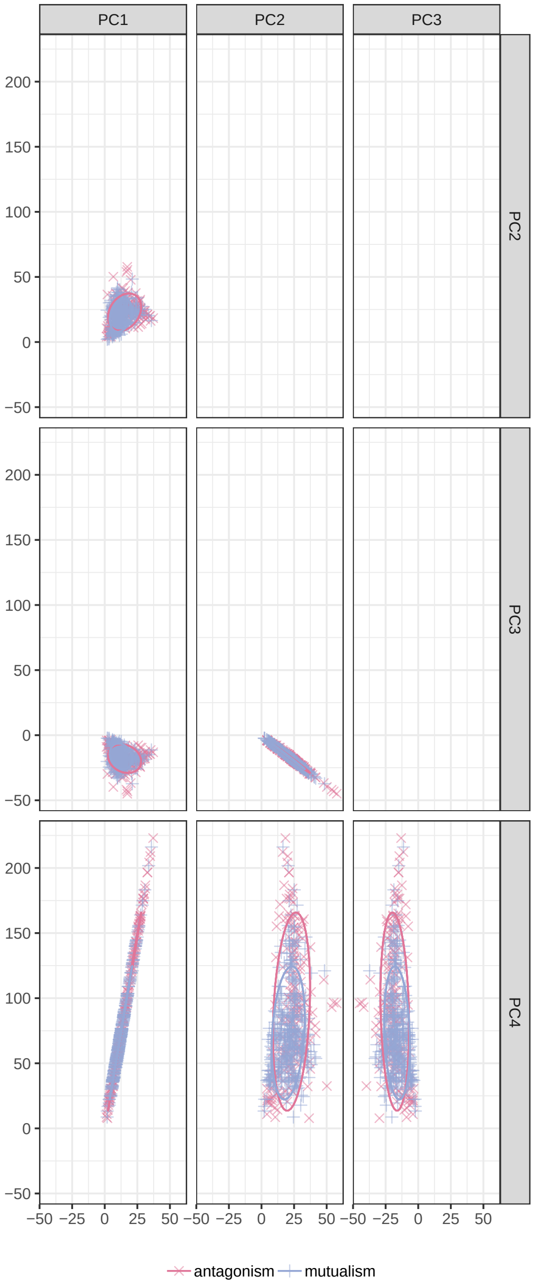


Figure G: PCA using only measures of nestedness and modularity.

# S9 Alternative Ecological Data

In an attempt to address the large variation in ecological networks, in fig. H we replot the ecological networks using only cases where there are multiple networks published by the same group. Often, these are networks in similar environmental conditions and were collected using similar methods over a relatively constrained amount of time. Moreover, because networks that meet these criteria also tend to be more recently published, they also tend to be larger, on average, than older, lower-quality networks.

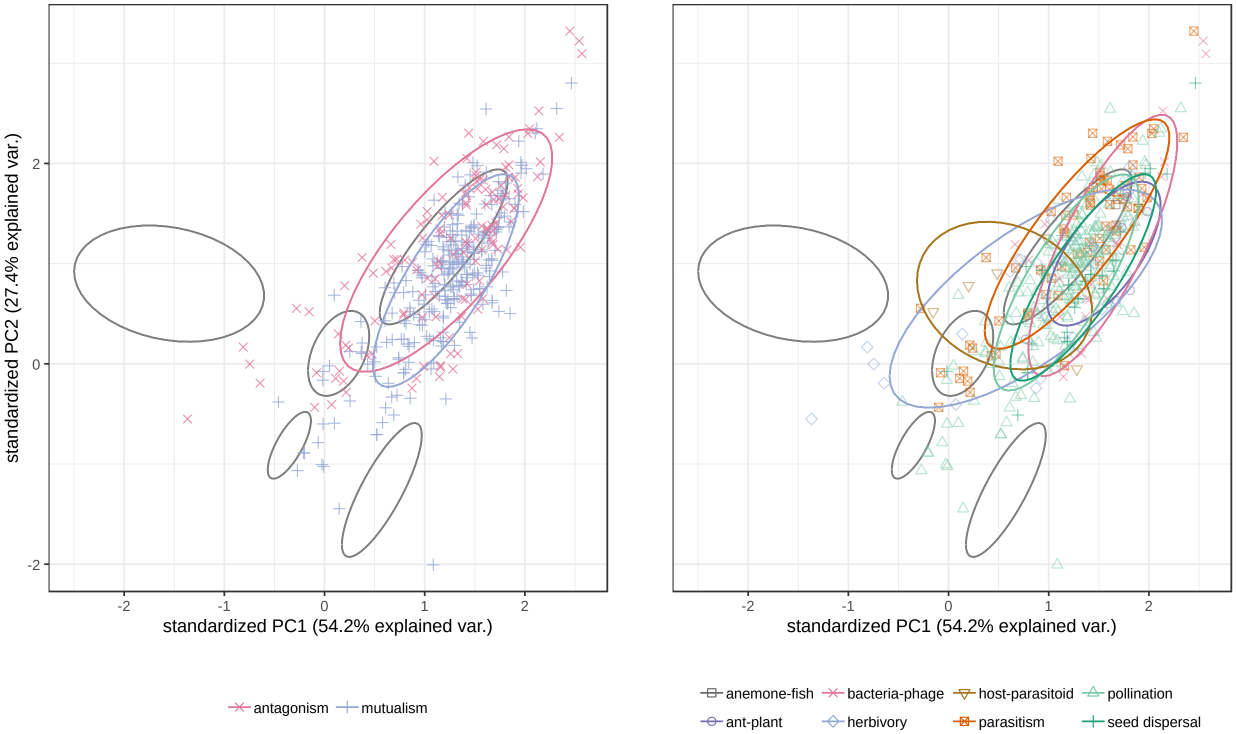


Figure H: As Figure 3 of the main text, but using only multiple networks collected by the same groups.

### S9.1 More Dimensions

Perhaps there is separation in our results, but not within the first two principal component dimensions. In fig. I we plot each pairwise combination of dimensions for the PCA from the main text (Note that here we are only plotting the ecological networks, but we are still projecting them into the space defined by the PCA defined by the non-ecological networks):

and the same for each pairwise combination of the first five dimensions of the full PCA presented in this supplement (fig. J):

For all cases, the level of overlap is substantially greater than that seen between the non-ecological networks.

Again, it is difficult to distinguish the clusters.

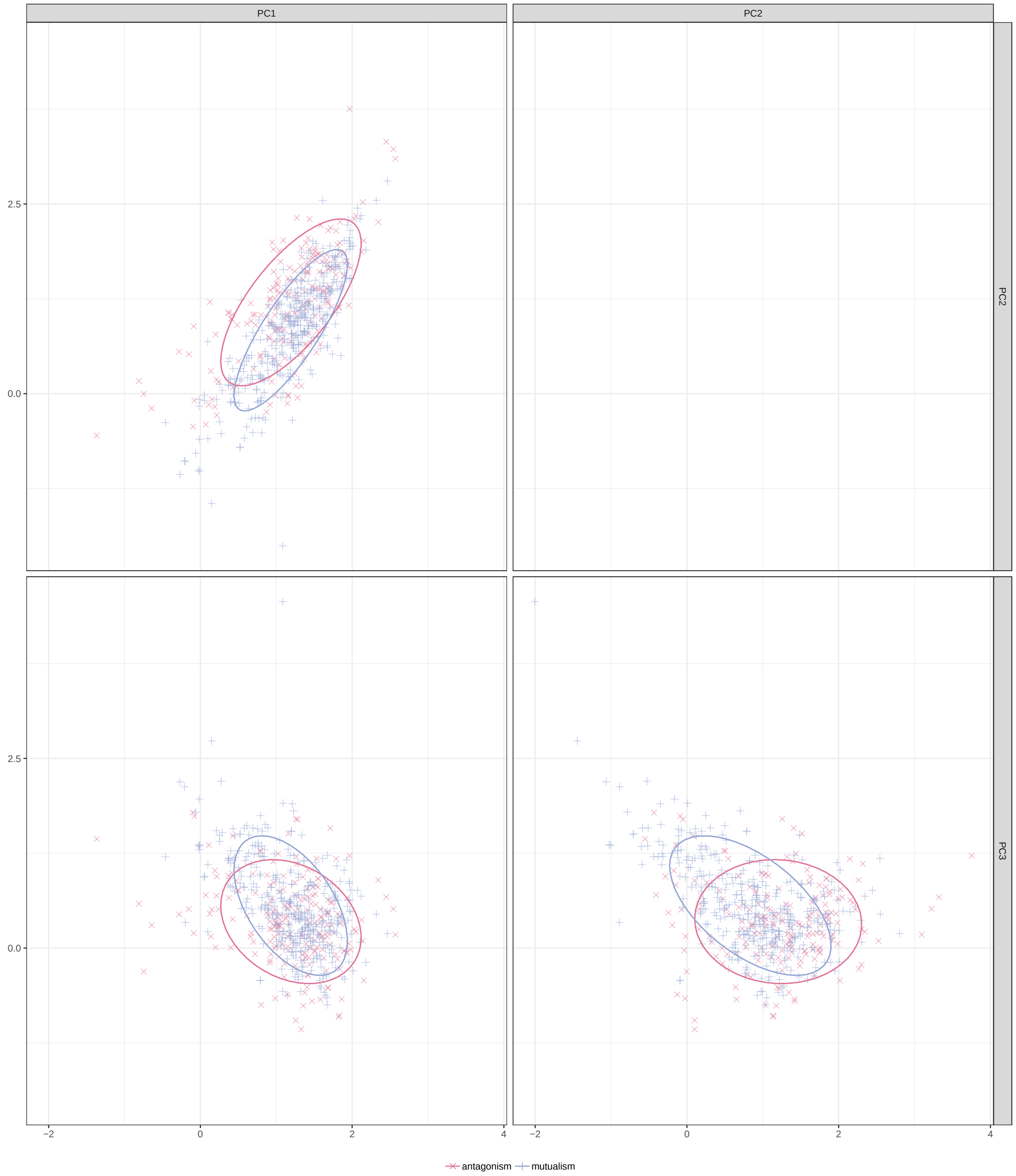


Figure I: Biplots for the three combinations of axes.

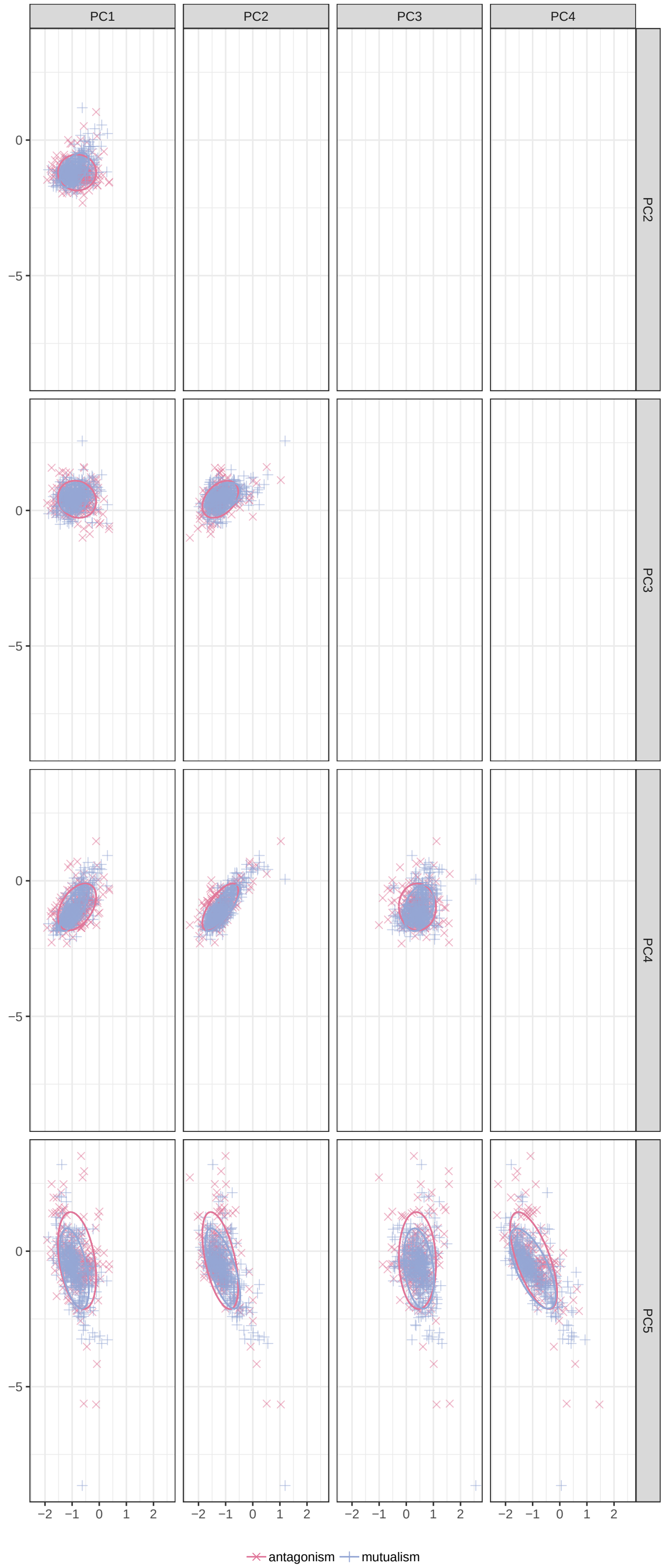


Figure J: Biplots for the first five components, using all metrics.

# S10 Including Ecological Data in the Fitting

Perhaps the lack of separation is due to our process of not including the ecological data in the model construction, thus leading to principal components which were not constructed to explain the variation within ecological networks. Though we believe this choice is stil justified (see the Note on Methodology (section S5), we include figures resulting from this approach here for comparison (again mirroring figures from the main text; figs. K and L):

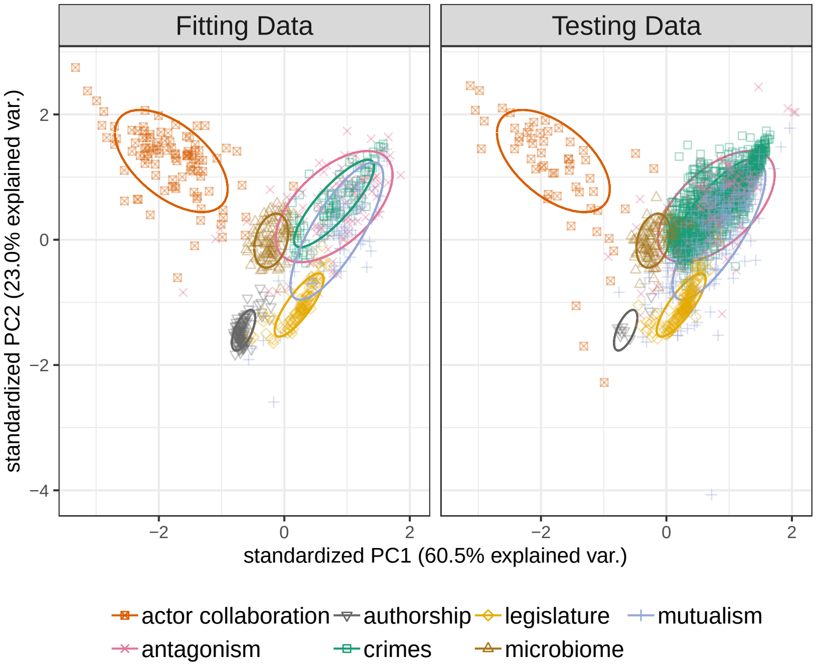


Figure K: As fig. A, but using using a principal component space defined with fitting data that includes ecological interaction networks.

As before, there is no separation between mutualistic and antagonisitic networks, which fall over the microbiome and crime networks.

Similar results are obtained when restricting to the ”high quality” ecological datasets (note here that we had to reduce our sample size for the fitting dataset to the size of the smallest category: antagoinstic with 48 networks; figs. M and N)):

and when using the full set of metrics collected (figs. O and P):

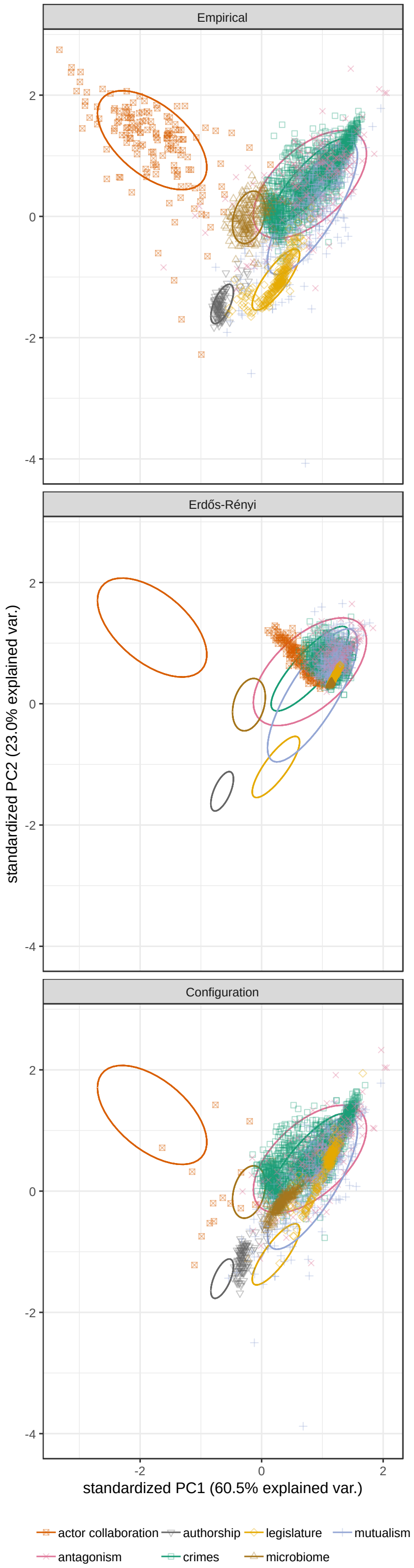


Figure L: As Figure 1 of the main text, but using using a principal component space defined with fitting data that includes ecological interaction networks.

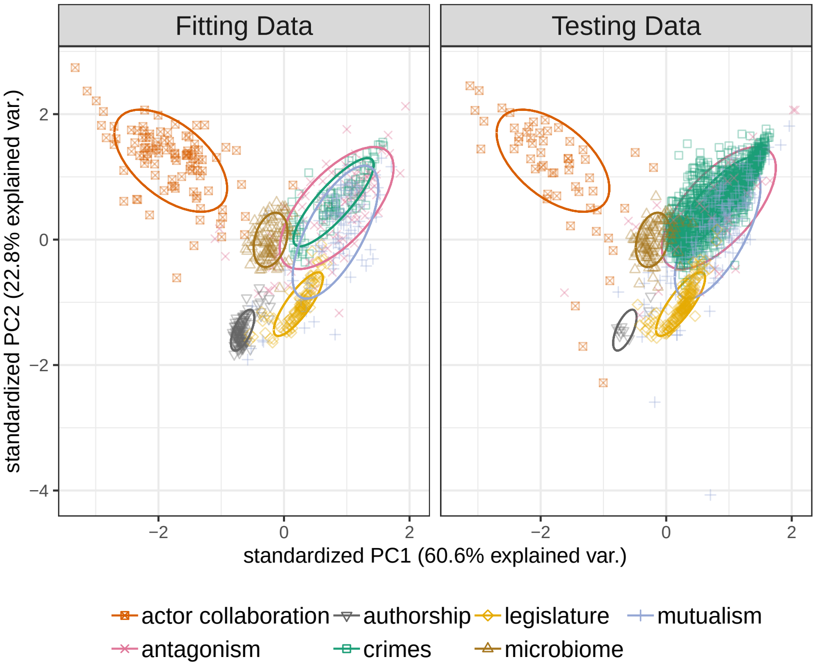


Figure M: As fig. A, but using using a principal component space defined with fitting data that includes high-quality ecological interaction networks.

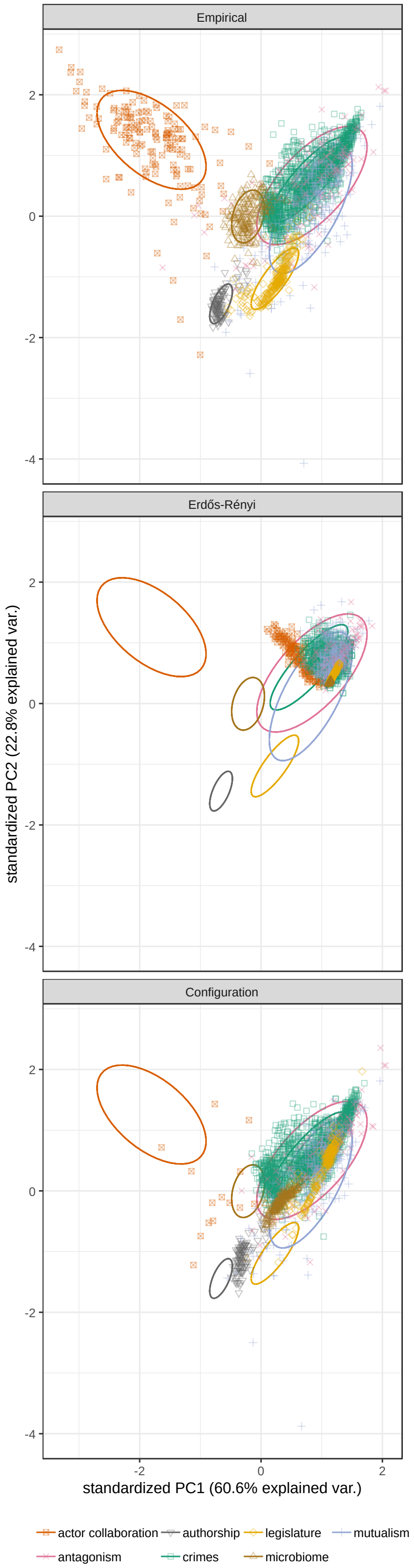


Figure N: As Figure 1 of the main text, but using using a principal component space defined with fitting data that includes high-quality ecological interaction networks.

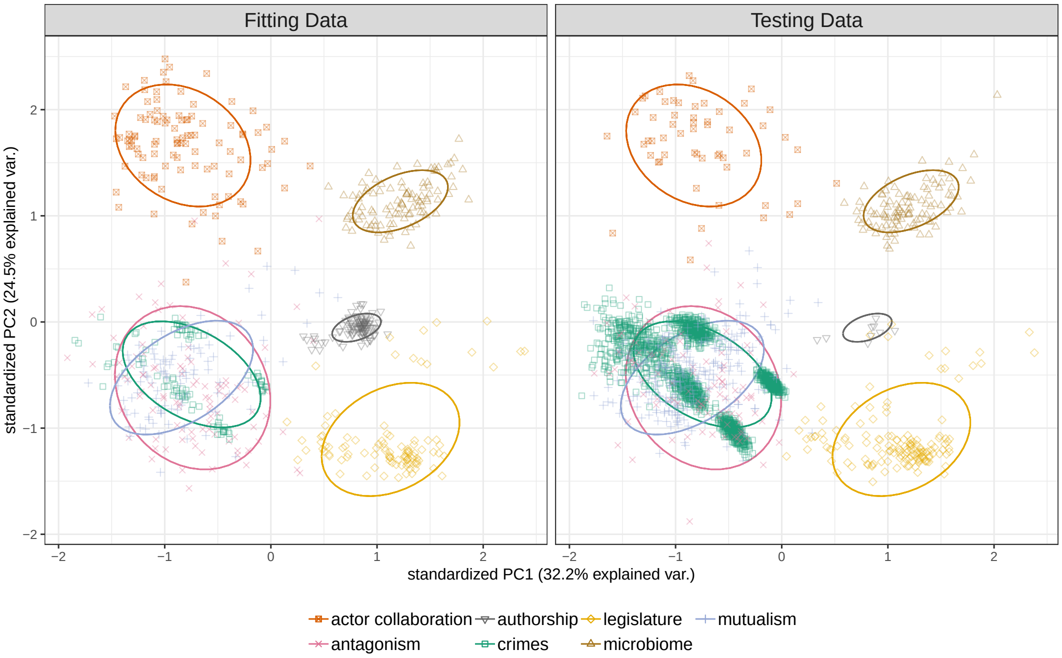


Figure O: As fig. A, but using using a principal component space defined with fitting data that includes high-quality ecological interaction networks and utilizing the full suite of metrics.

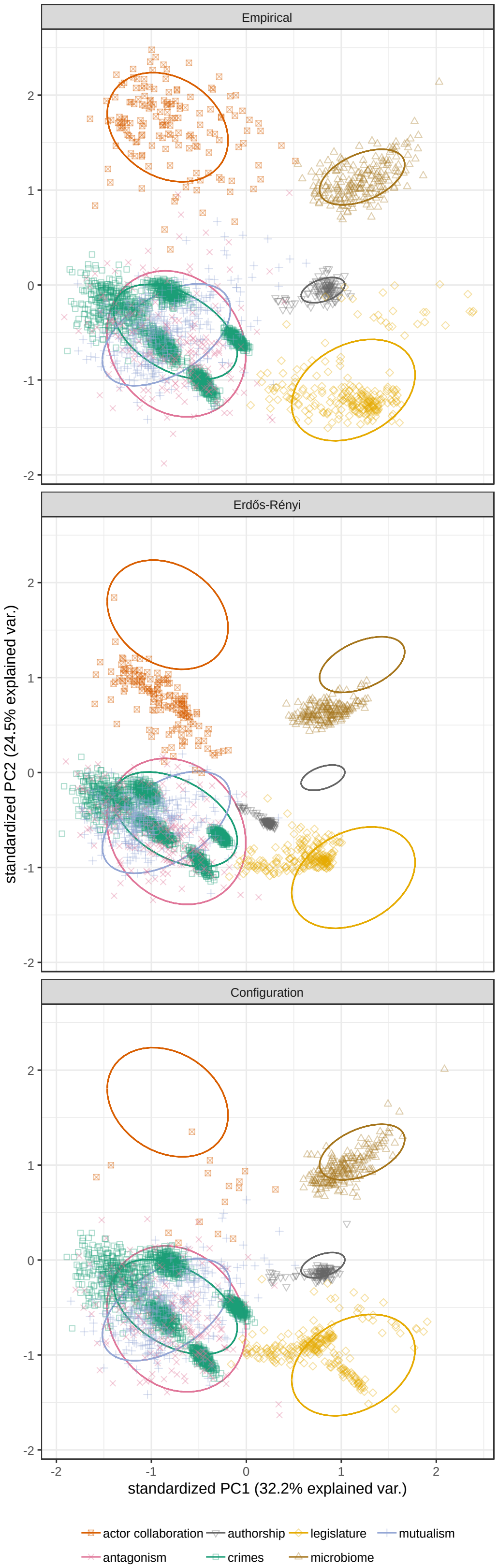


Figure P: As Figure 1 of the main text, but using using a principal component space defined with fitting data that includes high-quality ecological interaction networks and utilizing the full suite of metrics.

## S11 Machine Learning Approaches

As noted in the main text, Principal Component Analysis is not necessarily the best tool for addressing this problem, but it does have some advantages. In this section, we apply two alternative approaches from the machine learning literature: Random Forests and Gradient Boosted Regression Trees. In both cases, the degree of success is often represented through confusion matrices, where the predicted classification of the testing data is compared to the known correct classification. This provides a clear measure of sensitivity and specificity, but does not produce the visual map we present as a measure of PCA's success. Moreover, with these approaches, it doesn't make sense to do the ”ecological-data-agnostic” approach we apply in the main text — all classes must be present throughout the analysis.

In all cases below, we are able to get high specificity for both antagonistic and mutualistic ecological interaction networks, but we fall short on sensitivity. That is, when the models categorize something as an antagonistic interaction network, we can be quite sure that that classification is correct, yet the model is less successful at ensuring that all antagonistic ecological networks are detected.

### S11.1 Using same metrics as main text

#### S11.1.1 Random Forest

Table B: Random forest results using metrics from the main text.

| | actor collab. | antagonism | authorship | crimes | legislature | microbiome | mutualism |
|---|---|---|---|---|---|---|---|
| actor collab. | 34 | 2 | 0 | 0 | 0 | 0 | 0 |
| antagonism | 2 | 7 | 0 | 2 | 1 | 0 | 3 |
| authorship | 1 | 0 | 26 | 0 | 0 | 0 | 1 |
| crimes | 0 | 27 | 0 | 427 | 0 | 0 | 38 |
| legislature | 0 | 0 | 0 | 0 | 60 | 1 | 3 |
| microbiome | 1 | 1 | 0 | 0 | 0 | 50 | 0 |
| mutualism | 1 | 11 | 1 | 25 | 0 | 0 | 43 |
| Sensitivity | 0.87 | 0.15 | 0.96 | 0.94 | 0.98 | 0.98 | 0.49 |
| Specificity | 1.00 | 0.99 | 1.00 | 0.79 | 0.99 | 1.00 | 0.94 |
| Pos Pred Value | 0.94 | 0.47 | 0.93 | 0.87 | 0.94 | 0.96 | 0.53 |
| Neg Pred Value | 0.99 | 0.95 | 1.00 | 0.90 | 1.00 | 1.00 | 0.93 |
| Precision | 0.94 | 0.47 | 0.93 | 0.87 | 0.94 | 0.96 | 0.53 |
| Recall | 0.87 | 0.15 | 0.96 | 0.94 | 0.98 | 0.98 | 0.49 |
| F1 | 0.91 | 0.22 | 0.95 | 0.90 | 0.96 | 0.97 | 0.51 |
| Prevalence | 0.05 | 0.06 | 0.04 | 0.59 | 0.08 | 0.07 | 0.11 |
| Detection Rate | 0.04 | 0.01 | 0.03 | 0.56 | 0.08 | 0.07 | 0.06 |
| Detection Prevalence | 0.05 | 0.02 | 0.04 | 0.64 | 0.08 | 0.07 | 0.11 |
| Balanced Accuracy | 0.93 | 0.57 | 0.98 | 0.87 | 0.99 | 0.99 | 0.72 |

#### S11.1.2 Gradient Boosted Regression Trees

Table C: Gradient boosted regression tree results using metrics from the main text.

| | actor collab. | antagonism | authorship | crimes | legislature | microbiome | mutualism |
|---|---|---|---|---|---|---|---|
| actor collab. | 35 | 2 | 0 | 0 | 0 | 0 | 0 |
| antagonism | 0 | 1 | 0 | 1 | 0 | 0 | 3 |
| authorship | 2 | 1 | 27 | 0 | 0 | 0 | 2 |
| crimes | 0 | 31 | 0 | 436 | 1 | 0 | 47 |
| legislature | 0 | 0 | 0 | 0 | 60 | 1 | 3 |
| microbiome | 1 | 2 | 0 | 0 | 0 | 50 | 0 |
| mutualism | 1 | 11 | 0 | 17 | 0 | 0 | 33 |
| Sensitivity | 0.90 | 0.02 | 1.00 | 0.96 | 0.98 | 0.98 | 0.38 |
| Specificity | 1.00 | 0.99 | 0.99 | 0.75 | 0.99 | 1.00 | 0.96 |
| Pos Pred Value | 0.95 | 0.20 | 0.84 | 0.85 | 0.94 | 0.94 | 0.53 |
| Neg Pred Value | 0.99 | 0.94 | 1.00 | 0.93 | 1.00 | 1.00 | 0.92 |
| Precision | 0.95 | 0.20 | 0.84 | 0.85 | 0.94 | 0.94 | 0.53 |
| Recall | 0.90 | 0.02 | 1.00 | 0.96 | 0.98 | 0.98 | 0.38 |
| F1 | 0.92 | 0.04 | 0.92 | 0.90 | 0.96 | 0.96 | 0.44 |
| Prevalence | 0.05 | 0.06 | 0.04 | 0.59 | 0.08 | 0.07 | 0.11 |
| Detection Rate | 0.05 | 0.00 | 0.04 | 0.57 | 0.08 | 0.07 | 0.04 |
| Detection Prevalence | 0.05 | 0.01 | 0.04 | 0.67 | 0.08 | 0.07 | 0.08 |
| Balanced Accuracy | 0.95 | 0.51 | 1.00 | 0.85 | 0.99 | 0.99 | 0.67 |

## S11.2 Using the full set of metrics

As with the PCA results listed above, using the full set of metrics improves our ability to distinguish ecological networks, but still not to the level we obtain with our nonecological datasets.

### S11.2.1 Random Forest

Table D: Random forest results using all metrics.

| | actorcollaboration | antagonism | authorship | crimes | legislature | microbiome | mutualism |
|---|---|---|---|---|---|---|---|
| actorcollaboration | 38 | 1 | 0 | 0 | 0 | 0 | 0 |
| antagonism | 1 | 21 | 0 | 1 | 1 | 0 | 11 |
| authorship | 0 | 0 | 27 | 0 | 0 | 0 | 0 |
| crimes | 0 | 10 | 0 | 446 | 1 | 0 | 7 |
| legislature | 0 | 0 | 0 | 0 | 59 | 0 | 1 |
| microbiome | 0 | 0 | 0 | 0 | 0 | 51 | 0 |
| mutualism | 0 | 17 | 0 | 7 | 0 | 0 | 72 |
| Sensitivity | 0.97 | 0.43 | 1.00 | 0.98 | 0.97 | 1.00 | 0.79 |
| Specificity | 1.00 | 0.98 | 1.00 | 0.94 | 1.00 | 1.00 | 0.96 |
| Pos Pred Value | 0.97 | 0.60 | 1.00 | 0.96 | 0.98 | 1.00 | 0.75 |
| Neg Pred Value | 1.00 | 0.96 | 1.00 | 0.97 | 1.00 | 1.00 | 0.97 |
| Precision | 0.97 | 0.60 | 1.00 | 0.96 | 0.98 | 1.00 | 0.75 |
| Recall | 0.97 | 0.43 | 1.00 | 0.98 | 0.97 | 1.00 | 0.79 |
| F1 | 0.97 | 0.50 | 1.00 | 0.97 | 0.98 | 1.00 | 0.77 |
| Prevalence | 0.05 | 0.06 | 0.03 | 0.59 | 0.08 | 0.07 | 0.12 |
| Detection Rate | 0.05 | 0.03 | 0.03 | 0.58 | 0.08 | 0.07 | 0.09 |
| Detection Prevalence | 0.05 | 0.05 | 0.03 | 0.60 | 0.08 | 0.07 | 0.12 |
| Balanced Accuracy | 0.99 | 0.70 | 1.00 | 0.96 | 0.98 | 1.00 | 0.88 |

### S11.2.2 Gradient Boosted Regression Trees

Table E: Gradient boosted regression tree results using all metrics.

| | actor collab. | antagonism | crimes | legislature | mutualism |
|---|---|---|---|---|---|
| actor collab. | 3 | 0 | 0 | 0 | 0 |
| antagonism | 0 | 24 | 2 | 0 | 5 |
| crimes | 0 | 13 | 450 | 1 | 12 |
| legislature | 0 | 0 | 0 | 8 | 0 |
| mutualism | 0 | 11 | 1 | 0 | 72 |
| Sensitivity | 1.00 | 0.50 | 0.99 | 0.89 | 0.81 |
| Specificity | 1.00 | 0.99 | 0.83 | 1.00 | 0.98 |
| Pos Pred Value | 1.00 | 0.77 | 0.95 | 1.00 | 0.86 |
| Neg Pred Value | 1.00 | 0.96 | 0.98 | 1.00 | 0.97 |
| Precision | 1.00 | 0.77 | 0.95 | 1.00 | 0.86 |
| Recall | 1.00 | 0.50 | 0.99 | 0.89 | 0.81 |
| F1 | 1.00 | 0.61 | 0.97 | 0.94 | 0.83 |
| Prevalence | 0.00 | 0.08 | 0.75 | 0.01 | 0.15 |
| Detection Rate | 0.00 | 0.04 | 0.75 | 0.01 | 0.12 |
| Detection Prevalence | 0.00 | 0.05 | 0.79 | 0.01 | 0.14 |
| Balanced Accuracy | 1.00 | 0.74 | 0.91 | 0.94 | 0.89 |

## S11.3 Directly Parsing Ecological Networks

In the above examples, we compare non-ecological classification to that for ecological networks (as we do in the main text). In principal, such a comparison is not as relevant when using machine learning approaches such as these. Instead, we can just plug in the two (or more) types directly. The results are not qualitatively different from above, but the difficulties of classification are more apparent.

### S11.3.1 Random Forest

Table F: Random forest results for directly distinguishing ecological network types

| | antagonism | mutualism |
|---|---|---|
| antagonism | 29 | 13 |
| mutualism | 19 | 76 |

| | |
|---|---|
| Sensitivity | 0.60 |
| Specificity | 0.85 |
| Pos Pred Value | 0.69 |
| Neg Pred Value | 0.80 |
| Precision | 0.69 |
| Recall | 0.60 |
| F1 | 0.64 |
| Prevalence | 0.35 |
| Detection Rate | 0.21 |
| Detection Prevalence | 0.31 |
| Balanced Accuracy | 0.73 |

### S11.3.2 Gradient Boosted Regression Trees

Table G: Gradient boosted regression tree results for directly distinguishing ecological network types

| | antagonism | mutualism |
|---|---|---|
| antagonism | 31 | 12 |
| mutualism | 17 | 77 |

| | |
|---|---|
| Sensitivity | 0.65 |
| Specificity | 0.87 |
| Pos Pred Value | 0.72 |
| Neg Pred Value | 0.82 |
| Precision | 0.72 |
| Recall | 0.65 |
| F1 | 0.68 |
| Prevalence | 0.35 |
| Detection Rate | 0.23 |
| Detection Prevalence | 0.31 |
| Balanced Accuracy | 0.76 |

## S11.4 Directly Parsing Ecological Networks—Subcategorizations

Here, we repeat the above analysis with the subcategorization of ecological interaction network type. As can be seen below, some sub-types tend to have high specificity, while others have high sensitivity, but in no cases are both high as was the case for the non-ecological data.

### S11.4.1 Random Forest

Table H: Random forest results for directly distinguishing subcategorized ecological network types

| | ant-plant | bacteria-phage | host-parasitoid | host-parasite | plant-herbivore | plant-pollinator | seed-disperser |
|---|---|---|---|---|---|---|---|
| ant-plant | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| bacteria-phage | 0 | 3 | 0 | 0 | 1 | 0 | 1 |
| host-parasitoid | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| host-parasite | 0 | 2 | 0 | 11 | 1 | 1 | 0 |
| plant-herbivore | 0 | 0 | 1 | 0 | 1 | 1 | 0 |
| plant-pollinator | 2 | 2 | 5 | 15 | 6 | 76 | 6 |
| seed-disperser | 0 | 0 | 0 | 1 | 1 | 0 | 3 |
| Sensitivity | 0.00 | 0.43 | 0.00 | 0.41 | 0.10 | 0.97 | 0.30 |
| Specificity | 1.00 | 0.98 | 1.00 | 0.96 | 0.98 | 0.42 | 0.98 |
| Pos Pred Value | | 0.60 | | 0.73 | 0.33 | 0.68 | 0.60 |
| Neg Pred Value | 0.99 | 0.97 | 0.96 | 0.87 | 0.93 | 0.93 | 0.95 |
| Precision | | 0.60 | | 0.73 | 0.33 | 0.68 | 0.60 |
| Recall | 0.00 | 0.43 | 0.00 | 0.41 | 0.10 | 0.97 | 0.30 |
| F1 | | 0.50 | | 0.52 | 0.15 | 0.80 | 0.40 |
| Prevalence | 0.01 | 0.05 | 0.04 | 0.19 | 0.07 | 0.56 | 0.07 |
| Detection Rate | 0.00 | 0.02 | 0.00 | 0.08 | 0.01 | 0.54 | 0.02 |
| Detection Prevalence | 0.00 | 0.04 | 0.00 | 0.11 | 0.02 | 0.80 | 0.04 |
| Balanced Accuracy | 0.50 | 0.71 | 0.50 | 0.69 | 0.54 | 0.70 | 0.64 |

### S11.4.2 Gradient Boosted Regression Trees

Table I: Gradient boosted regression tree results for directly distinguishing subcategorized ecological network types

| | ant-plant | bacteria-phage | host-parasitoid | host-parasite | plant-herbivore | plant-pollinator | seed-disperser |
|---|---|---|---|---|---|---|---|
| ant-plant | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| bacteria-phage | 0 | 3 | 0 | 0 | 1 | 0 | 0 |
| host-parasitoid | 0 | 0 | 1 | 0 | 0 | 0 | 0 |
| host-parasite | 0 | 2 | 0 | 13 | 0 | 1 | 0 |
| plant-herbivore | 0 | 0 | 1 | 0 | 2 | 2 | 0 |
| plant-pollinator | 2 | 2 | 4 | 13 | 5 | 74 | 7 |
| seed-disperser | 0 | 0 | 0 | 1 | 2 | 1 | 3 |
| Sensitivity | 0.00 | 0.43 | 0.17 | 0.48 | 0.20 | 0.95 | 0.30 |
| Specificity | 1.00 | 0.99 | 1.00 | 0.97 | 0.98 | 0.47 | 0.97 |
| Pos Pred Value | | 0.75 | 1.00 | 0.81 | 0.40 | 0.69 | 0.43 |
| Neg Pred Value | 0.99 | 0.97 | 0.96 | 0.89 | 0.94 | 0.88 | 0.95 |
| Precision | | 0.75 | 1.00 | 0.81 | 0.40 | 0.69 | 0.43 |
| Recall | 0.00 | 0.43 | 0.17 | 0.48 | 0.20 | 0.95 | 0.30 |
| F1 | | 0.55 | 0.29 | 0.60 | 0.27 | 0.80 | 0.35 |
| Prevalence | 0.01 | 0.05 | 0.04 | 0.19 | 0.07 | 0.56 | 0.07 |
| Detection Rate | 0.00 | 0.02 | 0.01 | 0.09 | 0.01 | 0.53 | 0.02 |
| Detection Prevalence | 0.00 | 0.03 | 0.01 | 0.11 | 0.04 | 0.76 | 0.05 |
| Balanced Accuracy | 0.50 | 0.71 | 0.58 | 0.73 | 0.59 | 0.71 | 0.63 |

## S12 Code availability

All code used to run these analyses was written in ‘R‘ [R Core Team, 2018] with the use of several packages [Csardi and Nepusz, 2006, Dormann et al., 2009, 2008, Dormann, 2011, Wickham, 2017b, Bache and Wickham, 2014, Liaw and Wiener, 2002, Wickham, 2017c, Robinson, 2017, Wickham, 2017b,a, Dahl, 2016]. This code is made available through a public Git repository associated with this project (`http://git.io/f4y4o`).

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