Appendix from R. P. Rohr and J. Bascompte, "Components of Phylogenetic Signal in Antagonistic and Mutualistic Networks"

Mathematical Derivation of the Matching-Centrality Model (Eq. [1])

A theoretical framework similar to our model (eq. [1]) describing how interaction strength in food webs depends on species traits was first introduced by Rossberg et al. (2010). Here, we provide a conceptually similar model but with two main differences. First, our model works for the probability of existence of trophic/mutualistic links between species pairs as opposed to the strength of the interaction. Second, instead of considering the general framework of a quadratic form, we directly applied the singular valued decomposition on the matrix containing the logit of linking probabilities.

Our derivation works as follows. Let $\mathbf{P}_{ij}$ be the matrix containing the linking probabilities between pairs of species, that is, $\mathbf{P}_{ij}$ is the probability that there is a trophic/mutualsitic link between species i and j. Now, we consider the logit of all these linking probabilities and define the matrix $\mathbf{M}$ by $M_{ij} = \text{logit}(\mathbf{P}_{ij}) = \log(\mathbf{P}_{ij}/(1 - \mathbf{P}_{ij}))\Sigma$. In general, the matrix $\mathbf{M}$ is a rectangular matrix of size $S_1 \times S_2$, where S_1 is the number of prey/plants species and S_2 the number of predator/animals species. Now, instead of using the general framework of Rossberg et al. (2010, eq. [3]), we apply directly the singular value decomposition (SVD) on matrix $\mathbf{M}$. The SVD (see Watkins 2010) is the factorization of $\mathbf{M}$ into a product of three matrices, $\mathbf{M} = \mathbf{VDF}$, where

$$\mathbf{V} = \begin{pmatrix} | & | & & | \\ \mathbf{v}^1 & \mathbf{v}^2 & \cdots & \mathbf{v}^S \\ | & | & & | \end{pmatrix}, \mathbf{D} = \begin{pmatrix} \delta_1 & & & \\ & \delta_2 & & \\ & & \ddots & \\ & & & \delta_S \end{pmatrix}, \mathbf{F} = \begin{pmatrix} - & \mathbf{f}^1 & - \\ - & \mathbf{f}^2 & - \\ & \vdots & \\ - & \mathbf{f}^S & - \end{pmatrix}. \tag{A1}$$

The matrix $\mathbf{D}$ is a diagonal matrix made of nonnegative numbers $\delta_1, \ldots, \delta_S$, called the singular value of $\mathbf{M}$; $\mathbf{V}$ is a matrix of orthogonal column vectors $(\mathbf{v}^1, \ldots, \mathbf{v}^S)$; and $\mathbf{F}$ is a matrix of orthogonal row vectors $(\mathbf{f}^1, \ldots, \mathbf{f}^S)$. Here, $S = \min(S_1, S_2)$. Note that SVD is unique, that is, the singular values are unique up to a common scaling factor, and the vectors are also unique up to their orientation and length in the space.

Expanding this matrix product, we obtain the following expression:

$$\mathbf{M} = \mathbf{v}^1\delta^1\mathbf{f}^1 + \mathbf{v}^2\delta^2\mathbf{f}^2 + \cdots + \mathbf{v}^S\delta^S\mathbf{f}^S. \tag{A2}$$

Note that we use the following nonstandard convention for the products between two vectors: $\mathbf{v}^1\delta^1\mathbf{f}^1$ is a matrix of size $S_1 \times S_2$, with the element ij given by $v_i^1\delta^1 f_j^1$. Now, the next step resides in decomposing each singular vector in its components parallel and perpendicular to the unitary vector $(\mathbf{1})$, that is,

$$\mathbf{v}^i = \underbrace{\tilde{\mathbf{v}}^i}_{\perp 1} + \underbrace{\hat{\mathbf{v}}^i}_{\|1} \text{ and } \mathbf{f}^i = \underbrace{\tilde{\mathbf{f}}^i}_{\perp 1} + \underbrace{\hat{\mathbf{f}}^i}_{\|1}. \tag{A3}$$

With this decomposition, the matrix $\mathbf{M}$ is then given by

$$\begin{aligned} \mathbf{M} = \; &\tilde{\mathbf{v}}^1\delta^1\tilde{\mathbf{f}}^1 + \tilde{\mathbf{v}}^2\delta^2\tilde{\mathbf{f}}^2 + \cdots + \tilde{\mathbf{v}}^S\delta^S\tilde{\mathbf{f}}^S \ldots \\ &+ \hat{\mathbf{v}}^1\delta^1\tilde{\mathbf{f}}^1 + \hat{\mathbf{v}}^2\delta^2\tilde{\mathbf{f}}^2 + \cdots + \hat{\mathbf{v}}^S\delta^S\tilde{\mathbf{f}}^S \ldots \\ &+ \tilde{\mathbf{v}}^1\delta^1\hat{\mathbf{f}}^1 + \tilde{\mathbf{v}}^2\delta^2\hat{\mathbf{f}}^2 + \cdots + \tilde{\mathbf{v}}^S\delta^S\hat{\mathbf{f}}^S \ldots \\ &+ \hat{\mathbf{v}}^1\delta^1\hat{\mathbf{f}}^1 + \hat{\mathbf{v}}^2\delta^2\hat{\mathbf{f}}^2 + \cdots + \hat{\mathbf{v}}^S\delta^S\hat{\mathbf{f}}^S. \end{aligned} \tag{A4}$$

The last degree of freedom that we have is the length of the vectors. To ensure that the elements of the vectors $\tilde{\mathbf{v}}^i$ and $\tilde{\mathbf{f}}^i$ are on the same scale, we impose $\|\tilde{\mathbf{v}}^i\| = S_1^{1/2}$, $\|\tilde{\mathbf{f}}^i\| = S_2^{1/2}$.

By writing $\hat{\mathbf{v}}^i$ and $\hat{\mathbf{f}}^i$ in the form $\hat{\mathbf{v}}^i = \sigma_v^i \mathbf{1}$ and $\hat{\mathbf{f}}^i = \sigma_f^i \mathbf{1}$, we can simplify the expression:

$$
\begin{aligned}
\mathbf{M} = \; & \tilde{\mathbf{v}}^1 \delta^1 \tilde{\mathbf{f}}^1 + \tilde{\mathbf{v}}^2 \delta^2 \tilde{\mathbf{f}}^2 + \cdots + \tilde{\mathbf{v}}^S \delta^S \tilde{\mathbf{f}}^S \ldots \\
& + \mathbf{1} \underbrace{(\sigma_v^1 \delta^1 \tilde{\mathbf{f}}^1 + \sigma_v^2 \delta^2 \tilde{\mathbf{f}}^2 + \cdots + \sigma_v^S \delta^S \tilde{\mathbf{f}}^S) \ldots}_{=\tilde{\mathbf{f}}^*} \\
& + \underbrace{(\tilde{\mathbf{v}}^1 \delta^1 \sigma_f^1 + \tilde{\mathbf{v}}^2 \delta^2 \sigma_f^2 + \cdots + \tilde{\mathbf{v}}^S \delta^S \sigma_f^S) \mathbf{1}}_{=\tilde{\mathbf{v}}^*} \ldots \\
& + \mathbf{1} \underbrace{(\sigma_v^1 \delta^1 \sigma_f^1 + \sigma_v^2 \delta^2 \sigma_f^2 + \cdots + \sigma_v^S \delta^S \sigma_f^S) \mathbf{1}}_{=m} .
\end{aligned}
\tag{A5}
$$

Now, we restrict the first row of equation (A5) to the term with the largest value for δ^i (which by reordering and without loss of generality is δ^1). We obtain the following approximation:

$$
\mathbf{M} \approx \tilde{\mathbf{v}}^1 \delta^1 \tilde{\mathbf{f}}^1 + \tilde{\mathbf{v}}^* \mathbf{1} + \mathbf{1} \tilde{\mathbf{f}}^* + m,
\tag{A6}
$$

which at the component levels reads

$$
\mathbf{M}_{ij} \approx \tilde{v}_i^1 \delta^1 \tilde{f}_j^1 + \tilde{v}_i^* + \tilde{f}_j^* + m.
\tag{A7}
$$

By rewriting the first term of the right side, we obtain our final equation,

$$
\mathbf{M}_{ij} \approx -\frac{\delta^1}{2}\left(\tilde{v}_i^1 - \tilde{f}_j^1\right)^2 + \tilde{v}_i^* + \frac{\delta^1}{2}\left(\tilde{v}_i^1\right)^2 + \tilde{f}_j^* + \frac{\delta^1}{2}\left(\tilde{f}_j^1\right)^2 + m,
\tag{A8}
$$

which is equivalent to our equation [1], with the following correspondences: $\lambda = \delta^1/2$, $v_i = \tilde{v}_i^1$, $f_i = \tilde{f}_i^1$, $\delta_1 v_i^* = \tilde{v}_i^* + \delta^1/2(\tilde{v}_i^1)^2$, and $\delta_2 f_i^* = \tilde{f}_i^* + \delta^1/2(\tilde{f}_i^1)^2$.

Finally, we need to scale and constrain the vectors $\mathbf{v}^*$ and $\mathbf{f}^*$. It would be possible to add the same quantity to all components of vector $\mathbf{v}^*$, simultaneously subtract the same quantity to all components of vector $\mathbf{f}^*$, and let equation (A8) be invariant. This is a major issue when estimating these values with a Monte Carlo Markov chain. However, this does not change the phylogenetic signal. Thus, for practical reasons, we set $\mathbf{v}^* \perp \mathbf{1}$ and $\mathbf{f}^* \perp \mathbf{1}$. As previously, we scale these two vectors such that $\|\mathbf{v}^*\| = S_1^{1/2}$ and $\|\mathbf{f}^*\| = S_2^{1/2}$. In this way, their components are on the same scale, and δ_1 and δ_2 can be compared.

Table A1. Difference in mean phylogenetic strength across network component

	Food webs		Mutualistic networks		Pollinator networks		Seed-disperser networks	
	Mean difference	P	Mean difference	P	Mean difference	P	Mean difference	P
Matching (predator/animals) vs. matching (prey/plant)	−.167	*.061*	.057	**.036**	.077	**.033**	.028	.514
Matching (predator/animals) vs. centrality (predator/animals)	.026	.741	.121	**<.001**	.129	**<.001**	.108	**.005**
Matching (predator/animals) vs. centrality (prey/plant)	.024	.754	.111	**<.001**	.122	**<.001**	.094	*.055*
Matching (prey/plant) vs. centrality (predator/animals)	.194	**.006**	.063	**.005**	.052	**.033**	.080	*.075*
Matching (prey/plant) vs. centrality (prey/plant)	.192	**.005**	**.054**	**.040**	.046	*.085*	.066	.219
Centrality (predator/animals) vs. centrality (prey/plant)	−.002	.968	−.010	.653	−.007	.696	−.014	.770

Note: For each network type, the difference in mean phylogenetic strength between all pairs of network component is provided. P values were estimated using a t-test. P values <.05 are indicated in boldface type; P values from .05 to .1 are indicated in italic type.

Table A2. Difference in mean phylogenetic strength across network type

	Matching				Centrality			
	Predators/animals		Prey/plants		Predators/animals		Prey/plants	
	Mean difference	P	Mean difference	P	Mean difference	P	Mean difference	P
Food webs vs. mutualistic	−.001	.993	.224	**.001**	.094	**.036**	.086	**.036**
Food webs vs. pollinator	−.015	.843	.229	**.001**	.088	**.046**	.083	**.037**
Food webs vs. frugivore	.021	.776	.216	**.002**	.103	**.039**	.091	*.092*
Mutualistic vs. pollinator	−.014	.675	.005	.862	−.006	.683	−.003	.895
Mutualistic vs. frugivore	.022	.499	−.008	.846	.009	.755	.005	.918
Pollinator vs. frugivore	.036	.342	−.013	.757	.015	.594	.008	.860

Note: For each network component, the difference in mean phylogenetic strength between all pairs of network type is provided. P values were estimated using a t-test. P values <.05 are indicated in boldface type; P values from .05 to .1 are indicated in italic type.

Literature Cited Only in the Appendix

Rossberg, A. G., A. Brännström, and U. Dieckmann. 2010. How trophic interaction strength depends on traits. Theoretical Ecology 3:13–24.

Watkins, D. S. 2010. The singular value decomposition. Pages 259–288 *in* Fundamentals of matrix computations. 3rd ed. Wiley, New York.